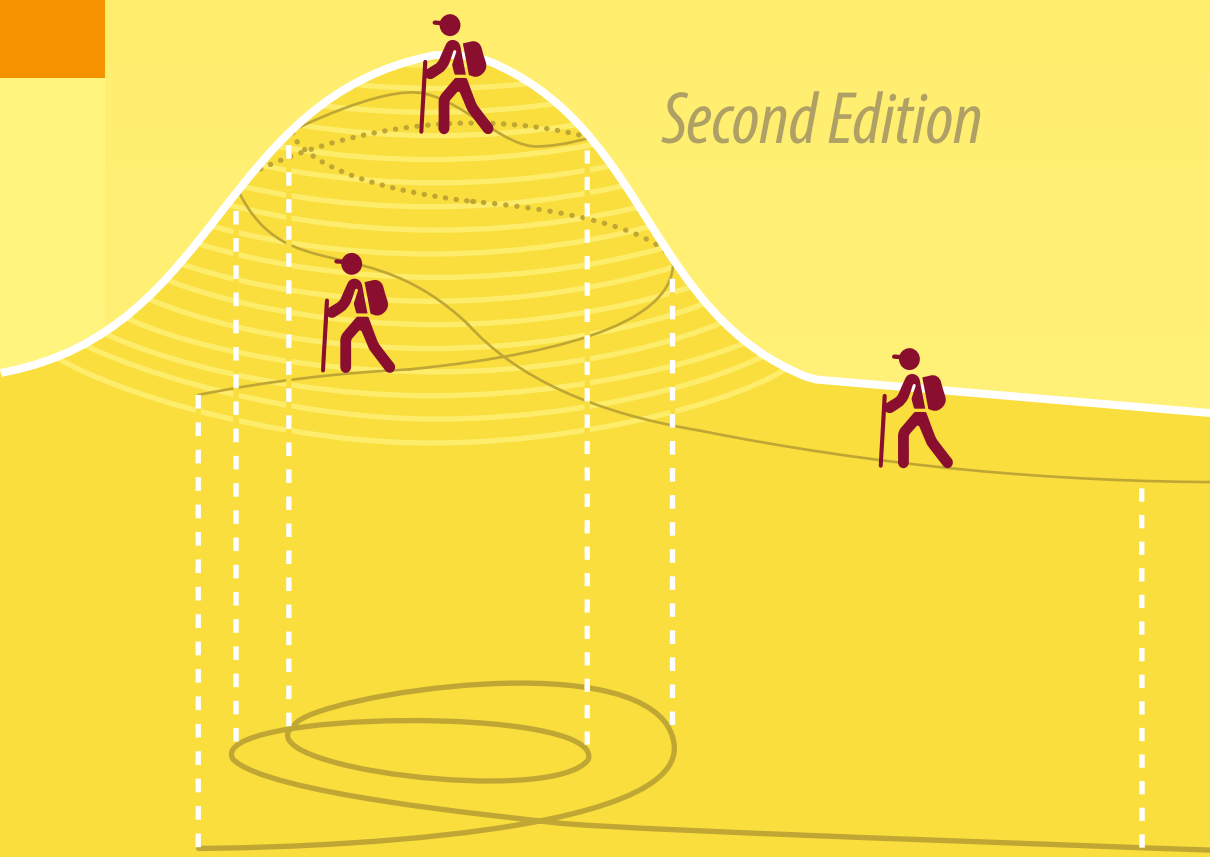
Stanley J. Miklavcic

An Illustrative Guide to Multivariable and Vector Calculus

Second Edition



Springer

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Stanley J. Miklavcic

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Second Edition

In collaboration with Ross A. Frick

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To my children Arya, Nadia, Jacob, and David.

Preface to the Second Edition

Returning to this textbook after a reasonably long absence of six-seven years, it became obvious that the original decision to produce a slim volume had some significant consequences. Some desirable if not important information was left out. Some explanations were far too brief and hence ambiguous (a generous description). And, too great a burden was placed on readers to follow up on subject matter themselves by solving in-text exercises. These shortcomings, as well as others, have been addressed in this revised edition.

All chapters have been reviewed, with Sects. 1.A, 1.C, 2.B, 2.G, 2.H, 5.C and 5.D having been all but completely rewritten. Many of the other sections have also been revised to a lesser degree, with some material moved to more appropriate places. Several discussion points (*e.g.*, in Sects. 1.C, 2.G and 5.C) have been extended and many explanatory statements elaborated on and clarified. Some considerable amount of new material has also been added. In some cases, the additional material has been included to fill gaps, including an introductory discussion on the ordinary derivative in Sect. 1.C and some useful integration information in Sect. 4.J. In other cases, new material has been added to provide a more complete study of a particular topic. Examples of the latter include an alternative method for evaluating second and higher order derivatives of composite functions in Sect. 2.G, a new Sect. 5.G, expounding on the summation convention in vector analysis, and in Sect. 3.E a motivational discussion on the use of a change of variables as a direct way of solving partial differential equations (a method of solution featured in many of the practical exercises). These changes account for most of the 70 or more additional pages of text.

There are now fewer in-text exercises (*Mastery Checks*). Essentially, the deleted exercises have been replaced by fully solved examples (35 additional detailed examples). It is my hope that the more balanced and favorable ratio of examples : exercises (87:61, compared with the previous ratio of 52:93) will provide better guidance for the student reader. A less obvious change can also be noted in the character of the Mastery Checks remaining; these have been selected to better match the character and difficulty of the solved examples.

Finally, a major change concerns the Supplementary problems. Those end-of-chapter sections have been condensed in order to conserve space. Many of the original, first edition problems that were of similar character but numbered individually, have now been combined and identified as parts (a), (b), etc. of single problems. Despite this consolidation, the total number of Supplementary problems has increased following the addition of over 70 new problems to give a total of approximately 200 problems across the five chapters. In this second edition I have also taken the trouble to distinguish, with an asterisk (*), the more difficult problems from the more straightforward ones. This should help both the self-directed student reader and the instructor, who may wish to assign assignment or examination questions. As with the first edition, a fully detailed book of solutions to all Mastery Check and Supplementary problems is available to instructors upon request.

Acknowledgements

My colleague and friend, Mr. Ross A. Frick, responsible for typing up most of the first edition, was unable to accompany me on this part of the journey. Nevertheless, it was impossible to take up the task of editing, especially when it came to the intricate formatting of new figures, without constantly reflecting on the magnificent job he did with the first edition. So, in an inspirational sense Ross contributed here too. I hope that my latex editing of this second edition does justice to the quality and style of Ross's superb efforts.

I am exceedingly grateful for the feedback I received on the first edition from the many students and teachers who have diligently pointed out a wide range of typographical, graphical, textual and mathematical errors that pervaded the book. I do believe these have now been corrected (I am hoping that I have not introduced too many new errors in the process). I particularly want to express my sincere gratitude to Mr. Wei Ming Ong, Mr. Lindsay Dylan Adcock, Dr. Sandeep Santhosh Kumar, and especially Dr. Farah Atour whose suggestions, reflections and otherwise useful comments have guided my own efforts through this second edition.

Adelaide, Australia Stanley J. Miklavcic
September 2025

Preface to the First Edition

This book originated as a set of lectures prepared for courses given by me at the University of Linköping in Sweden and at the University of South Australia in Australia. At Linköping University the material (apart from Sect. 3.E) was delivered in a second year, single semester course (14 weeks, 2 two-hour lectures per week) to engineering students, with the first half focused on the differential calculus of real-valued multivariable functions, while the second half was divided between integral calculus and vector calculus. At the University of South Australia the subject was delivered in two separate semester courses (12 weeks, 2 two-hour lectures per week), the first of which was offered to second year engineering, science and mathematics students and featured differential and integral calculus, including an introduction to partial differential equations. The second course, taken mostly by third year mathematics and science students, dealt with vector calculus, although only the first five weeks of that course was covered by the material in this book.

The lectures generally were so well received by students that it was thought the material might appeal to a wider audience. Having taken the decision to convert my notes into a book, I aimed for a document of manageable size rather than generate yet another bulky tome on calculus. The result is a book that students can carry easily to and from class, can take out and leaf through on the library lawn, or in a booth of a pub, or while lying on the banks of a river waiting for the fish to bite.

Very many ideas in mathematics are more readily conveyed and more easily appreciated when presented visually. This is certainly true of multivariable and vector calculus, and as my lecture material took advantage of many visual devices, I sought to capture the spirit if not the body of these same devices in printed form. Consequently, the majority of concepts are introduced and explained with the support of figures and graphics as well as the generous use of colour. Indeed, colour is used to highlight specific pieces of information, to emphasize relationships between variables in different equations, and to distinguish different roles or actions. The inevitable issue of colour blindness was raised in the course of the book's development. To minimize difficulties, colour typesetting has been configured to allow for some degree of differentiation even by those readers with impaired colour vision.

In addition, colour has been implemented so as only to benefit one's understanding, and *not* as an essential condition for understanding.

The book is self-contained and complete as an introduction to the theory of the differential and integral calculus of both real-valued and vector-valued multivariable functions. The entire material is suitable as a textbook in its own right for one to two, semester-long courses in either the second year or third year of University studies, and for students who have already completed courses in single variable calculus and linear algebra. Some selection of content may be necessary depending on student need and time available. For instance, as the topic of partial differential equations (PDEs) is normally offered as a separate course to mathematics students, Sect. 3.E can be skipped in a multivariable calculus course. On the other hand, a course in PDEs is not always included in engineering and science curricula, so Sect. 3.E is a pragmatic, albeit brief, introduction to the subject, particularly as its focus is on solving PDEs in simple cases. Alternatively, because of its illustrative emphasis, the book can also perform the role of a reference text to complement one of the more standard textbooks in advanced calculus, such as [5], thus providing the student with a different visual perspective.

Consequent to the ambition of producing a portable book, the reader should not be surprised that some areas of the calculus are not covered in detail. One other notable sacrifice is mathematical rigour. There are very few proofs included and those that have been are deliberately sketchy, included only to give students a rational justification for, or to illustrate the origin of, an idea. Consequently, students of pure mathematics may want to complement this book with one that offers a deeper analysis, such as [6].

Within each chapter is a sequence of Mastery Checks, exercises on the topic under discussion that are usually preceded by solved examples. Students are encouraged to attempt these Mastery Checks and keep a record of their solutions for future reference. To reinforce the ideas, additional exercises appear at the end of each chapter to supplement the Mastery Checks. Solutions to both sets of exercises are available from the publisher. I have limited the number of problems in order to restrict the size of the book, assuming that students would have access to auxiliary exercises in more standard treatises. All the same, the book contains over 90 Mastery Checks and over 120 Supplementary Exercises, many with multiple parts.

The reader should be aware that I have made use of mathematical symbols (such as $\Rightarrow$ and $\exists$) and abbreviations (w.r.t., 3D) in place of text, a common practice in mathematics texts and research literature. A glossary of definitions can be found at the end of the book. Wherever they appear in the book they should be read as the pieces of text they replace. Finally, for easy reference a summary of some key formulae covering various topics in multivariable and vector calculus is given on Page xiii.

Acknowledgements

In drafting this book I had great pleasure in working closely with my colleague Ross A. Frick who was instrumental in turning my lecture material and supplementary notes into book form. His skill with LATEX and MATLAB® was critical in this endeavour. I would also like to thank Dr. Loretta Bartolini, Mathematics Editor at Springer, for her strong support and encouragement of this venture and for her efficient handling of the publication of this book.

I will forever be indebted to my partner Julie for her patience and enduring support over the many, many months of editing and re-editing to which this book was subjected. It is no exaggeration to say that without her understanding the task of completing this book would have been a far greater challenge than it has been.

Lastly, I would like to thank the students who have taken my course over the years, particularly those (now graduate) students who gave feedback on the notes prior to their publication. Their general enthusiasm has been an absolutely essential factor in getting the book to this point. I hope that future students of this important area of mathematics will also enjoy and be inspired by what this little volume has to offer.

Adelaide, Australia Stanley J. Miklavcic
December 2019

Competing Interests The author has no competing interests to declare that are relevant to the content of this manuscript.

Important Formulae

Multivariable Calculus

- Suppose $f, g, h \in C^1$ and $w = f(u, v)$ where $u = g(x, y)$ and $v = h(x, y)$, then the partial derivative of w with respect to x is given by $\frac{\partial w}{\partial x} = \frac{\partial f}{\partial u}\frac{\partial g}{\partial x} + \frac{\partial f}{\partial v}\frac{\partial h}{\partial x}$, and similarly for the partial derivative of w with respect to y.
- Suppose $f \in C^3$ at the point (a, b), then for points (x, y) in a neighborhood of (a, b) the function f has the following Taylor approximation:

$$f(x, y) = f(a, b) + f_x(a, b)\Delta x + f_y(a, b)\Delta y + \frac{1}{2}Q(\Delta x, \Delta y) + R(\Delta x, \Delta y)$$

  where Q is the quadratic form,

$$Q(\Delta x, \Delta y) = f_{xx}(a, b)(\Delta x)^2 + 2f_{xy}(a, b)\Delta x\Delta y + f_{yy}(a, b)(\Delta y)^2$$

  and R is a remainder term of order $((\Delta x^2 + \Delta y^2)^{3/2})$.
- $f = f(x, y, z) \in C^2$, is a solution of Laplace's equation in domain $D \subset \mathbb{R}^3$ if f satisfies

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} = 0.$$

- The Jacobian for the transformation $(x, y) \mapsto (u, v)$:

$$J = \frac{\partial(x, y)}{\partial(u, v)} = \begin{vmatrix} \frac{\partial x}{\partial u} & \frac{\partial y}{\partial u} \\ \frac{\partial x}{\partial v} & \frac{\partial y}{\partial v} \end{vmatrix}$$

- Orthogonal curvilinear coordinate systems and their corresponding change of variables:

1. Polar coordinates: $r \geq 0$ and $0 \leq \theta \leq 2\pi$; Jacobian, $J = r$.

$$\{x = r\cos\theta, \quad y = r\sin\theta\}$$

2. Cylindrical polar coordinates: $r \geq 0$, $0 \leq \theta \leq 2\pi$ and $z \in \mathbb{R}$; Jacobian, $J = r$.

$$\{x = r\cos\theta, \quad y = r\sin\theta, \quad z = z\}$$

3. Spherical polar coordinates: $\rho \geq 0$, $0 \leq \theta \leq 2\pi$, $0 \leq \phi \leq \pi$; Jacobian, $J = \rho^2\sin\phi$.

$$\{x = \rho\sin\phi\cos\theta, \quad y = \rho\sin\phi\sin\theta, \quad z = \rho\cos\phi\}$$

- A level set to a function $f(x, y)$ is the set $\{(x, y) : \text{s.t.} f(x, y) = C\}$ for some real constant C. The gradient of f is always normal to a level set of f.
- An iterated integral of a function of two variables over a y-simple domain $D = \{(x, y) : a \leq x \leq b; g_1(x) \leq y \leq g_2(x)\}$

$$\iint_D f(x, y)\, \mathrm{d}A = \int_a^b \mathrm{d}x \int_{g_1(x)}^{g_2(x)} f(x, y)\, \mathrm{d}y.$$

- An iterated integral of a function of two variables over a x-simple domain $D = \{(x, y) : c \leq y \leq d; h_1(y) \leq x \leq h_2(y)\}$

$$\iint_D f(x, y)\, \mathrm{d}A = \int_c^d \mathrm{d}y \int_{h_1(y)}^{h_2(y)} f(x, y)\, \mathrm{d}x.$$

- For a bijective transformation $D \ni (x, y) \mapsto (u, v) \in E$ with Jacobian determinant, $J \neq 0$, the double integral of $f(x, y) = F(u, v)$ is

$$\iint_D f(x, y)\, \mathrm{d}x\mathrm{d}y = \iint_E F(u, v) \left| \frac{\partial(x, y)}{\partial(u, v)} \right| \mathrm{d}u\mathrm{d}v.$$

Vector Calculus

- In terms of a general, 3D curvilinear coordinate system $\{\xi_1, \xi_2, \xi_3\}$, with unit vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ (*s.t.* $\boldsymbol{a}_i$ points in the direction of increasing ξ_i), and scale factors h_1, h_2, h_3, the gradient, divergence and curl operations on scalar ($\phi \in C^1$) and vector ($\mathbf{F} \in C^1$) fields, respectively, take the form

$$\nabla\phi = \frac{1}{h_1}\frac{\partial\phi}{\partial\xi_1}\mathbf{a}_1 + \frac{1}{h_2}\frac{\partial\phi}{\partial\xi_2}\mathbf{a}_2 + \frac{1}{h_3}\frac{\partial\phi}{\partial\xi_3}\mathbf{a}_3$$

$$\nabla\cdot\mathbf{F} = \frac{1}{h_1h_2h_3}\left[\frac{\partial}{\partial\xi_1}(h_2h_3F_1) + \frac{\partial}{\partial\xi_2}(h_1h_3F_2) + \frac{\partial}{\partial\xi_3}(h_1h_2F_3)\right],$$

$$\nabla\times\mathbf{F} = \frac{1}{h_1h_2h_3}\begin{vmatrix} h_1\mathbf{a}_1 & h_2\mathbf{a}_2 & h_3\mathbf{a}_3 \\ \frac{\partial}{\partial\xi_1} & \frac{\partial}{\partial\xi_2} & \frac{\partial}{\partial\xi_3} \\ h_1F_1 & h_2F_2 & h_3F_3 \end{vmatrix}$$

For *Cartesian* coordinates $\{\xi_1,\xi_2,\xi_3\} = \{x_1,x_2,x_3\} = \{x,y,z\}$, $h_1 = h_2 = h_3 = 1$, and $\mathbf{a}_1 = \mathbf{e}_1 = \mathbf{i}$; $\mathbf{a}_2 = \mathbf{e}_2 = \mathbf{j}$; $\mathbf{a}_3 = \mathbf{e}_3 = \mathbf{k}$.
For *cylindrical* coordinates $\{\xi_1,\xi_2,\xi_3\} = \{r,\theta,z\}$, $h_1 = 1$, $h_2 = r$, $h_3 = 1$, and $\mathbf{a}_1 = \hat{r} = (\cos\theta, \sin\theta, 0)$; $\mathbf{a}_2 = \widehat{\theta} = (-\sin\theta, \cos\theta, 0)$; $\mathbf{a}_3 = \mathbf{e}_3 = \mathbf{k}$.
For *spherical* coordinates $\{\xi_1,\xi_2,\xi_3\} = \{\rho,\theta,\phi\}$, $h_1 = 1$, $h_2 = \rho$, $h_3 = \rho\sin\phi$, and $\mathbf{a}_1 = \widehat{\rho} = (\cos\theta\sin\phi, \sin\theta\sin\phi, \cos\phi)$; $\mathbf{a}_2 = \widehat{\theta} = (-\sin\theta, \cos\theta, 0)$; $\mathbf{a}_3 = \widehat{\phi} = (\cos\theta\cos\phi, \sin\theta\cos\phi, -\sin\phi)$.

- A C^1 vector field $\mathbf{F} = \mathbf{F}(\boldsymbol{r})$ defined in some domain $D \subset \mathbb{R}^3$ is said to be

  1. solenoidal in D, if $\nabla\cdot\mathbf{F} = 0$ in D;
  2. irrotational in D, if $\nabla\times\mathbf{F} = 0$ in D;
  3. conservative in D, if $\mathbf{F} = \nabla\phi$ in D for some C^2 real-valued function $\phi = \phi(\boldsymbol{r})$.

- Some useful vector identities. Suppose $\psi, \phi : R^3 \to R$ and $h : R \to R$ are C^1 scalar-valued functions, $\mathbf{f}, \mathbf{g} : R^3 \to R^3$ are C^1 vector-valued functions, $\mathbf{r} = (x, y, z)$ is a position vector of length $r = |\mathbf{r}| = \sqrt{x^2+y^2+z^2}$ and $\mathbf{c}$ is a constant vector.

(1) $\nabla(\phi\psi) = \psi\nabla\phi + \phi\nabla\psi$
(2) $\nabla\cdot(\phi\mathbf{f}) = \phi\nabla\cdot\mathbf{f} + \mathbf{f}\cdot\nabla\phi$
(3) $\nabla\times(\nabla\phi) = 0$
(4) $\nabla\cdot(\nabla\times\mathbf{f}) = 0$
(5) $\nabla\times(\nabla\times\mathbf{f}) = \nabla(\nabla\cdot\mathbf{f}) - \nabla^2\mathbf{f}$
(6) $\nabla\cdot\mathbf{r} = 3$
(7) $\nabla h(r) = \frac{dh}{dr}\frac{\mathbf{r}}{r}$
(8) $\nabla\cdot(h(r)\mathbf{r}) = 3h(r) + r\frac{dh}{dr}$
(9) $\nabla\times(h(r)\mathbf{r}) = 0$
(10) $\nabla(\mathbf{c}\cdot\mathbf{r}) = \mathbf{c}$
(11) $\nabla\cdot(\mathbf{c}\times\mathbf{r}) = 0$
(12) $\nabla\times(\mathbf{c}\times\mathbf{r}) = 2\mathbf{c}$
(13) $\nabla\times(\phi\mathbf{f}) = \phi\nabla\times\mathbf{f} + \nabla\phi\times\mathbf{f}$
(14) $\nabla(\mathbf{f}\cdot\mathbf{g}) = (\mathbf{f}\cdot\nabla)\mathbf{g} + (\mathbf{g}\cdot\nabla)\mathbf{f} + \mathbf{f}\times(\nabla\times\mathbf{g}) + \mathbf{g}\times(\nabla\times\mathbf{f})$

(15) $\nabla \cdot (\mathbf{f} \times \mathbf{g}) = \mathbf{g} \cdot (\nabla \times \mathbf{f}) - \mathbf{f} \cdot (\nabla \times \mathbf{g})$
(16) $\nabla \times (\mathbf{f} \times \mathbf{g}) = \mathbf{f}(\nabla \cdot \mathbf{g}) - \mathbf{g}(\nabla \cdot \mathbf{f}) + (\mathbf{g} \cdot \nabla)\mathbf{f} - (\mathbf{f} \cdot \nabla)\mathbf{g}$

- Vector integration

1. Line integral of $\mathbf{f} = \mathbf{f}(\mathbf{r})$ over $\Gamma = \{\mathbf{r} = \mathbf{r}(t) : a \leq t \leq b\}$:

$$\int_{\Gamma} \mathbf{f} \cdot \mathrm{d}\mathbf{r} = \int_{a}^{b} \mathbf{f}(\mathbf{r}(t)) \cdot \frac{d\mathbf{r}}{dt} \mathrm{d}t$$

2. Surface integral of $\mathbf{f} = \mathbf{f}(\mathbf{r})$ over $S = \left\{\mathbf{r} = \mathbf{r}(u, v) : (u, v) \in D \subset \mathbb{R}^2\right\}$ with unit surface normal $\mathbf{N}$:

$$\iint_{S} \mathbf{f} \cdot \mathrm{d}\mathbf{S} = \iint_{S} \mathbf{f} \cdot \mathbf{N} \mathrm{d}S = \iint_{D} \mathbf{f}(\mathbf{r}(u, v)) \cdot \left(\frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v} \right) \mathrm{d}u \mathrm{d}v$$

3. Green's theorem for $\mathbf{f} = (f_1, f_2) \in C^1$ over a finite 2D region D bounded by a positively oriented closed curve Γ:

$$\oint_{\Gamma} \mathbf{f} \cdot \mathrm{d}\mathbf{r} = \oint_{\Gamma} (f_1 \mathrm{d}x + f_2 \mathrm{d}y) = \iint_{D} \left(\frac{\partial f_2}{\partial x} - \frac{\partial f_1}{\partial y} \right) \mathrm{d}A$$

4. Gauss's theorem (divergence theorem) for $\mathbf{f} \in C^1$ over a finite 3D region V bounded by smooth closed surface S with outward pointing, unit surface normal, $\mathbf{N}$:

$$\iiint_{V} (\nabla \cdot \boldsymbol{f}) \mathrm{d}V = \oiint_{S} \boldsymbol{f} \cdot \boldsymbol{N} \mathrm{d}S$$

5. Stokes's theorem for $\mathbf{f} \in C^1$ defined on a smooth surface S with unit surface normal $\mathbf{N}$ and bounded by a positively oriented, closed curve Γ:

$$\iint_{S} (\nabla \times \mathbf{f}) \cdot \mathrm{d}\mathbf{S} = \iint_{S} (\nabla \times \mathbf{f}) \cdot \mathbf{N} \mathrm{d}S = \oint_{\Gamma} \mathbf{f} \cdot \mathrm{d}\mathbf{r}$$

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Chapter 1

Vectors and Functions

Many mathematical properties possessed by functions of several variables are couched in both geometric and algebraic terms, with the occasional reference to fundamental set theory. In this introductory chapter, some of the basic concepts falling within these categories and needed in later chapters will be reviewed, starting with vector algebra. This is followed by a short review of some essential concepts from set theory, employed throughout the book. These will help establish many foundation concepts in both the differential and integral calculus. Coordinate systems and the notion of level sets are also discussed. Once again, both topics find application in differential and integral multivariable calculus, as well as in vector calculus.

It goes without saying that multivariable calculus is largely built on the foundations of single-variable calculus. Consequently, this chapter also contains a brief review of the differential calculus as it pertains to single-variable functions. This review begins in Section 1.C, but continues in Chapters 2, 3, and 4 as needed.

Lastly, to help appreciate the behaviour of multivariable functions defined on two or higher dimensional domains, it is useful to visualize the graph of a function, or at least its domain of definition. Some people are more hard-wired to visual cues and visual information, while others are more comfortable with abstract ideas. Whatever your preference, being able to draw figures is always an advantage. As such, in this chapter we shall also review some basic 3D graphs and show how to draw them using MATLAB®or equivalent software. In the event, the reader is unable to access software solutions, a subsection which may hopefully illustrate by example how one can obtain a picture of a region or of a function graph directly from a mathematical formula or

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equation is also included. While it is not possible to offer a general procedure that works in all cases, some of the steps that I will go through may be applicable in other instances.

1.A Some Vector Algebra Essentials

I. Vectors and unit vectors in 3-space

In three dimensions, a (constant) vector will be represented by three independent numbers; in two dimensions, only two independent numbers will be needed. In what will soon be referred to as a Cartesian coordinate system, a (constant) vector in $\mathbb{R}^3$,

$$\boldsymbol{v} \;=\; (\alpha, \beta, \gamma) \;=\; \alpha\mathbf{i} + \beta\mathbf{j} + \gamma\mathbf{k} \;=\; \alpha\mathbf{e}_1 + \beta\mathbf{e}_2 + \gamma\mathbf{e}_3$$

(see also Section 1.B) has three components: α, β, and γ, where α, β, and γ are real numbers, referred to as the x-, y-, and z-components, respectively, relative to a well-defined *point of reference* or *origin*.

For example, measured from the origin, if $\alpha = 1$, $\beta = -2$, and $\gamma = 2$, then $\boldsymbol{v}$ is a vector with a component of unit magnitude in the positive x-direction, a component with magnitude of 2 units in the negative y-direction and a component of magnitude 2 units in the positive z-direction.

The components of $\boldsymbol{v}$ also determine the vector's magnitude. Two applications of Pythagoras's theorem show that the magnitude of $\boldsymbol{v}$ is

$$|\boldsymbol{v}| = \sqrt{\alpha^2 + \beta^2 + \gamma^2}.$$

The vector $\boldsymbol{v}$ above has been written in the three most common forms used in textbooks. The first form simply shows the component values (scalars) along the three respective x-, y-, and z-directions, without explicit reference to those directions. In the second and third forms, the mutually orthogonal directions are included explicitly, represented by the *unit* vectors $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$ or by $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ in $\mathbb{R}^3$. For application purposes the vectors $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ (or equivalently $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$) are arranged in what is referred to as a right-handed system as depicted in Figure 1.1, mimicking the arrangement of the extended *thumb, forefinger, and middle finger*, respectively(!), of a person's right hand. The unit vectors themselves may be expressed in component form as $\mathbf{i} = (1, 0, 0)$, $\mathbf{j} = (0, 1, 0)$, and $\mathbf{k} = (0, 0, 1)$, each directed to points one unit from a nominal point of origin $(0, 0, 0)$, in their defined directions.

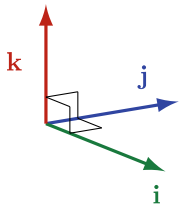


Figure 1.1 Unit vectors **i**, **j**, **k** in a right-handed, Cartesian coordinate system.

We shall refer to vectors using any of the three equivalent forms, depending on what is appropriate. For example, a point P in $\mathbb{R}^3$ will usually be designated in its position component form (α, β, γ), but circumstances may dictate it more appropriate to refer to P in the directed vector form, $\alpha\mathbf{i} + \beta\mathbf{j} + \gamma\mathbf{k}$, and graphed as a vector drawn from the origin to that location.

Multiplying a vector $\boldsymbol{v}$ with a scalar, a, will return a new vector with either the same direction if the scalar is positive, or the opposite direction if the scalar is negative. In either case, the resulting vector has different magnitude (Figure 1.2). Such scalings will be employed in Chapter 5 where we will need vectors of unit magnitude derived from vectors of non-unit magnitude. For example, to produce a vector of unit magnitude (a unit vector), $\boldsymbol{N}$, having the same direction as the (arbitrary) vector $\boldsymbol{v}$ in 3D, we employ a scaling $a\boldsymbol{v}$, where $a > 0$ satisfies

$$|\boldsymbol{N}| = |a\boldsymbol{v}| = |a||\boldsymbol{v}| = a\sqrt{\alpha^2 + \beta^2 + \gamma^2} = 1, \ \textit{i.e.}, \ a = \frac{1}{\sqrt{\alpha^2 + \beta^2 + \gamma^2}}.$$

Thus, we see that to construct a unit vector in the direction of a specific vector $\boldsymbol{v}$, we simply divide $\boldsymbol{v}$ by its length: $\boldsymbol{N} = \dfrac{\boldsymbol{v}}{|\boldsymbol{v}|}$.

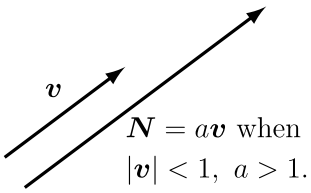


Figure 1.2 The unit vector in the case when $|\boldsymbol{v}| < 1$ and $a = 1/|\boldsymbol{v}| > 1$.

Combining two vectors by addition or subtraction is effected by simple addition or subtraction of the vectors' corresponding components. For example, given two vectors in $\mathbb{R}^3$,

$$\boldsymbol{u} = (a_1, a_2, a_3) \quad \text{and} \quad \boldsymbol{v} = (b_1, b_2, b_3),$$

their addition and subtraction define new vectors, also in $\mathbb{R}^3$, given by

$$\boldsymbol{u}+\boldsymbol{v}=\begin{cases}(a_1+b_1,a_2+b_2,a_3+b_3),\\(a_1+b_1)\mathbf{i}+(a_2+b_2)\mathbf{j}+(a_3+b_3)\mathbf{k},\end{cases}$$

and

$$\boldsymbol{u}-\boldsymbol{v}=\begin{cases}(a_1-b_1,a_2-b_2,a_3-b_3),\\(a_1-b_1)\mathbf{i}+(a_2-b_2)\mathbf{j}+(a_3-b_3)\mathbf{k}.\end{cases}$$

Geometrically, these added or subtracted vectors are graphed using the tail-to-head method. In the case of addition, the tail of vector $\boldsymbol{v}$ is placed at the head of vector $\boldsymbol{u}$, with the new vector being the vector drawn from the *tail* of $\boldsymbol{u}$ to the *head* of $\boldsymbol{v}$. In the case of subtraction, the same method applies except that $-\boldsymbol{v}$ is used instead of $\boldsymbol{v}$.

II. The product of two vectors in 3-space

Again, suppose $\boldsymbol{u}$ and $\boldsymbol{v}$ are two non-parallel but otherwise arbitrary vectors in $\mathbb{R}^3$:

$$\boldsymbol{u}=(a_1,a_2,a_3)\quad \boldsymbol{v}=(b_1,b_2,b_3).$$

There are two particular *product* operations that may be applied to $\boldsymbol{u}$ and $\boldsymbol{v}$ and that we will utilize on many occasions. These are the *vector* and *scalar* products. From them very useful information about the vectors can be extracted.

(i) The so-called *vector* or *cross* product, whose operation is denoted by the symbol $\times$, in the right-hand coordinate system of Figure 1.1 satisfies the conditions that

$$\mathbf{i}\times\mathbf{j}=\mathbf{k};\quad \mathbf{j}\times\mathbf{k}=\mathbf{i};\quad \mathbf{k}\times\mathbf{i}=\mathbf{j},$$

with negative signs introduced on the right-hand sides of these identities if the vectors on the left-hand sides are interchanged. In addition, we have the identities

$$\mathbf{i}\times\mathbf{i}=\mathbf{j}\times\mathbf{j}=\mathbf{k}\times\mathbf{k}=\mathbf{0}.$$

With these rules established and with help of the distribution law, the vector product of two arbitrary vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ becomes

$$\begin{aligned}\boldsymbol{u}\times\boldsymbol{v} &= (a_1\mathbf{i}+a_2\mathbf{j}+a_3\mathbf{k})\times(b_1\mathbf{i}+b_2\mathbf{j}+b_3\mathbf{k})\\ &= a_1b_1\mathbf{i}\times\mathbf{i}+a_1b_2\mathbf{i}\times\mathbf{j}+a_1b_3\mathbf{i}\times\mathbf{k}\\ &\quad +a_2b_1\mathbf{j}\times\mathbf{i}+a_2b_2\mathbf{j}\times\mathbf{j}+a_2b_3\mathbf{j}\times\mathbf{k}\\ &\quad +a_3b_1\mathbf{k}\times\mathbf{i}+a_3b_2\mathbf{k}\times\mathbf{j}+a_3b_3\mathbf{k}\times\mathbf{k},\\ &= (a_2b_3-a_3b_2)\mathbf{i}+(a_3b_1-a_1b_3)\mathbf{j}+(a_1b_2-a_2b_1)\mathbf{k}. \quad (1.1)\end{aligned}$$

A shorthand way of writing (and remembering) the vector product, particularly the various combinations of factors and their signs appearing in the resulting three components, is by evaluating

the 3×3 determinant comprised of three sets of "row elements": the unit vectors $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$, the components of $\boldsymbol{u}$: $\{a_1, a_2, a_3\}$, and the components of $\boldsymbol{v}$: $\{b_1, b_2, b_3\}$, *appearing* ***only*** *in this order in the array*:

$$\begin{aligned} \boldsymbol{w} &= \boldsymbol{u} \times \boldsymbol{v} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} \\ &= (a_2 b_3 - a_3 b_2)\mathbf{i} + (a_3 b_1 - a_1 b_3)\mathbf{j} + (a_1 b_2 - a_2 b_1)\mathbf{k}. \end{aligned} \tag{1.2}$$

The first noteworthy property of the vector product, proved below, is that it produces a vector, $\boldsymbol{w}$, that is *perpendicular to both* $\boldsymbol{u}$ and $\boldsymbol{v}$. The relationship between the three vectors is shown schematically in Figure 1.6.

Secondly, it's easily verified (either by direct evaluation or using the properties of the determinant) that $\boldsymbol{u} \times \boldsymbol{v}$ is antiparallel to $\boldsymbol{v} \times \boldsymbol{u}$. That is, $\boldsymbol{v} \times \boldsymbol{u} = -\boldsymbol{u} \times \boldsymbol{v}$.

A third very useful property of the vector product is based on its magnitude. The magnitude of the vector product of two vectors

$$|\boldsymbol{u} \times \boldsymbol{v}| = |\boldsymbol{w}| = \left| \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} \right| = \sqrt{(a_2 b_3 - a_3 b_2)^2 + \cdots}$$

gives the *area* of a *plane parallelogram* whose two adjoining, non-parallel sides are defined by the directions and lengths of the vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ (Figure 1.3).

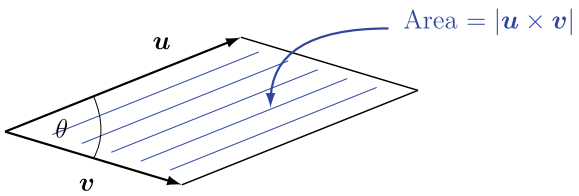


Figure 1.3 The $\boldsymbol{u} \times \boldsymbol{v}$ parallelogram.

On the other hand, referring to the figure itself and using simple plane geometry, the area of the parallelogram and hence the magnitude of the vector product can be shown to be

$$|\boldsymbol{w}| = |\boldsymbol{u}||\boldsymbol{v}| \sin\theta, \tag{1.3}$$

where θ is the (acute) angle between $\boldsymbol{u}$ and $\boldsymbol{v}$ lying in the plane they define.

(ii) The other type of product between two vectors, whose operation is denoted by the symbol $\cdot$, is the *scalar* or *dot* product. This product, not to be confused with ordinary scalar multiplication, is defined by a different set of conditions. Again, in a Cartesian coordinate system these conditions are

$$\mathbf{i}\cdot\mathbf{j} = \mathbf{j}\cdot\mathbf{k} = \mathbf{k}\cdot\mathbf{i} = 0;$$
$$\mathbf{i}\cdot\mathbf{i} = \mathbf{j}\cdot\mathbf{j} = \mathbf{k}\cdot\mathbf{k} = 1.$$

These equations are statements of the fact that the three unit vectors are mutually orthogonal and have magnitude unity. Correspondingly, the scalar product between two arbitrary vectors becomes

$$\begin{aligned}\boldsymbol{u}\cdot\boldsymbol{v} &= (a_1\mathbf{i}+a_2\mathbf{j}+a_3\mathbf{k})\cdot(b_1\mathbf{i}+b_2\mathbf{j}+b_3\mathbf{k})\\ &= a_1b_1\mathbf{i}\cdot\mathbf{i}+a_1b_2\mathbf{i}\cdot\mathbf{j}+a_1b_3\mathbf{i}\cdot\mathbf{k}\\ &\quad + a_2b_1\mathbf{j}\cdot\mathbf{i}+a_2b_2\mathbf{j}\cdot\mathbf{j}+a_2b_3\mathbf{j}\cdot\mathbf{k}\\ &\quad + a_3b_1\mathbf{k}\cdot\mathbf{i}+a_3b_2\mathbf{k}\cdot\mathbf{j}+a_3b_3\mathbf{k}\cdot\mathbf{k},\\ &= a_1b_1+a_2b_2+a_3b_3. \qquad (1.4)\end{aligned}$$

Working backwards from Equation (1.4) and using their component definitions, we can confirm that the unit vectors $\mathbf{i}$, $\mathbf{j}$, and $\mathbf{k}$ do indeed satisfy the above conditions.

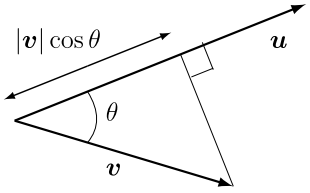


Figure 1.4 The projection of $\boldsymbol{v}$ onto $\boldsymbol{u}$.

Notice that in contrast to the vector product, the scalar product simply produces a scalar quantity, a number. The important role of the scalar product, as a measure of how closely aligned two vectors are, can be exploited in a variety of ways. Indeed, if we again denote the (acute) angle between the vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ by θ (Figure 1.4), then we find (see Mastery Check 1.1 or see [13] Ch 2) that the scalar product may be defined equivalently by

$$\boldsymbol{u}\cdot\boldsymbol{v} = |\boldsymbol{u}||\boldsymbol{v}|\cos\theta, \qquad (1.5)$$

from which we may uniquely obtain the angle between the two vector directions:

$$\cos\theta = \frac{\boldsymbol{u}\cdot\boldsymbol{v}}{|\boldsymbol{u}||\boldsymbol{v}|} = \frac{a_1b_1+a_2b_2+a_3b_3}{|\boldsymbol{u}||\boldsymbol{v}|}. \qquad (1.6)$$

If the vectors are parallel or antiparallel, then one vector, say $\boldsymbol{u}$, is a scalar multiple of the other: $\boldsymbol{u} = t\boldsymbol{v}$ so

$$\cos\theta = \frac{t\boldsymbol{v}\cdot\boldsymbol{v}}{|t\boldsymbol{v}||\boldsymbol{v}|} = \frac{t|\boldsymbol{v}|^2}{|t||\boldsymbol{v}|^2} = \frac{t}{|t|} = \pm 1.$$

Thus, $\boldsymbol{u}\cdot\boldsymbol{v} = \pm|\boldsymbol{u}||\boldsymbol{v}|$, *i.e.*, $\theta = 0$ or π.

If $\theta = \dfrac{\pi}{2}$, then the vectors are orthogonal and $\boldsymbol{u}\cdot\boldsymbol{v} = 0$. For non-aligned vectors, the scalar product may also be used to determine the projection of one vector in the direction of a second, as illustrated in Figure 1.4.

Employing Eq (1.5) using the component definition of *vector* product, Eq (1.2), it may now easily be verified that $\boldsymbol{w}\cdot\boldsymbol{u} = \boldsymbol{w}\cdot\boldsymbol{v} = 0$, which confirms our earlier statement that $\boldsymbol{w}$ is orthogonal to both $\boldsymbol{u}$ and $\boldsymbol{v}$. We will make extensive use of these products in Chapter 2 (Sections 2.E and 2.G) and throughout Chapter 5.

Remarks

Naively, the vector and scalar products are different generalizations to vectors of the operation of multiplication of scalars. However, the connection to ordinary multiplication does not extend to the latter's properties.

- In contrast to ordinary multiplication, the vector product operation does not satisfy either the commutative law or the associative law. However, it does satisfy the distributive law.
- Although the scalar product does satisfy the commutative and distributive laws, it does not satisfy the associative law.

■ Example 1.1:

Vectors $\boldsymbol{u} = (1, 2, 0)$ and $\boldsymbol{v} = (4, 3, 0)$ lie in the xy-plane.

(a) Verify that the vector product $\boldsymbol{u}\times\boldsymbol{v}$ is a vector orthogonal to the xy-plane.

(b) Verify that $\boldsymbol{v}\times\boldsymbol{u} = -\boldsymbol{u}\times\boldsymbol{v}$.

(c) Determine the vector $\boldsymbol{w}$ having magnitude equal to the length of the projection of $\boldsymbol{v}$ onto $\boldsymbol{u}$, with the direction of $\boldsymbol{u}$.

Solution:

(a) The vector product is given by

$$\boldsymbol{u}\times\boldsymbol{v} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 1 & 2 & 0 \\ 4 & 3 & 0 \end{vmatrix} = (0-0)\mathbf{i} + (0-0)\mathbf{j} + (3-8)\mathbf{k} = -5\mathbf{k}.$$

As this vector has only a component in the z-direction, it is orthogonal to the xy-plane.

(b) Switching the order of vector components gives

$$\boldsymbol{v}\times\boldsymbol{u}=\begin{vmatrix}\mathbf{i}&\mathbf{j}&\mathbf{k}\\4&3&0\\1&2&0\end{vmatrix}=0\mathbf{i}+0\mathbf{j}+\big(8-3\big)\mathbf{k}=+5\mathbf{k}=-\left(\boldsymbol{u}\times\boldsymbol{v}\right).$$

(c) We need to perform two calculations. Firstly, we need to determine a unit vector in the direction of $\boldsymbol{u}$. Secondly, we need to determine the length of the projection of $\boldsymbol{v}$ onto the direction of $\boldsymbol{u}$. The first calculation gives

$$\boldsymbol{N}=\frac{\boldsymbol{u}}{|\boldsymbol{u}|}=\frac{(1,2,0)}{\sqrt{1+4+0}}=\frac{1}{\sqrt{5}}(1,2,0).$$

The second calculation is effected using the scalar product:

$$|\boldsymbol{v}|\cos\theta=|\boldsymbol{v}|\frac{\boldsymbol{u}\cdot\boldsymbol{v}}{|\boldsymbol{u}||\boldsymbol{v}|}=\frac{\boldsymbol{u}\cdot\boldsymbol{v}}{|\boldsymbol{u}|}=\frac{4+6+0}{\sqrt{5}}=2\sqrt{5}.$$

The product of the above two results (magnitude times direction) gives the desired vector $\boldsymbol{w}$,

$$\boldsymbol{w}=|\boldsymbol{v}|\cos\theta\;\boldsymbol{N}=2\sqrt{5}\;\frac{(1,2,0)}{\sqrt{5}}=(2,4,0).$$

■

✍ Mastery Check 1.1:

Let $\boldsymbol{u}$ and $\boldsymbol{v}$ be directed vectors from a point C to respective points A and B, and let θ be the acute angle between the vectors at C. By completing the triangle ABC and using the fact that $|\boldsymbol{v}|^2=\boldsymbol{v}\cdot\boldsymbol{v}$ prove, *i.e.* derive, Eq (1.5).

Hint: Employ the cosine rule of trigonometry.

✍

III. A plane in 3-space

The equation of a plane in $\mathbb{R}^3$, expressed mathematically as

$$P=\{(x,y,z):ax+by+cz=d;\;\;a,b,c\text{ not all zero }\},$$

can be determined knowing either

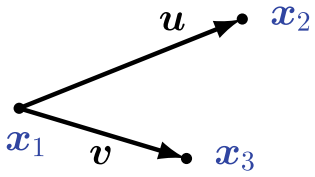


Figure 1.5 Construction of vectors $\boldsymbol{u}$ and $\boldsymbol{v}$.

(a) three non-collinear points on the plane; or
(b) one point and two non-parallel vectors lying parallel to the plane.

On the one hand, if we are given three coplanar points, $\boldsymbol{x}_i = (x_i, y_i, z_i)$, where $i = 1, 2, 3$, we can construct two vectors, $\boldsymbol{u}$ and $\boldsymbol{v}$, lying in the plane as in Figure 1.5 by subtracting the respective components of those points:

$$\begin{aligned} \boldsymbol{u} &= \boldsymbol{x}_2 - \boldsymbol{x}_1 = \big(x_2 - x_1, y_2 - y_1, z_2 - z_1\big), \\ \boldsymbol{v} &= \boldsymbol{x}_3 - \boldsymbol{x}_1 = \big(x_3 - x_1, y_3 - y_1, z_3 - z_1\big). \end{aligned}$$

Provided $\boldsymbol{x}_1$, $\boldsymbol{x}_2$, and $\boldsymbol{x}_3$ are not collinear, then $\boldsymbol{u}$ and $\boldsymbol{v}$ will not be superimposed or even parallel and, as discussed in II(i),

$$\boldsymbol{w} = \boldsymbol{u} \times \boldsymbol{v} = (\alpha, \beta, \gamma)$$

will be a vector normal (*i.e.*, perpendicular) to both $\boldsymbol{u}$ and $\boldsymbol{v}$ and thus normal to the plane in which the $\boldsymbol{x}_i$ lie (Figure 1.6).

The alternative case III(b) is actually a variation of alternative III(a) where we are provided directly with the vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ with which to construct the orthogonal vector $\boldsymbol{w}$.

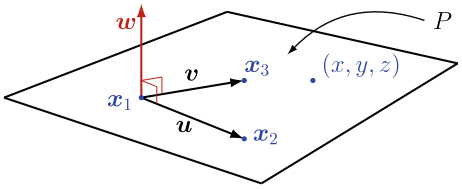


Figure 1.6 Construction of the plane P.

By convention, the direction of $\boldsymbol{w} = \boldsymbol{u} \times \boldsymbol{v}$ is given by the **right-hand rule**: *Take your right hand with fingers extended in the direction of* $\boldsymbol{u}$. *If you curl your fingers in the direction of* $\boldsymbol{v}$, *then your thumb will point in the direction of the resultant vector* $\boldsymbol{w}$. The vector product and its various geometric properties will play central roles in Sections 2.C and 5.D.

To construct the equation of the plane, suppose (x, y, z) is an arbitrary point in the plane P and let the given point be (x_1, y_1, z_1). As per the calculation above, we can determine a new vector joining the variable point (x, y, z) to the given point (x_1, y_1, z_1) by subtracting the respective components: $(x-x_1, y-y_1, z-z_1)$. By definition, this vector will lie in the plane whose equation we are to determine and thus be perpendicular to the previously determined normal vector, $\boldsymbol{w}$. Applying the scalar product of II(ii), we must then have that

$$\begin{aligned} \boldsymbol{w} \cdot \big(x - x_1, y - y_1, z - z_1\big) &= 0 \\ \implies \quad \alpha(x - x_1) + \beta(y - y_1) + \gamma(z - z_1) &= 0 \\ \implies \quad \alpha x + \beta y + \gamma z &= \mathcal{K}. \end{aligned}$$

The scalar product is thus instrumental in giving us the equation for the plane P with $a = \alpha$, $b = \beta$, $c = \gamma$, and $d = \mathcal{K}$.

This method of deriving the equation of a plane will be utilized in Sections 2.C and 5.D.

IV. A line in 3-space

The general equation of a line,

$$L = \left\{(x, y, z) : \frac{x - x_0}{a} = \frac{y - y_0}{b} = \frac{z - z_0}{c}\right\},$$

can be derived using analogous geometric reasoning to that used to deduce the plane equation. We need to know either

(a) two points on the line L, or

(b) one point on L and one vector parallel to L.

In the case of alternative IV(a), let (x_i, y_i, z_i), $i = 0, 1$, be the two given points on the line. As before, we construct the vector $\boldsymbol{u}$ directed from one point to the other by subtracting their respective coordinate components:

$$\boldsymbol{u} = \big(x_1 - x_0, y_1 - y_0, z_1 - z_0\big) = (\alpha, \beta, \gamma).$$

As the two points lie in the straight line L so too must the vector $\boldsymbol{u}$, as shown in Figure 1.7. In the alternative case IV(b), the vector $\boldsymbol{u}$ is already given so the above calculation is not needed and we can proceed with the next step.

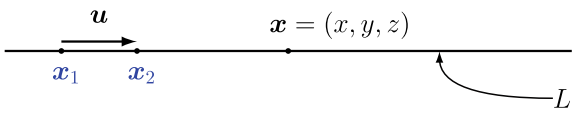


Figure 1.7 Vector $\boldsymbol{u}$ parallel to line L.

The equation of the line is most simply obtained by reasoning as follows: given a known point $\boldsymbol{x}_0 = (x_0, y_0, z_0)$ on L, then for an arbitrary point $\boldsymbol{x} = (x, y, z)$ to also be on L it must, by definition, be some distance away from $\boldsymbol{x}_0$ in the direction of $\boldsymbol{u}$. This is readily expressed by a simple vector addition equation

$$\boldsymbol{x} \;=\; \boldsymbol{x}_0 \;+\; t\,\boldsymbol{u}, \qquad t \in \mathbb{R}. \tag{1.7}$$

(fixed) starting point

scaling (continuous parameter)

direction of stepping

As indicated, this equation says that to determine an arbitrary point on the line $\boldsymbol{x}$ we begin at a convenient starting point $\boldsymbol{x}_0$ and continue in the direction $\boldsymbol{u}$ a (positive or negative) distance determined by the scalar $t \in \mathbb{R}$.

This simple vector equation is equivalent to the general line equation given earlier. We get the latter by splitting Equation (1.7) into its components and solving each component for the scalar variable t.

For later reference, we remark that a particularly important feature emerges from Equation (1.7), which is linear in the parameter t. If we treat each component individually as an equation expressing some function of t and take single-variable derivatives, we get three equations

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \alpha, \;\; \frac{\mathrm{d}y}{\mathrm{d}t} = \beta, \;\; \frac{\mathrm{d}z}{\mathrm{d}t} = \gamma.$$

Recombining these into a single vector equation, we arrive at the statement that the derivative with respect to the (line-generating) parameter t returns a vector which gives the direction of the line. In anticipation of later results, we refer to this as the equation of the *tangent vector*:

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{u} \quad \text{—the tangent vector.}$$

This last result is deceptively elementary. It underscores the very important fact that the first derivative with respect to the parameter that generates a curve in a higher dimensional space gives rise to a tangent vector. This will be demonstrated in Sections 5.A and 5.C , where the present straight line is generalized to a nonlinear curve.

V. The scalar triple product $\boldsymbol{u} \cdot (\boldsymbol{v} \times \boldsymbol{w})$

Let $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}$ be three non-parallel and non-coplanar vectors. These define the edges of a parallelepiped as shown in Figure 1.8.

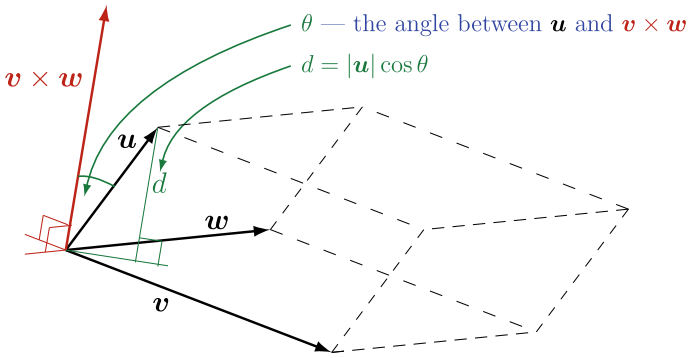


Figure 1.8 The $\boldsymbol{u}$, $\boldsymbol{v}$, $\boldsymbol{w}$ parallelepiped.

To form the scalar triple product, we first form the vector product of $\boldsymbol{v}$ and $\boldsymbol{w}$: $\boldsymbol{v} \times \boldsymbol{w}$, and then form the scalar product of that result with $\boldsymbol{u}$. The *magnitude* of the scalar triple product, which is found using II(i), is given by

$$\begin{aligned} |\boldsymbol{u} \cdot (\boldsymbol{v} \times \boldsymbol{w})| &= |\boldsymbol{u}||\boldsymbol{v} \times \boldsymbol{w}||\cos\theta| \\ &= |\boldsymbol{v} \times \boldsymbol{w}||\boldsymbol{u}||\cos\theta| \\ &= \underbrace{|\boldsymbol{v} \times \boldsymbol{w}|}\,\underbrace{||\boldsymbol{u}|\cos\theta|} \end{aligned}$$

area of the $(\boldsymbol{v}, \boldsymbol{w})$ parallelogram — perpendicular height, d

This gives the *volume of the parallelepiped* formed by the vectors $\boldsymbol{u}$, $\boldsymbol{v}$, and $\boldsymbol{w}$. If the vectors have the following component forms,

$$\begin{aligned} \boldsymbol{u} &= (a_1, a_2, a_3) &&= a_1\mathbf{i} + a_2\mathbf{j} + a_3\mathbf{k}, \\ \boldsymbol{v} &= (b_1, b_2, b_3) &&= b_1\mathbf{i} + b_2\mathbf{j} + b_3\mathbf{k}, \text{ and} \\ \boldsymbol{w} &= (c_1, c_2, c_3) &&= c_1\mathbf{i} + c_2\mathbf{j} + c_3\mathbf{k}, \end{aligned}$$

then, firstly, using the determinant expression in II(i), we have

$$\boldsymbol{v} \times \boldsymbol{w} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix} = (b_2c_3 - b_3c_2)\mathbf{i} + (b_3c_1 - b_1c_3)\mathbf{j} + (b_1c_2 - b_2c_1)\mathbf{k},$$

and consequently,

$$\begin{aligned}
&\boldsymbol{u}\cdot(\boldsymbol{v}\times\boldsymbol{w})\\
&=\big(a_1\mathbf{i}+a_2\mathbf{j}+a_3\mathbf{k}\big)\cdot\big((b_2c_3-b_3c_2)\mathbf{i}+(b_3c_1-b_1c_3)\mathbf{j}+(b_1c_2-b_2c_1)\mathbf{k}\big)\\
&=a_1(b_2c_3-b_3c_2)+a_2(b_3c_1-b_1c_3)+a_3(b_1c_2-b_2c_1)\\
&=\begin{vmatrix} a_1 & a_2 & a_3\\ b_1 & b_2 & b_3\\ c_1 & c_2 & c_3\end{vmatrix}.
\end{aligned}$$

Hence, the scalar triple product can be written succinctly in determinant form, but note that the notation *does not* mean that the determinant involves an absolute value! The determinant could be negative or positive; after all we are dealing here with vectors and angles. On the other hand, the *magnitude* of the scalar triple product, $|\boldsymbol{u}\cdot(\boldsymbol{v}\times\boldsymbol{w})|$, *does* involve an absolute value, which is taken after the determinant calculation is performed.

The scalar triple product and the interpretation of its magnitude as the volume of a parallelepiped play a central role in our discussion of multiple integrals in Section 4.H.

VI. The vector triple product $\boldsymbol{u}\times(\boldsymbol{v}\times\boldsymbol{w})$

As we noted on Page 4, the vector $(\boldsymbol{v}\times\boldsymbol{w})$ is perpendicular to both $\boldsymbol{v}$ and $\boldsymbol{w}$. Now suppose vector $\boldsymbol{u}$ is not coplanar with either $\boldsymbol{v}$ or $\boldsymbol{w}$. What happens if we form the vector cross product of vector $\boldsymbol{u}$ with $(\boldsymbol{v}\times\boldsymbol{w})$?

Following the same line of reasoning as above, the result will be a new vector which will be perpendicular to both $\boldsymbol{u}$ and $(\boldsymbol{v}\times\boldsymbol{w})$. Given that we have only three dimensions to play with (in $\mathbb{R}^3$), $\boldsymbol{u}\times(\boldsymbol{v}\times\boldsymbol{w})$ *must be a vector that lies in the plane defined by the original vectors* $\boldsymbol{v}$ *and* $\boldsymbol{w}$. Consequently, $\boldsymbol{u}\times(\boldsymbol{v}\times\boldsymbol{w})$ must be a linear combination of $\boldsymbol{v}$ and $\boldsymbol{w}$.

In fact, by twice applying the determinant formula for the cross product, it can easily be verified that

$$\boldsymbol{u}\times(\boldsymbol{v}\times\boldsymbol{w})=(\boldsymbol{u}\cdot\boldsymbol{w})\boldsymbol{v}-(\boldsymbol{u}\cdot\boldsymbol{v})\boldsymbol{w}.$$

■ Example 1.2:

Use the vector triple product to show that for an arbitrary vector $\boldsymbol{u}$

$$\mathbf{i}\times(\boldsymbol{u}\times\mathbf{i})+\mathbf{j}\times(\boldsymbol{u}\times\mathbf{j})+\mathbf{k}\times(\boldsymbol{u}\times\mathbf{k})=2\boldsymbol{u}.$$

Solution:

Applying the triple vector product to the first of the three terms on the left-hand side, we have

$$\mathbf{i} \times (\boldsymbol{u} \times \mathbf{i}) = (\mathbf{i} \cdot \mathbf{i})\, \boldsymbol{u} - (\mathbf{i} \cdot \boldsymbol{u})\, \mathbf{i} = \boldsymbol{u} - u_1 \mathbf{i},$$

which follows since $\mathbf{i}$ is a vector with magnitude 1 and $\mathbf{i} \cdot \boldsymbol{u} = u_1$. Consequently, the first term delivers the vector $\boldsymbol{u}$ itself minus a vector that only comprises the first component (lying in the x-direction). By symmetry, the second and third terms on the left-hand side of the given equation will similarly produce the vector $\boldsymbol{u}$ less a vector that only involves the y- and z-components of $\boldsymbol{u}$, respectively. Adding the three contributions gives the desired result,

$$3\boldsymbol{u} - u_1 \mathbf{i} - u_2 \mathbf{j} - u_3 \mathbf{k} = 3\boldsymbol{u} - \boldsymbol{u} = 2\boldsymbol{u}.$$

■

✍ **Mastery Check 1.2:**
For vectors $\boldsymbol{A} = a_1 \mathbf{i} + a_2 \mathbf{j} + a_3 \mathbf{k}$, $\boldsymbol{B} = b_1 \mathbf{i} + b_2 \mathbf{j}$, $\boldsymbol{C} = c_1 \mathbf{i}$, verify the vector triple product identity.

✍

The content of this section may seem elementary when applied to constant vectors and straight lines, but the concepts will prove to be quite important when generalized to multivariable scalar and vector function settings in which we deal with non-constant *vectors* and more general differential curves.

1.B Introduction to Sets

The aim with this book is to understand the workings of functions that depend on many variables. As such we need to be prepared to qualify and quantify the higher dimensional spaces on which the functions are defined: are those spaces finite? do they have holes? are the edges included? The need is greater when the functions are vector-valued and themselves occupy higher dimensional spaces. While the physical dimensions involved are limited to two or three, it is possible to visualize the spaces and so obtain whatever information is needed by visual means. This is a topic addressed in Section 1.E. In general, however, the spaces involved will not always be possible to

visualize. Consequently, we must rely on abstract mathematical descriptions that will assist us to nonetheless characterize the spaces involved. This is the rationale behind the present section. The topic concerned is set theory, which is itself an extensive branch of mathematics. Fortunately, only some elements of that subject are needed for our purposes.

We begin with some useful definitions. For more detailed information, it suffices for the reader to refer to standard texts on linear algebra. A good reference is [19].

Definition 1.1
Given that $\mathbb{R}^n = \mathbb{R} \times \mathbb{R} \times \cdots \times \mathbb{R}$ *is the set of all points* $\boldsymbol{x}$ *having* n *independent real components, then* $\boldsymbol{x} = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$ *(where* $x_i \in \mathbb{R}$*) defines a point in* n*-dimensional Cartesian space.*
Other notations in common use for a point in $\mathbb{R}^n$ *are:* $\underset{\sim}{x}$, $\vec{x}$, $\bar{x}$, *and* $\mathbf{x}$.

Example 1.3:

Define and illustrate the definitions of point sets in $\mathbb{R}^2$ and $\mathbb{R}^3$.

Solution:

First, recall our earlier statement about designating points in $\mathbb{R}^2$ and $\mathbb{R}^3$ in component form, (x, y, z). Then,

(a) the set of points in $\mathbb{R}^2$ is expressed as $\mathbb{R}^2 = \{(x, y) : x \in \mathbb{R}, y \in \mathbb{R}\}$; a single point with its defining pair of coordinates is shown in Figure 1.9(a);

(b) the set of points in $\mathbb{R}^3$ is denoted similarly as $\mathbb{R}^3 = \{(x, y, z) : x \in \mathbb{R}, y \in \mathbb{R}, z \in \mathbb{R}\}$; a single point with its defining triad of coordinates is shown in Figure 1.9(b).

■

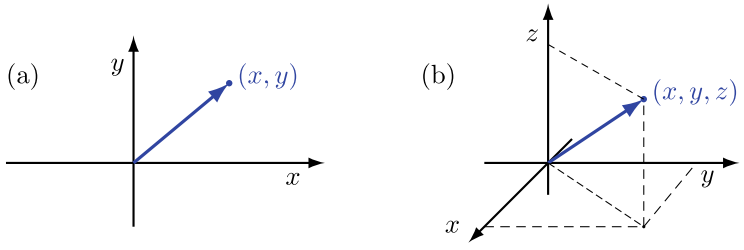


Figure 1.9 A point in (a) the 2D Cartesian plane and (b) the 3D Cartesian space.

It is not possible to provide a picture of $\boldsymbol{x} \in \mathbb{R}^n$ for $n > 3$ (nor $\mathbb{R}^n$ itself). However, this should not be a reason for concern as points in $\mathbb{R}^n$ behave mathematically the same as points in $\mathbb{R}^2$ and $\mathbb{R}^3$. That is, they follow the same set of rules. So it is enough to be familiar with points and point operations in $\mathbb{R}^2$ and $\mathbb{R}^3$, and then being able to generalize their properties. The most important point operations are listed below.

Vector algebra laws

Let $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}$.
At its most basic description, $\mathbb{R}^n$ is an example of a linear vector space which is characterized by the two properties of addition and scalar multiplication:

(a) $\boldsymbol{x} + \boldsymbol{y} = (x_1 + y_1, x_2 + y_2, \ldots, x_n + y_n) \in \mathbb{R}^n$.

(b) $\lambda \boldsymbol{x} = (\lambda x_1, \lambda x_2, \ldots, \lambda x_n) \in \mathbb{R}^n$.

As a direct generalization of the scalar product, Equation (1.4) of II(ii), points in $\mathbb{R}^n$ satisfy the so-called *inner product*,

(c) $\boldsymbol{x} \cdot \boldsymbol{y} = x_1 y_1 + \ldots + x_n y_n \in \mathbb{R}$ —$\mathbb{R}^n$ is called an *inner product space*.

Finally, there are the following generalizations to $\mathbb{R}^n$ of the two fundamental geometric measures:

(d) $|\boldsymbol{x}| = \sqrt{\boldsymbol{x} \cdot \boldsymbol{x}} = \sqrt{x_1^2 + \cdots + x_n^2}$ —the length of $\boldsymbol{x}$.

(e) $|\boldsymbol{x} - \boldsymbol{y}| = \sqrt{(x_1 - y_1)^2 + \cdots + (x_n - y_n)^2}$
—the distance between points.

With this distance property $\mathbb{R}^n$ is also a so-called *metric space*, since the distance between points is one measure or metric that allows a geometric characterization of a space.

Using the above definitions, one can prove the following fundamental relations satisfied by position vectors in $\mathbb{R}^n$. (See Example 1.4 and Mastery Check 1.3) These are useful in analysis to establish so-called order relations between vector quantities.

(f) Cauchy-Schwarz inequality:
$|\boldsymbol{x} \cdot \boldsymbol{y}| \leq |\boldsymbol{x}||\boldsymbol{y}|$; $\quad x_1 y_1 + \ldots + x_n y_n \leq \sqrt{x_1^2 + \ldots + x_n^2}\sqrt{y_1^2 + \ldots + y_n^2}$.

(g) Triangle inequality: $|\boldsymbol{x}+\boldsymbol{y}| \leq |\boldsymbol{x}|+|\boldsymbol{y}|$.

(h) The Cauchy-Schwarz inequality (f) means $-1 \leq \dfrac{\boldsymbol{x}\cdot\boldsymbol{y}}{|\boldsymbol{x}||\boldsymbol{y}|} \leq 1$.

Just as in $\mathbb{R}^2$ and $\mathbb{R}^3$, property (h) allows us to define an angle θ between vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ in $\mathbb{R}^n$ such that

$$\cos\theta = \frac{\boldsymbol{x}\cdot\boldsymbol{y}}{|\boldsymbol{x}||\boldsymbol{y}|}.$$

■ Example 1.4:

Prove the triangle inequality $|\boldsymbol{x}+\boldsymbol{y}| \leq |\boldsymbol{x}|+|\boldsymbol{y}|$:

$$\sqrt{(x_1+y_1)^2+\ldots+(x_n+y_n)^2} \leq \sqrt{x_1^2+\ldots+x_n^2}+\sqrt{y_1^2+\ldots+y_n^2}.$$

Solution:

We have, using the scalar product definition,

$$\begin{aligned} |\boldsymbol{x}+\boldsymbol{y}|^2 &= (\boldsymbol{x}+\boldsymbol{y})\cdot(\boldsymbol{x}+\boldsymbol{y}) \\ &= |\boldsymbol{x}|^2+|\boldsymbol{y}|^2+\boldsymbol{x}\cdot\boldsymbol{y}+\boldsymbol{y}\cdot\boldsymbol{x} \\ &= |\boldsymbol{x}|^2+|\boldsymbol{y}|^2+2\boldsymbol{x}\cdot\boldsymbol{y} \\ &\leq |\boldsymbol{x}|^2+|\boldsymbol{y}|^2+2|\boldsymbol{x}|.|\boldsymbol{y}| \quad \text{by Cauchy-Schwarz.} \end{aligned}$$

Thus $|\boldsymbol{x}+\boldsymbol{y}|^2 \leq \big(|\boldsymbol{x}|+|\boldsymbol{y}|\big)^2$, and by taking the square root of both sides of these positive quantities, we have our result. ■

✍ Mastery Check 1.3:

Prove the Cauchy-Schwarz inequality (f).

Hint: Consider the case $n = 2$ before tackling the general theorem. If you square $|\boldsymbol{x}\cdot\boldsymbol{y}|$ and $|\boldsymbol{x}||\boldsymbol{y}|$ and take the difference, you can argue that this difference is either zero or greater than zero, but never less than zero. This suggests that a proof might be possible by working backwards.

✍

Points and sets

In general $\mathbb{R}^n$, we can use vector algebra law (e), involving the distance between two points, $|\boldsymbol{x}-\boldsymbol{y}|$, to help generalize the "interval" concept to $\mathbb{R}^n$.

In $\mathbb{R}$, the inequality $|x-a| < \epsilon$ (which is equivalent to saying $a-\epsilon < x < a+\epsilon$) describes the set of all points $x \in \mathbb{R}$ which lie within ϵ of a on the real line. In $\mathbb{R}^n$, we have an analogous statement, but one involving a sphere rather than an interval:

Definition 1.2
Given $\boldsymbol{a} \in \mathbb{R}^n$*, an* **open sphere** $S_r(\boldsymbol{a}) \subset \mathbb{R}^n$ *centred at* $\boldsymbol{a}$ *and of radius* r *is the set of all points* $\boldsymbol{x} \in \mathbb{R}^n$ *that satisfy* $|\boldsymbol{x} - \boldsymbol{a}| < r$*:*

$$S_r(\boldsymbol{a}) = \{\boldsymbol{x} : \ |\boldsymbol{x} - \boldsymbol{a}| < r\}$$

for some $r \in \mathbb{R}$*. That is, the set of all points* $\boldsymbol{x} \in \mathbb{R}^n$ *which are no further than* r *from the given point* $\boldsymbol{a}$*.*

Remarks

* The open sphere is non-empty, since it contains $\boldsymbol{a}$, at least.
* In this context, $\boldsymbol{a}$ is called the *centre*, and r the *radius* of the open sphere.

The open sphere $S_r(\cdot)$ may now be used to define other point and set properties.

Definition 1.3
A point $\boldsymbol{x}$ *is called*

- *an* **interior point** *of a set* $M \subset \mathbb{R}^n$ *if there is an open sphere* $S_r(\boldsymbol{x}) \subset M$ *for some* $r > 0$*;*
- *an* **exterior point** *of a set* $M \subset \mathbb{R}^n$ *if there is an open sphere* $S_r(\boldsymbol{x}) \not\subset M$ *for some* $r > 0$*;*
- *a* **boundary point** *of a set* $M \subset \mathbb{R}^n$ *if for any* $r > 0$ *(no matter how small),* $S_r(\boldsymbol{x})$ *contains points in* M *and points not in* M*.*

These point definitions are illustrated in Figure 1.10. The reader should work through Example 1.5 and Mastery Check 1.4 to consolidate their understanding of these point definitions before going on to set-level concepts.

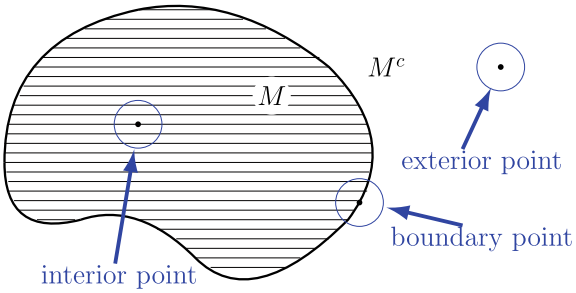


Figure 1.10 Interior, exterior, and boundary points to a set.

Example 1.5:

Let $M = \{(x, y) : 0 < x < 1, 0 < y < 1\}$. Draw a diagram of M on the Cartesian plane, showing the points $P_1(\frac{5}{6}, \frac{5}{6})$, $P_2(1, \frac{1}{3})$, and $P_3(-1, 1)$. Classify the points as either interior, exterior, or boundary.

Solution:

Figure 1.11 below shows the location of the points relative to set M.

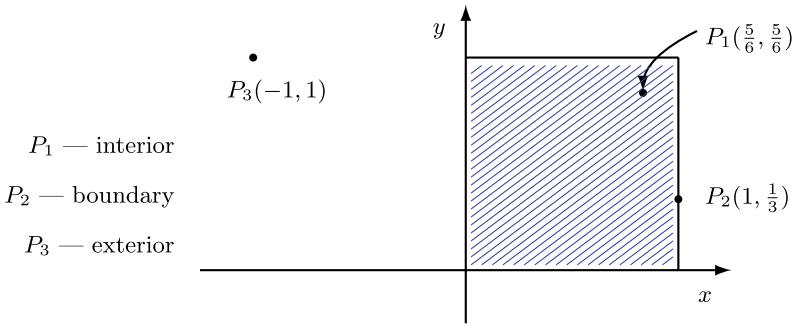


Figure 1.11 Points P_1, P_2, P_3 and set M.

Mastery Check 1.4:

Let $M = \left\{(x, y) : \dfrac{(x-1)^2}{4} + (y-1)^2 \leq 1\right\}$.

Draw a diagram of M showing the points $P_1(2, 1)$, $P_2(3, 1)$, and $P_3(-1, 2)$.

Classify the points as interior, exterior, or boundary.

We now establish a framework within which to categorize sets of points possessing common properties, according to Definition 1.3.

Definition 1.4

- *The set of all interior points of a set M is called the* **interior** *of M, and denoted* $\mathrm{Int}(M)$*:*

$$\mathrm{Int}(M) = \{\boldsymbol{x} : \boldsymbol{x} \in M \text{ and } S_r(\boldsymbol{x}) \subset M \text{ for some } r > 0\}.$$

- *The set of all points not in M is called the* **complement** *of M, and denoted M^c:*

$$M^c = \{\boldsymbol{x} : \boldsymbol{x} \notin M\}.$$

- *The set of all boundary points of a set M is called the* **boundary** *of M, and denoted ∂M.*

It follows from these definitions that $\mathrm{Int}(M^c) \subset M^c$, and if $\boldsymbol{x}$ is an exterior point to M, then $\boldsymbol{x} \in \mathrm{Int}(M^c) \subset M^c$.

The concept introduced in the next definition will play an important role in our analysis of multivariable functions.

Definition 1.5
A set M is called **open** *if it contains* **only** *interior points.*

Accordingly, a set M is an open set if for every point $\boldsymbol{x} \in M$ a positive radius r can be found such that $S_r(\boldsymbol{x})$ contains $\boldsymbol{x}$ and only other points in M. Also, only under the specific condition of set M being open is $\mathrm{Int}(M) = M$. Finally, an *open neighbourhood* of a point $\boldsymbol{a} \in M$ is an open set $W \subset M$.

Although we can utilize the notion of an open set to define a closed set (see Supplementary problem 1.11), it proves useful to invoke an independent concept to define a closed set, that of so-called *limit points*. In this way, we are able to introduce a concept that is central to our forthcoming discussion on limits.

Definition 1.6
A point $\boldsymbol{a}$ of a set M is said to be a **limit point** *of M if every open sphere $S_r(\boldsymbol{a})$ contains at least one point of M different from $\boldsymbol{a}$.*

This means that there are points in M that are arbitrarily close to $\boldsymbol{a}$. Hence, in approaching $\boldsymbol{a}$ from within M, we are always guaranteed to encounter

other points in M. It follows as an application of this important note that all points in an open interval on the real line are limit points.

Introducing limit points not only allows a convenient definition of a closed set but also useful as it allows us to prove a number of facts about closed sets, some of which are included as exercises at the end of this chapter. First the definition:

Definition 1.7
A set M of $\mathbb{R}^n$ is said to be **closed** *if it contains all its limit points.*

And, intimately related to this definition is the concept of set *closure*. For our purposes we invoke the following definition.

Definition 1.8
The **closure** *of a set M, denoted $\overline{M}$, is the union of $Int(M)$ with its boundary:*

$$\overline{M} = Int(M) \cup \partial M = \{\boldsymbol{x} : \boldsymbol{x} \in Int(M) \text{ or } \boldsymbol{x} \in \partial M\}.$$

Alternatively, $\overline{M}$ can be defined as the union of M and the set of all its limit points, L_M. It can be shown (see Supplementary problem 1.11) from this definition that (a) a closed set M is equal to its closure $\overline{M}$, and (b) that a set is closed *if and only if* it contains its boundary. Along this same line of thought, an alternative consequence of Definitions 1.5–1.8 is that the boundary of a set M contains those points that are in common with the closure of a set M and the closure of its complement, M^c. In other words,

$$\partial M = \{\boldsymbol{x} : \boldsymbol{x} \in \overline{M} \cap \overline{M^c}\}.$$

Next is the concept of set *boundedness*. This arises in the context of both differential and integral calculus of multivariable functions. As the term suggests, it essentially relates to a set being limited in geometric extent.

Definition 1.9
A set $M \subset \mathbb{R}^n$ is called **bounded** *if there exists a $K \in \mathbb{R}$ such that $|\boldsymbol{x}| < K$ for all $\boldsymbol{x} \in M$.*

Definition 1.5 is involved in the definition of derivatives in Chapter 2, while Definitions 1.4–1.9 are invoked in Chapter 3 and 4, although they are also used implicitly elsewhere.

The next definition is most useful when applied together with function behaviour to establish conditions that guarantee certain consequent function properties. We shall see this employed in practice in Sections 3.B, 4.A, and 4.D, but also 1.C.

Definition 1.10
A set $M \subset \mathbb{R}^n$ *is called* **compact** *if it is both* **closed** *and* **bounded**.

Example 1.6:

(a) Let $M = \{(x, y) : 0 < x < 1, 0 < y < 1\}$. What is the set ∂M?

(b) Is M bounded? If it is, find a number K such that $|\boldsymbol{x}| < K$ for all $\boldsymbol{x} \in M$?

(c) Is M compact? If it is not, write down the closure $\overline{M} = M \cup \partial M$.

Solution:

(a)

$$\partial M = \left\{(x, y) : (x, y) = \begin{matrix}(x, 0)\\(x, 1)\end{matrix}\right\} \text{ for } 0 \le x \le 1, = \left.\begin{matrix}(0, y)\\(1, y)\end{matrix}\right\} \text{ for } 0 \le y \le 1.\Big\}.$$

∂M thus comprises all points on the edges of the square (Figure 1.12).

For $|\boldsymbol{x}| \in M$, we must have $|\boldsymbol{x}| = \sqrt{x^2 + y^2} < \sqrt{1^2 + 1^2} = \sqrt{2}$.
(b) So, with $K = \sqrt{2}$, M is bounded.

(c) Since M is open (it doesn't contain boundary points), it is not compact.

However, $M \cup \partial M = \bar{M}$ is compact.
$\bar{M} = \left\{(x, y) : 0 \le x \le 1, 0 \le y \le 1\right\}$.

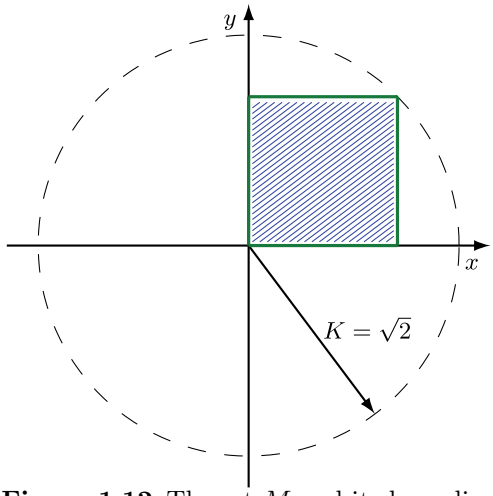


Figure 1.12 The set M and its bounding domain.

✍ Mastery Check 1.5:

Let $M = \left\{(x, y) : \dfrac{(x-1)^2}{4} + (y-1)^2 \leq 1\right\}$.

What is the set ∂M? Is M bounded? If it is, find a number K such that $|\boldsymbol{x}| < K$ for all $\boldsymbol{x} \in M$? Is M compact? If it is not, write down the closure $\overline{M} = M \cup \partial M$. Draw a diagram showing M, ∂M, and K.

✍

Lastly, to ensure a firm foundation for function concepts such as continuity and derivatives, we require the point sets on which functions are defined to be *connected*. In Sections 2.B and 5.C, this underlying set property will be applied (or assumed) in practice. For now, we can be satisfied with the following (for our purposes) equivalent definitions.

Definition 1.11
A set $M \subset \mathbb{R}^n$ is said to be **connected**

- *if M cannot be represented as the union of two or more disjoint open subsets of $\mathbb{R}^n$ (subsets A and B are disjoint if $A \cap B = \emptyset$); or*
- *if any two points $\boldsymbol{x}, \boldsymbol{y} \in M$ can be joined by a polygonal "curve" lying entirely in M (a polygonal "curve" is comprised of a finite number of end-to-end contiguous, straight line segments).*

For example, the set $M = \{x \ : \ 0 \leq x \leq 1\}$ is connected, while the set $S = \{x : x \in (0, 1) \cup (2, 3)\}$ is not a connected set. It can be shown that every open interval on the real line is an open connected set. By extension, using the distance function as the operational measure, it can be argued that every open disc is an open connected subset of $\mathbb{R}^2$, and every open sphere is an open connected subset of $\mathbb{R}^3$.

1.C Real-Valued Functions

Basic concepts and definitions

In Chapters 2, 3, and 4, we focus attention almost exclusively on scalar-valued functions of many variables. Then in Chapter 5, we extend the ideas developed in the earlier chapters to treat vector-valued functions. In both con-

texts, the following introduction to fundamental properties of single-variable and multivariable functions is invaluable. To start, we introduce some more notation. Moreover, we introduce a pictorial view of what functions do.

Definition 1.12
Consider a real-valued function f of n variables, where $n \geq 1$.
The **domain** *D_f of f is the set of all values of $\boldsymbol{x} \in \mathbb{R}^n$ for which f is defined (that is, for which f makes sense).*
The **range** *R_f of f is the set of all possible values of $y = f(\boldsymbol{x}) \in \mathbb{R}$ for all $\boldsymbol{x} \in D_f$.*

In our multivariable setting, $\boldsymbol{x} \in \mathbb{R}^n$ is the independent multivariable and $y \in \mathbb{R}$ is (still) the dependent scalar variable. It is common to find the following terminology used in textbooks. The independent variable, here $\boldsymbol{x} \in \mathbb{R}^n$, is sometimes referred to as the *pre-image* of y, while the dependent variable, here $y \in \mathbb{R}$, is called the *image* under f. The function f is alternatively referred to as a *mapping* from one set to another; or f is referred to as an *operation* that takes a point, here $\boldsymbol{x}$, to give a point y; or f is a *rule* that associates y with a point $\boldsymbol{x}$.

As far as mathematical notation is concerned, the mapping under f is either described *pointwise* (taking a point $\boldsymbol{x}$ and producing a value y):

$$f : \boldsymbol{x} \longmapsto y$$

or *set-wise* (mapping a set D_f to a set R_f):

$$f : D_f \subseteq \mathbb{R}^n \longrightarrow R_f \subseteq \mathbb{R}.$$

Both denotations will be used in this book.

In single-variable calculus, we have the following scenario:

Suppose $y = f(x)$. The Cartesian *graph* of f is the set of ordered pairs $\{(x, y = f(x))\} \in \mathbb{R}^2$ with $x \in D_f$, $y \in R_f$. This is shown in Figure 1.13 where the independent variable $x \in D_f$ and dependent variable $y \in R_f$ are plotted on mutually orthogonal axes.

This way of visualizing functions of one variable was introduced in the early 17th century by René Descartes [20], and is named the Cartesian representation in recognition. It is quite a useful means of illustrating function dependence and other function properties, especially for functions of one or two variables.

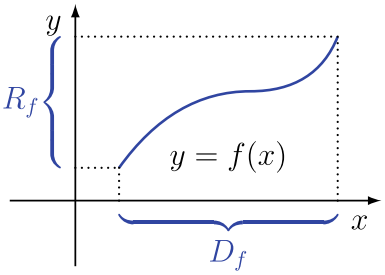


Figure 1.13 The Cartesian graph of $y = f(x)$.

The Cartesian diagram description ceases to be possible, however, for functions of more than two variables. For the latter cases, one resorts to simply considering a set-mapping picture, which nevertheless symbolizes the operational aspect of a function. The latter being a rule or a process that takes a point x from one set and associates it with a point y in another set. For the case $y = f(x)$, the depiction is a simple interval-to-interval map as shown in Figure 1.14.

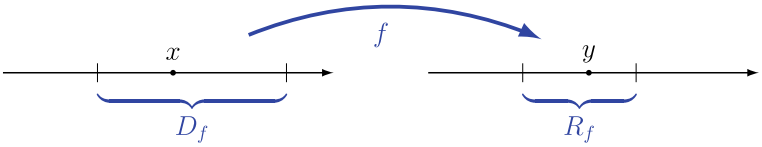


Figure 1.14 The set map of $D_f \subset \mathbb{R} \longrightarrow R_f \subset \mathbb{R}$.

For real-valued functions of many variables: $y = f(\boldsymbol{x}) = f(x_1, x_2, \ldots, x_n)$, the corresponding schematic representation is shown in Figure 1.15. The left-hand x-interval in the single-variable calculus case is replaced by an abstract $\boldsymbol{x}$-region for the multivariable case. For scalar-valued functions, the right-hand half of the schematic remains the same, represented by an interval on the real line.

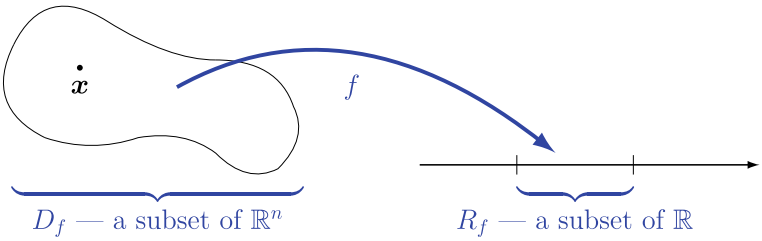


Figure 1.15 The set map of $D_f \subset \mathbb{R}^n \longrightarrow R_f \subset \mathbb{R}$.

Example 1.7:

Determine the domain and range of the function $f(x, y) = \sqrt[3]{y - x^2}$.

Solution:

We first recall from single-variable calculus that the real-valued function $s = t^{1/3}$ is defined for all t, since

$$\begin{aligned} &\text{if } t > 0, \text{ then } s > 0; \\ &\text{if } t < 0, \text{ then } s < 0; \\ &\text{if } t = 0 \text{ then } s = 0. \end{aligned}$$

In addition, we readily see that $y - x^2$ can take any real value. Combining these facts we deduce that f is defined everywhere. This implies that $D_f = \mathbb{R}^2$ and also that $R_f = \mathbb{R}$.

■

Example 1.8:

Determine the range and domain of $f(x, y) = \sin^{-1}(x^2 + y^2)$.

Solution:

Before considering this multivariable function, recall from single-variable calculus that within the intervals $-\dfrac{\pi}{2} \le z \le \dfrac{\pi}{2}$ and $-1 \le w \le 1$,

$$z = \sin^{-1} w \iff w = \sin z.$$

The graphs of these *inverse* functions, $\sin^{-1}$ and sin, are shown in Figure 1.16.

Note that in the present example $w = x^2 + y^2 \ge 0$, and therefore so too is $z \ge 0$. Consequently,

$$|w| \le 1 \implies |x^2 + y^2| \le 1 \implies 0 \le x^2 + y^2 \le 1.$$

This defines the unit disc in the xy-plane. That is, D_f is the unit disc (the unit circle and its interior).

Similarly, $|z| \le \dfrac{\pi}{2} \implies 0 \le z \le \dfrac{\pi}{2}$ since $z \ge 0$. So, $R_f = \left[0, \dfrac{\pi}{2}\right]$.

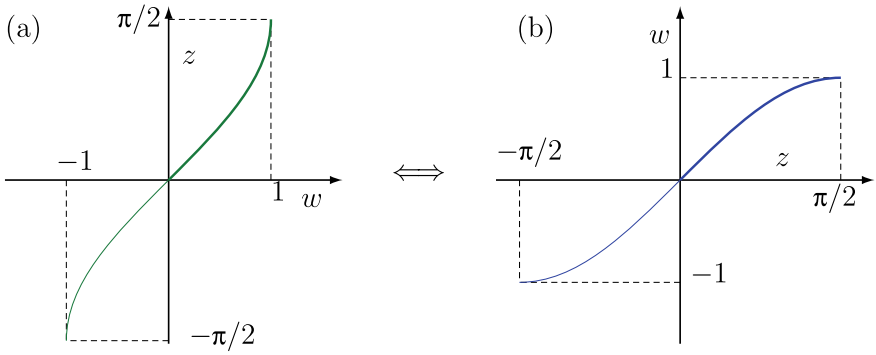


Figure 1.16 Graphs of the functions (a) $z = \sin^{-1} w$ and (b) $w = \sin z$.

■

✍ Mastery Check 1.6:

Find the (implied) domain and range of the following functions:

1. $f(x) = \sqrt{16 - x^4}$;
2. $f(x) = \dfrac{3 - x^2}{1 + x^2}$;
3. $\mathrm{gd}(x) = \sin^{-1}\big(\tanh(x)\big)$;
4. $f(x, y) = \sqrt{9 - x^2 - y^2}$;
5. $f(x, y) = \ln(x - y)$;
6. $f(x, y, z) = \ln(|z - x^2 - y^2|)$;
7. $f(x, y) = \ln(2 - e^{x^2+y^2})$.

(The function $\mathrm{gd}(x)$ is known as the Gudermannian function.)

✍

Limits and continuity

To lay the foundation for the next chapter's discussion on differentiation of multivariable functions, in this section we provide a brief review of the calculus for functions of one variable. One essential condition for differential calculus is that of *function continuity*. For multivariable functions this will be discussed in detail in Section 2.B. However, since the conditions underpinning continuity of a function of one variable are simpler to define and verify in practice while nevertheless being conceptually similar, we start with those fundamental concepts.

Function continuity is defined in terms of *limit* processes. In order to investigate such processes, we first need to guarantee their feasibility. This amounts to answering the following questions: What does it mean to take a limit and when is it possible to do so?

In Section 1.B, it was written that a point $\boldsymbol{a}$ of a set M is a limit point if any open sphere, no matter how small in radius, centred on that point contains

only points of M, apart from $\boldsymbol{a}$ itself. A particularly important application of this definition has shown that all points x of an open interval I on the real line are limit points. Moreover, open intervals of the real line are examples of open connected sets. From these facts, one concludes that open intervals of the real line contain no gaps. We thus imagine an open interval as being a *point set continuum* in the sense that we may move smoothly from one real value of the open interval to another without ever leaving the interval or encountering any holes. This property lays the foundation of and gives credibility to the mathematical expression: $x \to a$, which denotes the so-called *limit* process of the variable x "approaching" a fixed point a within an interval continuum on the real line. To be more precise, the properties possessed by an open interval give justification to the *direction-specific* limit expressions, $x \to a^-$ and $x \to a^+$, as meaning, respectively, the limit processes of approaching a fixed point a on the real line from "below" $(x < a)$ and from "above" $(x > a)$.

Intrinsic to these informal statements of approach to a point lies the often unstated—or at best *under*stated—understanding that it is *the approach process* itself that is of primary importance and not whether the final destination, or objective point, a, is reached. For example, to demonstrate the limit process $x \to 0^+$, we might consider, say, the following discrete sequence of positive x values: $\left\{1, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}, \ldots, \frac{1}{10}, \ldots, \frac{1}{100}, \ldots\right\}$, where each term in the sequence is smaller than its predecessor and the terms approach the value of zero, but 0 itself is not included in this sequence.

Turning now to the implications for a single-variable function defined on an interval domain $D_f \subset \mathbb{R}$, we shall see that the different approaches $x \to a^-$ and $x \to a^+$ for $x \in D_f$ can have different consequences, *independent of whether or not* $a \in D_f$. Meanwhile, we take explicit advantage of the idea of sequence sampling to define what is termed a *one-sided limit* (either $x \to a^+$ or $x \to a^-$).

Definition 1.13
A finite number A^+ (A^-) is called the one-sided limit of a function f as $x \to a^+$ $(x \to a^-)$ if, for ***any*** *sequence*

$$\{x_1, x_2, x_3, \ldots, x_n, \ldots\} \in D_f \quad s.t. \left\{ \begin{array}{c} a < x_{n+1} < x_n \\ (x_n < x_{n+1} < a) \end{array} \right\} \quad \forall\, n,$$

converging to a, the corresponding sequence

$$\Big\{f(x_1), f(x_2), \ldots, f(x_n), \ldots\Big\} \quad \textit{converges to} \quad A^+\,(A^-).$$

This one-sided limit is denoted $\lim\limits_{x \to a^+} f(x)$ $\left(\lim\limits_{x \to a^-} f(x)\right)$.

It follows from this definition that the above *direction-specific* processes, called *one-sided limits*, open up the possibility for two, potentially distinct, values of f: A^-, as $x \to a^-$ and A^+, as $x \to a^+$, respectively.

For instance, returning to the simple example above, suppose that $f(x) = 1/x$, then with the above sequence of x values, $\lim_{x\to a^+} f(x)$ would return the sequence $\{1, 2, 3, 4, 5, \ldots, 10, \ldots, 100, \ldots\}$. Notice that, in this example, $x = 0$ is not in the domain of f since $1/0$ is not defined. Nevertheless, the x values in the given sequence are perfectly legitimate, and so the limit process, with this well-defined set of x values, makes perfect sense, in terms of a legitimate mathematical query. Its implications are, of course, another matter, to be discussed below. Now consider the limit $x \to 0^-$, *i.e.*, approaching 0 from below. Here we might imagine a different (again non-unique) sequence of values x: $\{-1, -\frac{1}{2}, -\frac{1}{3}, -\frac{1}{4}, -\frac{1}{5}, \ldots, -\frac{1}{10}, \ldots, -\frac{1}{100}, \ldots\}$, where each term in the sequence is again smaller in magnitude than its predecessor and the terms again approach the value of zero, but this time from the negative direction; again, the value 0 is not included. Adopting this sequence, assuming $f(x) = 1/x$ as before, we find $\lim_{x\to a^-} f(x)$ returns the corresponding sequence in R_f: $\{-1, -2, -3, -4, -5, \ldots, -10, \ldots, -100, \ldots\}$. This sequence, while identical *in magnitude* to the previous sequence of f values, clearly tends towards a very different outcome (see the case $x = b$ in Figure 1.17(b)). This brings us to the following very important statement.

Definition 1.14
A function is said to possess a finite limit, A, at an interior point a of its domain $D_f \subset \mathbb{R}$, if both direction-specific *limits, approaching a from below ($x < a$) and from above ($x > a$), exist (**are finite**) and are equal. That is,*

$$\underbrace{\lim_{x\to a^-} f(x)}_{\left\{\begin{array}{c}\textit{left-hand-side}\\ \textit{limit of } f(x)\end{array}\right\}} = \underbrace{\lim_{x\to a^+} f(x)}_{\left\{\begin{array}{c}\textit{right-hand-side}\\ \textit{limit of } f(x)\end{array}\right\}} = A.$$

The equality of the two single-sided limits is summarized in the single statement

$$\lim_{x\to a} f(x) = A.$$

If either single-sided limit does not exist or if both exist but are not equal, then we say that the limit does not exist. In our simple explicit example, neither one-sided limit exists, as well as being mutually diverging, and so no limit exists in that case.

The definition explicitly assumes that $a \in D_f$ is in the interior of the given domain interval; this certainly allows the left-hand and right-hand limits to be well defined. However, if instead the domain were "punctured", that is, that it excluded just the point a, the one-sided limits in Definition 1.14 would still be feasible and so a limit may still exist (see the right-hand panel of Figure 1.17). On the other hand, if a were an endpoint of the domain interval, then only one of the two single-sided limits could possibly be evaluated. In that case, whether the limit exists depends solely on whether that one single-sided limit exists. Example 1.9 and Figure 1.17 aim to illustrate some, but not all, possible scenarios.

For future reference (Chapter 2), if $f(x)$ has limit A as $x \to a$, then the function $\alpha(x) = f(x) - A$ is said to be *infinitesimal* at $x = a$ and

$$f(x) = A + \alpha(x), \qquad \text{with} \qquad \lim_{x \to a} \alpha(x) = 0.$$

This definition doesn't specify the rate at which $\alpha(x)$ goes to zero. However, the rate can be determined by comparing α to another function. For example, $\alpha(x)$ is said to be a higher-order infinitesimal compared to $\beta(x)$, if $\dfrac{\alpha(x)}{\beta(x)} \to 0$ as $x \to a$. It is often convenient to employ as comparison functions $\beta(x) = (x - a)^m$ for some integer m. The integer m for which the ratio $\dfrac{\alpha(x)}{(x-a)^m}$ tends to a finite, nonzero value as $x \to a$, is said to be the order of the infinitesimal. We shall use these concepts to advantage in Section 2.D.

The limit considerations in Definition 1.14, existence and equality, are distinct from the question of what value f *actually* takes at $x = a$. The relationship between the limit values and $f(a)$ is outlined in the next definition.

Definition 1.15
A function is said to be **continuous** *at an interior point a of its domain $D_f \subset \mathbb{R}$ if*

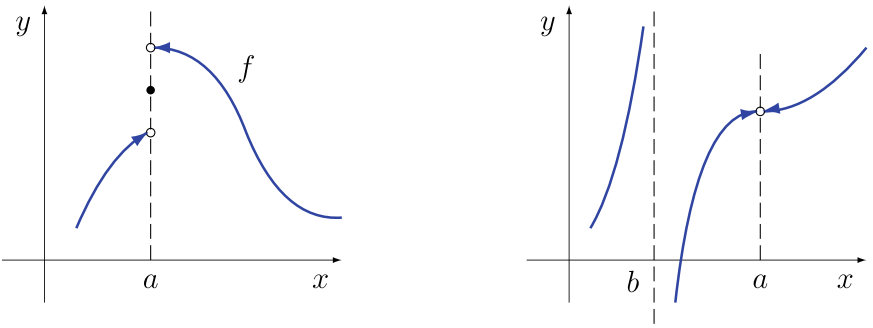
$$\lim_{x \to a} f(x) = f(a).$$

If either the limit fails to exist or the equality not satisfied, then f is said to be discontinuous at a.

Definition 1.15 thus stipulates that for function continuity, the common limit value, the aforementioned A in Definition 1.14, must also equal the value of the function f at $x = a$, $f(a)$. Of course, for function continuity a itself must now be a point in the domain of f, either as an interior point or as an endpoint.

The following example demonstrates graphically some different circumstances under which a limit of a function exists or does not exist, and how these relate to the left and right limits. Note the sole case of the function value actually being specified (solid dot) in the left-hand graph in Figure 1.17. Is either function continuous at a?

Example 1.9:



The limit does not exist at $x = a$.

The limit *does* exist at $x = a$, not at b.

Figure 1.17 When does a limit exist?

Following on from the two preceding definitions and subsequent discussion, we are brought to an important theorem on continuity at a point.

Theorem 1.1
A function f is continuous at an interior point a if and only if

$$\lim_{x \to a^-} f(x) = \lim_{x \to a^+} f(x) = f(a).$$

It might surprise the reader to know that a more practical mathematical restatement of Definition 1.15 (and similarly Theorem 1.1) takes the form of an implication involving a pair of inequalities. For *any* arbitrarily small positive

quantity ϵ, if a correspondingly small positive number δ, which may depend on ϵ, can be prescribed so that

$$0 < |x - a| < \delta,\ x, a \in D_f \quad \Longrightarrow \quad |f(x) - A| < \epsilon,\ \text{for some } \delta = \delta(\epsilon),$$

then the limit of f exists as $x \to a$ and is equal to A. While it may not appear so, this is actually a useful mathematical formulation that can be invoked in practice to prove the existence of a function limit or of function continuity. Graphically, this implication of inequalities can be represented as in Figure 1.18 below.

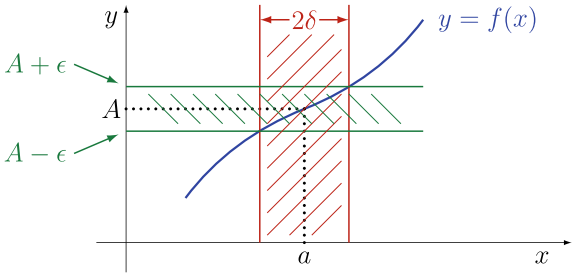


Figure 1.18 The ϵ–δ condition.

The schematic and the implication on which it is based can be interpreted as follows: if a certain degree of accuracy, $\epsilon > 0$, was specified, no matter how small, for finding the value of $f(x)$ close to A, then for this accuracy to be upheld x itself must be within $\delta > 0$ of the point a. Typically, the choice of δ will depend on ϵ. If ϵ is reduced then δ would also need to be reduced; reducing the width of the green strip implies that the red strip would also need to be reduced. The restriction imposed on x values is a sufficient condition for the restriction of f values. This formulation of a limit statement may be extended to reflect the condition of continuity by replacing A with $f(a)$. As will be seen in Section 2.B, the formulation can also be extended to a multivariable setting using the general distance formula. Finally, the formulation may be used to prove a number of results involving limits (addition, multiplication, division, etc. of limits) which are valid more generally. The reader is referred to the limit laws listed on Page 66 in Section 2.B.

The notion of continuity addressed in Definition 1.15 and Theorem 1.1 applies to an isolated point a in the domain of f, *i.e.*, they are valid pointwise. However, the concept has much greater significance and value if it can be extended to an open, connected subset of the function domain. In this case, we have the following definition.

Definition 1.16
A function f that is continuous at every point of a subset, D, of its domain $D \subset D_f \subset \mathbb{R}$, is said to be **continuous** *over that subset.*

Of course, the subset D could be the whole of the domain D_f.

Although we have been speaking of a single function, other functions may also be defined and continuous on the same interval. As certain results can be proved to apply more generally than for any specific function, it is convenient to introduce here a collective notation for the set of *all* continuous functions defined on a given interval D. We denote this set by $C(D)$ and refer to its members by the usual set member statement: $f \in C(D)$. The idea of collective sets of functions will be generalized in Section 2.H to represent those continuous functions whose derivatives are also continuous.

As a case in point, the following is a theorem that is applicable to any continuous function defined on a compact (closed and bounded) set. Although specifically expressed here in terms of single-variable functions defined on an interval, we will see the theorem restated in a multivariable setting in Section 3.B, where its usefulness will also be demonstrated. Its significant value will be further demonstrated in Sections 4.A and 4.B. For now, the reader should just note that the theorem combines the conditions of function continuity and domain compactness to deduce a very important function property.

Theorem 1.2
Let $f \in C(D)$ be any continuous function defined on a closed and bounded interval $D \subset D_f \subset \mathbb{R}$. Then f attains an absolute maximum and an absolute minimum value in D. That is, there exist points $x_L \in D$ and $x_U \in D$ such that

$$f(x_L) \leq f(x) \leq f(x_U) \text{ for all } x \in D.$$

A moment's thought and possibly some simple sketches will make this theorem intuitively obvious, which does not detract from its significance.

In later chapters, the ideas expressed above will be developed further and extended to higher dimensional cases as required. For the present, we close this discussion with a short catalogue of well-established results that can assist us in evaluating limits for single-variable and, in some cases, multivariable functions. Three of the squeeze relations listed below are featured in Figure 1.19. Example 2.5 demonstrates how they may be applied in practice.

Some useful standard limits:

$$* \lim_{x\to 0} \frac{\sin x}{x} = 1. \qquad * \lim_{x\to\infty} \frac{\ln x}{x^\alpha} = 0 \quad \text{for constant } \alpha > 0.$$

$$* \lim_{x\to 0} \frac{\tan x}{x} = 1. \qquad * \lim_{x\to 0} x^\alpha \ln x = 0 \quad \text{for constant } \alpha > 0.$$

$$* \lim_{t\to 0} \frac{\sin(xt)}{t} = x. \qquad * \lim_{t\to 0} \frac{\cos t - 1}{t} = 0.$$

Some useful squeeze relations:

(a) $\sin x < x < \tan x, \quad 0 < x < \dfrac{\pi}{2}.$

(b) $x < \mathrm{e}^x - 1 < \dfrac{x}{1-x}, \quad 0 < x < 1.$

(c) $\dfrac{x}{1+x} < \ln(1+x) < x$, for $x > -1, \neq 0.$

(d) $\mathrm{e}^x > 1 + x \quad \forall x \neq 0.$

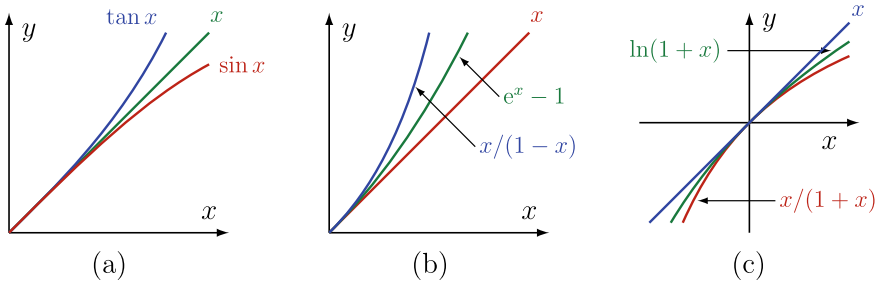


Figure 1.19 Graphs of various squeeze relations relative to $y = x$.

The ordinary or 1D derivative

The concepts reviewed thus far give insight into some of the qualitative properties of functions, but on their own they give limited information on function behaviour. The continuity condition effectively says that the graph of a continuous function may be drawn on paper without lifting one's pen, but it does not inform us if or where the function has kinks or cusps, or is increasing or decreasing. Theorem 1.2 informs us that a continuous function defined on a closed and bounded domain attains a maximum and a minimum, but it does not tell us where in the domain the maximum and minimum occur, nor does it tell us their values. These and other quantitative questions are answered with help of the derivative. For a single-variable function, the derivative measures the rate of change of that function at a specific point in the domain.

Since the derivative carries a sign, it also indicates the direction in which the function is headed. More specifically, the derivative, if it can be evaluated, gives the *slope* of the function at that point. As with the properties already reviewed, the derivative *at a point* is only defined by a *limit process*. It is not at all the case that one may simply "read off" the slope from a graph. Instead, as explained below, one considers a limiting sequence of special *linear approximations*.

The discussion below is useful groundwork for the more involved case of differentiation of functions of several variables. Not only is there a connection between the one- and the many-variable cases, the single-variable case is illuminative in that it may be readily illustrated on a 2D graph.

Consider the function $f : \mathbb{R} \to \mathbb{R}$ defined on a domain interval D_f as shown by the blue curve in Figure 1.20. In saying that f is differentiable at a point $x_0 \in D_f$ we mean that *geometrically* there exists a finite slope line that is tangent to the graph of $f(x)$ at x_0 (red line in Figure 1.20). The derivative of f *being* the slope of this tangent line. This quantitative measure is obtained by considering the limit of a sequence of secant lines, straight lines intersecting the graph at two points. The sequence of secant lines becoming better linear approximations to the curve as the two points get closer together. The slopes of these lines, which are equal to the slopes of the chords joining the two intersecting points, are calculated by taking ratios of differences in function values $\Big(f(x_0 + h) - f(x_0)\Big)$ to differences in x-values $\big((x_0 + h) - (x_0) = h\big)$. The secant lines are represented in Figure 1.20 by the thin black lines intersecting the graph at two points; one such pair of points, $(x_0, f(x_0))$ and $(x_0 + h, f(x_0 + h))$, is indicated. The mathematical statement of the limit process as $h \to 0$ is given in Definition 1.17.

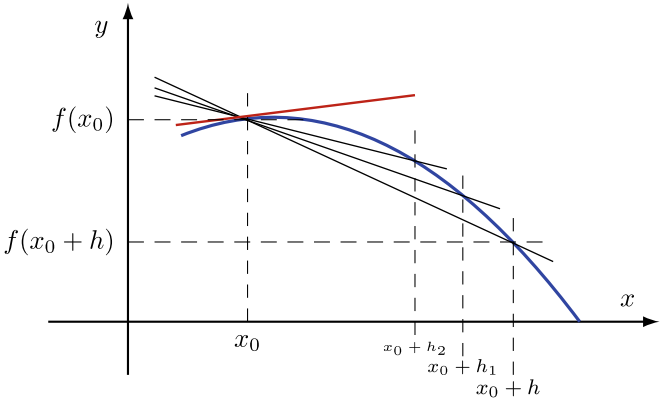


Figure 1.20 The graph of $y = f(x)$; a sequence of secant lines for $h > h_1 > h_2$; and the tangent line in the limit $h \to 0$.

Definition 1.17
Let $f \in C(D_f)$ be continuous on the open and connected domain $D_f \subset \mathbb{R}$ with open interval $(x_0, x_0 + h)$, a subset of D_f.
If the limit $\lim_{h\to 0} \dfrac{f(x_0+h)-f(x_0)}{h}$ *exists, it is called the* **derivative of f at x_0**, *and we write*

$$\left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_0} = f'(x_0) = \lim_{h\to 0} \frac{f(x_0+h)-f(x_0)}{h},$$

where $\left.\dfrac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_0}$ *is the* **slope** *of the tangent line to the* **graph** *of f at the point $\big(x_0, y_0 = f(x_0)\big)$.*
Equivalently, we may write

$$\left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_0} = \lim_{x\to x_0} \frac{f(x_0)-f(x)}{x_0-x};\ (x_0, x) \subset D_f.$$

Example 1.10:

From first principles, Definition 1.17, evaluate the derivative of the polynomial function $f(x) = x^3 - 6x^2 + 9x + 1$.

Solution:

This is an example of a nice function whose derivative exists everywhere in its domain $\mathbb{R}$.
To evaluate the limit in Definition 1.17, we first need $f(x+h) = (x+h)^3 - 6(x+h)^2 + 9(x+h) + 1$ and then we need to determine the ratio of the differences in function values to the difference in x-values, namely h:

$$\begin{aligned}\frac{f(x+h)-f(x)}{h} &= \frac{3x^2h + 3xh^2 + h^3 - 12xh - 6h^2 + 9h}{h} \\ &= 3x^2 - 12x + 9 + \left(3xh - 6h + h^2\right).\end{aligned}$$

Consequently, in the limit $h \to 0$ only the first three terms survive, the terms in the parentheses are at least proportional to h and vanish in the limit. This gives

$$f'(x) = 3x^2 - 12x + 9,$$

which is defined for all $x \in \mathbb{R}$.

A considerable amount of information can be extracted from this expression that was not immediately obvious from $f(x)$ itself. For instance, with a slight rewrite,

$$f'(x) = 3(x-1)(x-3),$$

we see that $f'(x)$ is zero at two points, $x = 1$ and $x = 3$. These are points where the function has a horizontal tangent and correspond to points where $f(x)$ is a local maximum $f(1) = 5$ and local minimum $f(3) = 1$, respectively.

We can also see that for $x < 1$ and for $x > 3$, the derivative is always positive, and hence the function is increasing on those semi-infinite intervals. For $1 < x < 3$, the derivative is negative and hence the function is decreasing in that interval. These features are shown in Figure 1.21.

■

Naturally, many differentiation laws or rules have been devised, and many explicit results derived for a large assortment of functions of one variable. This store of knowledge makes it largely unnecessary to apply the limit definition in most cases. We list without proof the major differentiation laws, which are assumed throughout the rest of the book.

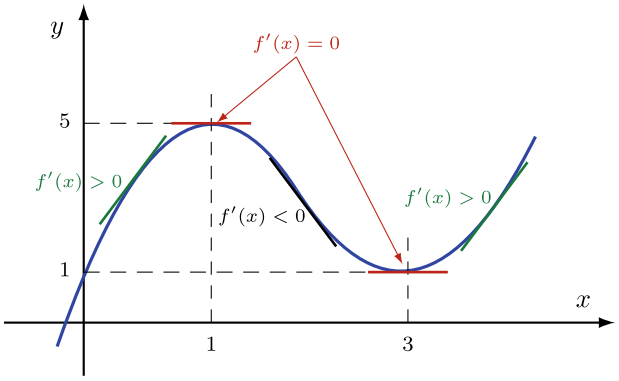


Figure 1.21 Graph of the polynomial function $f(x) = x^3 - 6x^2 + 9x + 1$ and some tangent lines.

Derivative rules: If f and g are two functions that are differentiable at a point x in a common domain, and if $g(x) \neq 0$, then the following sum, product, quotient, and chain rules results can be proved using the derivative definition.

(a) $\dfrac{\mathrm{d}}{\mathrm{d}x}(x^a) = ax^{a-1}$, for constant $a \in \mathbb{R}$

—power rule

(b) $\dfrac{\mathrm{d}}{\mathrm{d}x}(Af(x) + Bg(x)) = Af'(x) + Bg'(x)$, for constant $A, B \in \mathbb{R}$

—distribution law

(c) $\dfrac{\mathrm{d}}{\mathrm{d}x}\left(f(x)g(x)\right) = f'(x)g(x) + f(x)g'(x)$

—product rule

(d) $\dfrac{\mathrm{d}}{\mathrm{d}x}\left(\dfrac{f(x)}{g(x)}\right) = \dfrac{f'(x)g(x) - f(x)g'(x)}{(g(x)^2)}$

—quotient rule

(e) $\dfrac{\mathrm{d}}{\mathrm{d}x}\left(f\left(g(x)\right)\right) = f'\left(g(x)\right)g'(x)$

—chain rule

Despite the convenience created by these rules, it is still important to be mindful of the conditions under which a derivative is said to exist. Necessity becomes apparent in the pathological cases one may encounter. Either explicitly or implicitly, the existence of a derivative according to Definition 1.17 is conditional on the following essential criteria:

(i) the interval $x_0 < x < x_0 + h \subset D_f$

—$x_0, x_0 + h$ and points between are in the domain, D_f

(ii) $\lim\limits_{h\to 0^-} f(x_0 + h) = \lim\limits_{h\to 0^+} f(x_0 + h) = f(x_0)$

—the left limit equals the right limit which equals the function value at x_0
i.e., the function is continuous at x_0

(iii) Similarly, $\lim\limits_{h\to 0^-} \dfrac{f(x_0 + h) - f(x_0)}{h} = \lim\limits_{h\to 0^+} \dfrac{f(x_0 + h) - f(x_0)}{h}$

—the left and right limits of these ratios exist and are equal

The reason why these conditions are essential for the definition of a derivative is demonstrated by the following example.

■ Example 1.11:

Consider the function graphed in Figure 1.22. Determine whether function is differentiable everywhere.

Solution:

The function is continuous everywhere, so that conditions (i) and (ii) are satisfied. However, condition (iii) is not satisfied at one point, $x = 0$, since

$$\lim_{h\to 0^-} \frac{f(0+h) - f(0)}{h} = \lim_{h\to 0^-} \frac{(1-h) - 1}{h} = -1.$$

$$\lim_{h\to 0^+} \frac{f(0+h) - f(0)}{h} = \lim_{h\to 0^+} \frac{(1+h^{3/2}) - 1}{h} = \lim_{h\to 0^+} h^{1/2} = 0.$$

That is, the left limit is not equal to the right limit, implying that no derivative exists there.

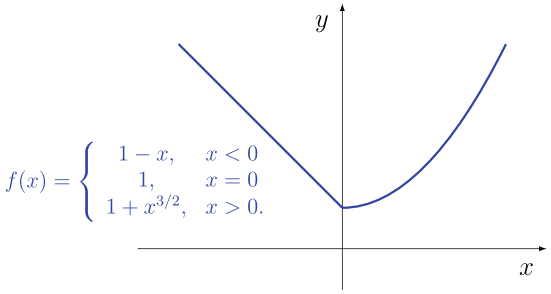


Figure 1.22 A function not everywhere differentiable.

■

A similar story exists for the function $f(x) = |x|$. Conditions (i) and (ii) are satisfied everywhere. At $x = 0$, however, although the left and right limits of (iii) exist, they are not equal, implying that no derivative exists there. Elsewhere (iii) is satisfied.

We have already mentioned that a function that fails to satisfy Condition (ii) at a point (Section 1.C), is said to be *discontinuous* at that point. There are different degrees of discontinuity depending on which equality is not satisfied. The "mildest" form of discontinuity arises if the single-sided limits agree but are not equal to the function value at that point. That type of discontinuity is referred to as a *removable discontinuity*. A somewhat more serious discontinuity, called an *ordinary discontinuity*, occurs if the single-sided limits do not agree (left panel of Figure 1.17), as in the case of the Heaviside step function:

$$f(x) = 0, \text{ for } x < 0, \quad f(x) = 1, \text{ for } x > 1.$$

Notwithstanding these cases of discontinuity, Example 1.11 demonstrates that continuity is a necessary but *not* a sufficient condition for differentiability. A point at which condition (iii) is not satisfied for a function is said to be a *singular* point or *singularity* of that function.

The author recognizes that it is not possible to cover in a brief review all the different and diverse aspects of single-variable differential calculus. Many of the important practical details and results have been left out to conserve space. The information that has been included simply provides context for the coming chapters. A similar story applies to a review of the integral calculus of functions of one variable given in Chapter 4, where only those concepts

necessary to engender reader understanding of multiple integration have been included. For additional information the reader is referred to any of the many dedicated and excellent texts on single-variable calculus including [1, 2, 4, 5].

1.D Coordinate Systems

Up until now we have represented points in $\mathbb{R}^2$ and $\mathbb{R}^3$ in terms of *Cartesian* coordinates (x, y) and (x, y, z) as in Example 1.3. However, problems arise that are better described in other coordinate systems. Such problems arise in both the differential and integral calculus (Sections 3.E, 4.E, and 4.H) and are usually suggested by the geometry of the region under consideration. The most common coordinate systems that we will encounter are the *polar coordinate* system in $\mathbb{R}^2$, and the *cylindrical* and *spherical coordinate* systems in $\mathbb{R}^3$. There are, however, other standard systems that can be useful in specific cases (see [18]), and even non-standard systems that may be useful to solve some problems (see Section 4.E). Nevertheless, it suffices for an introduction to discuss the more common alternative systems.

We begin with a few basic facts. First, the 2D Cartesian and polar coordinate systems have the same origin. Similarly, the 3D Cartesian, the cylindrical, and the spherical coordinate systems have a common origin. Second, the non-Cartesian coordinates are designed to uniquely identify and represent *every* point in $\mathbb{R}^2$ or $\mathbb{R}^3$, as do their Cartesian counterparts. That is, these coordinate systems span the whole of $\mathbb{R}^2$ and $\mathbb{R}^3$, respectively. Finally, the individual coordinate variables within each non-Cartesian system are independent of each other, just as the individual Cartesian coordinates are independent variables in the Cartesian system.

Polar coordinates

Consider an arbitrary point P in the plane with Cartesian coordinates (x, y). P's distance from the origin is

$$r = \sqrt{x^2 + y^2},$$

while the angle between P's position vector $\boldsymbol{r} = (x, y) \equiv x\mathbf{i} + y\mathbf{j}$ and the x-axis is given by

$$\tan\theta = \frac{y}{x}.$$

The unique inverse relation is given by the pair of equations

$$\left.\begin{array}{rcl} x &=& r\cos\theta \\ y &=& r\sin\theta \end{array}\right\} \quad \text{for} \quad 0 \le \theta \le 2\pi \text{ and } 0 \le r < \infty.$$

Thus, every point in $\mathbb{R}^2$ can be uniquely represented by the pair of so-called *polar* coordinates $(r, \theta) \in [0, \infty) \times [0, 2\pi]$[1], referred to a new orthogonal system, being a semi-infinite strip of width 2π. The geometric relationship between the two coordinate representations is shown in Figure 1.23(a).

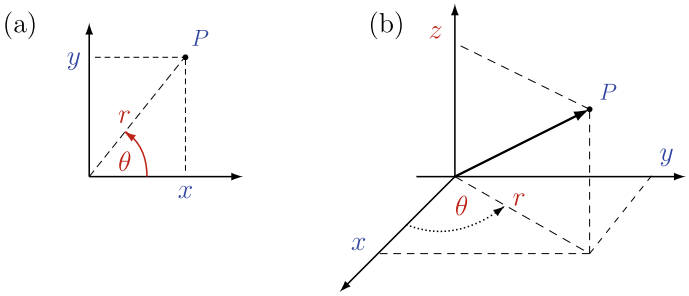


Figure 1.23 (a) 2D polar and (b) 3D cylindrical coordinates.

The distance D between two arbitrary points $P(x_1, y_1)$ and $Q(x_2, y_2)$ is then

$$\begin{aligned} D &= \left[(x_1 - x_2)^2 + (y_1 - y_2)^2\right]^{1/2} \\ &= \left[r_1^2 + r_2^2 - 2r_1 r_2 \cos(\theta_1 - \theta_2)\right]^{1/2}, \end{aligned}$$

where $x_i = r_i \cos\theta_i$ and $y_i = r_i \sin\theta_i$, $i = 1, 2$.

Cylindrical polar coordinates

An arbitrary point P in 3D is defined by Cartesian coordinates (x, y, z). The preceding case of plane polar coordinates is thus easily generalized to *cylindrical polar coordinates* in 3D by the inclusion of the Cartesian coordinate z to account for the third dimension.

We therefore have the relations

$$\begin{aligned} x &= r\cos\theta, \ y = r\sin\theta, \ z = z, \\ \text{for } \theta &\in [0, 2\pi], \quad r \in [0, \infty), \quad z \in (-\infty, \infty). \end{aligned}$$

The distance between any two points P and Q generalizes to

$$\begin{aligned} D &= \left[(x_x - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2\right]^{1/2} \\ &= \left[r_1^2 + r_2^2 - 2r_1 r_2 \cos(\theta_1 - \theta_2) + (z_1 - z_2)^2\right]^{1/2}. \end{aligned}$$

[1] The notation (r, θ) is convenient and will be employed often here without further comment, even though it conflicts with statements made in Section 1.A on notation; it does *not* mean that $\boldsymbol{r} = r\mathbf{i} + \theta\mathbf{j}$. The correct expression is $\boldsymbol{r} = r\cos\theta\mathbf{i} + r\sin\theta\mathbf{j}$.

Figure 1.23(b) shows the point P represented by the two alternative coordinate systems (x, y, z) and (r, θ, z). For future reference it is opportune to remark here that if we fix $r = a > 0$ and allow the remaining independent variables to span their respective domains, then the point P would trace out an infinite vertical cylinder of radius a with centreline coincident with the z-axis. On the other hand, if we fix $\theta = \theta_0$ and allow r and z to span their domains, then P would trace out a semi-infinite vertical plane, with one edge coinciding with the z-axis. The third option of fixing $z = z_0$ while allowing r and θ to span their domains reproduces the 2D polar system this time in the horizontal plane $z = z_0$. Note that in all three cases fixing one coordinate and allowing the remaining two to vary generates a surface in 3D. The reader should confirm these scenarios.

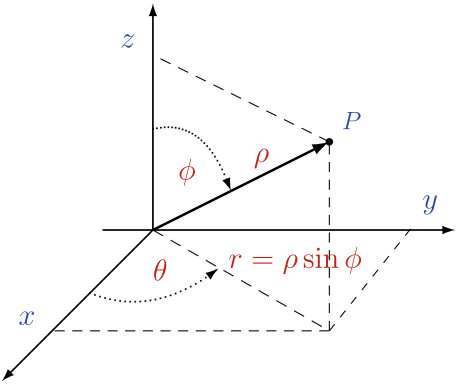


Figure 1.24 3D spherical coordinates.

Spherical polar coordinates

The second extension to 3D of polar coordinates is the *spherical polar* coordinate system. This is based on the idea of defining a point on a sphere in terms of latitude and longitude angles. To be precise, an arbitrary point P in $\mathbb{R}^3$ with Cartesian coordinates (x, y, z) is identified by the triplet of independent variables (ρ, ϕ, θ) defined by

$$\left.\begin{array}{rcl} x &=& \rho \sin\phi \cos\theta, \\ y &=& \rho \sin\phi \sin\theta, \\ z &=& \rho \cos\phi, \end{array}\right\} \qquad \begin{array}{l} 0 \le \rho < \infty, \\ 0 \le \phi \le \pi, \\ 0 \le \theta \le 2\pi, \end{array}$$

with the inverse relations

$$\rho^2 = x^2 + y^2 + z^2 = r^2 + z^2, \quad \tan\theta = \frac{y}{x},$$
$$\cos\phi = \frac{z}{(r^2 + z^2)^{1/2}} \quad \text{or} \quad \sin\phi = \frac{r}{\rho}.$$

Figure 1.24 illustrates how the variables are related geometrically. The origins of the angles ϕ and θ as $z-$axis and $x-$axis, respectively, are also indicated.

The distance between two arbitrary points P and Q in $\mathbb{R}^3$ is now expressed

$$D^2 = \rho_1^2 + \rho_2^2 - 2\rho_1\rho_2\cos(\phi_1 - \phi_2) - 2\rho_1\rho_2\sin\phi_1\sin\phi_2\big(\cos(\theta_1 - \theta_2) - 1\big).$$

As with the cylindrical coordinate system, all points in $\mathbb{R}^3$ can be uniquely represented in terms of the three independent coordinate variables (ρ, ϕ, θ). In this case, if we fix $\rho = a > 0$ and allow ϕ and θ to span their respective domains, then P would trace out a sphere of radius a. On the other hand, if we fix $\phi = \phi_0$ and allow ρ and θ to span their domains, then P would trace out the surface of an infinite cone, with apex at the origin, centreline aligned with the z-axis, and with surface at an angle ϕ_0 to the positive z-axis. The third option of fixing $\theta = \theta_0$ while allowing ρ and ϕ to span their domains produces a semi-infinite vertical plane with one edge coincident with the z-axis. The reader should again confirm these cases.

Higher dimensional polar coordinates

The spherical polar coordinate system may be extended in a natural way to represent points in higher dimensional spaces, $\mathbb{R}^n$ for $n \geq 4$. We shall leave to Supplementary problem 4.38 to show that the Cartesian coordinates of the position vector $\boldsymbol{r} = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$ may be represented by

$$\begin{aligned}
x_1 &= \rho\cos\theta_1, \\
x_2 &= \rho\sin\theta_1\cos\theta_2, \\
x_3 &= \rho\sin\theta_1\sin\theta_2\cos\theta_3, \\
x_4 &= \rho\sin\theta_1\sin\theta_2\sin\theta_3\cos\theta_4, \\
&\vdots \\
x_{n-1} &= \rho\sin\theta_1\sin\theta_2\ldots\sin\theta_{n-2}\cos\theta_{n-1}, \\
x_n &= \rho\sin\theta_1\sin\theta_2\ldots\sin\theta_{n-2}\sin\theta_{n-1}.
\end{aligned}$$

These transformation equations satisfy the condition $x_1^2 + x_2^2 + \cdots + x_n^2 = \rho^2$. The angles, all except θ_1 are defined on the interval $0 \leq \theta_i \leq 2\pi$ for $i = 2, \ldots, n$. The angle θ_1 is defined on the interval $0 \leq \theta_1 \leq \pi$. The spatial variable ρ is again defined on the interval $[0, \infty)$.

1.E Drawing or Visualizing Surfaces in $\mathbb{R}^3$

Throughout the book and indeed the subject generally, we will need to recognize, but also to sketch or otherwise visualize, areas and volumes embedded in $\mathbb{R}^2$ and $\mathbb{R}^3$, respectively. The ability to conceptualize regions in 2D and 3D makes the task of understanding multivariable function behaviour easier. Also, in the case of integration in Chapter 4, it simplifies the task of establishing integration limits that define the boundaries of a region. Lastly, being able to visualize structures in 3D can be helpful when checking the reasonableness of possible solutions to mathematical exercises.

Most of the examples and exercises to follow utilize MATLAB®in the visualization of various surfaces (using the "`surf`" function). However, the reader with access to other graphing software should be able to translate the programming information shown below into relevant code for their own graphing tool.

As an alternative, the following two examples illustrate how to piece together a picture of a graph with little or no reliance on software. A more detailed discussion of this manual approach (restricted to functions of a single variable) can be found in Chapter 5 of [5].

Example 1.12:
We shall consider here the graph of the function

$$f(x,y) = \frac{4x}{1+x^2+y^2} \quad \text{for} \quad (x,y) \in \mathbb{R}^2.$$

This function features in an exercise in a later chapter. For now we are just interested in determining the form taken by the function's graph,

$$G = \left\{(x,y,z) : (x,y) \in \mathbb{R}^2, z = f(x,y)\right\}.$$

In the steps that follow we will in essence dissect the function and with the pieces we obtain we will build up a picture of the graph.

Step 1: The first thing to note is the domain of definition. What you would be looking for are any restrictions or limitations on the independent variables as well as possible points where the function is not defined. In this case, the function is defined everywhere so the domain is the entire xy-plane.

Step 2: The second thing to do is to look for any zeros of the function. That is, we look for intercept points in the domain at which the function takes the value zero. Here, $f = 0$ when $x = 0$, that is, at all points along the y-axis.

Step 3: We now look for any symmetry. We note that the function is odd in x but even in y. The symmetry in x means that for any fixed y—which

means taking a cross-section of the graph parallel to the x-axis—howsoever the graph appears for $x > 0$, it will be inverted in the xy-plane for $x < 0$.

The symmetry in y means that for any fixed x (that is, a cross-section parallel to the $y-$axis) the graph will look the same on the left of $y = 0$ as on the right. Note, however, that because of the oddness in x, the graph will sit *above* the xy-plane for $x > 0$, but *below* the plane for $x < 0$.

So far, we have the impressions shown in Figure 1.25.

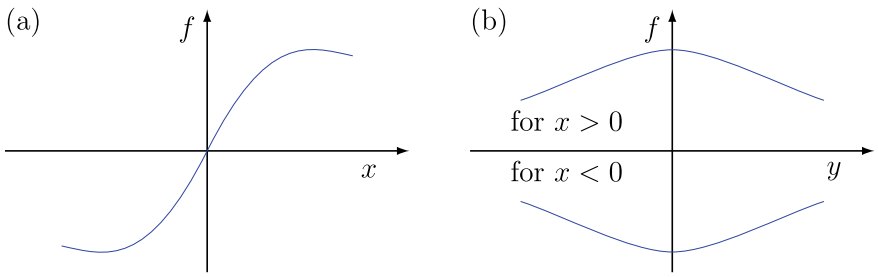


Figure 1.25 The function f is odd in x (a), but even in y (b).

Step 4: It is often instructive to look at small values of x and y.

Supposing $|x|$ to be very small compared to both 1 and y we see that f behaves as

$$f \approx \Big(\frac{4}{1+y^2}\Big)x \quad \text{as} \quad |x| \longrightarrow 0.$$

(The symbol $\approx$ means "approximately equal to" and indicates very close correspondence.) We see that f behaves linearly with respect to x, with a coefficient that depends on y. This is consistent with the fact that f is odd in x (Figure 1.25(a)).

Next, supposing $|y|$ to be very small compared to 1 and x, the function will tend to

$$f \approx \frac{4x}{1+x^2} \quad \text{as} \quad |y| \longrightarrow 0.$$

That is, f behaves very much as a constant with respect to y, dependent only on the given value of x. Again this is consistent with our finding that f is even in y: we would expect the function to be approximately constant for small $|y|$, as in Figure 1.25(b).

Step 5: We now consider the behaviour of f for large values of x and y, the "asymptotic" behaviour of f.

Again fixing y and taking $|x|$ very large compared with either 1 or y, the function will tend to behave as

$$f \approx \frac{4}{x} \longrightarrow 0 \quad \text{as} \quad x \longrightarrow \pm\infty.$$

The approach to zero will depend on the sign of x: approaching zero from *above* for $x > 0$ and from *below* for $x < 0$. (See Figure 1.26(a).)

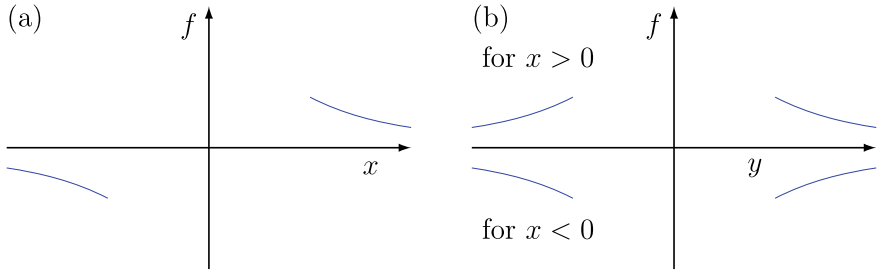


Figure 1.26 The behaviour of f for large $|x|$ (a), and large $|y|$ (b).

On the other hand, fixing x instead and taking $|y|$ very large compared to either 1 or x, we find that

$$f \approx \frac{4x}{y^2} \longrightarrow 0 \quad \text{as} \quad y \longrightarrow \pm\infty.$$

So the function again approaches zero. Note again the sign difference for positive and negative x (Figure 1.26(b)).

Now let's see if we can deduce something from this incomplete picture.

The function *is* zero along $x = 0$, and it *tends* to zero at large $|x|$ (and large $|y|$) and is nonzero in between.

Since the function does not have any singular behaviour anywhere in $\mathbb{R}^2$, we can conclude that there must be at least one point along $x > 0$ where the function peaks at some positive value, and similarly there must be at least one point along $x < 0$ where the function bottoms at some negative value. We are thus led to ...

Step 6: Investigate f for maxima and minima. This step we will leave until we have at our disposal the differentiation tools developed in the next chapter and applied in Chapter 3 (see Example 3.7). Nevertheless, even with just the above information obtained so far, we have enough to put together the sketch shown in our final Figure 1.27.

If we look at the curves running parallel to the $x-$axis we see that the extremities (large $|x|$) match the predictions in Figure 1.26(a), while the middle sections agree with the curves in Figure 1.25(a). Regarding the curves parallel to the y-axis, the extremes (large $|y|$) concur with Figure 1.26(b), while the sections crossing the x-axis agree with the lines in Figure 1.25(b).

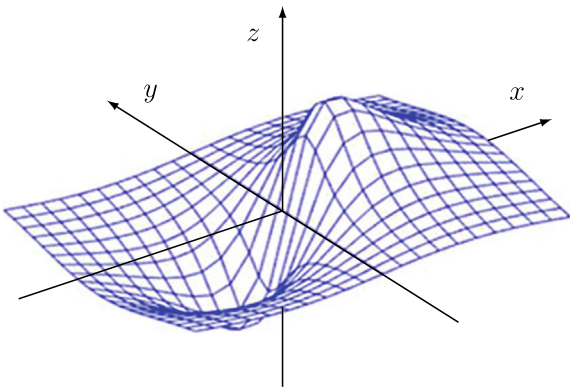


Figure 1.27 Putting it all together.

■

The next two examples relate to visualizing a sphere in 3D. The first attempts a visual construction without the assistance of graphing software, while the second demonstrates the use of MATLAB®.

■ Example 1.13:

Develop by stages the graph of the sphere of radius a centred at the origin.

Solution:

Section 1.D introduced the alternative, spherical polar coordinate system for representing points and objects in 3D. There, the results of holding one of the spherical polar coordinates fixed and allowing the other two coordinates to vary over their respective 1D domains were described. The idea of keeping one variable of three constant is one way to generate (figuratively or literally) a visual conception of a surface's shape. Although we know that in this example the shape is that of a sphere, we shall construct the shape assuming no prior knowledge, by applying the one-constant-variable idea to the Cartesian coordinate description.

We begin with the mathematical statement of the set of points making up the sphere: $S = \{(x, y, z) : x^2 + y^2 + z^2 = a^2,\ a > 0\}$. We note that even though all three Cartesian variables appear explicitly, the equation describes a surface S in $\mathbb{R}^3$ rather than a volume, Figure 1.28. That it is a surface can be deduced from the fact that the equation represents a constrained relation between the three variables, (x, y, z). They are no longer completely independent; one variable is considered a limited function of the other two.

We now build up a picture of the surface by successively fixing one of the variables, say z. Consider the case $z = 0$. The equation is then reduced to

one describing a subset of points satisfying $x^2 + y^2 = a^2$, which we recognize as the equation of a circle in the xy-plane. Note that the two equations ($z = 0$ and $x^2 + y^2 + z^2 = a^2$) is equivalent to setting *two* conditions on the *three* variables, thus generating a curve in $\mathbb{R}^2$. Another way of interpreting the physical result is that the two equations describe an *intersection of two surfaces*: the plane $z = 0$ cuts the sphere S giving rise to the subset of points that both surfaces have in common—the circle of radius a in the xy-plane.

For the sake of the argument suppose that $a > 2$. Then we may consider a sequence of fixed values of z, from 0 to a, *i.e.*, a sequence of intersecting planes, to generate a set of similar curves (*i.e.*, circles) in 3D. That is,

$$\begin{aligned} z = 0 &\implies x^2 + y^2 = a^2, \\ z = 1 &\implies x^2 + y^2 = a^2 - 1 < a^2, \\ z = 2 &\implies x^2 + y^2 = a^2 - 4 < a^2 - 1 < a^2, \\ z = a &\implies x^2 + y^2 = a^2 - a^2 = 0 \iff x = y = 0. \end{aligned}$$

These circles of diminishing radius are now plotted at their respective heights z to produce a skeletal image of the surface. The preceding curves are shown in the left-hand image in Figure 1.28. If necessary, one may similarly choose a discrete set of negative z to complete the underside of the skeletal sphere.

■

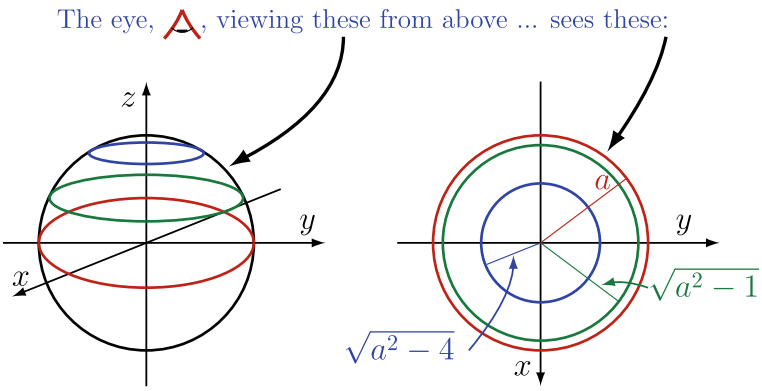


Figure 1.28 A skeletal construction of the sphere of radius a, and a few of its level sets.

In the execution of Example 1.13 we produced a number of circles, which admittedly lie at different heights. However, from the perspective of an observer placed well above the sphere we see the circles arranged in the plane as shown on the right-hand figure in Figure 1.28. Ignoring for the moment how they were arrived at, these curves, called *level sets*, represent the 2D point

sets (x, y) that are needed to produce those respective values of $\sqrt{a^2 - z^2}$. We will return to discuss level sets in detail in Section 1.F.

Example 1.14:

Repeat Example 1.13 but now using MATLAB® (Figure 1.29).

Solution:

This version of the MATLAB® code produces figures without axes.

```
figure(1)
[X,Y,Z]=sphere; % generates three 21X21 matrices for a unit
sphere
X=2.4*X; Y=2.4*Y; Z=2.4*Z; % sphere now has radius 2.4
surf(X,Y,Z), axis tight, axis off
figure(2)
[X,Y,Z]=sphere(100); % better definition with 100 segments
X=2.4*X; Y=2.4*Y; Z=2.4*Z;
map=[1,0,0;0,0.2,0;0,0,1]; % colours are red, dark green, blue
contour(X,Y,Z,[0,1,2]), axis off
colormap(map);
```

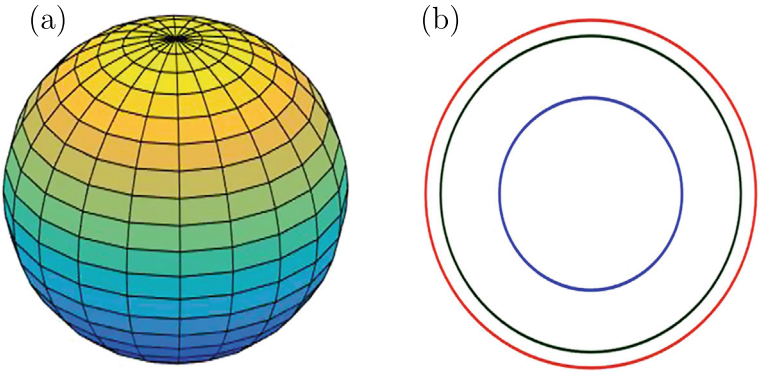


Figure 1.29 (a) The sphere of radius 2.4, and (b) its level sets.

Mastery Check 1.7:

Set up your own matrices in MATLAB® for the `surf` plot, as follows (or otherwise), and draw the sphere again:

```
r=2.4; theta=linspace(0,2*pi,21); phi=linspace(0,pi,21);
X=r*sin(phi')*cos(theta);
Y=r*sin(phi')*sin(theta);
Z=r*cos(phi')*ones(1,21);
surf(X,Y,Z)
```

■ Example 1.15:

Use MATLAB® to produce a graph of the circular cone: $S = \{(x, y, z) : z^2 = x^2 + y^2, -1 \leq x, y \leq 1\}$

Solution:

Let $0 \leq \theta \leq 2\pi$ and $0 \leq r \leq 1$, $\left.\begin{array}{rcl} x & = & r\cos\theta \\ y & = & r\sin\theta \end{array}\right\} \implies z = \pm r.$

This example illustrates why care should be exercised in cases involving squares. It is easy to forget that there is some ambiguity when taking the square root: see Figure 1.30.

The MATLAB® default figure format has tick marks with labels on the axes which suit most purposes, and there are simple functions for producing labels for the axes themselves, as shown in the sample code that follows.

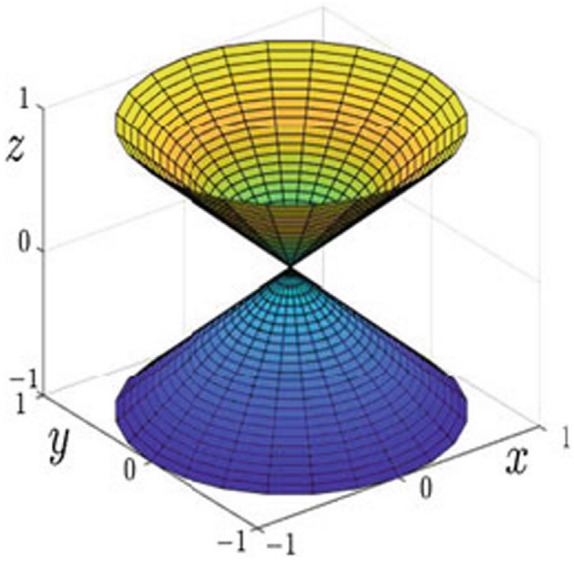


Figure 1.30 The graph of $z = \pm\sqrt{x^2 + y^2}$.

The MATLAB® code:

```
theta=linspace(0,2*pi,25);
r=linspace(0,1,25); % 25 intervals from 0 to 1
x=cos(theta')*r; y=sin(theta')*r; Z=sqrt(x.^2+y.^2);
surf(x,y,Z), hold on, surf(x,y,-Z)
xlabel('x'), ylabel('y'), zlabel('z')
```

However, the following may be used in place of the last line of code to produce clearer labels, given here for the x-axis, and easily adapted for the other two axes.

```
ax=gca; % Get the axis handle, call it 'ax'
xticks([-1,0,1]); % This sets the tick marks
% Place the new larger axis label at (0.6,-1.2,-1)
text(0.6,-1.2,-1,'$x$','interpreter','latex','fontsize',24)
% Overwrite the tick labels with blanks
ax.XAxis.TickLabels=' ',' ',' ';
% Place the new x-tick label '-1' at (-1,-1.2,-1)
text(-1,-1.2,-1,'-1','fontsize',16)
text(0,-1.2,-1,'0','fontsize',16)
text(1,-1.2,-1,'1','fontsize',16)
```

■

✍ Mastery Check 1.8:

Consider these conic sections for the case in Example 1.15:

1. Set $y = 0$ $\implies$ $z^2 = x^2 \implies z = \pm x$ —a pair of straight lines.
2. Set $y = 0.5$ $\implies$ $z^2 = x^2 + 0.25 \implies (z - x)(z + x) = 0.5^2$ —a hyperbola.
3. Set $z = 0.6$ $\implies$ $x^2 + y^2 = 0.6^2$ —a circle, radius 0.6.
4. Set $z = y + 0.25$ $\implies$ $x^2 + y^2 = y^2 + 0.5y + 0.0625$
   $\implies$ $y = 2x^2 - 0.125$ —a parabola.

Each of these curves may be generated using MATLAB®.
The task is to add in turn the groupings of lines of the following code to the end of the code for the cone, then use the "Rotate 3D" button on the MATLAB® figure to view the curves in space.

```
% the line pair
title('$z^2=x^2+y^2$','interpreter','latex')
x=linspace(-1,1,11)'; y=zeros(11,1); Z=x*ones(1,11);
surf(x,y,Z)
% the hyperbola
title('$z^2=x^2+y^2$','interpreter','latex')
x=linspace(-1,1,11)'; y=0.5*ones(11,1); Z=x*ones(1,11);
surf(x,y,Z)
% the circle
title('$z^2=x^2+y^2$','interpreter','latex')
x=linspace(-1,1,11); y=x; Z=0.6*ones(11);
surf(x,y,Z)
% the parabola
title('$z^2=x^2+y^2$','interpreter','latex')
x=linspace(-1,1,11)'; y=x; Z=(y+0.25)*ones(1,11);
surf(x,y,Z)
```

✍

Example 1.16:

How to draw an ellipsoid in MATLAB®.

Solution:

The following code produces the graph of the ellipsoid $\frac{x^2}{4^2}+\frac{y^2}{3^2}+\frac{z^2}{2^2}=1$ shown in Figure 1.31, whose semi-axes are $a=4$, $b=3$, and $c=2$. The MATLAB® code uses an elliptical parametrization,

$$x = 4\sin\phi\cos\theta, \quad y = 3\sin\phi\sin\theta, \quad x = 2\cos\phi,$$

which bears some similarities to the spherical coordinate transformation (Page 42) of the Cartesian coordinates.

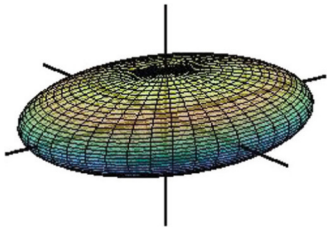


Figure 1.31 The graph of $\frac{x^2}{4^2}+\frac{y^2}{3^2}+\frac{z^2}{2^2}=1$.

This plot has been made partially transparent using the ‘‘FaceAlpha’’ property. The line commands are used to set x-, y-, z-axes.

```
theta=linspace(0,2*pi,41); phi=linspace(0,pi,41);
X=4*sin(phi')*cos(theta); Y=3*sin(phi')*sin(theta);
Z=2*cos(phi')*ones(1,41);
surf(X,Y,Z,'FaceAlpha',0.6), hold on
line([-5,0,0;5,0,0],[0,-5,0;0,5,0],[0,0,-5;0,0,5],...
'color','k','linewidth',2)
axis off
```

1.F Level Sets

In many areas of mathematics, physics, and engineering, there arise equations of the form

$$f(\boldsymbol{x}) = f(x_1,\ldots,x_n) = c$$

where c is a constant real scalar. Although this expression appears to place interest on the outcome of a function evaluation, its focus is actually on the values or points of the argument, $\boldsymbol{x}$, that give rise to the specific value c for f. This so-called *inverse* problem leads to the notion of a *level set*.

Definition 1.18
The set of all points $\boldsymbol{x} \in \mathbb{R}^n$ which give the constant value c for f is called a **level set**, *L, or more precisely, the c-***level set** *of f:*

$$L = \{\boldsymbol{x} \in D_f : f(\boldsymbol{x}) = c\}$$

Examples of level sets have already appeared in Figure 1.29 and more notably in Figure 1.28. Students often confuse a level set with the graph of a function. But as we have said, the former are concerned with the specific subset of points $\boldsymbol{x} = (x_1, x_2, \ldots)$ in the domain D_f, rather than what comes out of a function evaluation (except, of course, for the value c!). The aim of the examples in this section is to demonstrate how one might identify those points $\boldsymbol{x} \in D_f$ giving rise to specific values of f.

Example 1.17:

In $\mathbb{R}^2$, $\boldsymbol{x} = (x, y)$, and

$$L = \{(x, y) \in D_f : f(x, y) = c\}$$

is a *level curve*. For example, the level set $f(x, y) = x^2 + y^2 = 4$ is the set of points on the circle in the xy-plane (in $\mathbb{R}^2$) with centre $(0, 0)$ and radius 2. In contrast, the graph of $z = f(x, y)$ is a 3D object in $\mathbb{R}^3$.

In $\mathbb{R}^3$, $\boldsymbol{x} = (x, y, z)$, and

$$L = \{(x, y, z) \in D_f : f(x, y, z) = c\}$$

is a *level surface*. For example, the level set $f(x, y, z) = x^2 + y^2 + z^2 = 4$ is the set of points on the surface of the sphere in $\mathbb{R}^3$ with centre $(0, 0, 0)$ and radius 2.

■

As mentioned, determining the level set from the expression $f(\boldsymbol{x}) = c$ is an inverse problem. Sometimes, when f is given explicitly, as in Example 1.17 we are able to "solve" for one variable in terms of the others. For instance, in that 2D example, from $x^2 + y^2 = 4$ we obtain $y = \sqrt{4 - x^2}$, a semicircle

curve passing through $(0, 2)$, and $y = -\sqrt{4 - x^2}$, a semicircle curve passing through $(0, -2)$.

The next example shows how a 3D surface can give rise to level sets in different 2D planes.

Example 1.18:

Consider the circular paraboloid of Figure 1.32:

$$S = \{(x, y, z) : z = x^2 + y^2; -1 \leq x, y \leq 1\}.$$

Horizontal level sets arise for fixed values of z. The paraboloid is shown in Figure 1.32(a) together with the level sets (at the base of the figure) for $z = r^2,\ r = 0.5, 0.6, 0.7, 0.8, 0.9$.

Vertical level sets occur at fixed values of x or y. Shown in Figure 1.32(b) is the level set for $y = 0$.

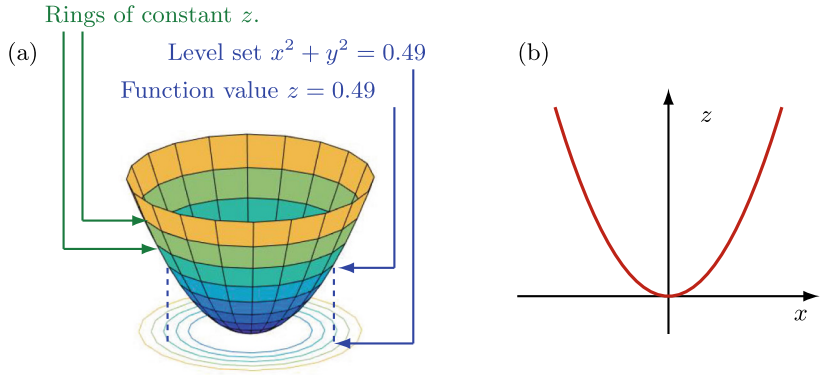


Figure 1.32 The paraboloid $z = x^2 + y^2$ (a), with level sets of two kinds in (a) and (b).

The basic figure in (a) was generated using this MATLAB® code:

```
theta=linspace(0,2*pi,21); % 20 intervals around the circle
r=linspace(0,1,11); % 10 intervals from 0 to 1
x=cos(theta')*r; y=sin(theta')*r; z=x.^2+y.^2;
% x, y and z are 21X11 matrices
surf(x,y,z), axis off
hold on % wait for the contours corresponding to
% the level sets at z=r^2; r=.5, .6, .7, .8, .9
contour(x,y,z,[0.25,0.36,0.49,0.64,0.81]) hold off.
```

A level set of the form: $g(x, y, z) = a\ constant$, is equivalent to declaring one variable a function of the other two variables, the points of which can, in principle at least, be plotted in a 3D diagram as we see in the next example. Note that the points of this 3D set, lying on a surface, reside in the domain of g and *not the graph of* g (which cannot be visualized as it resides in $\mathbb{R}^4$).

Example 1.19:

Consider the surfaces shown in Figure 1.33: $w = g(x, y, z) = z - f(x, y) = z - x^2 + y/5 = k$. Let k take the values $1, 2, 3, 4$.

The MATLAB® code:

```
X=ones(1,21)'*linspace(-1,1,21); Y=X';
Z=zeros(21,21);
for k=1:4
Z=X.^2+k-Y/5;
surf(X,Y,Z), hold on
end
xticks([-1,0,1]); yticks([-1,0,1]); zticks([0,1,2,3,4,5,6]);
text(0.6,-1.2,0,'$x$','interpreter','latex','fontsize',24)
text(-1.2,0.7,-0.1,'$y$','interpreter','latex','fontsize',24)
text(-1.2,1.1,4.5,'$z$','interpreter','latex','fontsize',24)
axis([-1 1 -1 1 0 6])
hold off
```

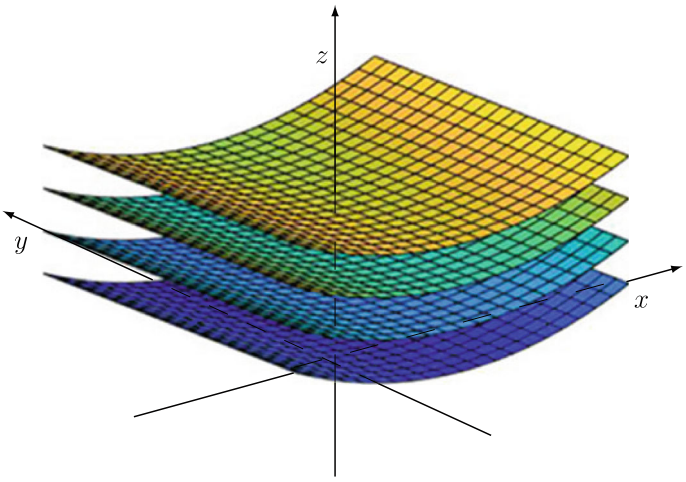


Figure 1.33 The level sets of $z - x^2 + y/5 = k$ for $k = 1, 2, 3, 4$.

✍ Mastery Check 1.9:

Consider $f(x,y) = \dfrac{x^3 - y^2}{x^2 - x}$ in the domain $D_f = \{(x,y) : x > 0,\ x \neq 1,\ y \geq 0\}$.
For what values of constant k can the level set $f(x,y) = k$ be solved for y as a function of x throughout D_f? Choose two such values for k, and plot the resulting curves for $0 < x < 1$ and $1 < x \leq 2$ in the same figure.

✍

1.G Supplementary Problems

§1.A.1. For arbitrary vectors $\boldsymbol{A}$ and $\boldsymbol{B}$ show that $|\boldsymbol{A} \times \boldsymbol{B}|^2 + |\boldsymbol{A} \cdot \boldsymbol{B}|^2 = |\boldsymbol{A}|^2 |\boldsymbol{B}|^2$.

2. Determine the three angles that each line through the origin $(0,0,0)$ and the points,

$$\text{(i)}\ \left(\sqrt{2},1,1\right), \quad \text{(ii)}\ (-1,2,2), \quad \text{(iii)}\ (2,-3,6),$$

respectively, make with the three coordinate axes.

3. Let point $P = (x_p, y_p, z_p)$ and line L be given. If $A = (x_0, y_0, z_0)$ is a known point on L, derive an expression for the perpendicular distance between P and L. Show that it can be expressed in terms of a vector cross product.

4. Show that the perpendicular distance, D, between a point $P = (x_p, y_p, z_p)$ and the plane $ax + by + cz + d = 0$ is

$$D = \frac{|ax_p + by_p + cz_p + d|}{\sqrt{a^2 + b^2 + c^2}}.$$

Hence, determine the shortest distance between $x + y + z = 3$ and the point $(1,2,-1)$.

5. Suppose three vectors $\boldsymbol{u}$, $\boldsymbol{v}$, $\boldsymbol{w}$ are such that $\boldsymbol{u} + \boldsymbol{v} + \boldsymbol{w} = \boldsymbol{0}$. Show that $\boldsymbol{u} \times \boldsymbol{v} = \boldsymbol{v} \times \boldsymbol{w} = \boldsymbol{w} \times \boldsymbol{u}$. With the aid of a diagram describe what this result means.

6. Let $\boldsymbol{x}_i = (x_i, y_i, z_i),\ i = 0,1,2,3$ be four non-coplanar points in $\mathbb{R}^3$, and let vectors $\boldsymbol{u}_i = \boldsymbol{x}_i - \boldsymbol{x}_0,\ i = 1,2,3$, be edges of the tetrahedron formed by those points. Consider the four vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}, \boldsymbol{d}$ with magnitudes in turn equal to twice the area of the four faces of the tetrahedron, and directions outwards and normal to those faces.

Express these vectors in terms of the $\boldsymbol{u}_i$ and hence show that $\boldsymbol{a} + \boldsymbol{b} + \boldsymbol{c} + \boldsymbol{d} = \boldsymbol{0}$.
(In Figure 1.34, regard the point (x_2, y_2, z_2) as being to the rear, without any loss of generality. Normal vectors $\boldsymbol{a}$ and $\boldsymbol{d}$ are shown.)

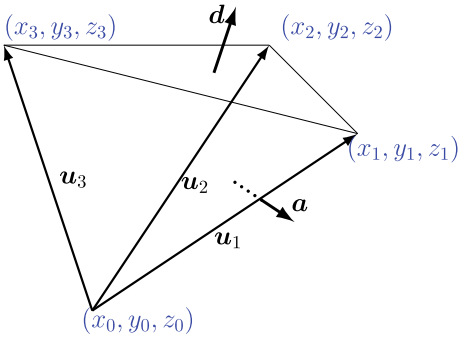


Figure 1.34 Four vectors in 3D space.

7. Let $\boldsymbol{u} = (a_1, a_2, a_3)$, $\boldsymbol{v} = (b_1, b_2, b_3)$, and $\boldsymbol{w} = (c_1, c_2, c_3)$ be vectors in 3D space.

(a) Show that $\boldsymbol{u} \cdot (\boldsymbol{v} \times \boldsymbol{w}) = (\boldsymbol{u} \times \boldsymbol{v}) \cdot \boldsymbol{w}$. That is, show that in the scalar triple product the "dot" and the "cross" can change places.

(b) Show that $\boldsymbol{u} \times (\boldsymbol{v} \times \boldsymbol{w}) = (\boldsymbol{u} \cdot \boldsymbol{w})\boldsymbol{v} - (\boldsymbol{u} \cdot \boldsymbol{v})\boldsymbol{w}$.

§1.B.8. Consider the points $\boldsymbol{a} = (1, -1, 2, 2)$, $\boldsymbol{b} = (3, 1, -1, 1)$, $\boldsymbol{c} = (-2, 0, 2, -1)$ in $\mathbb{R}^4$.

(a) Calculate the distances $|\boldsymbol{b} - \boldsymbol{a}|$, $|\boldsymbol{c} - \boldsymbol{b}|$, and $|\boldsymbol{a} - \boldsymbol{c}|$.

(b) Do either of the points $\boldsymbol{b}$ and $\boldsymbol{c}$ lie inside the open sphere $S_{3\sqrt{2}}(\boldsymbol{a})$?

(c) Find the angle θ between $\boldsymbol{b} - \boldsymbol{a}$ and $\boldsymbol{c} - \boldsymbol{a}$.

9. In $\mathbb{R}^n$, for what values of k is $\boldsymbol{b} = (k, k, k, ...)$ inside $S_r(\boldsymbol{a})$ when $\boldsymbol{a} = (1, 1, 1, ...)$?

10. Sketch the following regions and determine their boundaries. Also establish whether the regions are open or closed or neither.

(a) $\{(x, y) : |x| + |y| < 1\}$.
(b) $\{(x, y) : \max(|x|, |y|) < 1\}$.
(c) $\{(x, y) : x^2 \leq y \leq \sqrt{x}\}$.
(d) $\{(x, y) : 1 < (x-1)^2 + (y+1)^2 \leq 2\}$.
(e) $\{(x, y) : |x + 3y| \leq 3\}$.

*11. Prove the following statements about sets:

(a) The boundary of a set M is a closed set.

(b) A set M is closed $\iff$ $M = \overline{M}$.

(c) A set M is open $\iff$ $M = \text{Int}(M)$.

(d) A set M is closed $\iff$ its complement M^c is open.

(e) The union of any number of open sets is open, and any finite intersection of open sets is open.

(f) The intersection of any number of closed sets is closed, and any finite union of closed sets is closed.

12. If $\boldsymbol{x} = (x, y, z)$ and $|\boldsymbol{x}| = \sqrt{x^2 + y^2 + z^2}$, show that

$$\max(|x|, |y|, |z|) \le |\boldsymbol{x}| \le |x| + |y| + |z| \le \sqrt{3}|\boldsymbol{x}| \le 3\max(|x|, |y|, |z|)$$

*13. Suppose $a, b, c \in \mathbb{R}$ with $a, c \neq 0$. Show that the roots, $x_+, x_- \in \mathbb{R}$, of the quadratic equation $ax^2 + bx + c = 0$ satisfy the two-sided inequality

$$\frac{|c|}{|b| + \sqrt{|a||c|}} \le |x_\pm| \le \frac{|b| + \sqrt{|a||c|}}{|a|}.$$

Hint: Apply the triangle inequality (twice) to the formulae for the roots.

§1.C.14. Describe the implied domain D_f for each of the following functions: Is it (i) closed?, (ii) finite?, (iii) compact?

(a) $f(x, y, z) = \arcsin(x^2 + y^2 + z^2)$.
(b) $f(x, y, z) = \arcsin(x^2 + y^2)$.
(c) $f(x, y) = \arctan(x^2 + y^2)$.
(d) $f(x, y, z) = \ln(1 - |x + y + z|)$.

15. Apply the limit laws listed in Section 2.B on Page 66, or otherwise, to determine the following limits if they exist.

(a) $\lim\limits_{x\to-3} \dfrac{6 + 11x + 6x^2 + x^3}{x^2 - 9}$ (b) $\lim\limits_{x\to2} \dfrac{x^4 + 4x^3 - 8x - 32}{\sqrt{x-1} - 1}$ *(c) $\lim\limits_{x\to1} \dfrac{3 - \sqrt{x+8}}{\sqrt{x+1} - \sqrt{2}}$.

16. In addition to the standard limits and squeeze relations on Page 34, there is the following *Squeeze Theorem*: Suppose $f(x) \le g(x) \le h(x)$ for all x in an open set D. If $\lim_{x\to a} f(x) = \lim_{x\to a} h(x) = L$ for $a \in D$, then $\lim_{x\to a} g(x) = L$.
Use this result to determine $\lim_{x\to2^-} g(x)$ if f and h are continuous functions defined for all x in the open interval $(0, 2)$, and specifically for $x \neq 2$,

$$f(x) = \frac{x - 2}{8\left(\sqrt{2 + x} - \sqrt{6 - x}\right)} \quad \text{and} \quad h(x) = \frac{1}{x - 2} - \frac{4}{x^2 - 4}.$$

17. Use a squeeze relation to show that

$$\frac{1}{1 - a^2x^4} > \frac{\mathrm{e}^{-ax^2}}{(1 - ax^2)} > 1, \quad \text{for } 0 < x < \frac{1}{\sqrt{a}} \text{ and } a > 1.$$

18. Consider in turn the following functions $f : \mathbb{R} \longrightarrow \mathbb{R},\ x \mapsto f(x)$,

    (a) $f(x) = x^{2/3}$; (b) $f(x) = x^{4/3}$; (c) $f(x) = x^{1/2}$.

    In each case of f, by following the steps below determine whether the derivative of f exists at $x = 0$:

    (i) Check whether f exists at x=0 and at $x = 0+h$ (for h arbitrarily small).

    (ii) Check right and left limits to see whether f is continuous at $x = 0$.

    (iii) Check right and left limits to see whether f has a derivative at $x = 0$.

19. Consider the function $f : \mathbb{R} \longrightarrow \mathbb{R},\ x \mapsto (x-1)^\alpha,\ \alpha \in \mathbb{R}$. Decide from first principles for what values of α the derivative of f exists at $x = 1$.

§1.D.20. MATLAB® is able to plot functions expressed in 2D polar coordinates using a plotter called `ezpolar`. Use this function to plot the curves $r = 2\sin n\theta,\ 0 \le \theta \le 2\pi$, for $n = 2, 3, 4$, on separate graphs.

21. (a) Express the 2D polar function $r = 2a\sin\theta,\ 0 \le \theta \le \pi$, a constant, in Cartesian coordinates, and describe the curve.

    (b) What is the curve defined by $r = 2a\sin\theta,\ 0 \le \theta \le 2\pi$?

*22. *A curve in $\mathbb{R}^3$ can be sufficiently prescribed in terms of one independent parameter.*

    Represent all points on the curve of intersection of the plane $ax + by + cz = d$ with the unit sphere centred at the point (x_0, y_0, z_0) in terms of spherical coordinates, if the plane passes through the sphere's centre.

    Give conditions that must be satisfied by the constants a, b, c, d for the intersection to be possible and your representation valid.

    Hints: Set the origin for the spherical coordinate system to be at the sphere's centre. Select the longitude angle θ as the independent variable, then the latitude angle ϕ becomes a function of θ.

23. The surfaces $z^2 = 2x^2 + 2y^2$ and $z = y - 1$ intersect to create a closed curve. Use cylindrical coordinates to represent points on this curve.

*24. *A surface in $\mathbb{R}^3$ can be sufficiently prescribed in terms of two independent parameters.*

Represent all points on the plane $ax + by + cz = d$ within or coinciding with the sphere $x^2 + y^2 + z^2 = R^2$ in terms of spherical coordinates defined with respect to the origin at the sphere's centre.

Give conditions that must be satisfied by the constants a, b, c, d, R for the intersection to be possible and your representation valid.

*25 The surfaces $z = 1 + x + y$, $z = 0$, and $x^2 + y^2 = 1$ bound a closed volume, V. Represent all points in V and on its boundary in spherical coordinates. Be mindful of the domains of the respective independent variables.

§1.E.26. Use MATLAB® to reproduce Figure 1.35(a) of a one-sheeted elliptic hyperboloid,

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} - \frac{z^2}{c^2} = 1.$$

27. Use MATLAB® to reproduce Figure 1.35(b) which shows the graphs of the cylinders $x^2 - 2x + y^2 = 0$ and $z^2 - 2x = 0$ for $0 \le x \le 2$, $-2 \le y \le 2$, $-2 \le z \le 2$, plotted on the same axes.

28. Use MATLAB® to sketch the graph of the cone $x^2 + y^2 = xz$ for $-4 \le z \le 4$.

(a) (b)

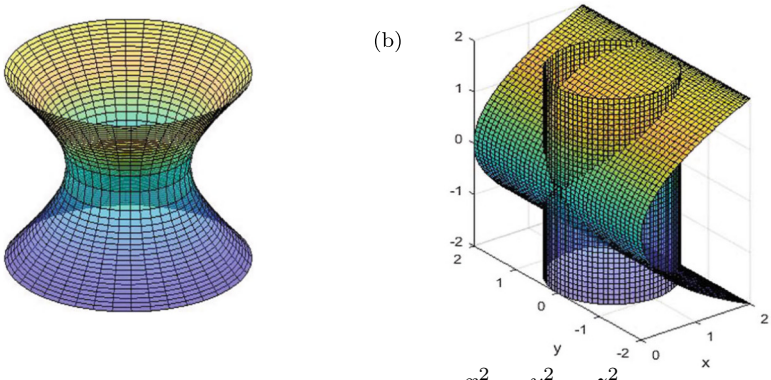


Figure 1.35 (a) The graph of $\frac{x^2}{a^2} + \frac{y^2}{b^2} - \frac{z^2}{c^2} = 1$; (b) two intersecting cylinders.

29. Describe and sketch the graphs of the following functions, $z = f(x, y)$, using ideas analogous to those described in Example 1.6.

(a) $z = \sqrt{1 - x^2 - y^2}$, for $x^2 + y^2 \leq 1$.
(b) $z = \sqrt{1 - y^2}$, for $|y| \leq 1, x \in \mathbb{R}$.
(c) $z = 1 - (x^2 + y^2)$, for $(x, y) \in \mathbb{R}^2$.
(d) $z = \dfrac{1 - \sqrt{x^4 + y^4}}{x^2 + y^2 + 1}$, for $(x, y) \in \mathbb{R}^2$.

§1.F.30. Consider the function $f(x, y, z) = \sin(xy) + \cos(yz)$, $-\frac{\pi}{2} \leq x, y, z \leq \frac{\pi}{2}$.
Use MATLAB® to draw the graphs of the level sets $x = 1$, $x = 2$; $y = 1$, $y = 2$; and $z = 1$, $z = 2$.

31. Sketch the level curves of the following functions and determine the conditions for the allowed constant values of f.

(a) $f(x, y) = x^2 + y^2 - 4x + 2y$.
(b) $f(x, y) = x^2 y$.
(c) $f(x, y) = x\sqrt{y^2 + 1}$.
(d) $f(x, y) = \dfrac{x}{x^2 + y^2}$.
(e) $f(x, y) = \dfrac{4x}{1 + x^2 + y^2}$.

32. Consider the function $f(x, y, z) = x^2 - y^2 + z^2$ defined for $D_f = \{(x, y, z) : |x| \leq 2,\ |y| < \infty,\ z \geq 0\}$.
Show that we may solve the level set $f(x, y, z) = k$ for z in terms of x and y for all $k \geq 4$. For the cases $k = 4, 6, 8$, draw the graphs for $|x| \leq 2,\ |y| \leq 2$, on the same figure.

33 Consider $F(w, x, y, z) = 36x^2 - 36y^2 - 4z^2 - 9w^2 = 0$. This is a level set in $\mathbb{R}^4$. Describe in words the precise subsets of this level set that arise from setting $x = 0,\ 1,\ 2,\ 3$. Use MATLAB® to draw the graphs for cases $x = 1,\ 2$, on the same axes. You may wish to use the `''FaceAlpha''` property (see Page 52).



Chapter 2

Differentiation of Multivariable Functions

Based on the limit definitions of continuity and the derivative for a function of one variable, as reviewed in Section 1.C, we begin the study of the differential calculus of real-valued, multivariable functions with a presentation of limits and continuity as applied to the same. The theory is developed over the course of the first three sections, which deal with differentiation proper. Considerable emphasis is placed on the geometric meaning of derivatives and of differentiability in general. In the process we introduce the core concept of the *gradient* of a function. This introduction concludes with a discussion of higher-order derivatives.

The focus of attention for the remaining sections of this chapter is divided between composite functions and the chain rule, implicit functions and implicit differentiation, and lastly Taylor polynomials and Taylor series. As these topics also arise in single variable calculus, each of the respective sections is preceded with a quick review of the 1D case. We dedicate a considerable amount of space to the first two of these topics in part because they are considerably more involved for multivariable functions than for single-variable functions.

With these foundation concepts established we put them to practical use in Chapter 3, where we discuss a fair assortment of applications.

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2.A Preliminary Remarks

In Section 1.C the derivative of a function $f(x)$ of one variable at a point $x_0 \in D_f$ was defined by the limit

$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x_0} = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}. \tag{2.1}$$

We saw that for this limit to exist at $x = x_0$ a number of conditions needed to be satisfied, including **(i)** that the points x near x_0 belong to the domain of f and **(ii)** that the function f be continuous at x_0. Continuity in turn requires the existence of yet another limit: $\lim_{x \to x_0} f(x)$. So, we have the third condition **(iii)** that the left-hand and right-hand, single-sided limits of f at x_0 be equal. These conditions are necessary to ensure the existence of the derivative limit. As a side note, we remark that the limit definition, Eq (2.1) makes sense ("rise over run", slope of a line, etc.) and is straightforward to implement. We are now confronted with the question: How does one generalize these concepts and processes to a function of two or more variables?

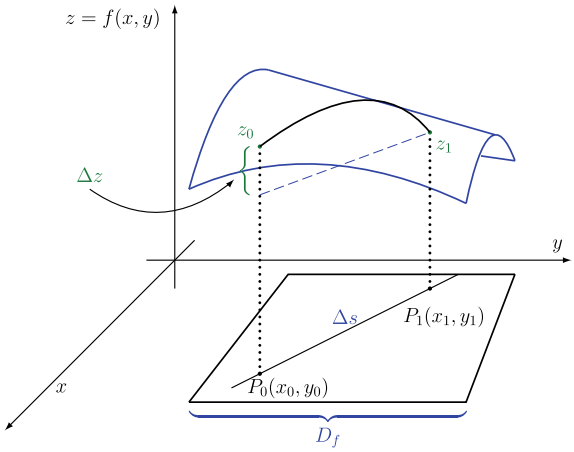


Figure 2.1 A 3D graph of a function of two variables.

An intuitive generalization of the limit definition for a function $f : \mathbb{R}^2 \to \mathbb{R}$ of two variables would look like

$$\lim_{P_1 \to P_0} \frac{f(x_1, y_1) - f(x_0, y_0)}{\sqrt{(x_1 - x_0)^2 + (y_1 - y_0)^2}}. \tag{2.2}$$

This too has the form of a limit of a ratio of difference of function values at two points to the distance between the two points, just as in the 1D case. Despite the expression's appeal, the question remains, if this limit were to exist should we then call it "the" derivative of f at point P_0? However, even before we contemplate an answer to this question, we first need to ask

what are the generalizations to $\mathbb{R}^2$ (or $\mathbb{R}^3$, ... , $\mathbb{R}^n$) of the existence criteria: **(i)**–**(iii)**?

A pictorial representation for the limit Eq (2.2) is shown in Figure 2.1. The factors to note are, firstly, the graph of f is a surface suspended in 3D; secondly, the domain D_f lies in the xy-plane; thirdly, the points P_0 and P_1 in D_f give rise to specific values $z_0 = f(x_0, y_0)$ and $z_1 = f(x_1, y_1)$, respectively; and finally, points on the line in the domain joining P_0 and P_1 give rise to points on the black curve in the graph of f.

For the limit in Eq (2.2) to even exist, questions corresponding to conditions **(i)-(iii)** first need to be addressed:

* do (x_0, y_0), (x_1, y_1), and "intervening" points belong to D_f?
* is f continuous at (x_0, y_0)?
* does $\lim\limits_{P_1 \to P_0} \dfrac{\Delta z}{\Delta s}$ exist, where $\Delta z = z_1 - z_0$, $\Delta s = \sqrt{\Delta x^2 + \Delta y^2}$?

Only thereafter can we ask the essential question of what Eq (2.2) actually gives us. This question is compelling given what can be derived from Figure 2.1. Obviously, the line P_1P_0 in the domain is but one particular choice of a line of approach to the point P_0. A different choice of approach line may give a very different result.

In the next three sections we will address the above questions, aiming to first establish a set of conditions for the existence of a limit, a definition of derivatives, a geometric understanding of what these tell us, and finally a way in which we may uniquely characterise the derivative of a function of several variables.

2.B Limits and Continuity

In Chapter 1 the pointwise limit of a function of one variable was explained in some detail, firstly in terms of left-hand and right-hand sequences of points converging to a given point and then in terms of the ϵ–δ condition for the existence of a limit depicted in Figure 1.18. As was already argued, the latter condition is not restricted to a one-dimensional model. Indeed, with the help of results from Section 1.B, it is that condition that will facilitate an immediate generalization of the limit and continuity definitions to functions of several variables. In what follows, the reader should keep in mind that the discussion (for the most part) pertains to specific and individual points in $\mathbb{R}^n$, *i.e.* the discussion too holds pointwise.

Definition 2.1
A function $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ *approaches a limit* L *as* $\boldsymbol{x} \to \boldsymbol{a}$ *for all points* $\boldsymbol{x}$ *in a* **neighbourhood** *of* $\boldsymbol{a}$ *belonging to* D_f *if, given any small positive number* ϵ*, another positive number* δ*, which may depend on* ϵ*, can be found such that if* $\boldsymbol{x}$ *is within a radius* δ *of* $\boldsymbol{a}$*, then* f *will be within a distance* ϵ *of* L*.*

In mathematical notation: Given any $\epsilon > 0$ *there exists a* $\delta > 0$ *such that whenever* $0 < |\boldsymbol{x} - \boldsymbol{a}| < \delta$ *then* $|f(\boldsymbol{x}) - L| < \epsilon$*. We write* $\lim\limits_{\boldsymbol{x} \to \boldsymbol{a}} f(\boldsymbol{x}) = L$*.*

As with functions of one variable, if it can be established that two functions, f and g, satisfy the conditions of this fundamental definition at a given point in a common domain, then a number of important results involving their combination follow. We refer to these as *limit laws* and apply them to all *well-behaved* functions.

Limit laws: If $\lim\limits_{\boldsymbol{x} \to \boldsymbol{a}} f(\boldsymbol{x}) = L, \quad \lim\limits_{\boldsymbol{x} \to \boldsymbol{a}} g(\boldsymbol{x}) = M \neq 0,$ then the following sum, product, quotient, convergence and composition results can be proved.

(a) $\lim\limits_{\boldsymbol{x} \to \boldsymbol{a}} \big(f(\boldsymbol{x}) + g(\boldsymbol{x})\big) = L + M$

(b) $\lim\limits_{\boldsymbol{x} \to \boldsymbol{a}} \big(f(\boldsymbol{x}).g(\boldsymbol{x})\big) = L.M$

(c) $\lim\limits_{\boldsymbol{x} \to \boldsymbol{a}} \dfrac{f(\boldsymbol{x})}{g(\boldsymbol{x})} = \dfrac{L}{M} \quad (M \neq 0)$

(d) $\lim\limits_{\boldsymbol{x} \to \boldsymbol{a}} f(\boldsymbol{x}) = \lim\limits_{\boldsymbol{x} \to \boldsymbol{a}} g(\boldsymbol{x})$ and $f(\boldsymbol{x}) \leq h(\boldsymbol{x}) \leq g(\boldsymbol{x})$ means that $\lim\limits_{\boldsymbol{x} \to \boldsymbol{a}} h(\boldsymbol{x})$ exists and equals L which equals M (a "squeeze theorem").

(e) If $F(t)$ is a continuous function at $t = L$ then

$$\lim_{\boldsymbol{x} \to \boldsymbol{a}} F\big(f(\boldsymbol{x})\big) = F\big(L\big) = F\big(\lim_{\boldsymbol{x} \to \boldsymbol{a}} f(\boldsymbol{x})\big).$$

That is, for continuous functions, F, we may interchange the limit and function composition operations.

Example 2.1:

Prove limit law (a) using the ϵ–δ concept in Definition 2.1.

Solution:

We may assume that, given $\epsilon_1 > 0$ and $\epsilon_2 > 0$, we have found numbers $\delta_1 > 0$ and $\delta_2 > 0$ such that $|f(\boldsymbol{x}) - L| < \epsilon_1$ whenever $|\boldsymbol{x} - \boldsymbol{a}| < \delta_1$, and $|g(\boldsymbol{x}) - M| < \epsilon_2$ whenever $|\boldsymbol{x} - \boldsymbol{a}| < \delta_2$.

For given arbitrarily small $\epsilon > 0$, let $\epsilon_1 = \epsilon_2 = \frac{1}{2}\epsilon$. Then, we have

$$\begin{aligned} |\big(f(\boldsymbol{x}) + g(\boldsymbol{x})\big) - \big(L + M\big)| &= |\big(f(\boldsymbol{x}) - L\big) + \big(g(\boldsymbol{x}) - M\big)| \\ &\leq |f(\boldsymbol{x}) - L| + |g(\boldsymbol{x}) - M| \\ &\qquad \text{by the triangle inequality,} \\ &< \epsilon_1 + \epsilon_2 = \epsilon \quad \text{provided both} \\ &\qquad |\boldsymbol{x} - \boldsymbol{a}| < \delta_1 \text{ and } |\boldsymbol{x} - \boldsymbol{a}| < \delta_2. \end{aligned}$$

Now with the choice $\delta = \min(\delta_1, \delta_2)$ we find

$$|\big(f(\boldsymbol{x}) + g(\boldsymbol{x})\big) - \big(L + M\big)| < \epsilon \text{ whenever } |\boldsymbol{x} - \boldsymbol{a}| < \delta.$$

Thus, we have proved that $\lim\limits_{\boldsymbol{x} \to \boldsymbol{a}} \big(f(\boldsymbol{x}) + g(\boldsymbol{x})\big) = L + M$.

■

Many of the other limit laws are similarly proved, a fact which the reader is encouraged to verify.

✍ Mastery Check 2.1:

Prove the limit laws (b)–(e).

Hint: For law (b), with the assumptions made in Example 2.3 together with the conditions $L, M \neq 0$, assume
$|\boldsymbol{x} - \boldsymbol{a}| < \delta = \min(\delta_1, \delta_2)$, and write $f(\boldsymbol{x}) = L + e_1(\boldsymbol{x})$, which implies $|e_1(\boldsymbol{x})| < \epsilon_1$, and similarly for g. Expand $f(\boldsymbol{x}).g(\boldsymbol{x})$ in terms of e_1 and e_2. Let $\epsilon_1 = \frac{1}{3}\epsilon/|M|$ and $\epsilon_2 = \frac{1}{3}\epsilon/|L|$ and consider $|f(\boldsymbol{x}).g(\boldsymbol{x}) - L.M| < \epsilon$.
For law (c), prove first that $\lim\limits_{\boldsymbol{x} \to \boldsymbol{a}} \dfrac{1}{g(\boldsymbol{x})} = \dfrac{1}{M}$ and then invoke law (b).

✍

The following example illustrates the use of the limit laws when a function is well-behaved both near and at a limit point.

■ Example 2.2:

Determine the limit value $L = \lim\limits_{(x,y)\to(1,\pi)} \dfrac{\cos(xy)}{1 - x - \cos y} = \lim\limits_{(x,y)\to(1,\pi)} \dfrac{g(x,y)}{h(x,y)}$, noting in particular that $\lim\limits_{(x,y)\to(1,\pi)} h(x,y) \neq 0$.

Solution:

This quotient involves functions that are continuous over all $\mathbb{R}^2$ and so satisfy the conditions for the validity of the standard limit laws. Applying the latter we find that

$$L = \frac{\lim_{(x,y)\to(1,\pi)} \cos(xy)}{\lim_{(x,y)\to(1,\pi)} (1 - x - \cos y)} = \frac{\cos(\pi)}{(1 - 1 - \cos \pi)} = \frac{-1}{+1} = -1.$$

Here, we have used, in order of application: the quotient, sum (denominator), composition (numerator and denominator), and product (numerator) laws. ■

Evaluating limits of other well-behaved functions $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ for $n \geq 2$, follows similar lines using similar procedures and rules as those used in the above example. In addition to the use of the limit laws, the reader can also make use of results from the study of limits of functions of one variable, some of which are listed on Page 34.

This brings us to the regrettable fact that not all functions are well-behaved at all points. For those functions that are ill-behaved at isolated points within so-called *punctured domains* (domains excluding the isolated point in question) or at points on the boundary of their domains, special handling is required. Functions that are unequivocally divergent at one or more points (*e.g.*, $1/(x^2 + y^2)$, which clearly diverges at $(0, 0)$) are not included in this discussion. The functions we refer to are those that characteristically take the form $0/0$ or $0 \cdot \infty$ or ∞/∞ at some point. These can be said to behave ambiguously, but more importantly not satisfy the conditions of the limit laws. For these functions, some of which are illustrated below, we must resort to applying the definition directly.

Definition 2.1 implicitly means that

* $\lim\limits_{\boldsymbol{x}\to\boldsymbol{a}} f(\boldsymbol{x})$ exists and is equal to L if $f \longrightarrow L$ *independently* of *how* $\boldsymbol{x}$ approaches $\boldsymbol{a}$!
* The limit L, if it exists, is unique!
* *No* limit of f exists if f has different limits when $\boldsymbol{x}$ approaches $\boldsymbol{a}$ along different curves!

The graphical depiction of Definition 2.1, in analogy with Figure 1.18, is shown in Figure 2.2.

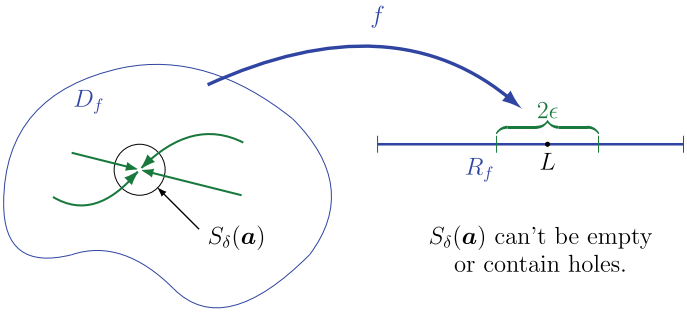


Figure 2.2 Schematic of the limit definition in 2D.

As in the 1D cases (Supplementary Problems 1.18 and 1.19), the idea of needing to consider limit values taken along multiple approaches is best illustrated by an example which demonstrates the failure to meet one or more of the above criteria.

Example 2.3:

Determine whether the limit $\lim\limits_{(x,y)\to(1,1)} \dfrac{x-y}{x-1}$ exists.

Solution:

This function takes the form $\dfrac{0}{0}$ at the limit point $(1,1)$, and is therefore undefined at $(1,1)$, although well-defined elsewhere. To see if a limit exists, we attempt to evaluate it by approaching the point $(1,1)$ along four different paths in the xy-plane, as shown in Figure 2.3.

$$
\begin{aligned}
y = x: &\quad \lim_{(1,1)} \frac{x-y}{x-1} = \lim_{(1,1)} \frac{0}{x-1} = 0.\\
y = 2-x: &\quad \lim_{(1,1)} \frac{x-y}{x-1} = \lim_{(1,1)} \frac{2(x-1)}{x-1} = 2.\\
y = x^2: &\quad \lim_{(1,1)} \frac{x-y}{x-1} = \lim_{(1,1)} \frac{x-x^2}{x-1} = -1.\\
y = 1: &\quad \lim_{(1,1)} \frac{x-y}{x-1} = \lim_{(1,1)} \frac{x-1}{x-1} = 1.
\end{aligned}
$$

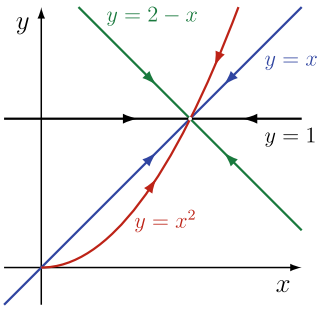


Figure 2.3 Different paths of approach to a limit point.

The resulting limiting values found by following these different paths are all different. And because they are different we conclude that no limit exists. Note that it is enough for *one* of these cases to give a different result for us to conclude that no limit exists. The graph of the function is shown in Figure 2.4. The point $(1,1)$ is the cusp where the two sheets of the function meet (along the dashed line). ■

The next exercise, for the reader to complete, is similar to this last example.

✍ Mastery Check 2.2:

Consider the function $f(x,y) = \dfrac{x^2+2y^2}{2x^2+y^2}$. Does $\lim\limits_{(x,y)\to(0,0)} f(x,y)$ exist?
Hint: Take limits along the lines $x = 0$, $y = x$, and finally along the line $y = kx$, and see if your limits agree.

✍

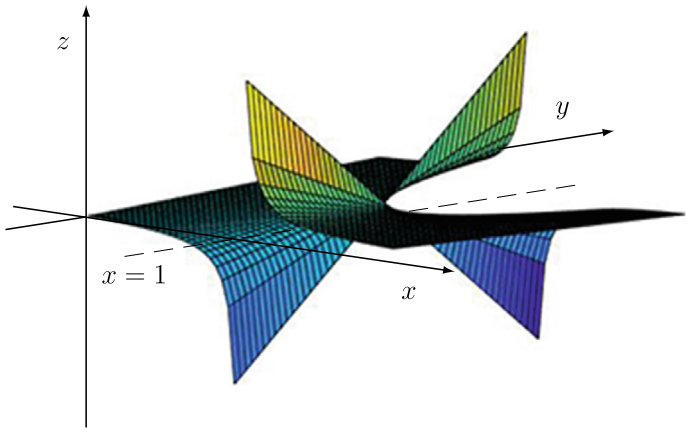


Figure 2.4 The graph of $z = \dfrac{x-y}{x-1}$, $x \in [0,1) \cup (1,2], 0 \le y \le 2$.

A warning against complacency accompanies the following Mastery Check. The student may be inclined to believe that equality of limit calculations along straight lines in $\mathbb{R}^2$ is a sufficient criterion for the existence of a limit. But this is not so!

✍ Mastery Check 2.3:

Consider the function $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$ defined by $f(x,y) = \dfrac{x^4y^2}{(x^4+y^2)^2}$, $(x,y) \neq (0,0)$.

Show that $\lim\limits_{(x,y)\to(0,0)} f(x,y)$ does not exist even though identical limit values are obtained along arbitrary straight lines through the origin. (Do not first draw the graph.)

Hint: Consider a simple nonlinear curve passing through the origin.

✍

Suppose a function $f(x,y)$ is well-defined everywhere except at a point (a,b), where it takes the ambiguous form $0/0$, making $f(x,y)$ undefined there. In order for the function to be well-defined everywhere, and ultimately continuous, it is necessary to complement the definition of $f(x,y)$ with a specific value at (a,b). For this to be possible it is necessary for the limit $\lim\limits_{(x,y)\to(a,b)} f(x,y)$ to actually exist. For the functions in Example 2.3 and Mastery Checks 2.2 and 2.4, it was readily discovered that no limit existed at the given points. Generally speaking, demonstrating that a limit does not exist requires no great effort; a few well-chosen approach paths resulting in different outcomes suffices to negate the existence of a limit. Now it is necessary to consider

the more difficult task of proving that a limit does indeed exist. As Mastery Check 2.4 demonstrated, it is not sufficient, although necessary, for the same result to be obtained from a few (or any finite number of) trial approach paths. The critical burden is to prove that a value obtained from those few trials *is* the value that will be obtained with all possible approach paths. One suggestion, based on the definition itself, is proposed in the next example.

■ Example 2.4:

Determine whether the limit $\lim\limits_{(x,y)\to(0,0)} \dfrac{x^3 - x^2y}{x^2 + y^2 + xy}$ exists.

Solution:

Note once again that the function is undefined at the limit point, here the origin $(0, 0)$. To begin with we can evaluate the limit by adopting various simple paths that pass through or approach the limit point.

$$\text{Along } y = 0: \quad \lim_{(0,0)} \frac{x^3 - x^2y}{x^2 + y^2 + xy} = \lim_{(0,0)} \frac{x^3}{x^2} = \lim_{x\to 0} x = 0.$$

$$\text{Along } x = 0: \quad \lim_{(0,0)} \frac{x^3 - x^2y}{x^2 + y^2 + xy} = \lim_{y\to 0} \frac{0}{y^2} = 0.$$

In fact, we get the same result along any straight line $y = kx$ that passes through the origin. So, since the limit, if it exists, is unique it must be 0!

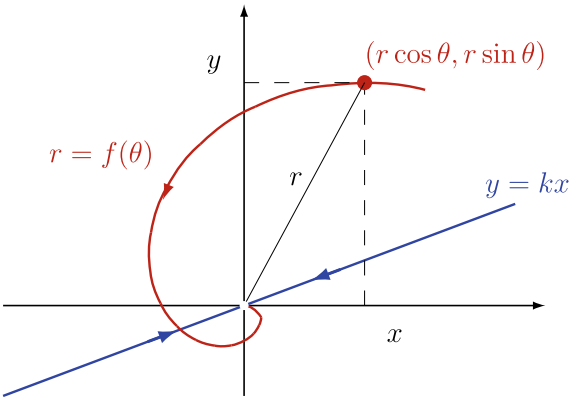


Figure 2.5 Example of conventional and unconventional paths to a limit point.

To prove that the limit exists and is indeed the value zero, consider an arbitrary curve in the plane that converges to (or passes through) the origin:

$r = f(\theta) \geq 0$, such that $x = h(\theta) = r(\theta)\cos\theta$, $y = g(\theta) = r(\theta)\sin\theta$. In general, points on the curve have distance to the origin that will be a function of θ. Tracing the curve we have $r \to 0$. Shown in Figure 2.5 is one of the cases $r \to 0$ as θ increases. However, any such path in the plane will do. Straight lines through the origin are simple examples of these.

Since we now trace this curve we can substitute the polar functions for x and y in the $\epsilon - \delta$ definition of the function limit (*i.e.*, we consider $|f(x,y) - L|$).

$$\begin{aligned}\left|\frac{x^3 - x^2y}{x^2+y^2+xy} - 0\right| &= \left|\frac{r^3\cos^3\theta - r^3\cos^2\theta\sin\theta}{r^2\cos^2\theta + r^2\cos^2\theta + r^2\cos\theta\sin\theta}\right| \\ &= \left|\frac{r^3\cos^2\theta(\cos\theta - \sin\theta)}{r^2(1+\cos\theta\sin\theta)}\right| \\ &= r\cos^2\theta\,\frac{|\cos\theta - \sin\theta|}{|1+\sin\theta\cos\theta|}\end{aligned}$$

(It is actually sufficient to stop here: the denominator is not zero and the numerator is bounded and proportional to r which $\to$ 0. Nevertheless we pursue this calculation a little further to demonstrate how ϵ and δ enter the analysis.) Using a few trigonometric identities we find that

$$\begin{aligned}\left|\frac{x^3 - x^2y}{x^2+y^2+xy} - 0\right| &= r\cos^2\theta\frac{\sqrt{2}|\cos\theta\cos(\pi/4) - \sin\theta\sin(\pi/4)|}{|1+\frac{1}{2}2\sin\theta\cos\theta|} \\ &\leq r\sqrt{2}\frac{|\cos(\theta+\pi/4)|}{|1+\frac{1}{2}\sin(2\theta)|} \\ &\leq r\frac{\sqrt{2}}{1/2} = 2\sqrt{2}r \;\longrightarrow\; 0 \text{ as } r \to 0.\end{aligned}$$

In the last set of calculations, working from the second to the third line using only known properties of trigonometric functions for arbitrary angles, we see that the numerator is less than or equal to 1, while the denominator is greater than or equal to 1/2.

Thus, given $\epsilon > 0$, however small, we find that the left-hand side will be smaller than ϵ provided r is smaller than $\delta = \dfrac{\epsilon}{2\sqrt{2}}$. Thus, the limit definition is satisfied:

$$\left|\frac{x^3 - x^2y}{x^2+y^2+xy} - 0\right| < \epsilon \quad \text{whenever} \quad r < \delta.$$

Given that we have invoked an arbitrary curve whose sole requirement is to pass through the limit point (the origin) the result is general, the limit exists, and is indeed 0. The surface itself is reproduced in Figure 2.6.

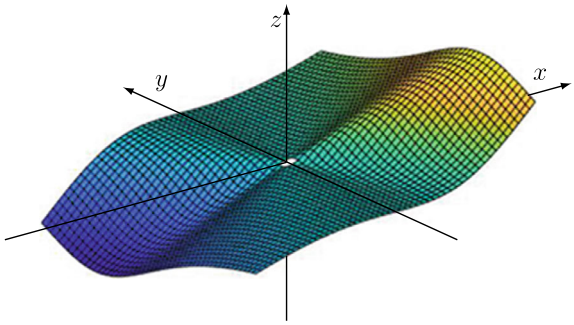


Figure 2.6 The graph of $z = \dfrac{x^3 - x^2y}{x^2 + y^2 + xy}$.

The reader is invited to attempt a similar calculation in this next Mastery Check.

✍ Mastery Check 2.4:

Consider the function $f(x, y) = \dfrac{x + y}{\ln(x^2 + y^2)}$ (which is undefined at $(0, 0)$).

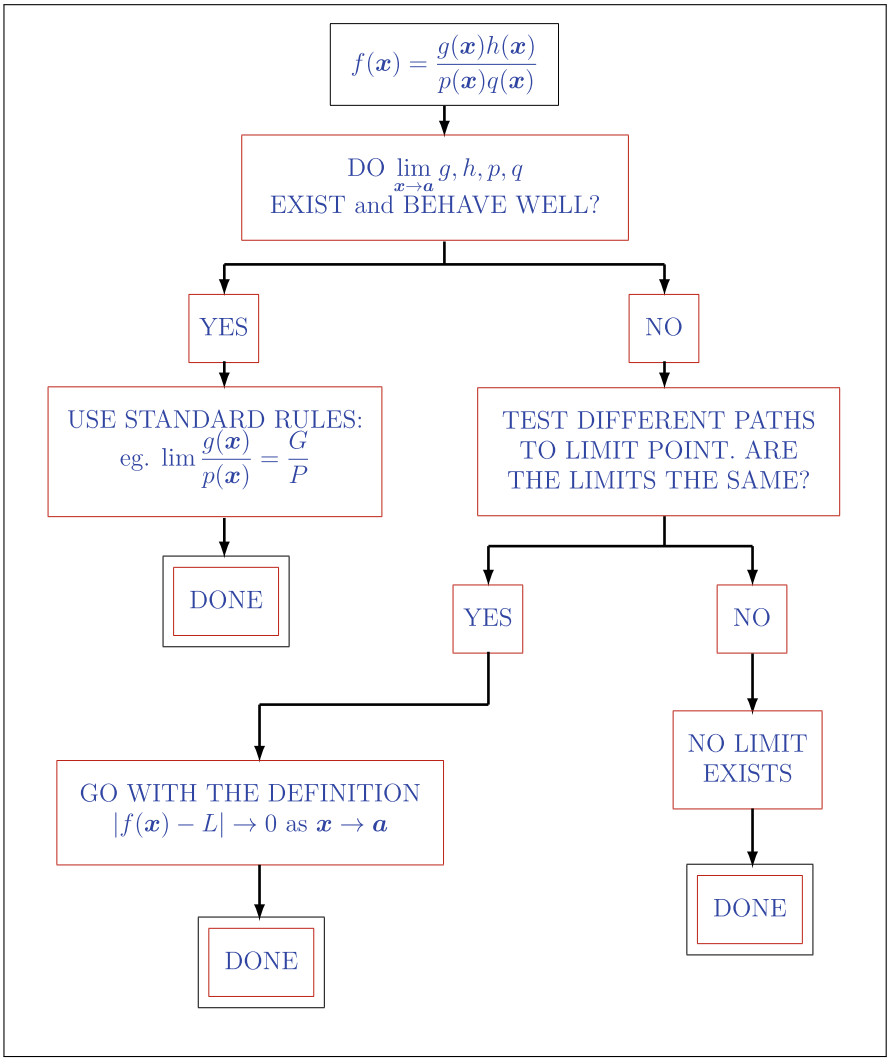
Determine whether $\lim\limits_{(x,y)\to(0,0)} f(x, y)$ exists and if so evaluate it. That is, verify that Definition 2.1 is satisfied.

Hint: Use the approach featured in Example 2.4. Standard limits are also useful.

The functions considered in Example 2.4 and Mastery Check 2.4 depend on two variables. Consequently, the limit calculations rely on lines and curves in the xy-plane, depending on one parameter. In particular, an arbitrary curve could be constructed using polar coordinates, fashioned as a function of one variable. In a completely analogous way, limits of functions of three variables may be considered using straight lines and curves in 3D. In the case of 3D limits, approaching a limit point along a straight line, $\boldsymbol{x} = \boldsymbol{x}_0 + t\boldsymbol{u}$ (as defined in Section 1.A), will revert to a limit involving a single parameter, t. Similarly, approaching a limit point along a more general curve in 3D can be effected using cylindrical or spherical coordinates to represent the curve, fashioned so that it too will only depend on *a single* parameter (this characteristic of curves in 3D was demonstrated in Supplementary Problem 1.22). Similar remarks hold for functions of four or more variables, although regrettably their domains cannot be visualized. In this context, see also Supplementary Problem 4.38.

In general, Flowchart 2.1 illustrates the sequence of steps one might consider taking to evaluate a limit.

Flowchart 2.1: How to work through a limit problem



As with functions of one variable, a multivariable function, whose finite limit, L, at a point $\boldsymbol{x}_0$ in its domain exists according to Definition 2.1, will moreover be continuous at that point if $f(\boldsymbol{x}_0) = L$. This pointwise proposition and its domain-wide version follow naturally from Definition 2.1. These propositions are summarized in the following, combined version of Definitions 1.14 and 1.15.

Definition 2.2

* *A function* $f : \mathbb{R}^n \to \mathbb{R}$ *whose limit at* $\boldsymbol{x}_0 \in D_f$ *exists, according to Definition 2.1, is* **continuous** *at* $\boldsymbol{x}_0$ *if* $\lim_{\boldsymbol{x}\to\boldsymbol{x}_0} f(\boldsymbol{x}) = f(\boldsymbol{x}_0)$.

* *A function* $f : \mathbb{R}^n \to \mathbb{R}$ *that is continuous at every point of its domain* $D_f \subset \mathbb{R}^n$ *is said to be* **continuous** *over that domain.*

2.C Partial Derivatives

Having understood the intricacies of limit processes for functions of many variables, we may now return to the question of whether the same principles can be applied to *ratios of differences*. That is to say, we have thus far addressed the first two of the three necessary criteria for the validity of a limit of the form Eq (2.2) and so are now better prepared to address the third point.

At this juncture, it is relevant to reflect on two seemingly conflicting observations related to Eq (2.2). Firstly, we have seen that in contemplating the existence of a limit of a multivariable function, it is not sufficient to consider a finite number of approach paths. Definition 2.1 effectively states that for the limit to exist it must be path independent. At the same time we have seen from the examples and exercises that graphs of *continuous* multivariable functions can be quite convoluted, undulating in various directions and perhaps even possessing cusps and edges. This tells us that we should not expect Eq (2.2), if the limit existed, to provide us with a unique number. In fact, quite the contrary, we should expect that choosing different paths of approach to a limit point in an expression like Eq (2.2) *will* deliver different values.

The two facts are contradictory. If a derivative is to be defined as a multidimensional limit it must be unique, but this seems impossible. This dilemma in turn begs the question of how to establish whether or not a function can be differentiated at a point and if so what property should be used to characterize its derivative, if it were to exist.

Surprisingly enough the foundation for – the beginning of – a resolution of this conundrum is the most elementary of extensions of the one-dimensional, *i.e.*, ordinary, derivative. This extension involves contemplating the existence of derivatives with respect to *one variable at a time*, keeping all other variables constant. Hence, we are led to the concept of *partial derivatives* of functions of many variables.

Definition 2.3
Let $\boldsymbol{x}_0 = (x_1^0, x_2^0, \ldots, x_n^0)$ *be an* **interior** *point or a* **boundary** *point of* D_f *of a continuous function* $f : \mathbb{R}^n \longrightarrow \mathbb{R}$.

* *If the limit* $\displaystyle\lim_{h\to 0} \frac{f(\boldsymbol{x}_0 + h\mathbf{e}_j) - f(\boldsymbol{x}_0)}{h}$
$\displaystyle= \lim_{h\to 0} \frac{f(x_1^0, \ldots, x_j^0 + h, \ldots, x_n^0) - f(x_1^0, \ldots, x_n^0)}{h}$ *exists, we call it the first* **partial derivative** *of* f *w.r.t.* x_j *at the point* $\boldsymbol{x}_0$ *and denote it* $\dfrac{\partial f}{\partial x_j}(\boldsymbol{x}_0)$.

* *If all* $\dfrac{\partial f}{\partial x_j}(\boldsymbol{x}_0)$, $j = 1, \ldots, n$, *exist then we say that* f *is* **partially differentiable at** $\boldsymbol{x}_0$.

* *We say* f *is* **partially differentiable in** D_f *if it is partially differentiable at* **every** *point* $\boldsymbol{x}_0 \in D_f$.

Remarks

* Equivalent notations for partial derivatives are:

$$\frac{\partial f}{\partial x_j}(\boldsymbol{x}_0), \quad D_j f(\boldsymbol{x}_0), \quad f_{x_j}(\boldsymbol{x}_0), \quad f_j(\boldsymbol{x}_0).$$

  Care should be exercised with the last option to avoid confusion (later) when dealing with vector-valued functions with components denoted by index subscripts.

* Given our statements at the start of this section, it is worth highlighting some important facts.

  (i) The limit expression appearing in Definition 2.3 is identical to the limit definition used in Section 1.C (Definition 1.17). It therefore represents the same *summary* expression stating the equality of two, single-sided limits: the left-hand limit must equal the right-hand limit.

(ii) The limit in Definition 2.3 is one of n *one*-dimensional limits of a multivariable function defined on $\mathbb{R}^n$, and *not* an n-dimensional limit in a $\mathbb{R}^n$ setting, as in the case of Definition 2.1.

(iii) With these n one-dimensional limits there is no conflict of definitions; each such limit can return a different value for the same point $\boldsymbol{x}_0$ (see later in this section).

∗ As with the single variable case, functions for which any of the n partial derivative limits fails to exist at a point are said to be *singular* at that point. That is, a multivariable function may be continuous everywhere in its domain of definition, but need not be partially differentiable at every point in its domain.

The next example and Mastery Check (for the reader to attempt) demonstrate the typical approach. Note that in these calculations we make use of the squeeze propositions and standard limits from Section 1.C.

■ Example 2.5:

Use Definition 2.3 to determine the first partial derivative with respect to x of $f(x, y, z) = x^2 \mathrm{e}^{xy} + zx$ at an arbitrary point (x, y, z). That is, determine $\dfrac{\partial f}{\partial x}$.

Solution:

We note first that the function is well defined everywhere in $\mathbb{R}^3$ so that we need not concern ourselves about any issues brought by singular points.

For the task ahead we need both $f(x, y, z)$ and $f(x + h, y, z)$ in Definition 2.3, treating y and z as fixed coordinates, *i.e.*, as constants. The latter function becomes

$$f(x + h, y, z) = (x + h)^2 \mathrm{e}^{(x+h)y} + z(x + h) = (x^2 + 2xy + h^2)\mathrm{e}^{xy}\mathrm{e}^{hy} + zx + zh.$$

Consequently, the difference between the two functions is,

$$f(x + h, y, z) - f(x, y, z) = \left[\left(x^2 \mathrm{e}^{xy} + 2xy\mathrm{e}^{xy} + h^2 \mathrm{e}^{xy} \right) \mathrm{e}^{hy} + \cancel{zx} + zh \right] - \left[x^2 \mathrm{e}^{xy} + \cancel{zx} \right].$$

Dividing by h we simplify a few terms, while combining others,

$$\frac{f(x + h, y, z) - f(x, y, z)}{h} = x^2 \mathrm{e}^{xy} \frac{\left(\mathrm{e}^{hy} - 1 \right)}{h} + 2xy\mathrm{e}^{xy}\mathrm{e}^{hy} + h\mathrm{e}^{xy}\mathrm{e}^{hy} + z.$$

Now, using squeeze relation (b) from Page 34 in the following forms,

$$\begin{array}{rcccl} y & < & \dfrac{\mathrm{e}^{hy} - 1}{h} & < & \dfrac{y}{1 - hy}, \\ hy + 1 & < & \mathrm{e}^{hy} & < & \dfrac{hy}{1 - hy} + 1 = \dfrac{1}{1 - hy}, \end{array}$$

we readily deduce that,

$$\lim_{h\to 0}\frac{\mathrm{e}^{hy}-1}{h}=y \quad ; \quad \lim_{h\to 0}\mathrm{e}^{hy}=1 \quad ; \quad \lim_{h\to 0}h\mathrm{e}^{hy}=0,$$

and so find,

$$\lim_{h\to 0}\frac{f(x+h,y,z)-f(x,y,z)}{h}=x^2y\mathrm{e}^{xy}+2x\mathrm{e}^{xy}+z,$$

as the first partial derivative of f with respect to x. ■

✍ Mastery Check 2.5:

Let $f(x,y,z)=xy+z\sin(yz)$. Use Definition 2.3 to determine the first partial derivative, $\dfrac{\partial f}{\partial y}$, at an arbitrary point (x,y,z).

Hint: Here, you might need to use standard limits (see Page 34).

✍

In the above Example (and Mastery Check) we could have arrived at the same result had we used the rules of differentiation for functions of one variable, provided we treated y and z (x and z in the Mastery Check) as if they were constants! In actual fact, Definition 2.3 effectively states precisely that: in taking the limit with respect to one variable, we treat *all other* variables as if they too were constants.

With the operation of partial differentiation being equivalent to ordinary differentiation keeping other variables constant, one can then conveniently apply all the known differentiation rules and results that have been developed from single variable calculus for all known differentiable functions of one variable. We demonstrate this very convenient operational equivalence with an example and leave it to Mastery Check 2.6 to reinforce the procedure.

■ Example 2.6:

Let $f(x,y,z)=\ln(1+\mathrm{e}^{xyz})=g\big(h(x,y,z)\big)$. Determine the partial derivatives $\dfrac{\partial f}{\partial x}$, $\dfrac{\partial f}{\partial y}$, and $\dfrac{\partial f}{\partial z}$.

Solution:

In each case we assume two variables are constant and differentiate with respect to the third using the chain rule of single-variable calculus:

$$\begin{aligned}
\frac{\partial f}{\partial x} &= \frac{\mathrm{d}g}{\mathrm{d}h}\frac{\partial h}{\partial x}=\frac{1}{1+\mathrm{e}^{xyz}}yz\mathrm{e}^{xyz},\\
\frac{\partial f}{\partial y} &= \frac{1}{1+\mathrm{e}^{xyz}}xz\mathrm{e}^{xyz},\\
\frac{\partial f}{\partial z} &= \frac{1}{1+\mathrm{e}^{xyz}}xy\mathrm{e}^{xyz}.
\end{aligned}$$

■

Mastery Check 2.6:

Find the (first-order) partial derivatives of the following functions with respect to each variable:

(a) $f(x,y,z) = \dfrac{x^2+y^2}{x^2-z^2}$;

(b) $f(s,t,u) = \sqrt{s^2t + stu + tu^2}$;

(c) $f(x,y,z) = y\sin^{-1}(x^2 - z^2)$;

(d) $f(u,v,w) = u^2 e^{uv^2w}$;

(e) $f(x,y,u,v) = x^2\sin(2y)\ln(2u+3v)$.

(f) $f(x,y,z,u) = \sin(3x)\cosh(2y) - \cos(3z)\sinh(2u)$.

Now that we can evaluate them, what are partial derivatives?

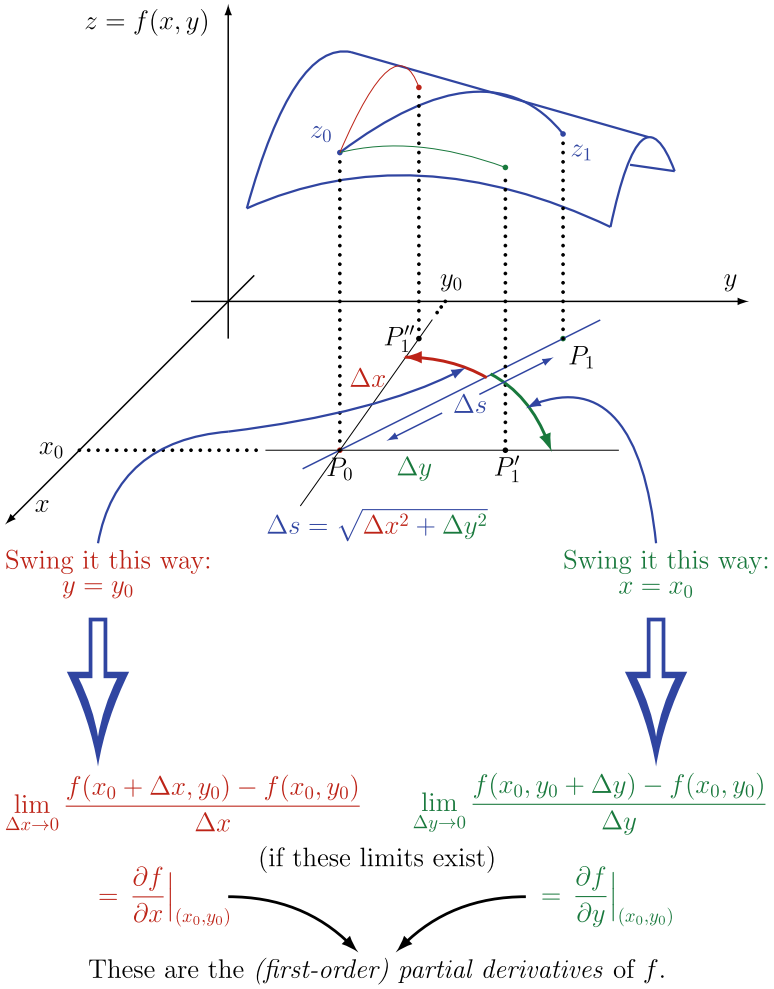


Figure 2.7 Partial derivatives of a function of two variables.

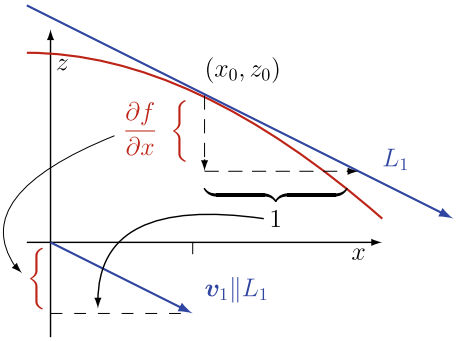
Although defining and calculating "the" derivative of a multivariable function is not as straightforward or even possible sometimes as naively suggested by Eq (2.2) and Figure 2.1, the partial derivatives of a multivariable function, if they exist, are well defined. So, how do they relate to our earlier discussion? Consider Figure 2.7, a modified version of Figure 2.1, which illustrates the special cases of the one-dimensional limits that define the partial derivatives of a function of two variables.

In Section 1.C we found that the one-dimensional limit defining the derivative at a point gave the slope of the line that was tangent to the graph of a function of one variable. Since partial derivatives are similarly defined as one-dimensional limits, the same interpretation holds for them in their respective one-dimensional orientations. Thus, referring to Figure 2.7, we deduce the following geometric interpretations of $\frac{\partial f}{\partial x}\Big|_0$, $\frac{\partial f}{\partial y}\Big|_0$:

$\frac{\partial f}{\partial x}\Big|_0$ — the *slope* of the *tangent line* L_1 to the red curve $f(x, y_0)$ at (x_0, y_0).

$\frac{\partial f}{\partial y}\Big|_0$ — the *slope* of the *tangent line* L_2 to the green curve $f(x_0, y)$ at (x_0, y_0).

In fact, by taking two orthogonal cross sections through the point $(x_0, y_0, f(x_0, y_0))$ on the graph, one parallel to the x-axis and one parallel to the y-axis, the following pictures emerge.



$$\boldsymbol{v}_1 = \mathbf{e}_1 + \frac{\partial f}{\partial x}\Big|_0 \mathbf{e}_3$$
$$\left(= \mathbf{i} + \frac{\partial f}{\partial x}\Big|_0 \mathbf{k} \right)$$

starting at the origin in the xz-plane.

Figure 2.8 A tangent vector and line in the x-direction.

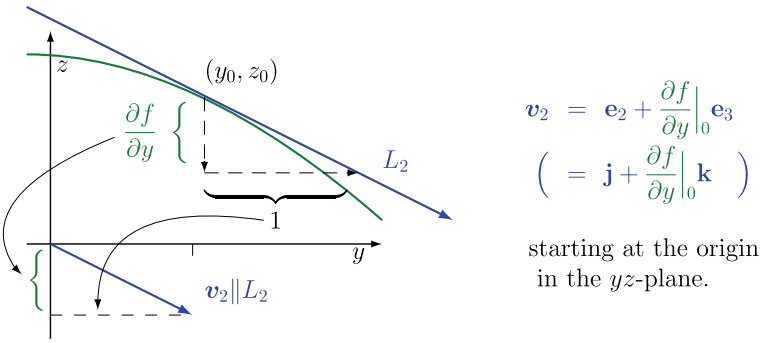


Figure 2.9 A tangent vector and line in the y-direction.

In the cross section parallel to the xz-plane, a vector parallel to line L_1 in Figure 2.8 is $\boldsymbol{v}_1$.

In the cross section parallel to the yz-plane, a vector parallel to line L_2 shown in Figure 2.9 is $\boldsymbol{v}_2$.

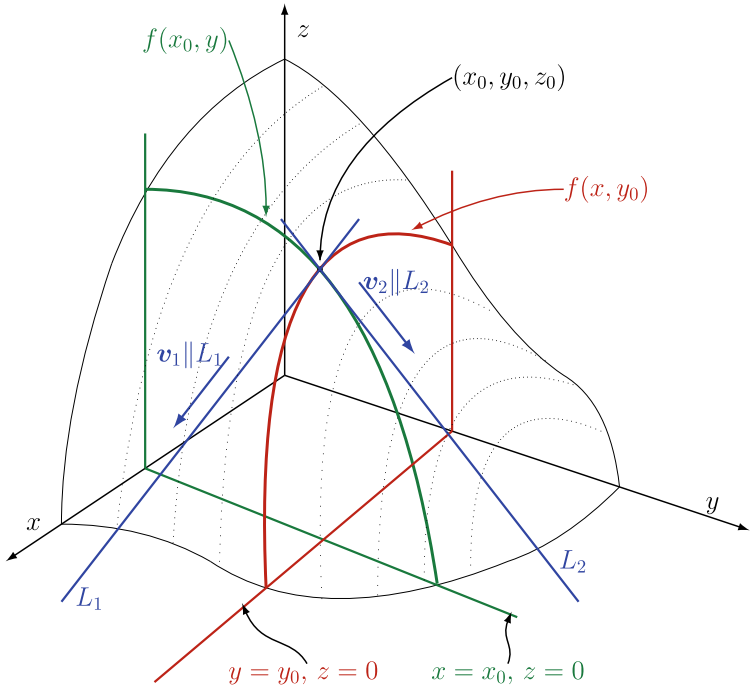


Figure 2.10 Tangent vectors and lines to a 3D function graph.

In the full 3D graph, the tangent lines L_1 and L_2, and corresponding vectors $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$, appear as in Figure 2.10. Compare the corresponding lines in this figure with those in Figures 2.7, 2.8, and 2.9 above.

Notice that $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ are not parallel to each other! The former has a component in the x-direction and no component in the y-direction, the latter has the opposite. This is typical of such tangent vectors even in higher dimensional cases. Being non-parallel is useful as these tangent vectors, $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$, can be used to define what is called a *tangent plane*, T, with normal vector $\boldsymbol{n}$:

$$\boldsymbol{n} = \boldsymbol{v}_1 \times \boldsymbol{v}_2 = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 1 & 0 & \left.\dfrac{\partial f}{\partial x}\right|_0 \\ 0 & 1 & \left.\dfrac{\partial f}{\partial y}\right|_0 \end{vmatrix} = -\left.\frac{\partial f}{\partial x}\right|_0 \mathbf{i} - \left.\frac{\partial f}{\partial y}\right|_0 \mathbf{j} + \mathbf{k}.$$

This plane, defined uniquely by $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$, in which lie the tangent lines L_1 and L_2, is consequently *tangent* to the surface $z = f(x, y)$ at (x_0, y_0, z_0). Moreover, the plane T, spanned by $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$, has the same *normal vector* as the *normal vector* to the graph of $z = f(x, y)$ at (x_0, y_0, z_0).

For future reference, notice that the existence of the tangent plane is contingent on the existence of the tangent vectors $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$, whose existence in turn is contingent on the existence of the partial derivatives, $\left.\frac{\partial f}{\partial x}\right|_0$, $\left.\frac{\partial f}{\partial y}\right|_0$!

The equation of this tangent plane can be found from the scalar vector product (see Pages 6 and 8)):

$$\boldsymbol{n} \cdot (\boldsymbol{x} - \boldsymbol{x}_0) = 0.$$

an arbitrary point *on* the plane.

the specific point on the plane that is also on the surface, f.

$$\begin{aligned} \implies \quad & \left.\frac{\partial f}{\partial x}\right|_0 (x - x_0) + \left.\frac{\partial f}{\partial y}\right|_0 (y - y_0) - (z - z_0) = 0 \\ \implies \quad & z - z_0 = \left.\frac{\partial f}{\partial x}\right|_0 (x - x_0) + \left.\frac{\partial f}{\partial y}\right|_0 (y - y_0). \end{aligned}$$

Example 2.7:

Determine a vector normal to the graph of $z = \arcsin(xy)$ at the point $(1, \frac{1}{2}, \frac{\pi}{6})$. Then determine the equation of the tangent plane to the graph at $(1, \frac{1}{2}, \frac{\pi}{6})$.

Solution:

The point $(1, \frac{1}{2})$ lies in the domain of the function, which is well defined and continuous there. Moreover, the partial derivatives are also well defined at

the point. Using the expression just derived for the normal vector in terms of partial derivatives, we get, firstly,

$$\begin{aligned} \frac{\partial f}{\partial x}\Big|_0 &= \left(\frac{y}{\sqrt{1-(xy)^2}}\right)\Big|_0 = \frac{1/2}{\sqrt{3}/2} = \frac{1}{\sqrt{3}}; \\ \frac{\partial f}{\partial y}\Big|_0 &= \left(\frac{x}{\sqrt{1-(xy)^2}}\right)\Big|_0 = \frac{1}{\sqrt{3}/2} = \frac{2}{\sqrt{3}}, \end{aligned}$$

and so,

$$\boldsymbol{n} = -\frac{\partial f}{\partial x}\Big|_0 \mathbf{i} - \frac{\partial f}{\partial y}\Big|_0 \mathbf{j} + \mathbf{k} = (-\mathbf{i} - 2\mathbf{j} + \sqrt{3}\mathbf{k})/\sqrt{3},$$

at $\boldsymbol{x}_0 = (1, \frac{1}{2}, \frac{\pi}{6})$. The equation of the tangent plane is then

$$-\frac{1}{\sqrt{3}}(x-1) - \frac{2}{\sqrt{3}}(y-\tfrac{1}{2}) + 1(z-\tfrac{\pi}{6}) = 0, \text{ or, } x + 2y - \sqrt{3}\,z = 2 - \pi\sqrt{3}/6.$$

Both normal vector $\boldsymbol{n}$ and tangent plane are shown in Figure 2.11.

■

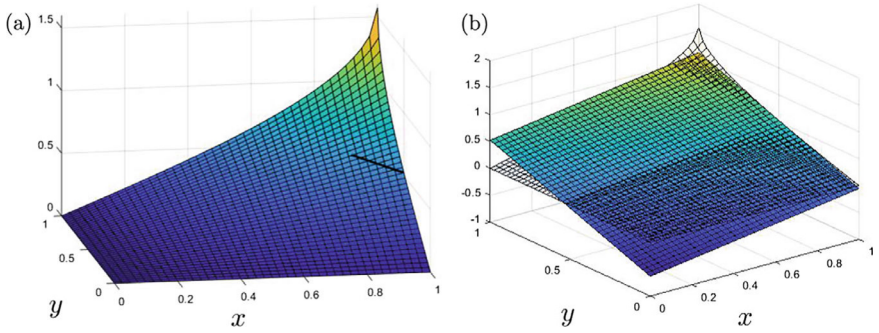


Figure 2.11 (a) $z = \arcsin(xy)$ with normal vector $\boldsymbol{n}$ at $(1, \frac{1}{2}, \frac{\pi}{3})$ and (b) $z = \arcsin(xy)$ and its tangent plane.

To further illustrate tangent plane calculations, we have a slightly more involved Mastery Check, which additionally offers an opportunity to apply knowledge from Section 1.A on vector algebra.

✍ Mastery Check 2.7:

Determine the equations of the tangent planes to the graph of $z = f(x, y) = \sqrt{x^2 + y^2}$, at the points $(0, 1, 1)$ and $(1, 0, 1)$. Then, determine the equation of their line of intersection.

✍

2.D Differentiability of $f : \mathbb{R}^n \longrightarrow \mathbb{R}$

Equipped with the knowledge and outcomes of the last section we are finally in a position to establish a convenient definition of differentiability for functions of many variables that logically generalizes the definition of differentiability of functions of one variable.

First, let us review what is meant geometrically and analytically by differentiability of a single-variable function, based solely on the existence of its derivative at a point.

In saying that $f : \mathbb{R} \longrightarrow \mathbb{R}$ is differentiable at a point $x_0 \in D_f \subset \mathbb{R}$ we mean, on the one hand, the *geometrical* condition that there exists a tangent line to the graph of $y = f(x)$ at the point x_0 (Figure 2.12):

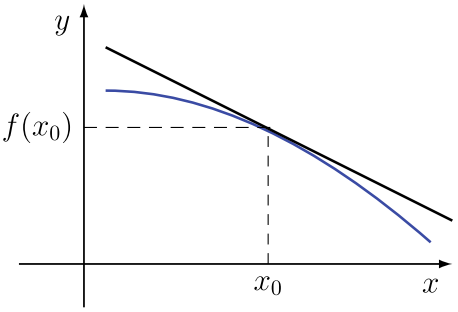


Figure 2.12 Tangent line to the graph of $f(x)$.

On the other hand, we also have the equivalent, *analytical* condition that:

$$\lim_{x\to x_0} \frac{f(x)-f(x_0)}{x-x_0} = c \quad \left(\; = \; \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_0 \right) \quad \text{exists,}$$

$$\iff \left| \frac{f(x)-f(x_0)-c(x-x_0)}{x-x_0} \right| \longrightarrow 0 \quad \text{as } x \to x_0,$$

$$\iff \frac{f(x)-f(x_0)-c(x-x_0)}{x-x_0} = \rho(x-x_0) \longrightarrow 0 \quad \text{as } x \to x_0.$$

The quantity ρ, referred to as an *infinitesimal* function, is generally a function of $(x - x_0)$ which $\longrightarrow 0$ as $x \to x_0$.

(To illustrate, the three terms in the parentheses in Example 1.10 represent ρ in that single variable case, with h taking the place of $x - x_0$.)

Rewriting the last equivalence statement, we conclude that $f(x)$ is differentiable at the point x_0,

$$\iff f(x) = f(x_0) + c(x-x_0) + \big(\Delta x\big)\rho(\Delta x),$$

provided $\lim_{\Delta x \to 0} \rho(\Delta x) = 0$,

$\iff$ the graph of f can be approximated by a line.

We are thus presented with an alternative condition of differentiability for a function of one variable that does not rely explicitly on the limit definition. The condition of differentiability conveniently takes both a geometric form and an analytic form. The uniqueness of the tangent line is also a crucial factor to keep in mind.

The generalization of this argument to a function of two or more variables is now reasonably straightforward with the tangent line approximation being replaced by a tangent *plane* approximation (or a tangent *hyper*plane approximation for the case of $n > 2$).

That is to say, in the two variable case $f(x, y)$ is differentiable at $(x_0, y_0) \in D_f \subset \mathbb{R}^2$ means *geometrically* that there exists a tangent plane to the graph of $z = f(x, y)$ at (x_0, y_0). Since a tangent plane is a function that is linear in the independent variables, we expect the analytical definition of differentiability to be concerned with approximations by linear functions of the form,

$$z = f(\boldsymbol{x}_0) + \phi(\boldsymbol{x} - \boldsymbol{x}_0; \boldsymbol{x}_0) = f(x_0, y_0) + c_1(x - x_0) + c_2(y - y_0),$$

where c_1 and c_2 are real constants. While there are several ways to formulate the analytic definition, all forms are equivalent. Two equivalent forms are presented in the definition below which is also phrased in the general case of a function of n variables.

Definition 2.4
Let $f : \mathbb{R}^n \longrightarrow \mathbb{R}$. f is said to be **differentiable** *at an interior point $\boldsymbol{x}_0 \in D_f$ if there exist n real constants $\{c_i\}_{i=1}^n$ and* ***either****,*

- *a scalar function $\rho(\boldsymbol{x} - \boldsymbol{x}_0; \boldsymbol{x}_0)$, for which $\lim_{\boldsymbol{\Delta x} \to 0} \rho(\boldsymbol{\Delta x}; \boldsymbol{x}_0) = 0$, so that*
  $f(\boldsymbol{x}) = f(\boldsymbol{x}_0) + \sum_{i=1}^n c_i(x_i - x_i^0) + |\boldsymbol{x} - \boldsymbol{x}_0|\rho(\boldsymbol{x} - \boldsymbol{x}_0; \boldsymbol{x}_0)$
  for $\boldsymbol{x}$ near $\boldsymbol{x}_0$,

or*,*

- *n scalar functions $\alpha_i(\boldsymbol{x} - \boldsymbol{x}_0; \boldsymbol{x}_0)$, $i = 1, .., n$, for which $\lim_{\boldsymbol{\Delta x} \to 0} \alpha_i(\boldsymbol{\Delta x}; \boldsymbol{x}_0) = 0$ for all $i = 1, .., n$, so that*
  $f(\boldsymbol{x}) = f(\boldsymbol{x}_0) + \sum_{i=1}^n c_i(x_i - x_i^0) + \sum_{i=1}^n \alpha_i(\boldsymbol{x} - \boldsymbol{x}_0; \boldsymbol{x}_0)(x_i - x_i^0)$
  for $\boldsymbol{x}$ near $\boldsymbol{x}_0$.

Remarks

* A function for which no linear approximation can be defined at a point is said to be **singular** at that point.
* The common feature of the two expressions in Definition 2.4 is the existence of a tangent plane

$$z = f(\boldsymbol{x}_0) + \phi(\boldsymbol{x} - \boldsymbol{x}_0; \boldsymbol{x}_0) = f(\boldsymbol{x}_0) + \sum_{i=1}^{n} c_i (x_i - x_i^0).$$

  The definition then effectively says that a function of n variables is differentiable if it can be approximated by a linear function, with a correction term that has a higher order dependence on the small quantity $|\boldsymbol{x} - \boldsymbol{x}_0|$ and that vanishes in the limit of $\boldsymbol{x} \to \boldsymbol{x}_0$. Corresponding statements apply to the alternative expression involving the functions α_i. Functions ρ and α_i are termed *infinitesimal* functions (Section 1.C) as they vanish in the limit $\boldsymbol{x} \to \boldsymbol{x}_0$ faster than $|\boldsymbol{x} - \boldsymbol{x}_0|$.
* It can readily be shown that the tangent plane at a differentiable point of function f is unique. This follows by first assuming the existence of two such linear approximations, $z = f(\boldsymbol{x}_0) + \phi(\boldsymbol{x} - \boldsymbol{x}_0)$ and $z = f(\boldsymbol{x}_0) + \psi(\boldsymbol{x} - \boldsymbol{x}_0)$, and then showing that if both fulfill the conditions of Definition 2.4 then they must be equal: $\phi = \psi$.
* Applying either expression in Definition 2.4 in Definition 2.3 of partial derivatives, it is clear that the constants $\{c_i\}_{i=1}^n$ are the n partial derivatives of the function $f(\boldsymbol{x})$ evaluated at the point $\boldsymbol{x}_0$: $c_i = \left.\dfrac{\partial f}{\partial x_i}\right|_{\boldsymbol{x}_0}$.
  Hence, the linear function $\phi(\boldsymbol{x} - \boldsymbol{x}_0; \boldsymbol{x}_0)$ becomes,

$$\phi(\boldsymbol{x} - \boldsymbol{x}_0; \boldsymbol{x}_0) = \left.\frac{\partial f}{\partial x_1}\right|_{\boldsymbol{x}_0} (x_1 - x_1^0) + \cdots + \left.\frac{\partial f}{\partial x_n}\right|_{\boldsymbol{x}_0} (x_n - x_n^0).$$

* The bi-linear functional, $\boldsymbol{\Phi}_{\boldsymbol{x}_0}$, acting first on function f and then on point $\boldsymbol{x} \in \mathbb{R}^n$, produces the real scalar $\phi(\boldsymbol{x}; \boldsymbol{x}_0) \in \mathbb{R}$. Its first action on f alone gives *the derivative of the multivariable function f at $\boldsymbol{x}_0$*. Later, this will be given a special name and denoted in a special way, but for now we may simply acknowledge $\Phi_{\boldsymbol{x}_0} f$ as the n-component vector derivative,

$$\boldsymbol{\Phi}_{\boldsymbol{x}_0} f = \left(\left.\frac{\partial f}{\partial x_1}\right|_{\boldsymbol{x}_0}, \left.\frac{\partial f}{\partial x_2}\right|_{\boldsymbol{x}_0}, \cdots, \left.\frac{\partial f}{\partial x_n}\right|_{\boldsymbol{x}_0} \right).$$

  This vector is the natural extension to a function of n variables of the ordinary derivative of a function of one variable.
* Although it is more relevant to the discussions in Section 2.I and Chapter 3, it is appropriate to say a word or two about the function ρ (in both the 1D and nD cases). For $\boldsymbol{x} \neq \boldsymbol{x}_0$, a rearrangement

of the equation in Definition 2.4 provides an expression for the function $\rho(\boldsymbol{\Delta x}; \boldsymbol{x}_0)$ as the ratio of the difference between f and its linear approximation, to $|\boldsymbol{\Delta x}|$,

$$\rho(\boldsymbol{\Delta x}; \boldsymbol{x}, \boldsymbol{x}_0) = \frac{f(\boldsymbol{x}) - f(\boldsymbol{x}_0) - \phi(\boldsymbol{x} - \boldsymbol{x}_0)}{|\boldsymbol{\Delta x}|}.$$

For this to vanish in the limit $|\Delta \boldsymbol{x}| \to 0$ it must be of nonlinear order in $|\Delta \boldsymbol{x}|$.

* In general, the infinitesimal functions α_i are not uniquely identified (see next example). However, we shall see in Section 2.I that additional conditions enable us to specify a particular choice.
* In summary, we see that Definition 2.4 means that $f : \mathbb{R}^n \to \mathbb{R}$ is differentiable at $\boldsymbol{x}_0$ if,

$$\lim_{\boldsymbol{\Delta x} \to 0} \frac{f(\boldsymbol{x}_0 + \boldsymbol{\Delta x}) - f(\boldsymbol{x}_0) - \sum_{i=1}^{n} \left.\frac{\partial f}{\partial x_i}\right|_{\boldsymbol{x}_0} \Delta x_i}{|\boldsymbol{\Delta x}|} = 0.$$

We clarify the above remarks with an example.

Example 2.8:

Consider the function $f(x, y) = xy^2$ and the point $\boldsymbol{x}_0 = (-2, 1)$. Using Definition 2.4, identify the partial derivatives and the infinitesimal functions, ρ, α_1 and α_2.

Solution:

We introduce $\boldsymbol{h} = (h, k)$ to form the nearby point $\boldsymbol{x} = \boldsymbol{x_0} + \boldsymbol{h} = (-2+h, 1+k)$. Then

$$\begin{aligned} f(\boldsymbol{x}_0 + \boldsymbol{h}) - f(\boldsymbol{x}_0) &= (-2+h)(1+k)^2 - (-2)1^2 \\ &= (-2+h)(1+2k+k^2) + 2 \\ &= (h - 4k) + (-2k^2 + 2hk + hk^2). \end{aligned}$$

In the last expression on the right-hand side, the two pairs of parentheses separate the linear contribution, $\phi(h, k) = h - 4k$, from the remaining nonlinear contribution. From the latter contribution we may construct our ρ function

$$\rho(\boldsymbol{h}; \boldsymbol{x}_0 + \boldsymbol{h}, \boldsymbol{x}_0) = \frac{-2k^2 + 2hk + hk^2}{\sqrt{h^2 + k^2}}$$

which vanishes in the limit $|\boldsymbol{h}| = \sqrt{h^2 + k^2} \to 0$ since the numerator is at least quadratic in h and k while the denominator is of linear order. Alternatively, from the nonlinear contribution we may identify (nonuniquely) the α_i functions:

$$\alpha_1 h + \alpha_2 k = \left(2k + k^2\right) h + (-2k)\, k.$$

We see that both α_1 and α_2 vanish at $h = k = 0$. Note, however, that in this example the alternative identification, $\alpha_1 = 0$ and $\alpha_2 = (-2k + 2h + hk)$ would also work. From the linear approximation, ϕ, we read off the partial derivatives $\left(\dfrac{\partial f}{\partial x}, \dfrac{\partial f}{\partial y}\right)\Big|_{(-2,1)} = (1, -4)$.

■

The existence of the partial derivatives evaluated at point $\boldsymbol{x}_0$, $\left\{ \dfrac{\partial f}{\partial x_i}\Big|_{\boldsymbol{x}_0} \right\}_{i=1}^{n}$ can at best guarantee the continuity of the function $f(\boldsymbol{x})$ at $\boldsymbol{x}_0$, *in the respective single-variable directions*. It does not ensure continuity of $f(\boldsymbol{x})$ generally. We see this from the definition of the partial derivatives. On the other hand, the condition of differentiability at a point (existence of a tangent plane) *does ensure continuity* at that point. Obviously we also see that differentiability at a point guarantees the existence of partial derivatives at that point. We summarize these observations in the following two-point theorem.

Theorem 2.1
Let $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ *be* **differentiable** *at an interior point* $\boldsymbol{x}_0 \in D_f$*, then*

- f *is continuous at that point,*
- f *is partially differentiable at that point.*

Our statements preceding Theorem 2.1 show that the converses of these two propositions are not true in general. A function continuous at a point is not necessarily differentiable, and a function partially differentiable at a point need not be differentiable there. This makes sense when considering functions with edges as illustrated in Figure 2.13. See also Mastery Check 2.8.

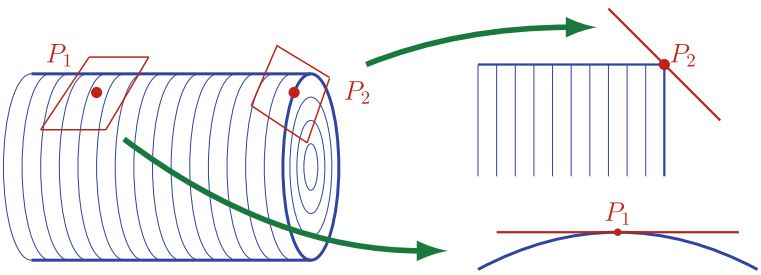


Figure 2.13 The relation between partial differentiability and differentiability.

Naturally, the important question to ask is what conditions *are* sufficient to ensure differentiability? This is answered in the next important theorem.

Theorem 2.2
A continuous function $f : \mathbb{R}^n \to \mathbb{R}$ *with* **continuous partial derivatives** $\dfrac{\partial f}{\partial x_i}$ *in a neighbourhood* M *of a point* $\boldsymbol{x}_0 \in D_f$ *is* **differentiable** *at* $\boldsymbol{x}_0$.

A proof of this important theorem follows the argument below.

■ **Proof:**
Suppose $\boldsymbol{x}_0 + \boldsymbol{h}$, with $\boldsymbol{h} = (h_1, \ldots, h_n)$ where $|\boldsymbol{h}| = \sqrt{h_1^2 + \ldots + h_n^2} \ll 1$, to be a point within the neighbourhood M of $\boldsymbol{x}_0$, and let all n partial derivatives of f exist and be continuous in M. Indulging in a little elaborate notation, define the vector increment

$$\boldsymbol{h}^{(i)} \quad = \quad (h_1, h_2, \ldots, h_{n-i}, \underbrace{0, 0, \ldots, 0}_{i \text{ zeros}}), \quad i = 0, \ldots, n.$$

So that $\boldsymbol{h}^{(0)} = \boldsymbol{h}$ and $\boldsymbol{h}^{(n)} = \boldsymbol{0}$.
Possessing i component zeros it follows that $|\boldsymbol{h}^{(i)}| \leq |\boldsymbol{h}|$, so $\boldsymbol{x}_0 + \boldsymbol{h}^{(n-i)}$ is also a point in M. We then have,

$$\begin{aligned} f(\boldsymbol{x}_0 + \boldsymbol{h}) - f(\boldsymbol{x}_0) &\doteq f\left(\boldsymbol{x}_0 + \boldsymbol{h}^{(0)}\right) - f\left(\boldsymbol{x}_0 + \boldsymbol{h}^{(n)}\right), \\ &= \sum_{i=1}^{n} \left[f\left(\boldsymbol{x}_0 + \boldsymbol{h}^{(i-1)}\right) - f\left(\boldsymbol{x}_0 + \boldsymbol{h}^{(i)}\right) \right], \end{aligned}$$

adding and subtracting intermediate terms

$$= \sum_{i=1}^{n} h_i \left(\frac{\partial f}{\partial x_i} \right)\Bigg|_{\boldsymbol{x}_0 + \overline{\boldsymbol{h}}^{(n-i)}},$$

by the mean value theorem applied to each [∼] term in the sum and since the partial derivatives exist in M

where $\overline{\boldsymbol{h}}^{(j)} = (h_1, h_2, \ldots, h_{n-j-1}, \theta_{n-j} h_{n-j}, 0, 0, \ldots, 0)$ with constants $0 < \theta_{n-j} < 1$, for $j = 0, \ldots, n-1$. Since the partial derivatives are continuous in M it follows that there exist infinitesimal functions $\alpha_i(\boldsymbol{h}; \boldsymbol{x}_0)$ satisfying $\alpha_i \to 0$ as $|\boldsymbol{h}| \to 0$, such that

$$\left(\frac{\partial f}{\partial x_i} \right)\Bigg|_{\boldsymbol{x}_0 + \overline{\boldsymbol{h}}^{(n-i)}} = \left(\frac{\partial f}{\partial x_i} \right)\Bigg|_{\boldsymbol{x}_0} + \alpha_i(\boldsymbol{h}; \boldsymbol{x}_0).$$

Consequently,

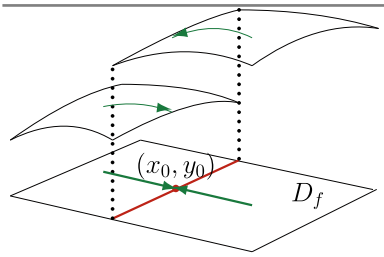
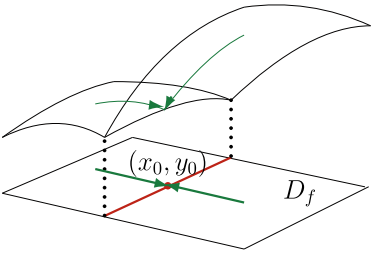
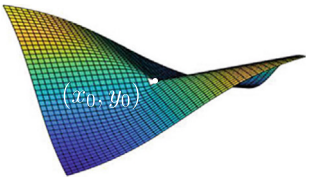
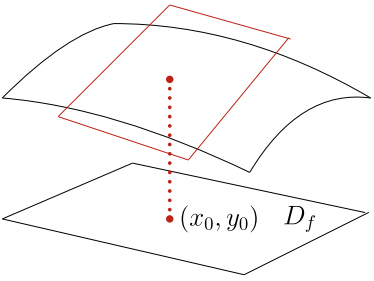
$$f(\boldsymbol{x}_0 + \boldsymbol{h}) - f(\boldsymbol{x}_0) = \sum_{i=1}^{n} h_i \left(\frac{\partial f}{\partial x_i} \right)\Bigg|_{\boldsymbol{x}_0} + \sum_{i=1}^{n} h_i \alpha_i,$$

and so f is differentiable at $\boldsymbol{x}_0$.

■

It may assist the reader to work through a version of the above argument for a function of only two variables, $f(x, y)$.

Table 2.1: A pictorial table of differentiable functions (not exhaustive)

Function	Diff'ble ats (x_0, y_0)?	Why or why not?
	*No*	Limit does not exist at points on the red line. Function is not continuous. No tangent plane.
	*No*	Limit exists and function is continuous across the red line. But not *all* partial derivatives exist. No tangent plane.
	*No*	[*Mastery Check 2.8*] The function is continuous; all partial derivatives exist but they are *not continuous* at one point. No tangent plane!
	**Yes**	Function is continuous, *all* partial derivatives exist and are continuous at (x_0, y_0). There exists a unique tangent plane!

Theorem 2.1 on the continuity of partial derivatives as a sufficient condition for differentiability inspires the pictorial interpretation in Figure 2.13, which depicts a cylinder lying on its side. At point P_1, which is a point on the curved side of the cylinder, the function describing the surface is partially differentiable - the partial derivatives in the two orthogonal directions (in the horizontal plane) exist and are continuous - and consequently the function is differentiable there. However, at point P_2, which is a point on the edge of the base of the cylinder, the function has limited partial differentiability (only in one direction) and so is not differentiable there. Table 2.1 reinforces the arguments for and against differentiability with a few more illustrative examples.

So, it appears that for $f : \mathbb{R} \longrightarrow \mathbb{R}$, the function is differentiable at a point if the derivative exists, but for $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$, the partial derivatives must not only exist at a point, they must also *be continuous* in an open circle about the point for the function to be differentiable there. The following example and Mastery Check aim to make this clear.

Example 2.9:

Consider the function $f : \mathbb{R}^2 \to \mathbb{R}$, defined by

$$f(x,y) = \begin{cases} x \arctan(y/x), & \text{for } x \neq 0,\ y \in \mathbb{R}, \\ 0, & \text{for } x = 0,\ y \in \mathbb{R}. \end{cases}$$

We first investigate the continuity of f, and then the existence and continuity of the partial derivatives f_x and f_y along the y-axis, for $y \neq 0$.

The function is in fact continuous for all points on the y-axis since

$$\lim_{x\to 0} f(x,y) = \lim_{x\to 0} x \arctan(y/x) = 0 = f(0,y),$$

because $|\arctan(y/x)| < \pi/2$.

Now consider the continuity of the two partial derivatives,

$$f_x = \arctan(y/x) - \frac{xy}{x^2+y^2} \text{ and } f_y(x,y) = \frac{x^2}{x^2+y^2}, \text{ for } x, y \neq 0,$$

at $x = 0$.

Consider the half line $y > 0$. Taking the right-hand limit $x \to 0^+$ at constant y of f_x, we have $\lim\limits_{x\to 0^+} f_x = \frac{\pi}{2} - 0 = \frac{\pi}{2}$, while the left-hand limit gives $\lim\limits_{x\to 0^-} f_x = -\frac{\pi}{2} + 0 = -\frac{\pi}{2}$.

Similarly, on the lower half line $y < 0$, we find $\lim\limits_{x\to 0^+} f_x = -\frac{\pi}{2} + 0 = -\frac{\pi}{2}$ and $\lim\limits_{x\to 0^-} f_x = \frac{\pi}{2} - 0 = \frac{\pi}{2}$. Thus, the limit of f_x does not exist and f_x is

not continuous at $x = 0$ for any $y \neq 0$. In fact, f_x has what we've termed a discontinuity of the first kind at $x = 0$ for $y \neq 0$.

On the other hand, $\lim_{x\to 0^+} f_y = \lim_{x\to 0^-} f_y = 0$, for any $y \neq 0$, and the limit exists. Given additionally that for any $y \neq 0$, $f_y(0, y) = 0$, we see that f_y is continuous along the line $x = 0$ for $y \neq 0$.

The reader may want to analyse what happens when $y = 0$.

■

✍ Mastery Check 2.8:

Consider the function $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$ defined by

$$f(x, y) = \begin{cases} \dfrac{xy}{\sqrt{x^2 + y^2}}, & \text{for } x, y \neq 0, \\ 0, & \text{for } x = y = 0. \end{cases}$$

whose graph appears in Figure 2.14. We wish to investigate the behaviour of f near $(0, 0)$.

(1) Find the two partial derivatives for $(x, y) \neq (0, 0)$.

(2) Show using Definition 2.3 that both partial derivatives are *zero* at $(0, 0)$. Therefore, *if it were to exist* the tangent plane at $(0, 0)$ *would coincide with the plane* $z = 0$.

(3) Show that the partial derivatives are not continuous at $(0, 0)$ by considering the following limits:

$$\lim_{x\to 0}\left(\lim_{y\to 0}\frac{\partial f}{\partial x}\right), \quad \lim_{y\to 0^-}\left(\lim_{x\to 0}\frac{\partial f}{\partial x}\right), \quad \lim_{y\to 0^+}\left(\lim_{x\to 0}\frac{\partial f}{\partial x}\right).$$

(A similar result holds for the other derivative.)

Given your result, do you expect the tangent plane to exist?

(4) Putting your last result aside, assume the existence of the supposed tangent plane from (2) in Definition 2.4, and determine $\rho(\Delta\boldsymbol{x})$ in the expression

$$f(\boldsymbol{x}) = f(\boldsymbol{x}_0) + \phi(\boldsymbol{x} - \boldsymbol{x}_0) + |\boldsymbol{\Delta x}|\rho(\boldsymbol{\Delta x})$$

for points $\boldsymbol{x}$ lying on the line $y = x \neq 0$.

(Assume $|\Delta\boldsymbol{x}| = \sqrt{\Delta x^2 + \Delta y^2}$ with $\Delta y = \Delta x$).

Use this result to decide independently of (3) whether a tangent plane exists.

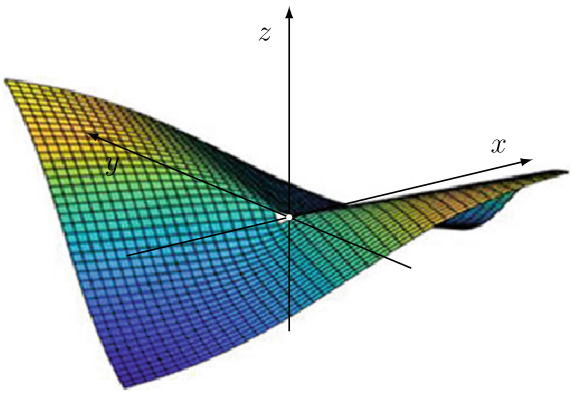


Figure 2.14 The graph of $z = \dfrac{xy}{\sqrt{x^2+y^2}}$, $x, y \neq 0$.

2.E Directional Derivatives and the Gradient

The directional derivative

Thus far we have established that the partial derivatives of a function $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$ at a point (x_0, y_0) in its domain have the properties that:

$$\left.\frac{\partial f}{\partial x}\right|_{(x_0,y_0)} = \text{the rate of change (that is, the slope) of } f \text{ in the (positive) } x\text{-direction at } (x_0, y_0).$$

$$\left.\frac{\partial f}{\partial y}\right|_{(x_0,y_0)} = \text{the rate of change (that is, the slope) of } f \text{ in the (positive) } y\text{-direction at } (x_0, y_0).$$

The derivative definitions specifically identify the two lines of approach to the limit point $\boldsymbol{x}_0$ and tell us a good deal about the function behaviour in two orthogonal directions, but not in other directions. Of course, in principle, there is nothing special about these directions; they have been singled out because of our choice of coordinate system. It is legitimate to ask under what conditions is it possible to determine the rate of change of f in some other direction, such as the direction of the vector $\boldsymbol{u}$ drawn in Figure 2.15, and how does one then proceed?

To answer this question it suffices to consider a function of two variables. The result may then be generalized to higher dimensions.

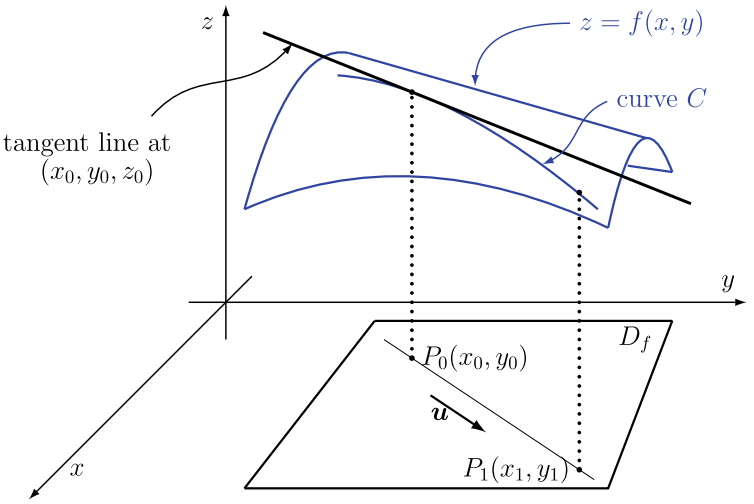


Figure 2.15 The tangent vector in an arbitrary direction.

Suppose $f(x, y)$ is *differentiable* at the point $P_0 = (x_0, y_0)$ and suppose we wanted the rate of change of f in an arbitrary direction $\boldsymbol{u} = (u, v)$ in the xy-plane. From our previous account, that f is differentiable at P_0 ensures that f is continuous and that the partial derivatives of f exist and are also continuous in a neighborhood of P_0. These conditions favor a revisit to the limit definition in Equation (2.2) on Page 64 as the presence of each of the quantities concerned is valid in the context. In addition, the unit vector $\boldsymbol{u} = (u, v)$ can be used to define the line along which we will consider taking a limit to P_0. Suppose $P_1 = (x_1, y_1)$ is a point on that line and consider the limit $P_1 \to P_0$.

From our vector algebra review in Section 1.A (Page 10) we have that the vector, $\overrightarrow{P_0P_1}$, joining the two points in the plane can be expressed,

$$\overrightarrow{P_0P_1} \quad = \quad \boldsymbol{x}_1 - \boldsymbol{x}_0 \quad = \quad \underset{(\ \Delta x\ ,\ \Delta y\ )}{(x_1 - x_0, y_1 - y_0)} \quad = \quad \underbrace{t}_{\text{scalar multiplier}} \,.\, \underbrace{\boldsymbol{u}}_{\text{unit vector in direction } \overrightarrow{P_0P_1}} \quad = \quad t\,.(u, v).$$

From this we see that we can reformulate the approach $\boldsymbol{x}_1 \to \boldsymbol{x}_0$ as a real scalar limit $t \to 0$, given that there is no change in the direction of approach. Inserting the above into the limit expression, Equation (2.2) for the derivative of f, may be rewritten as in the following definition.

Definition 2.5
The derivative limit:

$$\lim_{\boldsymbol{x}_1 \to \boldsymbol{x}_0} \frac{f(x_1, y_1) - f(x_0, y_0)}{|\boldsymbol{x}_1 - \boldsymbol{x}_0|} = \lim_{\boldsymbol{x}_1 \to \boldsymbol{x}_0} \frac{f(x_0 + tu, y_0 + tv) - f(x_0, y_0)}{|t\boldsymbol{u}|} = \lim_{t \to 0} \frac{f(x_0 + tu, y_0 + tv) - f(x_0, y_0)}{|t|},$$

with $|\boldsymbol{u}|=1$, *if it exists, is called* **the directional derivative of** f **at** (x_0, y_0) **in the direction of** $\boldsymbol{u}$.

Commonly used notations for the directional derivative include

$$D_{\boldsymbol{u}} f(\boldsymbol{x}_0) \text{ and } \frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{u}}(\boldsymbol{x}_0),$$

each of which feature the function, f, the point of application, $\boldsymbol{x}_0$, and the direction vector, $\boldsymbol{u}$.

To calculate the directional derivative, there are two alternatives. We can use the above definition, which may be necessary if the function is *not continuous, but possesses a finite limit at* $\boldsymbol{x}_0$ or *not differentiable at* $\boldsymbol{x}_0$. Alternatively, we can defer to the following theorem.

Theorem 2.3
If $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$ *is a differentiable function, then*

$$D_{\boldsymbol{u}} f(\boldsymbol{x}_0) = \frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{u}}(\boldsymbol{x}_0) = \frac{\partial f}{\partial x}\Big|_{\boldsymbol{x}_0} u + \frac{\partial f}{\partial y}\Big|_{\boldsymbol{x}_0} v.$$

For functions that satisfy the condition of differentiability, this theorem is easy to prove.

■ **Proof:**
In light of Definition 2.4, for a function f of variable $\boldsymbol{x} \in \mathbb{R}^n$ differentiable means

$$\frac{f(\boldsymbol{x}_0 + t\boldsymbol{u}) - f(\boldsymbol{x}_0)}{t} = \frac{1}{t}\left(f(\boldsymbol{x}_0) + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}\Big|_{\boldsymbol{x}_0} tu_i + t\rho(t) - f(\boldsymbol{x}_0)\right)$$

$$= \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}\Big|_{\boldsymbol{x}_0} u_i + \rho(t) \longrightarrow \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}\Big|_{\boldsymbol{x}_0} u_i \quad \text{as } t \to 0, \text{since } \rho(t) \to 0.$$

■

Although the pictorial representation may not be possible in $\mathbb{R}^n$, it is nevertheless obvious how one may extend Definition 2.5 to define the directional derivative of a function of n variables, $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ at a point $\boldsymbol{x}_0 = (x_1^0, \ldots, x_n^0)$ in the direction $\boldsymbol{u} = (u_1, \ldots, u_n)$. Similarly, Theorem 2.3 and its proof may also be extended easily. The n-variable version of Theorem 2.3 takes the form

$$D_{\boldsymbol{u}} f(\boldsymbol{x}_0) = \frac{\partial f}{\partial x_1}\Big|_{\boldsymbol{x}_0} u_1 + \frac{\partial f}{\partial x_2}\Big|_{\boldsymbol{x}_0} u_2 + \cdots + \frac{\partial f}{\partial x_n}\Big|_{\boldsymbol{x}_0} u_n \tag{2.3}$$

where $\boldsymbol{u} = (u_1, u_2, \ldots, u_n)$ and $|\boldsymbol{u}| = 1$.

It is easy to verify that applying the definition (or theorem) to the particular case of $\boldsymbol{u}$ being one of the coordinate vectors ($\mathbf{i}$ or $\mathbf{j}$ in $\mathbb{R}^2$; $\mathbf{i}$, $\mathbf{j}$, or $\mathbf{k}$ in $\mathbb{R}^3$; or $\boldsymbol{e}_j$ in higher dimensional cases of $\mathbb{R}^n$), simply returns the partial derivative of f in that variable. Moreover, since $\dfrac{\partial f}{\partial x_j}\Big|_{\boldsymbol{x}_0}$ gives the slope of the tangent line to the graph of f at $\boldsymbol{x}_0$ in the x_j direction, it follows that $D_{\boldsymbol{u}} f(\boldsymbol{x}_0)$ gives the slope of the graph of f at $\boldsymbol{x}_0$ in the direction of $\boldsymbol{u}$. Incidentally, it pays to remember that as a consequence of the definition of differentiability, $D_{\boldsymbol{u}} f(\boldsymbol{x}_0)$ also gives the slope of the *tangent plane* to the graph of f in the direction $\boldsymbol{u}$.

Gradient of a scalar function

Let's look a little more closely at what is used to calculate the directional derivative of a differentiable function. In the general case of $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ Equation (2.3) can be interpreted as the scalar product of two vectors:

$$\begin{aligned} D_{\boldsymbol{u}} f(\boldsymbol{x}_0) &= \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}\Big|_{\boldsymbol{x}_0} u_i \\ &= \underbrace{\left(\frac{\partial f}{\partial x_1}\Big|_{\boldsymbol{x}_0}, \frac{\partial f}{\partial x_2}\Big|_{\boldsymbol{x}_0}, \ldots, \frac{\partial f}{\partial x_n}\Big|_{\boldsymbol{x}_0} \right)}_{\text{a vector called } \ldots} \cdot \overbrace{(u_1, u_2, \ldots, u_n)}^{\text{direction of interest}} \end{aligned}$$

$\ldots$ the gradient of f at $\boldsymbol{x}_0$.

At a general point $\boldsymbol{x} \in D_f$ we have the formal definition:

Definition 2.6
The **vector gradient** *of a function* $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ *at a point* $\boldsymbol{x} \in D_f$ *is defined as*

$$\text{grad} f(\boldsymbol{x}) \;=\; \Big(\frac{\partial f}{\partial x_1}\Big|_{\boldsymbol{x}}, \frac{\partial f}{\partial x_2}\Big|_{\boldsymbol{x}}, \ldots, \frac{\partial f}{\partial x_n}\Big|_{\boldsymbol{x}}\Big) \;\equiv\; \boldsymbol{\nabla} f(\boldsymbol{x})$$

— *we say* "grad f" or "del f".

Using this new notation, the directional derivative of a differentiable function $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ at a point $\boldsymbol{x}_0$ in the direction $\boldsymbol{u}$, is conveniently expressed as the scalar product of the gradient of f evaluated at $\boldsymbol{x}_0$ and the *unit* vector $\boldsymbol{u}$.

$$D_{\boldsymbol{u}} f(\boldsymbol{x}_0) = \text{grad}\, f(\boldsymbol{x}_0) \cdot \boldsymbol{u} = \boldsymbol{\nabla} f(\boldsymbol{x}_0) \cdot \boldsymbol{u}.$$

■ **Example 2.10:**
Consider the function $f(x, y, z) = xy^3 + yz^2$. What is the directional derivative of f at the point $\boldsymbol{x}_0 = (1, 2, -1)$ in the direction $\boldsymbol{u} = 2\mathbf{e}_1 + \mathbf{e}_2 + 2\mathbf{e}_3$?

Solution:

The gradient of f at an arbitrary point $\boldsymbol{x}$ is $\boldsymbol{\nabla} f = y^3\mathbf{e}_1 + (3xy^2 + z^2)\mathbf{e}_2 + 2yz\mathbf{e}_3$. At the point $\boldsymbol{x}_0 = (1, 2, -1)$ this vector becomes $\boldsymbol{\nabla} f(\boldsymbol{x}_0) = 8\mathbf{e}_1 + 13\mathbf{e}_2 - 4\mathbf{e}_3$. Meanwhile, the unit vector $\boldsymbol{N}$ in the direction of $\boldsymbol{u} = 2\mathbf{e}_1 + \mathbf{e}_2 + 2\mathbf{e}_3$ is,

$$\boldsymbol{N} = \frac{\boldsymbol{u}}{|\boldsymbol{u}|} = \frac{2}{3}\mathbf{e}_1 + \frac{1}{3}\mathbf{e}_2 + \frac{2}{3}\mathbf{e}_3.$$

Hence, the directional derivative we require is the scalar product of these vectors:

$$\boldsymbol{\nabla} f \cdot \boldsymbol{N} = \big(8\mathbf{e}_1 + 13\mathbf{e}_2 - 4\mathbf{e}_3\big) \cdot \big(\frac{2}{3}\mathbf{e}_1 + \frac{1}{3}\mathbf{e}_2 + \frac{2}{3}\mathbf{e}_3\big) = 7.$$

To get some perspective on this result, compare this with the slope of f at $\boldsymbol{x}_0$ in the x-direction: $\dfrac{\partial f}{\partial x}\Big|_0 = 8$, in the y-direction: $\dfrac{\partial f}{\partial y}\Big|_0 = 13$; and in the z-direction: $\dfrac{\partial f}{\partial z}\Big|_0 = -4$.

■

Remarks — Some all-important facts about the gradient, $\boldsymbol{\nabla} f$:

* The gradient of a function f is what was regarded, in the fifth remark following Definition 2.4, as *the derivative of* $f : \mathbb{R}^n \to \mathbb{R}$. That is to say, the linear functional map, $\boldsymbol{\Phi}_{\boldsymbol{x}_0} f$, referred to earlier is what we have now defined as the *gradient of the function* f: $\boldsymbol{\Phi}_{\boldsymbol{x}_0} f \equiv \boldsymbol{\nabla} f(\boldsymbol{x}_0)$.

Henceforth, we shall drop the $\mathbf{\Phi} f$ notation in favor of the more conventional notation $\boldsymbol{\nabla} f$ (or, on occasion, grad$f$) as the derivative of a function of n variables.

* We reiterate that $\boldsymbol{\nabla} f(\boldsymbol{x})$ is the generalization to functions of several variables of the ordinary derivative $\mathrm{d}g/\mathrm{d}x$ for a function g of one variable, x. As an example of this, in $1D$, were a function g to satisfy the condition $\dfrac{\mathrm{d}g}{\mathrm{d}x} = 0$ for *all* $x \in D_g$ then $g(x) = \text{const}$.

  The nD version of this reads as follows. Only if a differentiable function $f : \mathbb{R}^n \longrightarrow \mathbb{R}$, satisfies the *vector* equation

  $$\boldsymbol{\nabla} f = \mathbf{0}, \textit{ at all points } \boldsymbol{x} \textit{ in an open subset of } D_f,$$

  would $f(\boldsymbol{x})$ then be constant in that subset. This follows easily from the following argument about f's inferred variable dependence:

$$\left.\begin{array}{c}\boldsymbol{\nabla} f(x,y,z) = \mathbf{0} \\ \forall \boldsymbol{x} \in D_f\end{array}\right\} \Longrightarrow \left\{\begin{array}{lcl}\dfrac{\partial f}{\partial x} = 0 & \Rightarrow & f = f(y,z) \\ \dfrac{\partial f}{\partial y} = 0 & \Rightarrow & f = f(x,z) \\ \dfrac{\partial f}{\partial z} = 0 & \Rightarrow & f = f(x,y)\end{array}\right\} \Longrightarrow f(x,y,z) = \text{const.}$$

* The above condition is <u>not</u> the same as $\boldsymbol{\nabla} f = \mathbf{0}$ at an *isolated* point $\boldsymbol{x}_0$. This is not a sufficient condition for f to be a constant. Nevertheless, the case when $\boldsymbol{\nabla} f = \mathbf{0}$ at one or more *isolated* points has significant practical implications. We shall follow up on these in Section 3.A.

* Earlier in this chapter it was argued that the partial derivative $\dfrac{\partial f}{\partial x_j}$ at a point $\boldsymbol{x}$ gives the slope of the graph of f in the direction of coordinate x_j. In this section we have found that the slope of the graph of f at $\boldsymbol{x}$ in an arbitrary direction $\boldsymbol{u}$ is given by the directional derivative $D_{\boldsymbol{u}} f(\boldsymbol{x}) = \boldsymbol{\nabla} f(\boldsymbol{x}) \cdot \boldsymbol{u}$. Applying the Cauchy-Schwarz inequality Eq. (1.B), to this scalar product, we find

  $$|D_{\boldsymbol{u}} f(\boldsymbol{x})| = |\boldsymbol{\nabla} f(\boldsymbol{x}) \cdot \boldsymbol{u}| \leq |\boldsymbol{\nabla} f(\boldsymbol{x})|\,|\boldsymbol{u}| = |\boldsymbol{\nabla} f(\boldsymbol{x})|\,,$$

  since $\boldsymbol{u}$ is a unit vector. It therefore follows that the slope of the graph of f at $\boldsymbol{x}$ in any direction is *bounded* (in magnitude, above and below) by $|\boldsymbol{\nabla} f(\boldsymbol{x})|$, and hence *the maximum rate of change of* f, $|D_{\boldsymbol{u}} f(\boldsymbol{x})| = |\boldsymbol{\nabla} f(\boldsymbol{x})|$, occurs when $\boldsymbol{u}$ is in the exact same $(+)$ or exact opposite $(-)$ direction to $\boldsymbol{\nabla} f(\boldsymbol{x})$.

  Consequently, at a point $\boldsymbol{x} \in D_f$, the differentiable function

  $$f : \mathbb{R}^n \longrightarrow \mathbb{R} \left\{\begin{array}{c}\text{increases} \\ \text{decreases}\end{array}\right\} \text{most } \textit{rapidly} \text{ in the direction of } \pm\boldsymbol{\nabla} f(\boldsymbol{x}).$$

∗ The gradient's direction is also an important quantitative feature that will be utilized often in the coming chapters. Suppose the function $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ is differentiable at a point $\boldsymbol{x}$ and that $\boldsymbol{\nabla} f(\boldsymbol{x}) \neq \mathbf{0}$. Then, $\boldsymbol{\nabla} f(\boldsymbol{x})$ is a vector which is *normal* to the level set $f(\boldsymbol{x}) =$ *a constant*. That is,

$$\left\{ \begin{array}{l} \left(\dfrac{\partial f}{\partial x}, \dfrac{\partial f}{\partial y}\right) \\ \left(\dfrac{\partial f}{\partial x}, \dfrac{\partial f}{\partial y}, \dfrac{\partial f}{\partial z}\right) \end{array} \right\} \text{is normal to the} \left\{ \begin{array}{l} \text{level curve in } \mathbb{R}^2 \\ \text{level surface in } \mathbb{R}^3 \end{array} \right\} \text{ of } f.$$

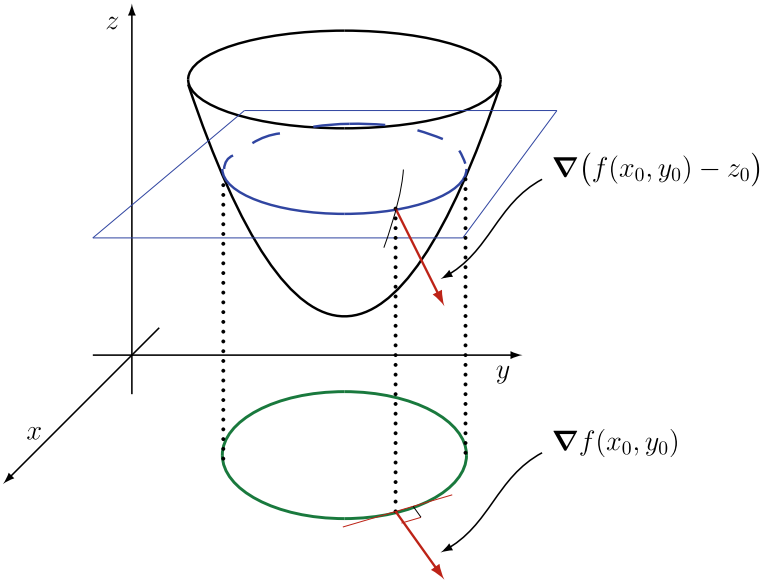


Figure 2.16 Comparison of the gradient applied in 2D and 3D circumstances.

Figure 2.16 illustrates the difference between the 2D and 3D situations, both involving the same function. In one case, we are concerned with the level set of $f(x, y)$, while the other case involves the level set of $f(x, y) - z$. To be precise, shown in the figure is the 3D vector,

$$\boldsymbol{\nabla}\big(f(x, y) - z\big)\Big|_0 = \frac{\partial f}{\partial x}\Big|_0 \mathbf{i} + \frac{\partial f}{\partial y}\Big|_0 \mathbf{j} - \mathbf{k},$$

which is normal to the surface in $\mathbb{R}^3$, $f(x, y) - z = C$, at (x_0, y_0, z_0) for some constant C, while the 2D vector

$$\boldsymbol{\nabla} f(x, y)\Big|_0 = \frac{\partial f}{\partial x}\Big|_0 \mathbf{i} + \frac{\partial f}{\partial y}\Big|_0 \mathbf{j},$$

is normal to the 2D level curve, $f(x, y) = c$ at (x_0, y_0) in the xy-plane, for some constant c.

The next two examples demonstrate precisely the distinction illustrated in Figure 2.16. The first involves a normal vector and a tangent plane in 3D, while the second example involves four dimensional objects.

Example 2.11:

Find the equation of the tangent plane to the level surface $f(x, y, z) = 2$ at the point $(1, 1, \pi)$, where $f(x, y, z) = xy\cos(z) + 3x$.

Solution:

The level surfaces of $w = f(x, y, z)$ are given by

$$xy\cos(z) + 3x = c. \qquad \text{— this is a surface in } \mathbb{R}^3.$$

According to theory, $\boldsymbol{\nabla} f$ is a normal vector to $f(x, y, z) = c$.

$$\boldsymbol{\nabla} f = (y\cos z + 3, x\cos z, -xy\sin z), \quad \text{and} \quad \boldsymbol{\nabla} f(1, 1, \pi) = (2, -1, 0) = \boldsymbol{n}_3.$$

The tangent plane to $f = c = 2$ at $(1, 1, \pi)$ is

$$\boldsymbol{n}_3 \cdot (\boldsymbol{x} - \boldsymbol{x}_0) = 0 \iff (2, -1, 0) \cdot (x - 1, y - 1, z - \pi) = 0.$$

That is, $2(x - 1) - (y - 1) = 0$, or $2x - y - 1 = 0$.
Notice that $\boldsymbol{n}_3$ is a 3-component vector and so lies in $\mathbb{R}^3$. Despite the absence of z in its equation, the tangent plane also resides in $\mathbb{R}^3$. The level surface, normal vector and tangent plane are shown in Figure 2.17.

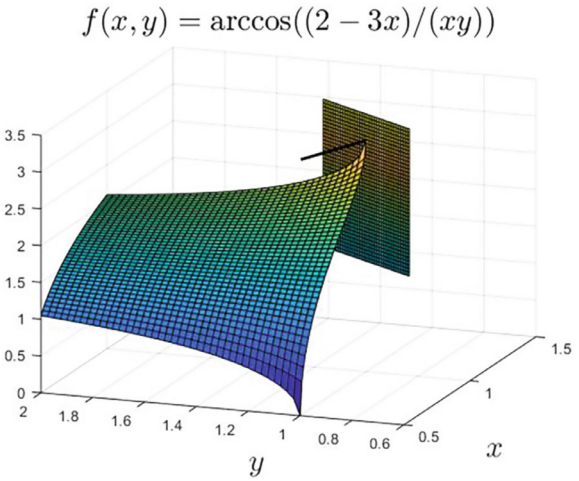


Figure 2.17 The level surface $xy\cos(z) + 3x = 2$, in a neighborhood of $(1, 1, \pi)$, and its normal vector and tangent plane at $(1, 1, \pi)$.

■

In contrast, the next example, although still involving the same function, cannot be visualised as all of its elements reside in $\mathbb{R}^4$.

Example 2.12:

Find the equation of the tangent plane to the level surface of $w = f(x, y, z)$ at the point $(1, 1, \pi)$, where $f(x, y, z) = xy\cos(z) + 3x$.

Solution:

The graph of $w = f(x, y, z)$ is the same as the level set of the four-variable object

$$g(x, y, z, w) = f(x, y, z) - w = 0. \qquad \text{— this is a surface in } \mathbb{R}^4.$$

We can now use the gradient again, this time the 4D version.

$$\begin{aligned} \boldsymbol{\nabla}_4 g &= \frac{\partial g}{\partial x}\boldsymbol{e}_1 + \frac{\partial g}{\partial y}\boldsymbol{e}_2 + \frac{\partial g}{\partial z}\boldsymbol{e}_3 + \frac{\partial g}{\partial w}\boldsymbol{e}_4 \\ &= \frac{\partial f}{\partial x}\boldsymbol{e}_1 + \frac{\partial f}{\partial y}\boldsymbol{e}_2 + \frac{\partial f}{\partial z}\boldsymbol{e}_3 - \boldsymbol{e}_4. \end{aligned}$$

At the point $(1, 1, \pi)$, $w = f = 2$, so (using the last result) the normal to $g = 0 = \text{const.}$ at $(1, 1, \pi, 2)$ is

$$\boldsymbol{n}_4 = (2, -1, 0, -1)$$

and the tangent plane is

$$\boldsymbol{n}_4 \cdot (\boldsymbol{x} - \boldsymbol{x}_0) = 0 \iff (2, -1, 0, -1) \cdot (x - 1, y - 1, z - \pi, w - 2) = 0.$$

That is, $2(x - 1) - (y - 1) - (w - 2)$, or $w = 2x - y + 1$.
Notice that here $\boldsymbol{n}_4$ is a 4-component vector and so lies in $\mathbb{R}^4$. Once again, even though z does not appear in the equation for the tangent plane, it formally involves 4 variables and so resides in $\mathbb{R}^4$. ■

Further examples of gradient calculations and potential uses are demonstrated in the next two exercises for the reader to pursue.

✍ Mastery Check 2.9:

What is the unit normal to the surface $xy^2z^3 = 4$ at the point $(1, 2, 1)$?
(Note that given all the topics discussed so far, this normal vector can be obtained in two ways. So, you can confirm your answer by attempting both approaches.)

✍

Mastery Check 2.10:
Determine the equation of the line L that passes through the point $(4, 4, \frac{1}{2})$ and that is normal to the surface

$$z = f(x, y) = x^2 + y^2.$$

2.F Higher-Order Derivatives

By now the reader will have correctly surmised that, just as in the single-variable case, higher-order derivatives are possible for functions of many variables.

Indeed, if

(a) $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ is a continuous function of $x_1, x_2, \ldots, x_n$, and

(b) some given partial derivative $\dfrac{\partial f}{\partial x_i}$ exists and is itself a continuous (not necessarily differentiable) function of $x_1, x_2, \ldots, x_n$,

then $\dfrac{\partial f}{\partial x_i}$ can itself be considered a function of $\boldsymbol{x}$ (independent of f).

For a convenient explanation, we shall refer to this particular derivative as $g(\boldsymbol{x})$ $\left(\equiv \dfrac{\partial f}{\partial x_i}(\boldsymbol{x}) \right)$. We can now consider the partial derivatives of g just as we had done with f:

Definition 2.7
If $\dfrac{\partial g}{\partial x_j} \equiv \lim\limits_{h \to 0} \dfrac{g(x_1, \ldots, x_j + h, \ldots, x_n) - g(x_1, \ldots, x_j, \ldots, x_n)}{h}$ *exists it is called* **a second-order partial derivative of** f. *More specifically, it is a second-order mixed partial derivative of* f *w.r.t.* x_i *and* x_j.

In terms of the original f we have that

$$\frac{\partial g}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\partial f}{\partial x_i}\right) \equiv \frac{\partial^2 f}{\partial x_j \partial x_i}$$

— this is the notation used (mostly) in this book

differentiate first w.r.t. x_i then w.r.t. x_j

Note that there are other ways to denote the second derivative. For example, for the function, $f(x, y)$, of two variables, three alternative notations,

$$\frac{\partial^2 f}{\partial y \partial x} = f_{xy} = f_{12},$$

are in common use, each of which describes the particular second-order partial derivative, where one first differentiates with respect to x and then with respect to y. The reader should exercise some care in interpreting the different notations. Notice the different order in which x and y appear in the first expression compared to the second expression, even though they refer to the same sequence of derivative operations.

We are now obliged to explain what higher partial derivatives are. For this explanation it suffices to remain with the function of two variables, $f(x, y)$. If $\left.\frac{\partial f}{\partial x}\right|_{(x_0,y_0)}$ is the slope of the tangent to f at (x_0, y_0) in the direction of x, then, just as in the single-variable case, $\left.\frac{\partial^2 f}{\partial x^2}\right|_{(x_0,y_0)}$ is the rate of change of the slope in this same direction. This second derivative is therefore a measure of *the curvature* of f in this direction. On the other hand, $\left.\frac{\partial^2 f}{\partial y \partial x}\right|_{(x_0,y_0)}$ is the rate of change of the x-directional slope in the y-direction.

The following is a convenient and useful result for continuous functions that possess continuous partial derivatives, which relieves some of the stress of interpreting notation as well as the need to keep track of the order in which derivatives are taken.

Theorem 2.4
Suppose $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ *is continuous and* $\dfrac{\partial f}{\partial x_i}$, $i = 1, 2, \ldots, n$ *exist and are continuous in* $S_r(\boldsymbol{x}) \subset D_f$, *and that both* $\dfrac{\partial^2 f}{\partial x_i \partial x_j}$ *and* $\dfrac{\partial^2 f}{\partial x_j \partial x_i}$ *exist and are continuous at* $\boldsymbol{x} \in D_f$. *Then* $\dfrac{\partial^2 f}{\partial x_i \partial x_j} \equiv \dfrac{\partial^2 f}{\partial x_j \partial x_i}$ *at* $\boldsymbol{x} \in D_f$.

(For the standard proof, see a standard text book such as [5] or [6].)

The conditions of Theorem 2.4 are highlighted in Figure 2.18. Note the distinction between the requirements of continuity *at a point* for the second derivatives and continuity *in a neighborhood of that point* required of the function and its first derivatives.

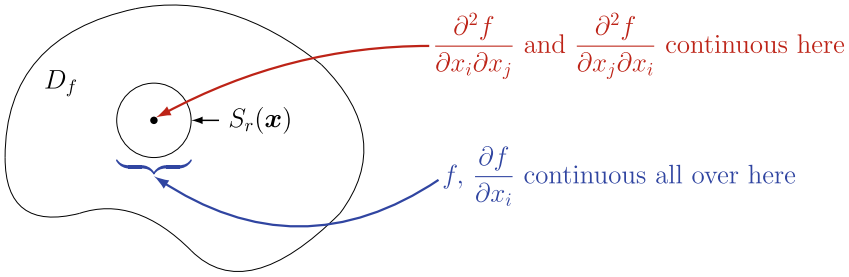


Figure 2.18 Conditions for the equivalence of mixed partial derivatives.

Of course, if conditions sufficient for the existence of the limits exist we may apply Definition 2.7 to define still higher-order partial derivatives of f. Then, if conditions of continuity of the function and all its partial derivatives up and including order $(n-1)$ are satisfied in a neighborhood of a point in the domain of f, Theorem 2.4 can be invoked to ensure the existence and continuity at that point of partial derivatives of order n. Moreover, Theorem 2.4 also ensures that mixed partial derivatives with respect to the same variables, irrespective of the sequence in which the derivatives are taken, will be the same. Figure 2.19 illustrates the scope of possibilities of higher-order partial derivatives for a function *of just two variables*.

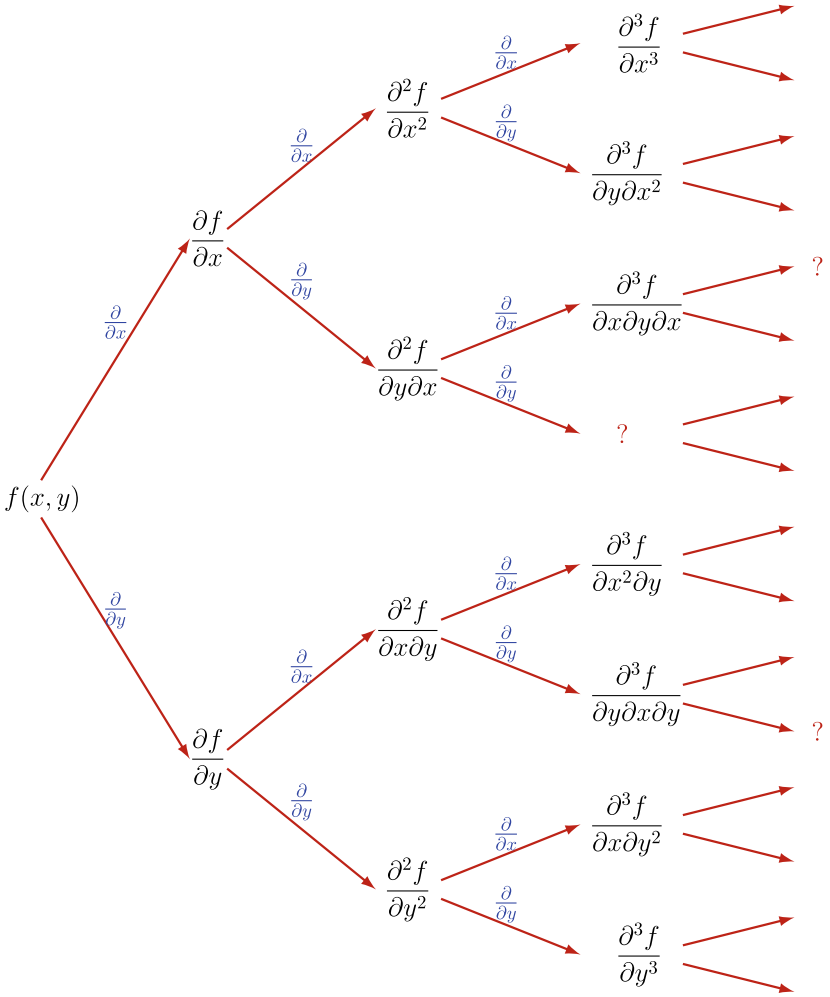


Figure 2.19 A chart of possible derivatives of $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$.

Note the pattern, at successive levels of partial derivatives, that is reflected by the arrow convention in Figure 2.19. The reader may attempt to answer the following questions:

(a) What derivatives are expected to appear in place of the question marks shown in the Figure?
(b) What is the maximum number of unique partial derivatives of third order?
(c) Which of the third order derivatives are potentially equal? What about for a function of n variables?

Generally speaking, second order partial derivatives, if they exist, will be much more complicated than first partial derivatives. One exception to this

otherwise general feature, exemplified in the first exercise below, arises when the multivariable function is a finite sum of low order powers of the independent variables. In general, however, the inevitable increase in complexity of high order partial derivatives is typically accompanied by an increase in the potential for errors. Consequently, a proportional increase in care is advised when tackling problems involving higher derivatives.

As we had done in Chapter 1 (Section 1.C), we now have cause to define new collective sets of differentiable functions whose partial derivatives comply with the conditions outlined in Theorem 2.4. We shall find that many propositions apply equally well to all functions that share the same properties of continuity of partial derivatives. Classifying functions according to their common derivative properties is so consequential that we formally introduce, through the following dedicated definition, a convenient notation.

Definition 2.8
A function $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ *with* **continuous partial derivatives** *up to and including order* m *(0,1,2,...,*m*) in an open subset of* D_f *is said to be of class* C^m.

The class $C(D)$ of continuous functions defined on a domain D, introduced in Section 1.C, may now be identified as the new class $C^0(D)$. As an example of a proposition relevant to all functions of a given class, we could now re-express Theorem 2.4 in the simple statement:

$$f \in C^2(D) \quad \Longrightarrow \quad \frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}, \quad \text{for all } \boldsymbol{x} \in D.$$

Example 2.13:

Verify that for $f(x, y) = 2 - x^2 y - xy^2$, the mixed derivatives $\dfrac{\partial^2 f}{\partial x \partial y}$ and $\dfrac{\partial^2 f}{\partial y \partial x}$ are equal. Sketch the graph of $f(x, y)$.

Solution:

The process begins with determining the two first order partial derivatives.

$$\begin{aligned} \frac{\partial f}{\partial x} &= \frac{\partial}{\partial x}\left(2 - x^2 y - xy^2\right) = -2xy - y^2, \\ \frac{\partial f}{\partial y} &= \frac{\partial}{\partial y}\left(2 - x^2 y - xy^2\right) = -x^2 - 2xy. \end{aligned}$$

This leads to four possible 2nd order derivatives, only two of which, the mixed 2nd order partial derivatives, are required. These are

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x}\Big(-x^2 - 2xy\Big) = -2x - 2y,$$
$$\frac{\partial^2 f}{\partial y \partial x} = \frac{\partial}{\partial y}\Big(-2xy - y^2\Big) = -2x - 2y,$$

which are of course equal. The equality of the mixed 2nd order partial derivatives is hence verified. The graph of the function, generated in MATLAB®, is reproduced in Figure 2.20 below.

■

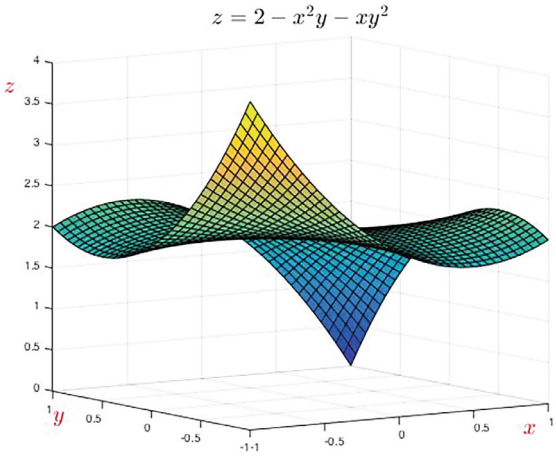


Figure 2.20 The graph of $z = 2 - x^2y - xy^2$ from Example 2.13.

✍ Mastery Check 2.11:

Determine all partial derivatives of order 2 of $f(x, y) = \arctan\left(\frac{x}{y}\right)$.

Specify any points where f or its derivatives are not defined.

✍

The next example and Mastery Check further demonstrate calculations involving second derivatives. The solutions of these problems, however, also demonstrate the process of finding *multivariable antiderivatives*. Note that the solutions make use of the fact that the functions to be determined are at least of class C^2.

■ Example 2.14:

Determine all C^2 functions $f(x, y)$ which satisfy the partial derivative conditions

$$\frac{\partial f}{\partial x} = xye^x + 1, \quad \frac{\partial f}{\partial y} = (x - 1)e^x + 1.$$

Solution:

First, we check to see whether $\dfrac{\partial^2 f}{\partial y \partial x} = \dfrac{\partial^2 f}{\partial x \partial y}$. This will support the case that a C^2 function exists with the given first partial derivatives (*i.e.*, whether f is of class C^2).

$$\frac{\partial^2 f}{\partial y \partial x} = x\mathrm{e}^x, \qquad \frac{\partial^2 f}{\partial x \partial y} = \mathrm{e}^x + (x-1)\mathrm{e}^x = x\mathrm{e}^x.$$

Since this ensures that a function $f(x, y)$ is worth seeking, we may now look for antiderivatives. This can be pursued in either of two ways. We could do a partial integration of each of the given equations and compare results, or we could partially integrate one of the equations, then differentiate the result with respect to the other variable(s) and then compare that new derivative with the one already given. Here we shall take the second course.

From the first of the given equations, integrating with respect to x, treating y as a constant we get

$$z = y(x\mathrm{e}^x - \mathrm{e}^x) + x + g(y),$$

where $g(y)$ is some as yet unknown and therefore arbitrary function of y alone. Note that in differentiating with respect to x this arbitrary function of y – *not just an arbitrary constant* – vanishes.

Now, we differentiate w.r.t. y and use the second of the given conditions to find $g(y)$.

$$\frac{\partial f}{\partial y} = (x\mathrm{e}^x - \mathrm{e}^x) + \frac{\mathrm{d}g}{\mathrm{d}y}(y) = (x-1)\mathrm{e}^x + 1.$$

Comparing the expressions we see that $\dfrac{\mathrm{d}g}{\mathrm{d}y} = 1 \Rightarrow g(y) = y + C$, and hence

$$z = f(x, y) = xy\mathrm{e}^x - y\mathrm{e}^x + x + y + C$$

for some constant C (which is truly a scalar constant and not a function).

We can now check to see if our analysis is at least formally correct by differentiating and comparing with one or both original equations:

$$\frac{\partial f}{\partial x} = xy\mathrm{e}^x + 1, \quad \frac{\partial f}{\partial y} = (x-1)\mathrm{e}^x + 1,$$

as required.

■

As in the above example, in the three exercises of the next Mastery Check, the first task is to confirm that a C^2 function is indeed possible by verifying the equality of second derivatives. Only if that condition is met is it feasible to attempt finding the scalar function.

✍ **Mastery Check 2.12:**
Determine all C^2 functions $f(x, y)$ such that

(a) $\dfrac{\partial f}{\partial x} = 2x \sin x^2, \quad \dfrac{\partial f}{\partial y} = \cos y.$ (b) $\dfrac{\partial f}{\partial x} = 2x + y, \quad \dfrac{\partial f}{\partial y} = 2y + x.$

(c) $\dfrac{\partial f}{\partial x} = x + 3yx^2, \quad \dfrac{\partial f}{\partial y} = x^3 + xy.$

✍

2.G Composite Functions and the Chain Rule

We now come to a topic which many find challenging. However, the subject is so important in a multivariable calculus course as well as in applications that we will devote some considerable space to it.

What are *composite functions*? These are functions *of functions* of one or more independent variables. The relationships between the functions and their variable dependencies can be readily represented by *ball-and-stick diagrams* (see below). Although we will retain function names in our analyses, the ball-and-stick diagrams show the relationships between dependent and independent variables. However, the reader should bear in mind that the functions themselves actually provide the links between the variables. These links are illustrated with the help of *domain-and-range diagrams*, which serve to aid understanding not only of the dependencies but also of the conditions that must be satisfied for the composite functions to be defined.

What then is the *chain rule*? The simple fact that this is the process by which one differentiates composite functions is rather unhelpful at this point. It will be necessary to examine various cases, in increasing order of complexity, for this statement to have meaning.

As for illustrating the chain rule — as distinct from visualizing composite functions — we take advantage of the notion that derivatives describe rates of change and so imagine a derivative to represent the regulated flow of water through a sluice gate or *floodgate* from one water reservoir to another. The chain rule, which involves sums of products of derivatives, we shall represent by *floodgate diagrams*: an arrangement of reservoirs fitted with floodgates to regulate water flow. The net flow of water out through the final gate will

depend on which gates above it are open (the variables), by how much (the partial derivatives), how two or more flow rates reinforce (the products), and in what combinations (the sums).

In this context, probably more so than in any other, it is important to distinguish between the independent variable that is involved in a partial derivative and others that are held fixed. To this end we will use notation such as

$$\left(\frac{\partial f}{\partial x}\right)_y \quad \text{and} \quad \left(\frac{\partial F}{\partial u}\right)_v$$

to refer to partial derivatives (here w.r.t. x and u, respectively) and the independent variables that are kept constant (here y and v, respectively).

Case 1

This is the simplest example which the student would have encountered in their single-variable calculus course. It nevertheless exhibits all the features inherent in the more complicated multivariable cases to follow. Accordingly, the format we follow in this discussion is repeated in the latter cases. Within this format we itemize the variable dependence of the functions involved including their domains and ranges, the composite function and its domain and range, and finally the appropriate chain rule for derivatives of the composite function.

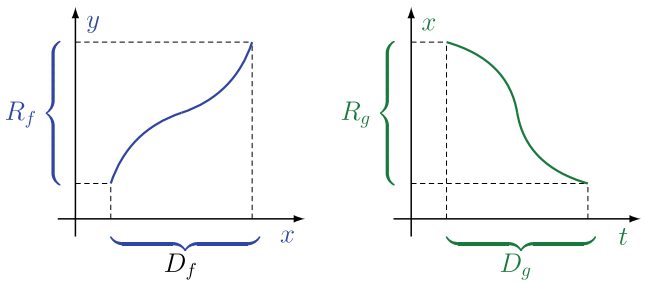


Figure 2.21 The graphs of $y = f(x)$ and $x = g(t)$.

Consider two functions $f, g \in C^1(\mathbb{R})$ of one variable.

$$\begin{array}{rcl} f : \mathbb{R} & \longrightarrow & \mathbb{R} \\ x & \longmapsto & y = f(x), \end{array} \qquad \begin{array}{rcl} g : \mathbb{R} & \longrightarrow & \mathbb{R} \\ t & \longmapsto & x = g(t). \end{array}$$

The domains and ranges of these are shown in Figure 2.21 above. From these functions we form the composite function of the independent variable t:

$$y = F(t) = \big(f \circ g\big)(t) = f\big(g(t)\big).$$

composite function

"f composed with g"

f is a function of g, which is a function of t

The composite function F may be represented schematically by the ball-and-stick diagram in Figure 2.22. In this case f may be called the *outer* or *exterior* function, while g is the *inner* or *interior* function. The diagram (as with the more complex ones to follow) indicates that the variable y depends on x, which in turn depends on t. Thus, a variation in t leads to a variation in x, which leads to a variation in y.



Figure 2.22 Ball-and-stick model for $f\big(g(t)\big)$ in Case 1.

The domain and range of F, which are based on the sets D_g, R_g, D_f, and R_f, must be such that F makes sense. Examine Figure 2.23, from left to right, noting the termini (start and end points) of the arrows.

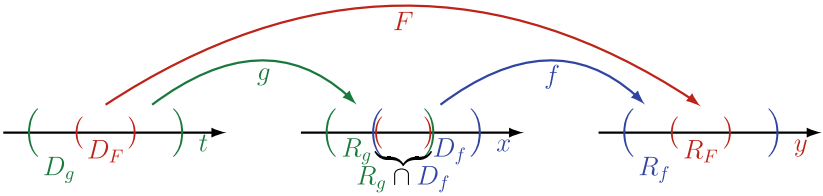


Figure 2.23 Conditional definition of D_F and R_F.

From the figure follow two set relations and one critical set constraint: the domain of F is a subset of the domain of g, the range of F is a subset of the range of f, and then there must be a non-empty intersection of the range of g and domain of f. In set notation these are summarized as follows.

$$\left.\begin{array}{rl} \text{Domain of } F: & D_F \subseteq D_g \\ \text{Range of } F: & R_F \subseteq R_f \end{array}\right\} \text{ An important condition: } R_g \cap D_f \neq \emptyset.$$

The derivative of F w.r.t. t is given by the chain rule and can be represented schematically by the *floodgate* diagram in Figure 2.24.

In constructing the relevant floodgate diagram for any given case we aim to compile and represent all the term- and factor-wise contributions to a chain rule derivative. The objective is the net outflow at the bottom.

$$\begin{aligned} \frac{\mathrm{d}F}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\big(f \circ g\big)(t) \\ &= \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{x=g(t)} \cdot \frac{\mathrm{d}g}{\mathrm{d}t}\Big|_{t} \\ &= \left\{\begin{array}{c}\text{derivative}\\ \text{of } f\\ \text{evaluated}\\ \text{at } x = g(t)\end{array}\right\} \times \left\{\begin{array}{c}\text{derivative}\\ \text{of } g\\ \text{evaluated}\\ \text{at } t\end{array}\right\} \end{aligned}$$

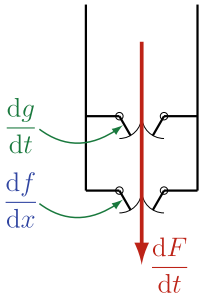


Figure 2.24 The floodgate diagram for $\mathrm{d}F/\mathrm{d}t$.

In this case the final flow rate out through the bottom gate of the reservoir $\left(\frac{\mathrm{d}F}{\mathrm{d}t}\right)$ is dependent not only on the flow rate from the x-reservoir to the y-reservoir $\left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)$ but also on the flow rate from the t-reservoir to the x-reservoir $\left(\frac{\mathrm{d}g}{\mathrm{d}t}\right)$: one reinforces (multiplies) the other.

A final note concerns the notation used to represent and describe the chain rule derivative. The more commonly seen notation is

$$\frac{\mathrm{d}y}{\mathrm{d}t} = \frac{\mathrm{d}y}{\mathrm{d}x} \cdot \frac{\mathrm{d}x}{\mathrm{d}t}.$$

Although it is intuitive and appealing to express the chain rule in this way (admittedly it is convenient sometimes), this notation can be problematic in some cases.

Case 2

The system in Case 1 is one that is taken up in a single variable calculus course and so is a system most students will recognize. We now move on to more complicated functional arrangements that is particular to multivariable functions. As was remarked earlier, to illustrate the parallels between the

different cases, the format for the following discussion remains identical to that for Case 1.

Consider the outer function f as before, but now suppose that the inner function g is a function of two variables.

$$\begin{array}{rcl} f : \mathbb{R} & \longrightarrow & \mathbb{R} \\ x & \longmapsto & y = f(x) \end{array} \qquad \begin{array}{rcl} g : \mathbb{R}^2 & \longrightarrow & \mathbb{R} \\ (s,t) & \longmapsto & x = g(s,t) \end{array}$$

The respective domains and ranges are shown schematically in Figure 2.25.

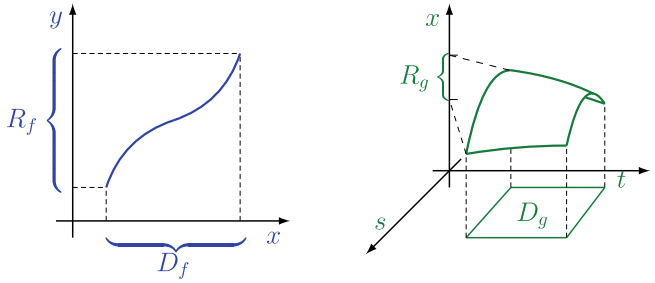


Figure 2.25 The graphs of $y = f(x)$ and $x = g(s,t)$.

The composite function of the two independent variables, s and t, is

$$y = F(s,t) = \big(f \circ g\big)(s,t) = f\big(g(s,t)\big).$$

The composite function can here too be represented schematically by a ball-and-stick diagram, but this time a *branch* diagram (Figure 2.26). The variable y depends on x, which depends on s and t. Consequently, a variation in s or t leads to a variation in x, which leads in turn to a variation in y.

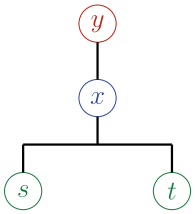


Figure 2.26 Ball-and-stick for $f\big(g(s,t)\big)$ in Case 2.

The domain and range of F, which are again determined by D_g, R_g, D_f, and R_f, are such that F makes sense (Figure 2.27).

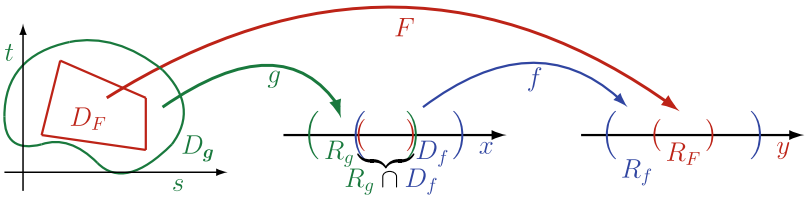


Figure 2.27 Conditional definition of D_F and R_F.

We once again find two set relations and the same set constraint.

$$\left.\begin{array}{rl} \text{Domain of } F: & D_F \subseteq D_g \\ \text{Range of } F: & R_F \subseteq R_f \end{array}\right\} \text{ An important condition: } R_g \cap D_f \neq \emptyset.$$

That is, the domain of F is not bigger than, and can be smaller than, the domain of g, and the range of F is not bigger than and can be smaller than the range of f. All is dictated by the size of $R_g \cap D_f$.

The derivatives of F w.r.t. s and t are now *partial derivatives* given by the chain rule, and represented by their respective *floodgate diagrams*: Figures 2.28 and 2.29.

$$\left(\frac{\partial F}{\partial s}\right)_t = \frac{\partial}{\partial s}(f \circ g)(s,t)$$
$$t \text{ — held fixed}$$
$$= \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=g(s,t)} \cdot \left(\frac{\partial g}{\partial s}\right)_t$$
$$\left\{\begin{array}{c}\text{full}\\ \text{derivative}\\ \text{of } f\\ \text{evaluated}\\ \text{at } x=g(s,t)\end{array}\right\} \times \left\{\begin{array}{c}\text{partial}\\ \text{derivative}\\ \text{of } g\\ \text{evaluated}\\ \text{at } (s,t)\end{array}\right\}$$

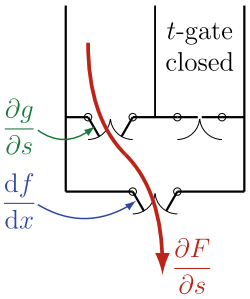


Figure 2.28 The floodgate diagram for $\partial F/\partial s$.

$$\left(\frac{\partial F}{\partial t}\right)_s = \frac{\partial}{\partial t}(f \circ g)(s,t)$$
$$s \text{ — held fixed}$$
$$= \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=g(s,t)} \cdot \left(\frac{\partial g}{\partial t}\right)_s$$
$$\left\{\begin{array}{c}\text{full}\\ \text{derivative}\\ \text{of } f\\ \text{evaluated}\\ \text{at } x=g(s,t)\end{array}\right\} \times \left\{\begin{array}{c}\text{partial}\\ \text{derivative}\\ \text{of } g\\ \text{evaluated}\\ \text{at } (s,t)\end{array}\right\}$$

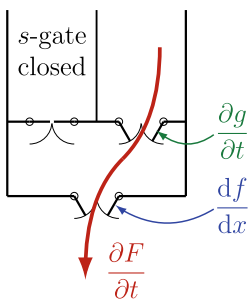


Figure 2.29 The floodgate diagram for $\partial F/\partial t$.

In this case (in contrast with Case 1) the partial derivatives of F mean that one variable is kept fixed, and thus its associated gate remains closed, giving no contribution to the flow out through the bottom floodgate.

We demonstrate how this case works with an example and leave the reader with an exercise to consolidate their understanding.

Example 2.15:

Consider the functions $f : x \longrightarrow y = f(x)$ and $g : (s,t) \longrightarrow x = g(s,t)$. Identify the domain D_F of the composite function $F : (s,t) \longrightarrow y = \big(f \circ g\big)(s,t)$ and determine the derivatives, $\left(\dfrac{\partial F}{\partial s}\right)_t$ and $\left(\dfrac{\partial F}{\partial t}\right)_s$, when $f(x) = \ln x$ and $g(s,t) = s(1-t^2)$.

Solution:

The domain of f is $D_f = \{x : x > 0\}$, while the range of g is $R_g = \{x : x \in \mathbb{R}\}$. The intersection is $R_g \cap D_f = \{x : x = s(1-t^2) > 0\}$. Therefore, $D_F = \{(s,t) : (s > 0 \text{ and } |t| < 1) \cup (s < 0 \text{ and } |t| > 1)\}$.

$$\left(\frac{\partial F}{\partial s}\right)_t = \frac{\mathrm{d}f}{\mathrm{d}x}\frac{\partial g}{\partial s} = \frac{1}{x}\bigg|_{x=s(1-t^2)}(1-t^2) = \frac{1}{s}.$$

$$\left(\frac{\partial F}{\partial t}\right)_s = \frac{\mathrm{d}f}{\mathrm{d}x}\frac{\partial g}{\partial t} = \frac{1}{x}\bigg|_{x=s(1-t^2)}(-2st) = -\frac{2t}{1-t^2}.$$

■

✍ Mastery Check 2.13:

Consider the function: $y = f(x) = \arcsin x$, where $x = g(s,t) = s^2 + \dfrac{1}{t}$. What are D_f, R_f, D_g, and R_g?
Determine where $y = F(s,t)$ makes sense, and then find (if possible) the partial derivatives $\left(\dfrac{\partial F}{\partial s}\right)_t$ and $\left(\dfrac{\partial F}{\partial t}\right)_s$.

Note: the final result should be expressed in terms of s and t!

✍

Case 3

Consider two functions $f, \boldsymbol{g} \in C^1(\mathbb{R}^2)$ of two variables.

$$f : \mathbb{R}^2 \longrightarrow \mathbb{R} \qquad \boldsymbol{g} : \mathbb{R}^2 \longrightarrow \mathbb{R}^2$$
$$(x,y) \longmapsto z = f(x,y) \qquad (s,t) \longmapsto \big(x = g_1(s,t), y = g_2(s,t)\big)$$

The composite function F of two variables s and t derived from f and $\boldsymbol{g}$ is

$$z = F(s,t) = \big(f \circ \boldsymbol{g}\big)(s,t) = f\big(g_1(s,t), g_2(s,t)\big).$$

This composite function is represented by the more elaborate branch model of dependent and independent variables shown in Figure 2.30.

This time z depends on x and y, and both x and y depend on s and t.

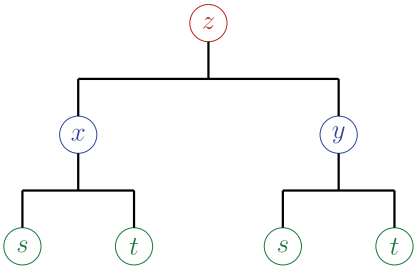


Figure 2.30 Ball-and-stick for $f\big(g_1(s,t), g_2(s,t)\big)$ in Case 3.

The domain and range of F, which are dictated by D_f and R_f, and $D_{\boldsymbol{g}}$ and $R_{\boldsymbol{g}}$, are such that F makes sense. In analogy with Case 1 and Case 2, the same set conditions and set constraint can be established from the depiction in Figure 2.31:

$$\left.\begin{array}{rl} \text{Domain of } F: & D_F \subseteq D_{\boldsymbol{g}} \\ \text{Range of } F: & R_F \subseteq R_f \end{array}\right\} \text{ An important condition: } R_{\boldsymbol{g}} \cap D_f \neq \emptyset.$$

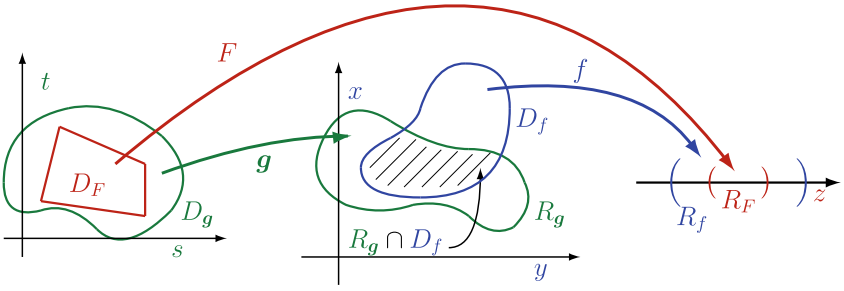


Figure 2.31 Conditional definition of D_F and R_F.

The partial derivatives of F w.r.t. s and t are given by the chain rule:

In each of the cases shown in Figures 2.32 and 2.33, both bottom floodgates $\left(\dfrac{\partial f}{\partial x} \text{ and } \dfrac{\partial f}{\partial y}\right)$ are open and contribute to the total flow, but with strengths that are modulated by the floodgates above them, that is, by the partial derivatives of g_1 and g_2.

$$\left(\frac{\partial F}{\partial s}\right)_t = \left(\frac{\partial f}{\partial x}\right)_y\Bigg|_{\substack{x=g_1(s,t)\\y=g_2(s,t)}} \cdot \left(\frac{\partial g_1}{\partial s}\right)_t + \left(\frac{\partial f}{\partial y}\right)_x\Bigg|_{\substack{x=g_1(s,t)\\y=g_2(s,t)}} \cdot \left(\frac{\partial g_2}{\partial s}\right)_t$$

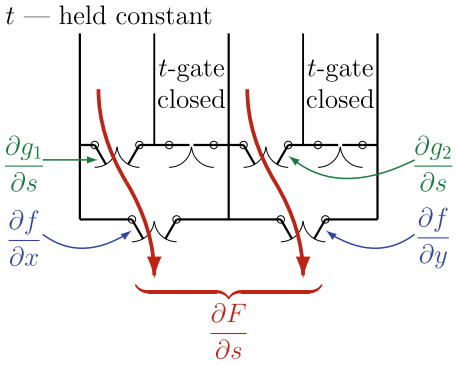


Figure 2.32 The floodgate diagram for $\partial F/\partial s$.

$$\left(\frac{\partial F}{\partial t}\right)_s = \left(\frac{\partial f}{\partial x}\right)_y\Bigg|_{\substack{x=g_1(s,t)\\y=g_2(s,t)}} \cdot \left(\frac{\partial g_1}{\partial t}\right)_s + \left(\frac{\partial f}{\partial y}\right)_x\Bigg|_{\substack{x=g_1(s,t)\\y=g_2(s,t)}} \cdot \left(\frac{\partial g_2}{\partial t}\right)_s$$

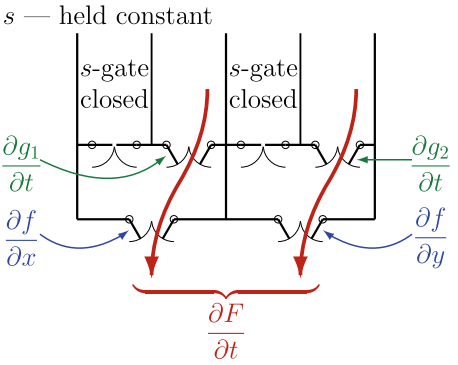


Figure 2.33 The floodgate diagram for $\partial F/\partial t$.

■ Example 2.16:

$F(s,t)$ is the composite function formed by the composition of $f(x,y) = x^2 + \mathrm{e}^{xy}$,

$$x = g_1(s,t) = \ln(s^2+t^2), \quad \text{and} \quad y = g_2(s,t) = \sin(st).$$

Determine the partial derivative $\left(\dfrac{\partial F}{\partial s}\right)_t$.

Solution:

To evaluate the first derivatives of the composite function $F(s,t)$ in this example we are presented with two options. We could first substitute the

functions $g_1(s,t)$ and $g_2(s,t)$ for x and y, respectively, in $f(x,y)$ to arrive at an explicit form for $F(s,t)$, and then partially differentiate with respect to s (or t). Alternatively, we could invoke the chain rule formulae for this class of composite function. Either approach will lead to the same end result. Pursuing the latter course we have, firstly,

$$\begin{aligned}
\frac{\partial f}{\partial x} &= 2x + y\mathrm{e}^{xy}, \quad ; & \frac{\partial f}{\partial y} &= x\mathrm{e}^{xy}, \\
\frac{\partial g_1}{\partial s} &= \frac{2s}{s^2+t^2}, \quad ; & \frac{\partial g_1}{\partial t} &= \frac{2t}{s^2+t^2}, \\
\frac{\partial g_2}{\partial s} &= t\cos(st), \quad ; & \frac{\partial g_2}{\partial t} &= s\cos(st).
\end{aligned}$$

Consequently, we have, for $\dfrac{\partial F}{\partial s}$:

$$\begin{aligned}
\left(\frac{\partial F}{\partial s}\right)_t &= \left(\frac{\partial f}{\partial x}\right)\Big|_{(g_1,g_2)} \frac{\partial g_1}{\partial s} + \left(\frac{\partial f}{\partial y}\right)\Big|_{(g_1,g_2)} \frac{\partial g_2}{\partial s}, \\
&= (2x + y\mathrm{e}^{xy})\Big|_{(g_1,g_2)} \frac{2s}{s^2+t^2} + (x\mathrm{e}^{xy})\Big|_{(g_1,g_2)} t\cos(st), \\
&= \left(2\ln(s^2+t^2) + \sin(st)\mathrm{e}^{\ln(s^2+t^2)\sin(st)}\right) \frac{2s}{s^2+t^2} \\
&\qquad + \ln(s^2+t^2)\mathrm{e}^{\ln(s^2+t^2)\sin(st)} t\cos(st).
\end{aligned}$$

A corresponding expression could be derived for $\left(\dfrac{\partial F}{\partial t}\right)_s$. No matter what form the intermediate steps take, the final result must be expressed in terms of the underlying variables s and t. To confirm the above result, the reader may wish to attempt the first option of differentiating

$$F(s,t) = \left(\ln(s^2+t^2)\right)^2 + \mathrm{e}^{\ln(s^2+t^2)\sin(st)}.$$

■

As is true of all cases considered explicitly, the example that was considered in this third case generalizes naturally to outer functions that depend on more than just two variables. Generalizations also allow the possibility of two or more inner variables. This is explored in the next Mastery Check which is a variant of this case with f being an outer function of three variables, x, y, and z, not just two. Each of the three variables is then a function of s and t.

✍ Mastery Check 2.14:

Consider the composite function formed by the composition of the following functions:

$$w = f(x,y,z) = \sqrt{1-x^2-y^2-z^2},$$
$$x = g_1(s,t) = \sin t, \quad y = g_2(s,t) = \cos s, \quad z = g_3(s,t) = \frac{s}{\sqrt{1-t^2}}.$$

Determine the domain and range of $\boldsymbol{g}(s,t) = (g_1(s,t), g_2(s,t), g_3(s,t))$ and the domain of $f(x,y,z)$ and establish that $D_f \cap R_g \neq 0$. Explore the pre-image of $D_f \cap R_g$, then determine the partial derivatives $\left(\dfrac{\partial F}{\partial s}\right)_t$ and $\left(\dfrac{\partial F}{\partial t}\right)_s$, at points where they and F make sense.

Note: The solution process is the same as in the previous example but with an additional pathway through the variable z. Consider how the floodgate and ball and stick models would look in this instance.

✍

Case 4

As a final example, consider two functions $f \in C^1(\mathbb{R}^3)$, $\boldsymbol{g} \in C^1(\mathbb{R}^2)$. This is a mixed case where the outer function, f, depends on an independent variable both directly, and indirectly through one or more inner functions.

$$\begin{array}{rcl} f : \mathbb{R}^3 & \longrightarrow & \mathbb{R} \\ (x,y,t) & \longmapsto & z = f(x,y,t) \end{array} \qquad \begin{array}{rcl} \boldsymbol{g} : \mathbb{R}^2 & \longrightarrow & \mathbb{R}^2 \\ (s,t) & \longmapsto & \big(x = g_1(s,t), y = g_2(s,t)\big) \end{array}$$

The composite function F of two variables s and t formed from f and $\boldsymbol{g}$ is

$$z = F(s,t) = f\big(g_1(s,t), g_2(s,t), t\big).$$

The ball-and-stick branch model appropriate for this example is shown in Figure 2.34 below. The direct feed, from t to z, may be a possible cause of confusion, depending on the user's choice of notation - see the end of this section for a demonstration.

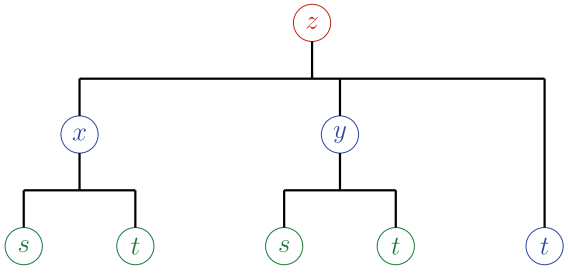


Figure 2.34 The complex ball-and-stick diagram for $f\big(g_1(s,t), g_2(s,t), t\big)$.

As in the previous three cases, the sets D_f, R_f, D_g, and R_g establish the domain and range of F so that F makes sense. However, this time there is the added complication of two domains for the independent variable t that f and $\boldsymbol{g}$ have in common. These domains will generally not be identical but must possess a region in common.

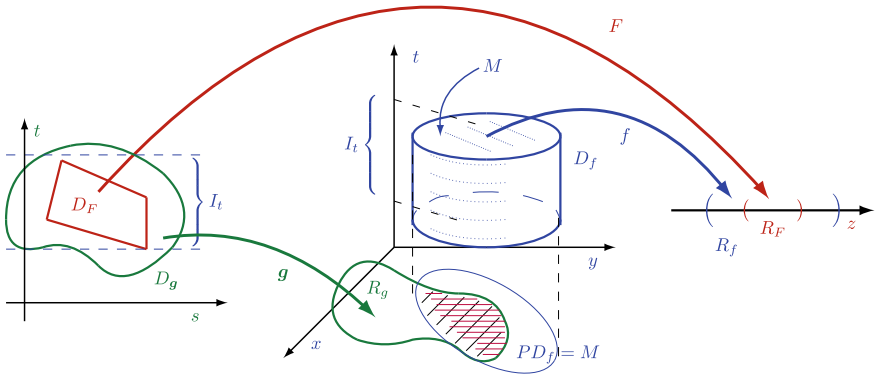


Figure 2.35 Conditional definition of D_F and R_F for $D_f = M \times I_t$.

While each new situation will require its own specific assessment, we can indicate what needs to be considered in regard to the complex inter-relationships between domains and ranges.

The simplest scenario, both to explain and to process, is one in which the domain D_f is shaped in the form of a cylinder, $M \times I_t$, where M is a subdomain in $\mathbb{R}^2$ for the x and y variables, while the t variable spans the (fixed) interval $I_t \subset \mathbb{R}$. I_t may either be finite or infinite in length and M itself may be a rectangular (*i.e.*, of the form $I_x \times I_y$), or a convex subset of $\mathbb{R}^2$, such as an elliptical disc. In any case, the projection of D_f onto the xy-plane will then simply be $PD_f = M$. These features are illustrated in the middle panel of Figure 2.35.

In this scenario the first and minimal condition to be satisfied for the validity of the composite function F is, as in Case 3,

$$PD_f \cap R_g = M \cap R_g \neq \emptyset.$$

This set intersection is depicted at the bottom of the middle panel by the black shaded region. A non-empty intersection ensures that at least some x and y values generated by $\boldsymbol{g}$ will be compatible with the requirements of the two first arguments of f. However, this alone is not the final determinant on permissable s and t values.

Turning to the third argument of f, in this simplest of cases an additional requirement is for the domain of $\boldsymbol{g}$ in the st-plane to have a region in common with the infinite strip $\mathbb{R} \times I_t$, also in the st-plane, generated by the interval I_t;

since s is not an explicit argument of f, any $t \in I_t$ may be coupled with any $s \in \mathbb{R}$. The left-hand panel of Figure 2.35 suggests this intersection. There is thus a second condition to satisfy, namely

$$(\mathbb{R} \times I_t) \cap D_g \neq \emptyset.$$

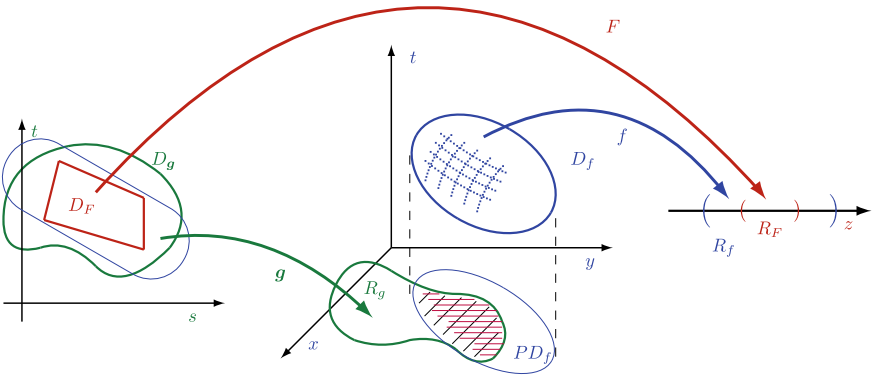


Figure 2.36 Conditional definition of D_F and R_F for convex $D_f \subset \mathbb{R}^3$.

Given that $(\mathbb{R} \times I_t) \cap D_g$ is a *subset* of D_g its image under $\boldsymbol{g}$ will in turn be a *subset* of $M \cap R_g$. This is indicated by the cross-shaded region in red in the xy-plane at the bottom of the middle panel of Figure 2.35.

With the two set restrictions we may formally establish the range and domain of composite F:

$$\left.\begin{array}{rll} \text{Domain of F:} & D_F & \subseteq D_g \cap (I_f \times \mathbb{R}) \\ \text{Range of F:} & R_F & \subseteq R_f \end{array}\right\},$$

subject to two necessary conditions,

$$R_g \cap PD_f \neq \emptyset \quad \text{and} \quad D_g \cap (I_f \times \mathbb{R}) \neq \emptyset.$$

Cases falling into this scenario class are relatively straightforward to characterize compared with cases involving more complicated D_f domains. A situation that is often encountered is when D_f is a finite, convex set in $\mathbb{R}^3$, for example an ellipsoid, such as that depicted in the middle panel of Figure 2.36. The allowed t-values will not be a fixed interval, but an interval of varied length generally depending on the other independent variables (x and y, here) as well as ultimately on s, as suggested by the schematic convex set in blue in the left-hand panel of Figure 2.36. Rather than attempt a general theoretical analysis that is likely to be confusing we examine this more complex scenario by means of an example.

Example 2.17:

Suppose $f(x,y,t) = \sqrt{1-x^2-y^2-t^2}$, with domain $D_f = \{(x,y,t) : x^2+y^2+t^2 \leq 1\}$.

Let $x = g_1(s,t) = s+t$ and $y = g_2(s,t) = t-s$, for $(s,t) \in D_g = [0,1]\times[0,1]$. Determine the domain of the composite function $F(s,t) = f(g_1(s,t), g_2(s,t), t)$.

Solution:

With the domain D_g being the unit square in the st-plane (see left-hand panel of Figure 2.37) it is easy to establish that

$$R_g = \{(x,y) : (-x \leq y \leq x,\ x \in [0,1]) \cup (x-2 \leq y \leq 2-x,\ x \in [1,2])\},$$

which is the diamond shaped region to the right of the y-axis in the right-hand panel of Figure 2.37. In comparison, the projection of D_f onto the xy-plane is the unit circle, which represents the extreme of allowed values of x and y.

The first of our conditions, $R_g \cap PD_f \neq \emptyset$, is thus satisfied, restricting possible values of x and y to the right-hand quarter segment of the unit circle, extending from the line $y = -x$ to the line $y = x$. This shown as the blue shaded region in the right-hand panel of Figure 2.37. The pre-image of this restricted set, $\boldsymbol{g}^{-1}(R_g \cap PD_f)$, is the quarter circle in the first quadrant of the st-plane, the blue shaded region in the left-hand panel of Figure 2.37.

Meanwhile, the allowed values of t, according to D_f, are restricted to the variable interval

$$-\sqrt{1-x^2-y^2} \leq t \leq \sqrt{1-x^2-y^2},$$

and so will depend on x and y. On the other hand, invoking the definitions of g_1 and g_2, we find that

$$\begin{aligned} 1 \geq t^2+x^2+y^2 &= t^2+g_1^2(s,t)+g_2^2(s,t), \\ &= t^2+2t^2+2s^2 \quad \Longrightarrow \quad 3t^2+2s^2 \leq 1, \end{aligned}$$

which describes the closed ellipse, E, in the st-plane (shown in red in the left-hand panel of Figure 2.37). Consequently, the (s,t) points allowed under conditions of both f and $\boldsymbol{g}$ belong to the subset,

$$D_g \cap E \subset \boldsymbol{g}^{-1}(R_g \cap PD_f).$$

The set $D_g \cap E$ hence defines the domain of the composite function F.

Consequently, not only must the domain of F be consistent with $R_g \cap PD_f$, but the allowed values of t can potentially lead to an even smaller valid subset of D_g (compare the red and blue-shaded regions in left-hand panel of

Figure 2.37). We will encounter similar considerations, in another context, in Section 4.G.

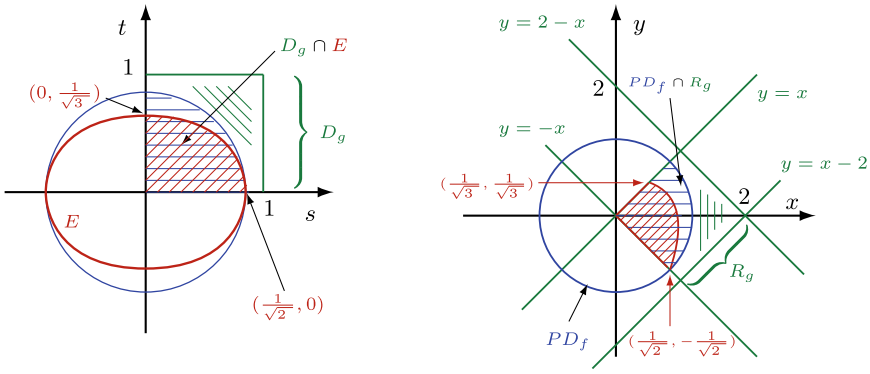


Figure 2.37 Domain, $D_g \cap E$, of the composite function $F(s,t)$.

The partial derivative of F with respect to s in this Case 4 is given by the chain rule, which is largely identical to the same derivative expression as in Case 3, except for the subscripts on the partial derivatives of f:

$$\left(\frac{\partial F}{\partial s}\right)_t = \left(\frac{\partial f}{\partial x}\right)_{y,t}\Bigg|_{\substack{x=g_1(s,t)\\y=g_2(s,t)}} \cdot \left(\frac{\partial g_1}{\partial s}\right)_t + \left(\frac{\partial f}{\partial y}\right)_{x,t}\Bigg|_{\substack{x=g_1(s,t)\\y=g_2(s,t)}} \cdot \left(\frac{\partial g_2}{\partial s}\right)_t$$

t — held constant

The corresponding floodgate model for $\left(\frac{\partial F}{\partial s}\right)_t$ is also effectively as appears in Case 3. On the other hand, the partial derivative of F with respect to t is given by a version of the chain rule that has three contributions (see Figure 2.38).

The indirect contribution to $\left(\frac{\partial F}{\partial t}\right)_s$ is as in the preceding case, but now there is an extra contribution from the direct dependence on t. This is reflected in Figure 2.38 by the fact that the reservoir above the floodgate $\left(\frac{\partial f}{\partial t}\right)_{x,y}$ has no other influences, while there are t-reservoirs that influence (multiply or reinforce) the other contributions.

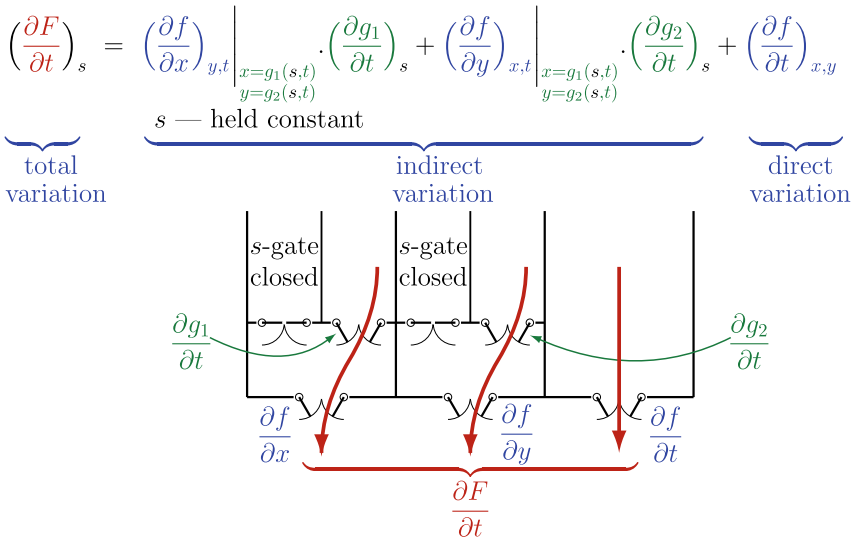


Figure 2.38 The floodgate diagram for $\partial F/\partial t$ in Case 4.

The reader should compare the above expression for the partial derivative $\left(\frac{\partial F}{\partial t}\right)_s$ with the expression one would write using the less precise notation that treats x, y, z, as both dependent and independent variables. With $z = F(s,t)$ and $z = f(x,y,t)$, the chain rule for the partial derivative with respect to t would then be written

$$\underbrace{\frac{\partial z}{\partial t}}_{\text{total variation}} = \underbrace{\frac{\partial z}{\partial x}\cdot\frac{\partial x}{\partial t} + \frac{\partial z}{\partial y}\cdot\frac{\partial y}{\partial t}}_{\text{indirect variation}} + \underbrace{\frac{\partial z}{\partial t}}_{\text{direct variation}}\cdot$$

We see that by being imprecise we arrive at an expression involving two terms with the same notation but which mean different things!

Choosing to refer to x, y, z as both functions and independent variables instead of just as independent variables, one should at least write the derivatives as

$$\frac{\partial z}{\partial t} = \left(\frac{\partial z}{\partial x}\right)_{y,t}\cdot\frac{\partial x}{\partial t} + \left(\frac{\partial z}{\partial y}\right)_{x,t}\cdot\frac{\partial y}{\partial t} + \left(\frac{\partial z}{\partial t}\right)_{x,y},$$

to partially distinguish the function dependencies.

We conclude the discussion on Case 4 with an example.

Example 2.18:

Consider the function $z = f(x, y, t) = xt\cos y$, where

$$x = g_1(s,t) = st + 1,\ \ y = g_2(s,t) = s^2 + t^2.$$

Let $\big(D_f\big)_t \subseteq \mathbb{R}^2$ denote the domain of f when t is held constant. Establish that $\big(D_f\big)_t \cap R_g \neq \emptyset$, and then determine the partial derivatives of $F(s,t) = \big(f \circ \boldsymbol{g}\big)(s,t)$ with respect to s and t.

Solution:

The problem statement does not restrict any of the variables x, y, s and t. Consequently, we shall assume the largest sets for which the functions make sense. In this example, $D_g = \mathbb{R}^2$ while $R_g = \mathbb{R} \times \mathbb{R}^+$ and $D_f = \mathbb{R}^3$ and $R_f = \mathbb{R}$. Consequently, the xy-domain of f at fixed t is $(D_f)_t = \mathbb{R} \times \mathbb{R}^+$.

Incidentally, this exercise is an example of our first, simpler situation of a cylindrical domain $D_f = I_t \times \mathbb{R}^2 = \mathbb{R}^3$, with $I_t = \mathbb{R}$. We note that according to our earlier notation $PD_f \cap R_g = \mathbb{R} \times \mathbb{R}^+$ and $D_g \cap (I_t \times \mathbb{R}) = \mathbb{R}^2$. Hence, all the set restrictions for non-empty set intersections are satisfied.

Regarding the partial derivatives, we have

$$\begin{aligned}
\left(\frac{\partial F}{\partial s}\right)_t &= \left(\frac{\partial f}{\partial x}\right)_{y,t}\left(\frac{\partial g_1}{\partial s}\right)_t + \left(\frac{\partial f}{\partial y}\right)_{x,t}\left(\frac{\partial g_2}{\partial s}\right)_t \\
&= (t\cos y)\big|_{g_1,g_2}.t + (-xt\sin y)\big|_{g_1,g_2}.2s \\
&= t^2\cos(s^2+t^2) - 2st(st+1)\sin(s^2+t^2). \\
\left(\frac{\partial F}{\partial t}\right)_s &= \left(\frac{\partial f}{\partial x}\right)_{y,t}\left(\frac{\partial g_1}{\partial t}\right)_s + \left(\frac{\partial f}{\partial y}\right)_{x,t}\left(\frac{\partial g_2}{\partial t}\right)_s + \left(\frac{\partial f}{\partial t}\right)_{x,y} \\
&= (t\cos y)\big|_{g_1,g_2}.s + (-xt\sin y)\big|_{g_1,g_2}.2t + (x\cos y)\big|_{g_1,g_2} \\
&= (2st+1)\cos(s^2+t^2) - 2t^2(st+1)\sin(s^2+t^2).
\end{aligned}$$

■

We have now completed our coverage of composite functions and their first partial derivatives. Of course, these four cases do not exhaust all possibilities. However, the reader will discover that more complicated cases of composite functions and their respective partial derivatives can be readily, if not easily, constructed by generalizing the expositions for the cases considered above.

Second derivatives and the chain rule. Method 1

Applications involving the chain rule are not limited to first partial derivatives. So, while it is essential to understand the chain rule in principle, a

Master Class in the practical use of the chain rule cannot be complete without a discussion of higher-order partial derivatives. In the author's experience, this is what most students find challenging.

On this topic we will explore two approaches to determining second order derivatives of composite functions, beginning first with what I refer to as a three-step process.

Although the method applies equally to other cases, by way of demonstration we consider Case 3:

$$\text{outer function, } f : \mathbb{R}^2 \longrightarrow \mathbb{R}, \quad \text{and inner function, } \boldsymbol{g} : \mathbb{R}^2 \longrightarrow \mathbb{R}^2$$

$$\implies \quad F(s,t) = \big(f \circ \boldsymbol{g}\big)(s,t) = f\big(g_1(s,t), g_2(s,t)\big).$$

The first partial derivative of F with respect to s is (as on Page 116):

$$\left(\frac{\partial F}{\partial s}\right)_t = \left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial g_1}{\partial s}\right)_t + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial g_2}{\partial s}\right)_t$$

For convenience, in the following we will suppress parentheses and their subscripts, trusting that the respective variable dependencies are clear.

If we now want a second derivative, say $\dfrac{\partial^2 F}{\partial t\, \partial s}$, then we must take note of two facts:

(a) $\dfrac{\partial F}{\partial s}$ is the sum of *products* of functions!

(b) $\dfrac{\partial f}{\partial x}$ and $\dfrac{\partial f}{\partial y}$ are *two new composite functions of* s and t! Let's denote these by K and H.

Hence, using

$$\frac{\partial f}{\partial x} = k\big(x(s,t), y(s,t)\big) = K(s,t), \quad \frac{\partial f}{\partial y} = h\big(x(s,t), y(s,t)\big) = H(s,t),$$

the first partial derivative of F with respect to s can be rewritten,

$$\frac{\partial F}{\partial s} = K(s,t).\frac{\partial g_1}{\partial s} + H(s,t).\frac{\partial g_2}{\partial s}.$$

In this guise, the first partial derivative is more clearly seen to be a sum of products of functions of s and t. Consequently, in taking a second partial derivative — any second partial derivative — we must take the following steps in the order given:

Step 1: use the product rule of differentiation;

Step 2: use the chain rule *again*, this time on K and H;

Step 3: express everything in terms of the independent variables of F.

As we said, these actions must be taken *in this order*!

Step 1: Differentiate the sum of products using the product rule

$$\begin{aligned}\frac{\partial^2 F}{\partial t\,\partial s} &= \frac{\partial}{\partial t}\Big(\frac{\partial F}{\partial s}\Big) = \frac{\partial}{\partial t}\Big(K(s,t)\frac{\partial g_1}{\partial s}\Big) + \frac{\partial}{\partial t}\Big(H(s,t)\frac{\partial g_2}{\partial s}\Big)\\ &= K(s,t)\frac{\partial^2 g_1}{\partial t\,\partial s} + H(s,t)\frac{\partial^2 g_2}{\partial t\,\partial s} + \frac{\partial K(s,t)}{\partial t}\cdot\frac{\partial g_1}{\partial s} + \frac{\partial H(s,t)}{\partial t}\cdot\frac{\partial g_2}{\partial s}\end{aligned}$$

product rule product rule

4 terms

The first two terms are finished.

Step 2: After the product rule, apply the *chain* rule (again) on the second two terms:

$$\begin{aligned}\frac{\partial K}{\partial t} &= \frac{\partial k}{\partial x}\cdot\frac{\partial g_1}{\partial t} + \frac{\partial k}{\partial y}\cdot\frac{\partial g_2}{\partial t} = \frac{\partial^2 f}{\partial x^2}\cdot\frac{\partial g_1}{\partial t} + \frac{\partial^2 f}{\partial y\,\partial x}\cdot\frac{\partial g_2}{\partial t}\cdot\\ \frac{\partial H}{\partial t} &= \frac{\partial h}{\partial x}\cdot\frac{\partial g_1}{\partial t} + \frac{\partial h}{\partial y}\cdot\frac{\partial g_2}{\partial t} = \frac{\partial^2 f}{\partial x\,\partial y}\cdot\frac{\partial g_1}{\partial t} + \frac{\partial^2 f}{\partial y^2}\cdot\frac{\partial g_2}{\partial t}\cdot\end{aligned}$$

Step 3: Finally, replace all the K and H factors with the f, g_1, and g_2 factors (with all derivatives of f evaluated at $x = g_1(s,t)$ and $y = g_2(s,t)$):

$$\begin{aligned}\frac{\partial^2 F}{\partial t\,\partial s} &= \frac{\partial f}{\partial x}\bigg|_{\substack{x=g_1\\y=g_2}}\frac{\partial^2 g_1}{\partial t\,\partial s} + \frac{\partial f}{\partial y}\bigg|_{\substack{x=g_1\\y=g_2}}\frac{\partial^2 g_2}{\partial t\,\partial s}\\ &\quad + \frac{\partial g_1}{\partial s}\left(\frac{\partial^2 f}{\partial x^2}\bigg|_{\substack{x=g_1\\y=g_2}}\frac{\partial g_1}{\partial t} + \frac{\partial^2 f}{\partial y\,\partial x}\bigg|_{\substack{x=g_1\\y=g_2}}\frac{\partial g_2}{\partial t}\right)\\ &\quad + \frac{\partial g_2}{\partial s}\left(\frac{\partial^2 f}{\partial x\,\partial y}\bigg|_{\substack{x=g_1\\y=g_2}}\frac{\partial g_1}{\partial t} + \frac{\partial^2 f}{\partial y^2}\bigg|_{\substack{x=g_1\\y=g_2}}\frac{\partial g_2}{\partial t}\right).\end{aligned}$$

For this example the second partial derivative has six terms in total!

We postpone showing an example while we explain an alternative approach to calculating second derivatives of composite functions.

Second derivatives and the chain rule. Method 2

In the preceding discussion emphasis was placed on the steps one needs to take in order to arrive at a second derivative of a composite function. There is, however, an alternative perspective that does have considerable merit and which is equivalent to the above.

We remain with the choice of Case 3:

$$\text{Outer function, } f : \mathbb{R}^2 \longrightarrow \mathbb{R}, \quad \text{and inner function, } \boldsymbol{g} : \mathbb{R}^2 \longrightarrow \mathbb{R}^2$$

$$\implies \quad F(s,t) = \big(f \circ \boldsymbol{g}\big)(s,t) = f\big(g_1(s,t), g_2(s,t)\big).$$

To summarize Method 1: we established that the first partial derivative of F with respect to s is

$$\frac{\partial F}{\partial s} = \frac{\partial f}{\partial x}.\frac{\partial g_1}{\partial s} + \frac{\partial f}{\partial y}.\frac{\partial g_2}{\partial s},$$

and we pointed out that both $\dfrac{\partial f}{\partial x}$ and $\dfrac{\partial f}{\partial y}$ were two new composite functions of s and t. In taking a second partial derivative we needed to (a) apply the product rule, and then (b) apply the chain rule an additional time on each of these functions.

The alternative method, that will now be explained, is based on the observation that at the intermediate point – *after taking the first derivative, but before any other action is taken* – both $\dfrac{\partial f}{\partial x}$ and $\dfrac{\partial f}{\partial y}$ are explicit functions of x and y, while $\dfrac{\partial g_1}{\partial s}$ and $\dfrac{\partial g_2}{\partial s}$ are explicit functions of s and t. Consequently, at this intermediate point (for the particular case studied) we find that $\dfrac{\partial F}{\partial s}$ is explicitly a function of *all four* variables, x, y, s, t. That is,

$$\frac{\partial F}{\partial s} = h(x, y, s, t),$$

where x and y will ultimately still be functions of s and t. So, at this intermediate point, the function $h(x, y, s, t)$ can be thought of as *one* composite function (of Class 4 studied earlier) possessing a branch diagram shown in Figure 2.39. Compare this diagram to that for the original composite function which was shown in Figure 2.34.

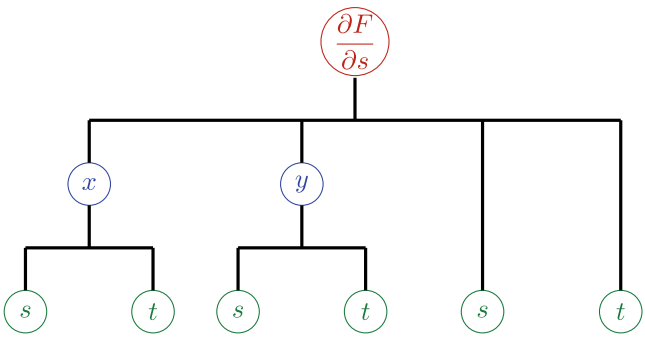


Figure 2.39 The complex ball-and-stick diagram for $h(x, y, s, t)$.

The second, mixed derivative of F, or *first* derivative of $\dfrac{\partial F}{\partial s}$, with respect to t, would then have the form, according to Case 4,

$$\frac{\partial^2 F}{\partial t \partial s} = \frac{\partial}{\partial t}\left(\frac{\partial F}{\partial s}\right) = \frac{\partial h}{\partial x}\frac{\partial g_1}{\partial t} + \frac{\partial h}{\partial y}\frac{\partial g_2}{\partial t} + \frac{\partial h}{\partial t}.$$

That is, we simply apply the chain rule *once*, as laid out in Case 4, to a function of *more* variables.

Similar considerations and outcomes apply to the first derivative $\dfrac{\partial F}{\partial t}$ which can be treated as another function of *four* variables $k(x, y, s, t)$. For example, the second pure derivative of F with respect to t, or the first partial derivative of $\dfrac{\partial F}{\partial t}$ with respect to t, would then be

$$\frac{\partial^2 F}{\partial t^2} = \frac{\partial k}{\partial x}\frac{\partial g_1}{\partial t} + \frac{\partial k}{\partial y}\frac{\partial g_2}{\partial t} + \frac{\partial k}{\partial t}.$$

Analogous considerations follow for the pure second derivative $\dfrac{\partial^2 F}{\partial s^2}$, and the other mixed second derivative $\dfrac{\partial^2 F}{\partial s \partial t}$.

In a sense, the first two steps of the three-step operation (the product rule followed by the chain rule) is replaced by a single, extended chain rule operation. A moment's thought will convince the reader that these second order derivatives may now similarly be treated as new functions of the same four variables and thus possess the same branch structure as the first order derivatives, since no additional variables are introduced. Higher order derivatives (of F) would then be evaluated in precisely the same way as in the above examples of second derivatives.

We illustrate both processes and their equivalence with an example, followed by a Mastery Check for the reader to attempt.

Example 2.19:

Evaluate $\dfrac{\partial^2 F}{\partial s \partial t}$ for the composite function $F(s,t) = \big(f \circ \boldsymbol{g}\big)(s,t) = f\big(g_1(s,t), g_2(s,t)\big)$
formed of

$$f(x,y) = \sin(x^2)y^3; \quad x = g_1(s,t) = s^2 - t^2; \quad \text{and} \quad y = g_2(s,t) = st.$$

Solution:

Following the suggestion of the floodgate model Figure 2.33, we have

$$\begin{aligned}\left(\frac{\partial F}{\partial t}\right)_s &= \left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial g_1}{\partial t}\right)_s + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial g_2}{\partial t}\right)_s \\ &= \cos(x^2)2xy^3.(-2t) + \sin(x^2)3y^2.(s).\end{aligned}$$

In the first method, the first two steps of the three-step method, the product rule + chain rule, we have

$$\begin{aligned}\frac{\partial}{\partial s}\left(\frac{\partial F}{\partial t}\right) &= \frac{\partial}{\partial s}\left[\cos(x^2)2xy^3.(-2t) + \sin(x^2)3y^2.(s)\right], \\ &= \frac{\partial}{\partial s}\left[2xy^3\cos(x^2)\right].(-2t) + \left(2xy^3\cos(x^2)\right).(0) \\ &\quad + \frac{\partial}{\partial s}\left[3y^2\sin(x^2)\right].(s) + \left(3y^2\sin(x^2)\right).(1),\end{aligned}$$

— the product rule is applied here, there are now 4 terms.

$$\begin{aligned}= \; & (-2t).\left[\frac{\partial}{\partial x}\left(2xy^3\cos(x^2)\right)\frac{\partial g_1}{\partial s} + \frac{\partial}{\partial y}\left(2xy^3\cos(x^2)\right)\frac{\partial g_2}{\partial s}\right] + \left(2xy^3\cos(x^2)\right).(0) \\ & + (s).\left[\frac{\partial}{\partial x}\left(3y^2\sin(x^2)\right)\frac{\partial g_1}{\partial s} + \frac{\partial}{\partial y}\left(3y^2\sin(x^2)\right)\frac{\partial g_2}{\partial s}\right] + \left(3y^2\sin(x^2)\right).(1)\end{aligned}$$

— the chain rule is applied here to the first and third terms, there are now 6 terms.

Evaluating the x and y derivatives we get

$$\begin{aligned}\frac{\partial^2 F}{\partial s \partial t} &= (-2t).\left[\left(2y^3\cos(x^2) - 4x^2y^3\sin(x^2)\right)\frac{\partial g_1}{\partial s} + 6xy^2\cos(x^2)\frac{\partial g_2}{\partial s}\right] \\ &+ \quad (s).\left[6xy^2\cos(x^2)\frac{\partial g_1}{\partial s} + 6y\sin(x^2)\frac{\partial g_2}{\partial s}\right] + 3y^2\sin(x^2). \qquad (2.4)\end{aligned}$$

The final step would involve a variable substitution using the expressions for the derivatives of g_1 and g_2 into Equation (2.4) and simplifying, and then

expressing the final result in terms of s and t. We leave this task to the reader. For the sake of our argument, we shall stop at this point since this last expression provides a more meaningful comparison with the alternative approach described below.

In the second method, we treat the first derivative $\dfrac{\partial F}{\partial t}$ *at the intermediate stage* as a function of *four* variables:

$$\frac{\partial F}{\partial t} = h(x, y, s, t) = -4xty^3 \cos(x^2) + 3sy^2 \sin(x^2).$$

Then

$$\begin{aligned} \frac{\partial^2 F}{\partial s \partial t} &= \frac{\partial h}{\partial x}\frac{\partial g_1}{\partial s} + \frac{\partial h}{\partial y}\frac{\partial g_2}{\partial s} + \frac{\partial h}{\partial s}, \\ &= \left[-4y^3 t\left(\cos(x^2) - 2x^2 \sin(x^2)\right) + 6sxy^2 \cos(x^2)\right]\frac{\partial g_1}{\partial s} \\ &\qquad + \left[-12xty^2 \cos(x^2) + 6ys \sin(x^2)\right]\frac{\partial g_2}{\partial s} + 3y^2 \sin(x^2). \quad (2.5) \end{aligned}$$

Term for term, one readily accounts for the equivalence of the two expressions. What is perhaps the most interesting aspect of this comparison is the origin of the difference of the two approaches. In Method 1 the second application of the chain rule is applied to each coefficient function. In Method 2 the single, but extended chain rule application is split across the two coefficient functions. Note the locations of $\dfrac{\partial g_1}{\partial s}$ and $\dfrac{\partial g_2}{\partial s}$ in Equations (2.4) and (2.5), and their respective coefficients. ■

As a last comment, the two methods just discussed are not limited to examples from Class 3. The ideas are applicable across all classes of composite functions. In particular, Method 2 generalizes intuitively to functions composed of more than two variables. For example, if an outer function has n independent outer variables (x, y, z, etc.) each of which depends on m inner variables (s, t, u, etc) through m inner functions, then the first derivative, treated as an intermediate, will be a function of $m + n$ variables. The reader should easily expand on this example to other cases.

We conclude this topic with a Mastery Check for the reader to pursue using either *or both* of the methods just discussed.

✍ Mastery Check 2.15:

Let $f(x, y) = x \cos y + y$, where $x = u(s, t) = st$, $y = v(s, t) = s^2 + t^2$. Determine $\dfrac{\partial^2 z}{\partial s \partial t}$.

✍

The Leibniz integral rule

A particularly important application of the chain rule is to differentiating an integral such as

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{a(t)}^{b(t)} h(x,t)\,\mathrm{d}x,$$

with respect to a parameter. Suppose h, a and b are C^1 functions and the indicated integral, as well as the integral of $\partial h/\partial t$, exists. The integral itself produces a function $z = F(t) = \big(f \circ \boldsymbol{g}\big)(t)$, which depends on t through three channels. Let's call these u, v and t, where u and v take the place of the upper and lower limits of the integral, and where

$$\begin{array}{rcl} f : \mathbb{R}^3 & \longrightarrow & \mathbb{R}, \\ (u,v,t) & \longmapsto & z = \displaystyle\int_v^u h(x,t)\,\mathrm{d}x, \\ & \text{and} & \boldsymbol{g} = \big(u = b(t), v = a(t)\big). \end{array}$$

The branch model relevant to this is shown in Figure 2.40. It is a somewhat simplified version of Case 4 on Page 119.

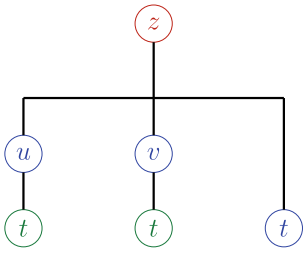


Figure 2.40 Ball-and-stick for $f\big(g_1(t), g_2(t), t\big)$.

Referring back to Case 4, the derivative of F with respect to t is then

$$\begin{aligned} \frac{\mathrm{d}F}{\mathrm{d}t} &= \left(\frac{\partial f}{\partial u}\right)\Bigg|_{(u=b(t),v=a(t),t)} \cdot \left(\frac{\mathrm{d}b}{\mathrm{d}t}\right) \\ &\quad + \left(\frac{\partial f}{\partial v}\right)\Bigg|_{(u=b(t),v=a(t),t)} \cdot \left(\frac{\mathrm{d}a}{\mathrm{d}t}\right) + \left(\frac{\partial f}{\partial t}\right)\Bigg|_{(u=b(t),v=a(t),t)}. \end{aligned}$$

The partial derivatives of f with respect to u and v are straightforward using the fundamental theorem of integral calculus:

$$g(x) \;=\; \pm\frac{dG}{dx} \Longleftrightarrow G(x) = \pm\int_c^x g(x')\mathrm{d}x'$$

where c is some constant. Thus,

$$\left(\frac{\partial f}{\partial u}\right)\Big|_{(b(t),a(t),t)} = h(b(t),t) \quad \text{and} \quad \left(\frac{\partial f}{\partial v}\right)\Big|_{(b(t),a(t),t)} = -h(a(t),t).$$

For the partial derivative of f with respect to t we use the definition:

$$\frac{f(u,v,t+\Delta t)-f(u,v,t)}{\Delta t} = \int_u^v \left[\frac{h\,(x,t+\Delta t)-h(x,t)}{\Delta t}\right]\mathrm{d}x.$$

where we are permitted to put everything under the one integral sign since f is C^1. Now, taking the limit $\Delta t \to 0$ we get

$$\frac{\partial f}{\partial t} \;=\; \int_u^v \frac{\partial h}{\partial t}(x,t)\,\mathrm{d}x.$$

All together, replacing u and v everywhere with $a(t)$ and $b(t)$, respectively, we have the very useful Leibniz rule,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{a(t)}^{b(t)} \quad & h(x,t)\mathrm{d}x \\ & = h\big(b(t),t\big)\cdot\left(\frac{\mathrm{d}b}{\mathrm{d}t}\right) - h\big(a(t),t\big)\cdot\left(\frac{\mathrm{d}a}{\mathrm{d}t}\right) + \int_{a(t)}^{b(t)} \frac{\partial h}{\partial t}(x,t)\mathrm{d}x\end{aligned}$$

■ Example 2.20:

We apply this rule to the following integrals. Note the use of the same process despite the different independent variables.

(1) Suppose $F(x) = \displaystyle\int_0^{x^2} \sin(u^2)\,\mathrm{d}u$. The independent variable, x only appears in the upper limit of the integral. Consequently, only the first of the three terms in the Leibniz rule in nonzero. In this case

$$\frac{\mathrm{d}b}{\mathrm{d}x} = 2x, \text{ and } h(b(x)) = \sin\left(\left(x^2\right)^2\right), \text{ giving } F'(x) = 2x\sin(x^4).$$

(2) Suppose $F(u) = \displaystyle\int_{1-\ln u}^{1} \mathrm{e}^{t^2}\,\mathrm{d}t$. Here, the independent variable, u, only appears in the lower limit. Hence, only the second of the three terms in the Leibniz derivative is nonzero. In this case we have

$$\frac{\mathrm{d}a}{\mathrm{d}u} = \frac{\mathrm{d}}{\mathrm{d}u}\,(1-\ln u) = -\frac{1}{u} \text{ and } h(a(u)) = \mathrm{e}^{(1-\ln u)^2}, \text{ so } F'(u) = \frac{1}{u}\mathrm{e}^{(1-\ln u)^2}.$$

(3) Suppose $F(t) = \int_{\sin t}^{\cos t} \mathrm{e}^{2xt}\,\mathrm{d}x$. The independent variable is t and appears in both limits as well as in the integrand function. Consequently, all three terms of Leibniz rule contribute to the overall derivative. We have,

$$\begin{aligned} \frac{\mathrm{d}b}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}(\cos t) = -\sin t, \text{ and } h(b(t)) = \mathrm{e}^{2x\cos t}, \text{ while} \\ \frac{\mathrm{d}a}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}(\sin t) = \cos t, \text{ and } h(a(t)) = \mathrm{e}^{2x\sin t}, \text{ so} \\ & F'(t) = -\mathrm{e}^{2t\cos t}\sin t - \mathrm{e}^{2t\sin t}\cos t + \int_{\sin t}^{\cos t} 2x\mathrm{e}^{2xt}\,\mathrm{d}x. \end{aligned}$$

■

It is worthwhile recognizing that because of the similarity between the definitions of ordinary and partial derivatives, the proof of the Leibniz differentiation rule admits a natural generalization to multivariable functions. In cases where the integration limits, a and b, are C^1 functions of x and y, say, while the integrand function, h, is a C^1 function of x, y, and t, the derivation and form of the Leibniz rule remains the same, but the derivatives become partial derivatives. For example, supposing that $F(x,y) = \int_{a(x,y)}^{b(x,y)} h(x,y,t)\mathrm{d}t$, where a, b and h are C^1 functions, then it follows that

$$\begin{aligned} \frac{\partial}{\partial x}\Big(F(x,y)\Big) &= h\big(x,y,b(x,y)\big)\cdot\Big(\frac{\partial b}{\partial x}\Big) \\ & \quad - h\big(x,y,a(x,y)\big)\cdot\Big(\frac{\partial a}{\partial x}\Big) + \int_{a(x,y)}^{b(x,y)} \frac{\partial h}{\partial x}(x,,y,t)\mathrm{d}t, \end{aligned}$$

with an analogous expression for the partial derivative with respect to y. It is easy to see how this might be generalized to multivariable functions of even more variables.

2.H Implicit Functions

Suppose we are given the following task: In each of the cases below express in closed form the variable y as a function of the remaining variables:

(a) $8y + 64x^2 = 0$;

(b) $2y^2 + 8y + 16z\sin x = 0$;

(c) $\ln|y| + y^3x + 20x^2 = w$.

I am as certain that you cannot complete task (c) as I am that you *can* complete tasks (a) and (b). Although task (c) is impossible, the equation suggests there is a functional relationship, at least in principle.

This last example introduces us to the notion of an implied or *implicit function*. In task (c) the equation suggests that y could be a function f of the variables x and w. What we shall do in this section is establish conditions under which such a function is defined, *at least locally*. Along the way we will derive a linear approximation to this unknown function of the independent variables that is valid near a given point. We will also derive explicit expressions and values for the derivative or derivatives of this implicit function evaluated at that point.

As before we explain by considering examples of increasing complexity. In each case we will also discuss an analogous linear problem. Since the arguments followed are based on linearization, we hope that the parallels will facilitate reader understanding.

We consider the following three problems:

1) $\mathrm{e}^{x+y} + xy = 0 \implies F(x,y) = 0$ — a level curve.

2) $\mathrm{e}^{x+y+z} - (x+y+z)^2 = 1 \implies F(x,y,z) = 0$ — a level surface.

3) $\begin{cases} e^{x+y+z} - (x+y+z)^2 - 1 = 0 \\ z\sin(xy) - x\cos(zy) = 0 \end{cases} \implies \begin{cases} F(x,y,z) = 0 \\ G(x,y,z) = 0 \end{cases}$

— a curve of intersection.

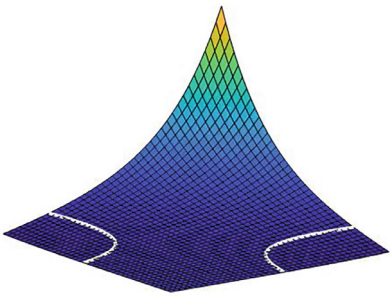


Figure 2.41 The graph of $z = \mathrm{e}^{x+y} + xy$ and the level set $F(x,y) = 0$.

Consider Problem 1). $F(x,y) = \mathrm{e}^{x+y} + xy = 0.$

This equation is nonlinear. Moreover, it cannot be manipulated to get y in terms of x. All the same, the equation suggests or implies a relationship of the form $y = f(x)$ even though f is unknown; the level curve described by $F(x,y) = 0$, determined numerically, is shown in Figure 2.41.

However, suppose we were not interested in F globally, but only in its behaviour locally. Then we may consider the linear approximation to $F(x, y) = e^{x+y} + xy$ for points (x, y) about a point (a, b) known to lie on the level curve $F(x, y) = 0$. The linear approximation is shown in Figure 2.42 and is developed below.

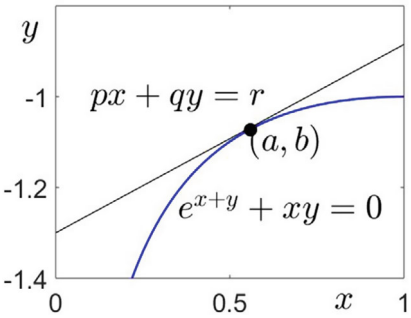


Figure 2.42 The level curve $e^{x+y} + xy = 0$ and its approximation valid near $(a, b) \approx (0.5, -1.1)$.

By way of introduction to the analysis of the more general nonlinear problem, we shall first reflect on what occurs in the special case of a straight line.

Consider the level set representing a line in 2D described by the general line equation (Figure 2.43):

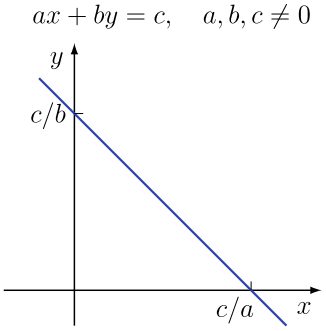


Figure 2.43 The line $G(x, y) = ax + by = c$.

If we divide both sides of this linear equation by b, the coefficient of y, and solve for y, we naturally get the equation of a line in standard, slope-intercept form.

$$y = -\frac{a}{b}x + \frac{c}{b} = mx + k,$$

where m is the *finite* slope, $m = -a/b \in (-\infty, \infty)$ *as long* as $b \neq 0$. This is the important point for what follows: *The coefficient, b, of the variable we solved for, y, cannot be zero.*

Now consider the more general nonlinear function, $F(x, y)$.

Suppose we are given that $\boldsymbol{a} = (a, b)$ is a point on the level curve,

$$L = \Big\{(x, y) \in \mathbb{R}^2 : \ F(x, y) = 0\Big\}.$$

If F is a C^1 function, then for any $(x, y) \in D_F$ *near* (a, b) (see Page 85) F may be written as,

$$F(x,y) \quad = \quad \cancelto{0}{F(a,b)} + \frac{\partial F}{\partial x}\Big|_{(a,b)}.(x-a) + \frac{\partial F}{\partial y}\Big|_{(a,b)}.(y-b) + |\Delta\boldsymbol{x}|\rho(\Delta\boldsymbol{x}),$$

where ρ is an infinitesimal function of $\Delta\boldsymbol{x} = \boldsymbol{x} - \boldsymbol{a}$, and its contribution is therefore small in magnitude compared to the linear terms for $|\Delta\boldsymbol{x}| \ll 1$.

Now let, in particular, point $\boldsymbol{x} = (x, y)$ be a point on the level curve, L, then both $F(x, y)$ and $F(a, b)$ are zero and we get

$$0 = \frac{\partial F}{\partial x}\Big|_{(a,b)}.(x-a) + \frac{\partial F}{\partial y}\Big|_{(a,b)}.(y-b) + \ |\Delta\boldsymbol{x}|\rho(\Delta\boldsymbol{x}),$$

or, equivalently,

$$\frac{\partial F}{\partial x}\Big|_{(a,b)}.x + \frac{\partial F}{\partial y}\Big|_{(a,b)}.y = \frac{\partial F}{\partial x}\Big|_{(a,b)}.a + \frac{\partial F}{\partial y}\Big|_{(a,b)}.b - |\Delta\boldsymbol{x}|\rho(\Delta\boldsymbol{x}).$$

Consequently, for $|\Delta\boldsymbol{x}| \ll 1$, the level curve $F(x, y) = 0$ may be approximated by the tangent line obtained upon neglecting the last term on the right-hand side of this last equation. The tangent line itself, an approximation to the level curve $F(x, y) = 0$ for $\boldsymbol{x} \in L$ near $\boldsymbol{a}$, takes the form of the general line equation.

$$\frac{\partial F}{\partial x}\Big|_{(a,b)}.x + \frac{\partial F}{\partial y}\Big|_{(a,b)}.y = \frac{\partial F}{\partial x}\Big|_{(a,b)}.a + \frac{\partial F}{\partial y}\Big|_{(a,b)}.b \quad \Longrightarrow \ px + qy = r.$$

This line is valid at all such points on the C^1 level set, exemplified by the three lines tangent to $F(x, y) = 0$ at the three points (x_1, y_1), (x_2, y_2) and (x_3, y_3) in Figure 2.44. However, of these three tangent lines (and similarly for other possible tangent lines at other points on L) only the tangent lines at (x_2, y_2) and (x_3, y_3) indicate that the level set equation, $F(x, y) = 0$, defines an implicit function $y = f(x)$ locally. The curve segment about the point (x_1, y_1) does not satisfy the important criterion for a function: that a given x value maps to a single y value (Page 25).

Whether $F(x, y) = 0$ defines $y = f(x)$ as an implicit function for (x, y) near point $(a, b) \in L$ can also be shown analytically using the tangent line equation. Now, as we saw with the above simple linear example, a sufficient condition for the existence of an implicit function f is for the coefficient, q, of the variable we wish to solve for, y, to be nonzero, $q \neq 0$.

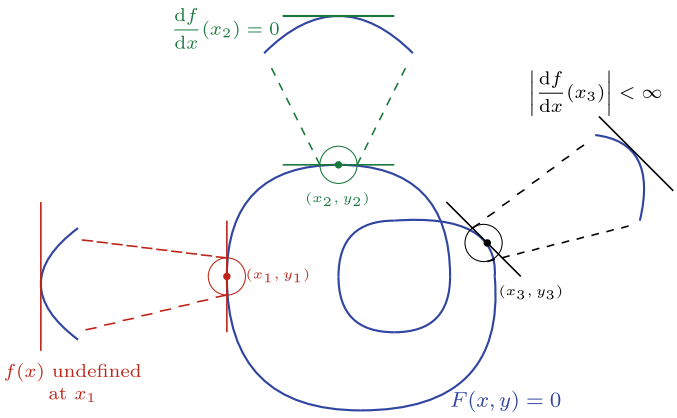


Figure 2.44 Three points of tangency on a nonlinear, level curve, $F(x, y) = 0$.

Hence, by dividing the general equation for the tangent line by $q \neq 0$, we obtain the slope-intercept expression for this same tangent line,

$$y = -(p/q)x + r/q, \qquad \text{provided} \qquad q \neq 0.$$

Apart from being the linear approximation to the implicit function graph at (a, b), it is also in the correct form to identify the slope of the graph at (a, b) and hence the derivative $f'(x)$ at the point $x = a$.

The key, take-home points from this discussion are that:

(1) solving for y in the differentiability equation for $F(x, y)$, for points $(x, y) \in L$ near point $(a, b) \in L$ is valid *as long as its coefficient*, $q = \dfrac{\partial F}{\partial y}\Big|_{(a,b)} \neq 0$;

(2) the linear approximation to the level curve $F(x, y) = 0$ may then be written

$$y = -\frac{\dfrac{\partial F}{\partial x}\Big|_{(a,b)}}{\dfrac{\partial F}{\partial y}\Big|_{(a,b)}} x + \frac{r}{q}, \qquad \text{for} \quad q \neq 0;$$

(3) from this we obtain the explicit value of the derivative of the implicit function, at the point of tangency,

$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=a} = -\frac{\left.\dfrac{\partial F}{\partial x}\right|_{(a,b)}}{\left.\dfrac{\partial F}{\partial y}\right|_{(a,b)}} \iff F \in C^1 \text{ at } (a,b), \text{ and } q = \left.\frac{\partial F}{\partial y}\right|_{(a,b)} \neq 0.$$

We explore these points further in an example and a Mastery Check.

Example 2.21:

Suppose the equation $x^3y + 2y^3x = 3$ defines y as a function f of x in the neighbourhood of the point $(1,1)$. Evaluate the derivative of f at $x = 1$, and the linear approximation to f near that point.

Solution:

Let $F(x,y) = x^3y + 2y^3x = 3$. Note that $F \in C^1 \; \forall \; (x,y) \in \mathbb{R}^2$. We then have

$$\frac{\partial F}{\partial x} = 3x^2y + 2y^3, \quad \frac{\partial F}{\partial y} = x^3 + 6xy^2.$$

We note $\dfrac{\partial F}{\partial y} \neq 0$ at $(1,1)$ (the sufficient condition for the existence of implicit f).

Thus, from our linear approximation we have

$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{(x=1)} = -\frac{\left.\dfrac{\partial F}{\partial x}\right|_{(1,1)}}{\left.\dfrac{\partial F}{\partial y}\right|_{(1,1)}} = -\frac{3+2}{1+6} = -\frac{5}{7}.$$

The linear approximation is therefore $y = -\dfrac{5}{7}x + c$. To determine c, we use the fact that the line passes through $(1,1)$, giving $y = -\dfrac{5}{7}x + \dfrac{12}{7}$.

■

Mastery Check 2.16:

Show that $x^y + \sin y = 1$ defines a function $y = f(x)$ in the neighbourhood of $(1,0)$, and evaluate $\dfrac{\mathrm{d}f}{\mathrm{d}x}$ at $(1,0)$. Determine a linear approximation to f, valid near $(1,0)$.

Consider Problem 2). $F(x, y, z) = \mathrm{e}^{x+y+z} - (x + y + z)^2 - 1 = 0.$

Suppose $\boldsymbol{a} = (a, b, c)$ is a point on the level surface,

$$L = \Big\{(x, y, z) : \ F(x, y, z) = 0.\Big\}$$

Our objective here is the same as in Problem 1: to determine conditions under which $F(x, y, z) = 0$ defines a function, $f(x, y)$, for points $\boldsymbol{x} = (x, y, z)$ on L near $\boldsymbol{a} = (a, b, c)$. As with Problem 1, the solution depends on the behaviour of $F(x, y, z)$ near the point $\boldsymbol{a}$ as well as on the existence of the linear approximation to F.

We again lead with a linear analogy. Consider the equation,

$$Ax \ + \ By \ + \ Cz \ = \ D, \qquad A, B, C, D > 0,$$

of the plane shown in Figure 2.45.

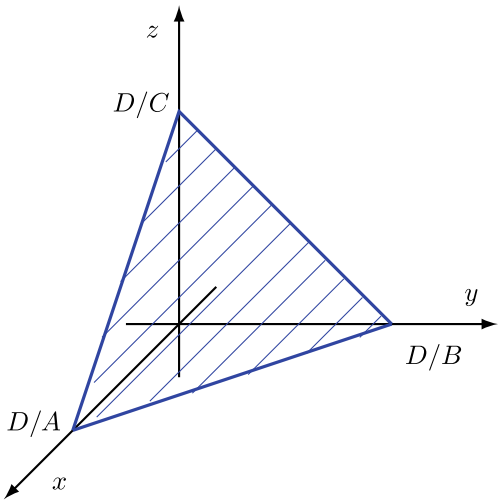


Figure 2.45 A segment of the plane $Ax + By + Cz = D$.

Dividing each term of this equation by C, the coefficient of z, and solving for z we get

$$z = \frac{D}{C} - \frac{A}{C}x - \frac{B}{C}y, \qquad \text{if } C \neq 0.$$

From this we read that the plane has (partial) slope $-A/C$ in the x-direction and (partial) slope $-B/C$ in y-direction; both slopes will be finite as long as $C \neq 0$. This is the key point of this analogy: *the coefficient, C, of the variable we wish to solve for, here it is z, cannot be zero.* The important implication is that subject to this condition the one variable, z, may be expressed in terms of the other two, x and y.

Keeping these points in mind, consider now the nonlinear function $F(x, y, z)$. We suppose that F is differentiable (*i.e.*, F is a C^1 function) at the point $\boldsymbol{a} = (a, b, c) \in L$. Then, according to Definition 2.4, differentiability implies that for points $\boldsymbol{x} = (x, y, z) \in D_F$ near point $\boldsymbol{a}$, $F(x, y, z)$ may be expressed as

$$F(\boldsymbol{x}) = \cancel{F(\boldsymbol{a})}^{\,0} + \left.\frac{\partial F}{\partial x}\right|_{\boldsymbol{a}}.(x-a) + \left.\frac{\partial F}{\partial y}\right|_{\boldsymbol{a}}.(y-b) + \left.\frac{\partial F}{\partial z}\right|_{\boldsymbol{a}}.(z-c) + |\boldsymbol{x}-\boldsymbol{a}|\rho(\boldsymbol{x}-\boldsymbol{a}),$$

where ρ again denotes an infinitesimal function of $\Delta\boldsymbol{x} = \boldsymbol{x} - \boldsymbol{a}$, giving a contribution that is small in magnitude compared with the linear terms. Choosing $\boldsymbol{x}$ to also be a point on the level set L near point $\boldsymbol{a}$, the expression simplifies further since $F(\boldsymbol{x}) = F(\boldsymbol{a}) = 0$ leading to

$$0 = \left.\frac{\partial F}{\partial x}\right|_{(a,b,c)}.(x-a) + \left.\frac{\partial F}{\partial y}\right|_{(a,b,c)}.(y-b) + \left.\frac{\partial F}{\partial z}\right|_{(a,b,c)}.(z-c) + |\boldsymbol{x}-\boldsymbol{a}|\rho(\boldsymbol{x}-\boldsymbol{a}).$$

So, for points $\boldsymbol{x} \in L$ such that $|\Delta\boldsymbol{x}| \ll 1$, the infinitesimal term may be neglected and the level surface can be approximated by the tangent plane equation,

$$\begin{aligned} \left.\frac{\partial F}{\partial x}\right|_{(a,b,c)}.x + \left.\frac{\partial F}{\partial y}\right|_{(a,b,c)}y + \left.\frac{\partial F}{\partial z}\right|_{(a,b,c)}.z &= \left.\frac{\partial F}{\partial x}\right|_{(a,b,c)}.a + \left.\frac{\partial F}{\partial y}\right|_{(a,b,c)}.b + \left.\frac{\partial F}{\partial z}\right|_{(a,b,c)}.c \\ &\Longrightarrow \quad Ax + By + Cz = D, \end{aligned}$$

which, as established in Definition 2.4, is a valid approximation for every differentiable point $\boldsymbol{a} \in L$. However, as in Problem 1, not all tangent planes are consistent with $F(x, y, z) = 0$ implying the existence of a function f of x and y. Only if the coefficient of z, $C = \left.\frac{\partial F}{\partial z}\right|_{(a,b,c)}$, is nonzero, may we divide all terms of the general tangent plane equation by C to obtain the tangent plane approximation to the graph of the implicit function, $z = f(x, y)$, for points (x, y) near (a, b). That is, provided $\left.\frac{\partial F}{\partial z}\right|_{(a,b,c)} \neq 0$, do we have

$$z = c - \frac{\left.\frac{\partial F}{\partial x}\right|_{(a,b,c)}}{\left.\frac{\partial F}{\partial z}\right|_{(a,b,c)}}.(x-a) - \frac{\left.\frac{\partial F}{\partial y}\right|_{(a,b,c)}}{\left.\frac{\partial F}{\partial z}\right|_{(a,b,c)}}.(y-b) \tag{2.6}$$

as the tangent plane approximation to $z = f(x, y)$ for points (x, y) in the neighborhood of (a, b). From this tangent plane equation we can read off the partial derivatives of the implicit function f evaluated at (a, b), namely

$$\left.\frac{\partial f}{\partial x}\right|_{(a,b)} = -\frac{\left.\frac{\partial F}{\partial x}\right|_{(a,b,c)}}{\left.\frac{\partial F}{\partial z}\right|_{(a,b,c)}} \quad \text{and} \quad \left.\frac{\partial f}{\partial y}\right|_{(a,b)} = -\frac{\left.\frac{\partial F}{\partial y}\right|_{(a,b,c)}}{\left.\frac{\partial F}{\partial z}\right|_{(a,b,c)}}$$

$$\Longleftrightarrow \qquad F \in C^1 \text{ at } (a,b,c), \text{ and } \left.\frac{\partial F}{\partial z}\right|_{(a,b,c)} \neq 0.$$

It follows that provided $\left.\frac{\partial F}{\partial z}\right|_{(a,b,c)} \neq 0$, both $\left.\frac{\partial f}{\partial x}\right|_{(a,b)}$ and $\left.\frac{\partial f}{\partial y}\right|_{(a,b)}$ will be *well defined* and the implicit function $f(x,y)$ will exist in a neighborhood of (a,b), approximated *locally* by the tangent plane described by Eq 2.6.

The parallels between the above argument and those expressed in Problem 1 should be clear. We consolidate the ideas in an example.

■ Example 2.22:

Show that the level surface, $F(x,y,z) = \mathrm{e}^{z-1} + zy + x - 2y^3 = 0$, passes through the point $\boldsymbol{a} = (0,1,1)$. Determine the tangent plane to the surface at $\boldsymbol{a}$ and determine whether the equation defines z as an implicit function of x and y in a neighborhood of $\boldsymbol{a}$.

Solution:

It is readily verified by substitution that the point $(0,1,1)$ lies on the level set $F(x,y,z) = 0$ since $F(0,1,1) = \mathrm{e}^{1-1} + 1.1 + 0 - 2.1^3 = 1 + 1 - 2 = 0$. Following the line of reasoning outlined above it is easy to see that

$$\begin{cases} \left.\frac{\partial f}{\partial x}\right|_{(0,1)} = -\dfrac{\left.\frac{\partial F}{\partial x}\right|_{(0,1,1)}}{\left.\frac{\partial F}{\partial z}\right|_{(0,1,1)}} = -\dfrac{1}{\left.(y + \mathrm{e}^{z-1})\right|_{(0,1,1)}} = -\dfrac{1}{2}, \\[2ex] \left.\frac{\partial f}{\partial y}\right|_{(0,1)} = -\dfrac{\left.\frac{\partial F}{\partial y}\right|_{(0,1,1)}}{\left.\frac{\partial F}{\partial z}\right|_{(0,1,1)}} = -\dfrac{z - 6y^2}{\left.(y + \mathrm{e}^{z-1})\right|_{(0,1,1)}} = \dfrac{5}{2}. \end{cases}$$

Consequently, invoking Eq 2.6 the equation of the tangent plane to the implicit function at $(0,1,1)$ is

$$\begin{aligned} z &= 1 + \left.\frac{\partial f}{\partial x}\right|_{(0,1)}.(x-0) + \left.\frac{\partial f}{\partial y}\right|_{(0,1)}.(y-1) = 1 - \frac{1}{2}x + \frac{5}{2}(y-1), \\ &\Longrightarrow x - 5y + 2z = -3 \end{aligned}$$

A normal vector to this plane is then

$$\left(-\left.\frac{\partial f}{\partial x}\right|_{(0,1)}, -\left.\frac{\partial f}{\partial y}\right|_{(0,1)}, +1\right) = \left(\frac{1}{2}, -\frac{5}{2}, +1\right) \Longrightarrow \boldsymbol{n} = \frac{1}{2}(1,-5,2).$$

Of course, the tangent plane is only possible because $\left.\dfrac{\partial F}{\partial z}\right|_{(0,1,1)} = 2 \neq 0$, which also guarantees that the implicit function $f(x, y)$ is well defined for points (x, y) near $(0, 1)$.

We take advantage of this exercise to revisit the gradient and its relation to level sets to give an alternative solution to the problem. According to the earlier discussion, the gradient

$$\boldsymbol{\nabla} F(x, y, z) = \left(\frac{\partial F}{\partial x}, \frac{\partial F}{\partial y}, \frac{\partial F}{\partial z}\right) = \left(1, z - 6y^2, y + \mathrm{e}^{z-1}\right),$$

is perpendicular to the level set $F(x, y, z) = 0$ at the point (x, y, z) (and points in the direction of increasing F). In particular, $\boldsymbol{\nabla} F(0, 1, 1) = (1, -5, 2)$ is a vector normal to the level set at the point $(0, 1, 1)$. It is also a vector normal to the tangent plane at that point. The latter is given by the scalar product,

$$\begin{aligned} \boldsymbol{\nabla} F(0,1,1) \cdot (x - 0, y - 1, z - 1) = 0 \quad &\Longrightarrow \quad x - 5(y - 1) + 2(z - 1) = 0, \\ &\Longrightarrow \quad x - 5y + 2z = -3. \end{aligned}$$

which is identical to the earlier result.

Incidentally, although the variables x, y, and z have been used throughout the above solution, it is good to remember that when (x, y, z) is used to refer to a point on the level set $F(x, y, z) = 0$, it is then *not* also a point on the tangent plane. Equivalently, when (x, y, z) is used to refer to an arbitrary point on the tangent plane, it will *not* also be a point on the level set. The *only* point the two surfaces have in common is the point $(0, 1, 1)$.

■

Consider Problem 3). $\begin{cases} F(x, y, z) = e^{x+y+z} - (x + y + z)^2 - 1 = 0 \\ G(x, y, z) = z \sin(xy) - x \cos(zy) = 0 \end{cases}$.

As with Problems 1 and 2, a parallel with a linear algebraic system also exists for Problem 3. For completeness, however, we review two linear examples, rather than just the one. The first linear problem concerns a system in $\mathbb{R}^2$, which is conceptually straightforward. The second problem concerns a system in $\mathbb{R}^3$ and is therefore the more dimensionally relevant example for the nonlinear problem to be addressed.

Suppose we have the situation posed in Figure 2.46: two lines in the plane intersecting at a point. The lines are represented mathematically by a 2×2

system of equations for the unknown values of x^* and y^* which represent the coordinates of the point of intersection.

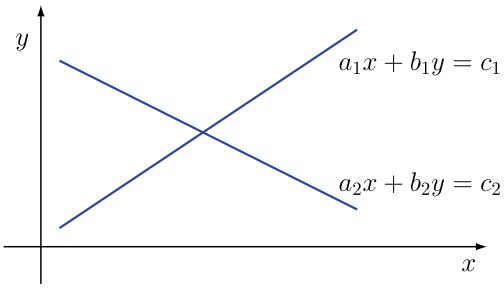


Figure 2.46 Two intersecting lines in $\mathbb{R}^2$.

This 2×2 matrix system can be solved for the coordinates of the point:

$$\begin{pmatrix} a_1 & b_1 \\ a_2 & b_2 \end{pmatrix} \begin{pmatrix} x^* \\ y^* \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \Longrightarrow \begin{pmatrix} x^* \\ y^* \end{pmatrix} = \frac{1}{a_1b_2 - a_2b_1} \begin{pmatrix} b_2 & -b_1 \\ -a_2 & a_1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$\Longrightarrow \quad x^* = \frac{c_1b_2 - c_2b_1}{a_1b_2 - a_2b_1} = \frac{\begin{vmatrix} c_1 & c_2 \\ b_1 & b_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}}, \qquad y^* = \frac{-c_1a_2 + c_2a_1}{a_1b_2 - a_2b_1} = \frac{\begin{vmatrix} a_1 & a_2 \\ c_1 & c_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}}$$

This system of equations has a unique solution *if and only if* the determinant of the *original* matrix is not equal to zero. Only then does the solution correspond to a single point in $\mathbb{R}^2$.

If, on the other hand, the determinant $a_1b_2 - a_2b_1$ were zero, then the two equations would be linearly dependent and either:

1) the two lines are separated but parallel and no solution exists (the numerator $\neq 0$), or

2) the lines are parallel and superimposed, in which case there is an infinite number of solutions (numerator $= 0$).

As in the earlier linear problems, the condition of a nonzero determinant is the important point to note.

Now consider the second of our linear problems, that of two arbitrary planes in $\mathbb{R}^3$.

$$\left.\begin{aligned} a_1x + b_1y + c_1z &= d_1 \\ a_2x + b_2y + c_2z &= d_2 \end{aligned}\right\} \quad \begin{array}{l} \text{two equations in} \\ \text{three unknowns: } x, y, \text{ and } z. \end{array}$$

Again, the objective is to determine whether the planes intersect or not, *i.e.* if there exists a solution to the pair of equations. If so, then the solution would correspond to a line of intersection: we have two equations and three unknowns, so two of the variables can be solved for in terms of the third. Choosing the third to be z we get,

$$\left.\begin{array}{rcl} a_1x + b_1y &=& d_1 - c_1z \\ a_2x + b_2y &=& d_2 - c_2z \end{array}\right\} \Longrightarrow \begin{pmatrix} a_1 & b_1 \\ a_2 & b_2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} d_1 - c_1z \\ d_2 - c_2z \end{pmatrix}$$

$$\Longrightarrow \quad \begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{a_1b_2 - a_2b_1} \begin{pmatrix} b_2 & -b_1 \\ -a_2 & a_1 \end{pmatrix} \begin{pmatrix} d_1 - c_1z \\ d_2 - c_2z \end{pmatrix}.$$

Again, this system has a unique solution

$$\Longleftrightarrow \text{ the determinant } = a_1b_2 - a_2b_1 \neq 0.$$

Once again, this is the determinant of the matrix of coefficients of x and y, the variables we are solving for.

For example, $\quad x = \dfrac{b_2(d_1 - c_1z) - b_1(d_2 - c_2z)}{a_1b_2 - a_2b_1}, \quad a_1b_2 - a_2b_1 \neq 0,$

$$\Longrightarrow x = \frac{b_2d_1 - b_1d_2}{a_1b_2 - a_2b_1} - \frac{b_2c_1 - b_1c_2}{a_1b_2 - a_2b_1}.z = k_1 - m_1z.$$

Similarly, we obtain $y = k_2 - m_2z$. Hence, combining these results we have

$$\left.\begin{array}{rcl} x &=& k_1 - m_1z \\ y &=& k_2 - m_2z \end{array}\right\} \Longrightarrow \quad \frac{x - k_1}{-m_1} = \frac{y - k_2}{-m_2} = z.$$

As expected, this last result is a well defined equation for a straight line in $\mathbb{R}^3$, *provided* $0 < |m_1|, |m_2| < \infty \iff a_1b_2 - a_2b_1 \neq 0$.

To summarize, the two equations for the two planes:

$$\left\{\begin{array}{rcl} a_1x + b_1y + c_1z &=& d_1 \\ a_2x + b_2y + c_2z &=& d_2 \end{array}\right.$$

define a *line of intersection* if the determinant of the *coefficients of the variables we wish to solve for, x and y, is nonzero*, *i.e.* provided $a_1b_2 - a_2b_1 \neq 0$. If the determinant were identically zero, then either:

1) the two planes are parallel and there is *no* solution, or

2) the two planes are parallel and superimposed, in which case there is an infinite number of solutions.

The two examples are essentially the same, they only differ in terms of dimensionality. The first example involves two lines determining a single *point* of intersection. The second involves two planes crossing to define a *line* of intersection. We could extend this to even higher dimensions: for example, two

four-dimensional hyperplanes intersecting to define a *plane* of intersection, but the key points are the same:

- *The determinant of coefficients of the variables to be solved for cannot be zero for the existence of a unique solution.*
- *If the determinant is zero, then either no solution exists (the surfaces are parallel) or there is an infinity of solutions (the surfaces coincide).*

Keeping the important points emerging from the two linear examples in mind, particularly the second two-plane system, we now consider the nonlinear problem:

$$F(x, y, z) = 0 \text{ and } G(x, y, z) = 0, \quad \text{for } x \in D_F \cap D_G, \tag{2.7}$$

for given (nonlinear) functions $F, G : \mathbb{R}^3 \to \mathbb{R}$.

The second linear, two-plane problem is but a special case of Equation (2.7), which according to the same principles, defines a set of points $\boldsymbol{x} = (x, y, z)$ the two level surfaces have in common. To be more precise, the system defines points, $\boldsymbol{x}$, that reside on a *curve of intersection*. In general, this will not be a straight line. Nevertheless, the same question may now be asked: under what conditions does the nonlinear system define a curve that can be expressed locally, near $\boldsymbol{a}$, in the form $\begin{cases} x &= f(z), \\ y &= g(z), \\ z &= z, \end{cases}$ with z as an independent variable?

As with Problems 1 and 2, the answer again depends on the behaviour of $F(x, y, z)$ and $G(x, y, z)$ about a known common point $\boldsymbol{a}$.

Suppose that $\boldsymbol{a} = (a, b, c)$ is a known point in common with the two level surfaces, *i.e.*, $F(a, b, c) = G(a, b, c) = 0$, and also suppose that F and G are differentiable at $\boldsymbol{a} = (a, b, c)$. Then, according to Definition 2.4, for points $\boldsymbol{x} = (x, y, z) \in D_F \cap D_G$ in the neighborhood of $\boldsymbol{a}$, these functions may be expressed as,

$$\begin{cases} F(\boldsymbol{x}) = \cancel{F(\boldsymbol{a})}^{\,0} + \dfrac{\partial F}{\partial x}\Big|_{\boldsymbol{a}}.(x-a) + \dfrac{\partial F}{\partial y}\Big|_{\boldsymbol{a}}.(y-b) + \dfrac{\partial F}{\partial z}\Big|_{\boldsymbol{a}}.(z-c) \\ \qquad\qquad + \quad |\boldsymbol{x}-\boldsymbol{a}|\rho_F(\boldsymbol{x}-\boldsymbol{a}), \\ G(\boldsymbol{x}) = \cancel{G(\boldsymbol{a})}^{\,0} + \dfrac{\partial G}{\partial x}\Big|_{\boldsymbol{a}}.(x-a) + \dfrac{\partial G}{\partial y}\Big|_{\boldsymbol{a}}.(y-b) + \dfrac{\partial G}{\partial z}\Big|_{\boldsymbol{a}}.(z-c) \\ \qquad\qquad + \quad |\boldsymbol{x}-\boldsymbol{a}|\rho_G(\boldsymbol{x}-\boldsymbol{a}), \end{cases}$$

where ρ_F and ρ_G are infinitesimal functions representing all higher order, nonlinear terms.

Selecting $\boldsymbol{x}$ now to be another, but otherwise arbitrary, point on both level surfaces and neglecting the higher order contributions compared to the linear terms for $|\Delta\boldsymbol{x}| = |\boldsymbol{x} - \boldsymbol{a}| \ll 1$, the nonlinear system of equations may be approximated by a system of linear approximations. Dropping the negligible terms involving the infinitesimal functions and rewriting to collect x and y terms on the left, the nonlinear system is approximated by the following linear system,

$$\begin{aligned} \frac{\partial F}{\partial x}\Big|_{\boldsymbol{a}}.(x-a) + \frac{\partial F}{\partial y}\Big|_{\boldsymbol{a}}.(y-b) &= -\frac{\partial F}{\partial z}\Big|_{\boldsymbol{a}}.(z-c) \\ \frac{\partial G}{\partial x}\Big|_{\boldsymbol{a}}.(x-a) + \frac{\partial G}{\partial y}\Big|_{\boldsymbol{a}}.(y-b) &= -\frac{\partial G}{\partial z}\Big|_{\boldsymbol{a}}.(z-c). \end{aligned}$$

These form a 2×2 matrix system:

$$\begin{pmatrix} \frac{\partial F}{\partial x}\Big|_{\boldsymbol{a}} & \frac{\partial F}{\partial y}\Big|_{\boldsymbol{a}} \\ \frac{\partial G}{\partial x}\Big|_{\boldsymbol{a}} & \frac{\partial G}{\partial y}\Big|_{\boldsymbol{a}} \end{pmatrix} \begin{pmatrix} (x-a) \\ \\ (y-b) \end{pmatrix} = \begin{pmatrix} -\frac{\partial F}{\partial z}\Big|_{\boldsymbol{a}}.(z-c) \\ -\frac{\partial G}{\partial z}\Big|_{\boldsymbol{a}}.(z-c) \end{pmatrix},$$

which can be solved for $(x-a)$ and $(y-b)$ in terms of $(z-c)$,

if and only if the determinant of the coefficient matrix,

$$\frac{\partial F}{\partial x}\Big|_{\boldsymbol{a}}.\frac{\partial G}{\partial y}\Big|_{\boldsymbol{a}} - \frac{\partial F}{\partial y}\Big|_{\boldsymbol{a}}.\frac{\partial G}{\partial x}\Big|_{\boldsymbol{a}} \neq 0.$$

This condition corresponds to the condition imposed in the second of our linear algebraic problems.

We digress briefly to introduce a handy notational definition based on the above *determinant of derivatives*. The notation is heavily utilized in the remaining pages of this section, but will also appear in later chapters in many related and also in some unrelated contexts (see Chapters 4 and 5 for more details). For the present, the very useful notation allows the many results to follow to be presented concisely.

Definition 2.9
The determinant of partial derivatives,

$$J(F,G)\big|_{\boldsymbol{a}} = \frac{\partial F}{\partial x}\Big|_{\boldsymbol{a}}.\frac{\partial G}{\partial y}\Big|_{\boldsymbol{a}} - \frac{\partial F}{\partial y}\Big|_{\boldsymbol{a}}.\frac{\partial G}{\partial x}\Big|_{\boldsymbol{a}} \equiv \frac{\partial(F,G)}{\partial(x,y)}\Big|_{\boldsymbol{a}},$$

is called the **Jacobian determinant** *of F and G with respect to variables x and y, evaluated at the point $\boldsymbol{a}$.*

Remarks

* For a 2×2 system the order in which the functions F and G *and* the variables x and y appear in the notation $\dfrac{\partial(F,G)}{\partial(x,y)}$ invariably determines which partial derivatives appear in the first term of the determinant; the second term, with a negative sign, has the partial derivatives switched. More generally speaking (see the next remark), the order of the terms, their signs and which partial derivatives appear are set by the standard determinant operation.

* The Jacobian determinant generalizes to higher dimensional systems of functions and variables. For example, the 3×3 system of functions F, G, H and variables x, y, z has Jacobian determinant:

$$\frac{\partial(F,G,H)}{\partial(x,y,z)} = \begin{vmatrix} \dfrac{\partial F}{\partial x} & \dfrac{\partial F}{\partial y} & \dfrac{\partial F}{\partial z} \\ \dfrac{\partial G}{\partial x} & \dfrac{\partial G}{\partial y} & \dfrac{\partial G}{\partial z} \\ \dfrac{\partial H}{\partial x} & \dfrac{\partial H}{\partial y} & \dfrac{\partial H}{\partial z} \end{vmatrix} \equiv \begin{vmatrix} \dfrac{\partial F}{\partial x} & \dfrac{\partial G}{\partial x} & \dfrac{\partial H}{\partial x} \\ \dfrac{\partial F}{\partial y} & \dfrac{\partial G}{\partial y} & \dfrac{\partial H}{\partial y} \\ \dfrac{\partial F}{\partial z} & \dfrac{\partial G}{\partial z} & \dfrac{\partial H}{\partial z} \end{vmatrix}.$$

* No absolute value signs are implied by the definition of the Jacobian determinant. Hence, $J(F,G)$ may be positive, negative or zero. In later applications where the absolute value of the Jacobian determinant is required, then absolute value signs will be introduced accordingly, as in $|J(F,G)|$, and the result will then be nonnegative.

Returning now to Problem 3, it can be readily verified that by inverting the coefficient matrix and using the Jacobian determinant definition multiple times, the variables x and y may be solved for in terms of the variable z. That is,

$$(x-a) = -\frac{\dfrac{\partial(F,G)}{\partial(z,y)}\Big|_{\boldsymbol{a}}}{\dfrac{\partial(F,G)}{\partial(x,y)}\Big|_{\boldsymbol{a}}}.(z-c), \qquad (y-b) = -\frac{\dfrac{\partial(F,G)}{\partial(x,z)}\Big|_{\boldsymbol{a}}}{\dfrac{\partial(F,G)}{\partial(x,y)}\Big|_{\boldsymbol{a}}}.(z-c),$$

for $\boldsymbol{x} = (x,y,z)$ in the neighborhood of $\boldsymbol{a} = (a,b,c)$, provided $\dfrac{\partial(F,G)}{\partial(x,y)}\Big|_{\boldsymbol{a}} \neq 0$.

Comparing these expressions with their linear counterparts in our linear, two-plane problem on Page 144 we recognize

$$\begin{cases} x-a &= m_1(z-c) \\ y-b &= m_2(z-c) \\ z-c &= z-c \end{cases}, \text{ with } m_1 = -\frac{\dfrac{\partial(F,G)}{\partial(z,y)}\Big|_{\boldsymbol{a}}}{\dfrac{\partial(F,G)}{\partial(x,y)}\Big|_{\boldsymbol{a}}}, \quad m_2 = -\frac{\dfrac{\partial(F,G)}{\partial(x,z)}\Big|_{\boldsymbol{a}}}{\dfrac{\partial(F,G)}{\partial(x,y)}\Big|_{\boldsymbol{a}}}$$

as equations representing the *tangent line* to the curve of intersection. The equations and the tangent line are well-defined provided $\left.\dfrac{\partial(F,G)}{\partial(x,y)}\right|_{\boldsymbol{a}} \neq 0$.

Whether the line is interpreted as a tangent line to the curve of intersection at the point $\boldsymbol{a} = (a,b,c)$, or as a linear approximation to the curve for points $\boldsymbol{x}$ near $\boldsymbol{a}$, it follows that provided m_1 and m_2 are finite, the curve of intersection representation in the form

$$x = f(z), \quad y = g(z), \quad z = z, \qquad \text{for } \boldsymbol{x} = (x,y,z) \text{ near } \boldsymbol{a} = (a,b,c). \tag{2.8}$$

is well defined for some implicit functions, $f(z)$ and $g(z)$, valid in a neighborhood of the point $\boldsymbol{a} = (a,b,c)$. Moreover, since the tangent line,

$$\begin{cases} x - a &= \left.\dfrac{\mathrm{d}f}{\mathrm{d}z}\right|_c .(z-c), \\ y - b &= \left.\dfrac{\mathrm{d}g}{\mathrm{d}z}\right|_c .(z-c), \\ z - c &= z - c, \end{cases}$$

is unique, by equating coefficients it follows that

$$\left.\frac{\mathrm{d}f}{\mathrm{d}z}\right|_c = -\frac{\left.\dfrac{\partial(F,G)}{\partial(z,y)}\right|_{\boldsymbol{a}}}{\left.\dfrac{\partial(F,G)}{\partial(x,y)}\right|_{\boldsymbol{a}}}, \qquad \left.\frac{\mathrm{d}g}{\mathrm{d}z}\right|_c = -\frac{\left.\dfrac{\partial(F,G)}{\partial(x,z)}\right|_{\boldsymbol{a}}}{\left.\dfrac{\partial(F,G)}{\partial(x,y)}\right|_{\boldsymbol{a}}}.$$

To summarize, the necessary conditions for the linear approximation equations to be valid and for the implicit functions f and g to exist are that

(1) *F and G be differentiable at $\boldsymbol{a} = (a,b,c)$;*

(2) *the Jacobian determinant $J = \dfrac{\partial(F,G)}{\partial(x,y)} \neq 0$ at (a,b,c).*

Condition (2) is the critical one to note; it involves *the determinant of the matrix of coefficients of the dependent variables*, here x and y. This is consistent with the preceding examples and is a general rule of thumb for establishing the existence of any implicit functions!

Example 2.23:

The surfaces, $F(x,y,z) = x^2 - y^2 - z^2 = -1$ and $G(x,y,z) = x^2 + 2y^2 + 3z^2 = 6$, intersect along a curve passing through the point $\boldsymbol{a} = (1,1,1)$. Determine the equation of the tangent line to this curve at $\boldsymbol{a}$.

Solution:

First, it is straightforward to confirm by substitution that $(1,1,1)$ is a point on both surfaces: $F(1,1,1) = 1-1-1 = -1$ and $G(1,1,1) = 1+2+3 = 6$. As both functions, F and G, are differentiable in $\mathbb{R}^3$, for any point $\boldsymbol{x}$ on the curve of intersection in the neighborhood of $\boldsymbol{a}$, it follows that,

$$\begin{aligned} \overset{-1}{\cancel{F(x,y,z)}} &= \overset{-1}{\cancel{F(1,1,1)}} + \boldsymbol{\nabla} F\big|_{\boldsymbol{a}} \cdot \big(\boldsymbol{x}-\boldsymbol{a}\big) + |\Delta\boldsymbol{x}|\rho_F(\Delta\boldsymbol{x}), \\ \underset{6}{\cancel{G(x,y,z)}} &= \underset{6}{\cancel{G(1,1,1)}} + \boldsymbol{\nabla} G\big|_{\boldsymbol{a}} \cdot \big(\boldsymbol{x}-\boldsymbol{a}\big) + |\Delta\boldsymbol{x}|\rho_G(\Delta\boldsymbol{x}), \end{aligned}$$

where

$$\boldsymbol{\nabla} F\big|_{\boldsymbol{a}} = (2x,-2y,-2z)\,\big|_{\boldsymbol{a}} = (2,-2,-2), \quad \boldsymbol{\nabla} G\big|_{\boldsymbol{a}} = (2x,4y,6z)\,\big|_{\boldsymbol{a}} = (2,4,6).$$

Then, to leading order, *i.e.*, neglecting the terms involving the infinitesimal functions compared to linear terms, the equations for F and G can be solved for x and y in terms of z to give the 2×2 system,

$$\begin{aligned} (2,-2,-2)\cdot(x-1,y-1,z-1) = 0 \quad &\Longrightarrow \quad x-y = z-1, \\ (2,4,6)\cdot(x-1,y-1,z-1) = 0 \quad &\Longrightarrow \quad x+2y = -3z+6, \end{aligned}$$

which in turn may be solved to obtain

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 4-z \\ 7-4z \\ 3z \end{pmatrix},$$

as the equation of the tangent line to the curve of intersection of $F=-1$ and $G=6$ at $(1,1,1)$. From this equation we can read off the derivatives, $\dfrac{\mathrm{d}f}{\mathrm{d}z}\Big|_{z=1} = -\dfrac{1}{3}$ and $\dfrac{\mathrm{d}g}{\mathrm{d}z}\Big|_{z=1} = -\dfrac{4}{3}$, whose finite values show that the curve of intersection may be represented in a neighborhood of the point $z=1$ by the well-defined equation set $\{x=f(z), y=g(z), z=z\}$.

As an aside, the principal problem in this exercise can also be solved by using gradient and level set properties, and the line equation.

The gradient $\boldsymbol{\nabla} F\big|_{\boldsymbol{a}}$ is orthogonal to the level set $F=-1$ at the point $\boldsymbol{a} = (1,1,1)$ and hence is orthogonal at $\boldsymbol{a}$ to every curve on $F=-1$ that passes through $\boldsymbol{a}$. Similarly, $\boldsymbol{\nabla} G\big|_{\boldsymbol{a}}$ is orthogonal to the level set $G=6$ at the point $\boldsymbol{a}$ and hence is orthogonal at $\boldsymbol{a}$ to every curve on that level set that passes through $\boldsymbol{a}$. On the other hand, the cross product

$$\boldsymbol{n} = \boldsymbol{\nabla} F\big|_{\boldsymbol{a}} \times \boldsymbol{\nabla} G\big|_{\boldsymbol{a}}$$

is a vector that is perpendicular to both gradient vectors (at that point) and hence must simultaneously be *parallel* to both level sets, $F=-1$ and

$G = 6$, (at that point). The vector $\boldsymbol{n}$ must therefore be *parallel to the curve of intersection at the point* $\boldsymbol{a} = (1, 1, 1)$!

From the definition of the vector cross product it is readily found that

$$\boldsymbol{n} = \boldsymbol{\nabla} F\big|_{\boldsymbol{a}} \times \boldsymbol{\nabla} G\big|_{\boldsymbol{a}} = (-4, -16, 12) = 4(-1, -4, 3).$$

With $\boldsymbol{n}$, the equation of the line tangent to the curve of intersection may be derived. To be specific, for any $\boldsymbol{x}$ on the tangent line (not on the curve of intersection itself) one has that $\boldsymbol{x} = \boldsymbol{a} + \boldsymbol{n}\, t$, where t is a scaling parameter:

$$\boldsymbol{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + 4 \begin{pmatrix} -1 \\ -4 \\ 3 \end{pmatrix} t = \quad \left\{ t = \frac{z-1}{12} \right\} \quad = \frac{1}{3} \begin{pmatrix} 4 - z \\ 7 - 4z \\ 3z \end{pmatrix},$$

in agreement with our earlier result.

■

In the next Mastery Check, we encounter a *fundamental property* of the Jacobian determinant (where it exists), namely its reciprocal property. The reader is likely familiar with the fact that in single-variable calculus, the ordinary derivative of a function of one variable, $y = f(x)$, satisfies the condition that

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \left(\frac{\mathrm{d}x}{\mathrm{d}y}\right)^{-1}, \qquad \text{provided } \frac{\mathrm{d}x}{\mathrm{d}y} \neq 0.$$

However, in multivariable calculus it is the *Jacobian* and *not* any individual partial derivative that exhibits this property.

Relaxing our stringent distinction between functions and variables, it is easily shown that if $u = f(x, y)$ and $v = g(x, y)$ and $x = h(u, v)$ and $y = k(u, v)$ then

$$\frac{\partial u}{\partial x} \neq \left(\frac{\partial x}{\partial u}\right)^{-1}, \qquad \left(i.e., \frac{\partial f}{\partial x} \neq \left(\frac{\partial h}{\partial u}\right)^{-1}\right).$$

Instead, in the following Mastery Check the reader will confirm (effectively) that

$$\frac{\partial(u, v)}{\partial(x, y)} = \left(\frac{\partial(x, y)}{\partial(u, v)}\right)^{-1}, \quad \text{provided } \frac{\partial(x, y)}{\partial(u, v)} \neq 0.$$

It will be discovered in later chapters that this property can be very useful when the route from one pair of variables to another, say $(x, y) \to (u, v)$, is more difficult or cumbersome to be made explicit than is the reverse route.

✍ Mastery Check 2.17:

Let $\begin{cases} F(x,y,z,w) &= x^2+y^3+xyz+wz=4, \\ G(x,y,z,w) &= w^2-z^2+x^2-y^2=0, \end{cases}$ and $(1,1,1,1)$ be a common point.

(a) Assume the two level set equations $F(x,y,z,w)=C_F$ and $G(x,y,z,w)=C_G$ define x and y as functions of z and w, where $x=f(z,w)$, $y=g(z,w)$. Derive a general expression for the Jacobian determinant $\dfrac{\partial(f,g)}{\partial(z,w)}$, in terms of the partial derivatives of arbitrary functions F and G.

(b) Evaluate the Jacobian for the above specific functions F and G at the point $(z,w)=(1,1)$.

(c) Assume now that the same two level set equations $F(x,y,z,w)=C_F$ and $G(x,y,z,w)=C_G$ define z and w as functions of x and y: $z=h(x,y)$, $w=k(x,y)$. Derive a general expression for the Jacobian determinant $\dfrac{\partial(h,k)}{\partial(x,y)}$, in terms of the partial derivatives of arbitrary functions F and G.

(d) Evaluate the Jacobian for the above specific functions F and G at the point $(x,y)=(1,1)$.

(e) Compare the general expressions for the Jacobian determinants from (a) and (c). In particular, determine the product $\dfrac{\partial(f,g)}{\partial(z,w)}\cdot\dfrac{\partial(h,k)}{\partial(x,y)}$. Confirm your answer using your results from (b) and (d).

✍

2.I Taylor's Formula and Taylor Series

On the one hand, the topic of Taylor series is but a natural if not prosaic extension of our earlier discussion on tangent plane approximations (Section 2.D). On the other hand, the subject of Taylor series and Taylor approximations is so incredibly useful in analysis and incredibly practical in computational applications that it is worth giving some consideration. The next chapter will highlight some examples of such applications. However, for the present we may consider this topic as a means of getting better approximations to functions, whether explicit or implicit. A convenient place to start is with the single-variable case.

The Taylor approximation for $F : \mathbb{R} \to \mathbb{R}$

Recall the properties of Taylor and Maclaurin polynomials for any single-variable function, $F : \mathbb{R} \to \mathbb{R}$: Let F possess a derivative of order $(n+1)$ in an open interval I containing a point t_0. Since, $F^{(n+1)}(t)$ exists, it follows that F and $F^{(k)}$, $k = 1, 2, \ldots, n$ exist and are continuous in I. Then the best polynomial approximation of order n to F for any t near $t_0 \in I$ is represented in the formula:

$$\begin{aligned} F(t) &= P_n(t) + E_{n+1}(t; t_0) \\ &= \left\{ F(t_0) + F'(t_0)(t-t_0) + \frac{F''(t_0)}{2}(t-t_0)^2 + \cdots \right. \\ &\qquad \left. + \frac{F^{(n)}(t_0)}{n!}(t-t_0)^n \right\} + E_{n+1}(t; t_0), \end{aligned}$$

where $P_n(t)$ is referred to as the *Taylor polynomial approximation* to F of order n, while

$$\begin{aligned} E_{n+1}(t; t_0) &= F(t) - P_n(t) \\ &= \frac{F^{(n+1)}(a)}{(n+1)!}(t-t_0)^{n+1}, \qquad a \in \big(\min(t_0, t), \max(t_0, t)\big) \end{aligned}$$

is called the *remainder*, being a measure of the difference between the true value of $F(t)$ and its approximation. The form for E_{n+1} quoted here is referred to as Lagrange's form (since other forms for the remainder have been defined).

Here are a few special cases of $P_n(t)$ for $n < \infty$:

(i) $P_1(t) = F(t_0) + F'(t_0)(t-t_0)$ — linear approximation

(ii) $P_2(t) = P_1(t) + \dfrac{F''(t_0)}{2}(t-t_0)^2$ — quadratic approximation

(iii) $P_3(t) = P_2(t) + \dfrac{F'''(t_0)}{3!}(t-t_0)^3$ — cubic approximation

(iv) $P_4(t) = P_3(t) + \dfrac{F^{(4)}(t_0)}{4!}(t-t_0)^4$ — quartic approximation

Remarks

* The existence of a linear approximation means there is a tangent line to $F(t)$ at $t = t_0$.

* A quadratic approximation is useful for critical-point analysis when $F'(t_0) = 0$, meaning that

$$F(t) - F(t_0) \approx \frac{F''(t_0)}{2}(t - t_0)^2 \quad \begin{matrix} > 0, & \text{— a minimum point} \\ < 0, & \text{— a maximum point.} \end{matrix}$$

* A cubic approximation means that there is a cubic curve osculating $F(t)$ at $x = t_0$. (What is that?)

* A quartic approximation may be useful in the uncommon cases when $F'(t_0) = F''(t_0) = F'''(t) = 0$, meaning that

$$F(t) - F(t_0) \approx \frac{F^{(4)}(t_0)}{4!}(t - t_0)^4 \quad \begin{matrix} > 0, & \text{— a minimum point} \\ < 0, & \text{— a maximum point.} \end{matrix}$$

Some functions have derivatives of all orders. Therefore, we can consider extending n without limit, $n \to \infty$. The above polynomial is then replaced by an infinite power series, provided it converges (absolutely) in some interval. Functions that can be differentiated an indefinite number of times and whose interval of convergence is the whole real line, for example, $\sin t$, $\cos t$, e^t, are called *analytic*.

The *Taylor series* representation of an analytic function $F(t)$ is defined as follows:

Definition 2.10
If there exists a $t_0 \in \mathbb{R}$ *and an* $R > 0$ *such that* $F(t) = \sum_{k=0}^{\infty} a_k (t - t_0)^k$ *converges for* $|t - t_0| < R$, *then this is the Taylor series of* F, *and* $a_k = \dfrac{F^{(k)}(t_0)}{k!}\ \forall k$.

What is especially important for the discussion to follow is the particular choice $t_0 = 0$. For this choice we have the well-known *Maclaurin polynomial*.

To be precise, if a single-variable continuous function $F : \mathbb{R} \to \mathbb{R}$ has a derivative of order $(n+1)$ in an open interval I containing $t = 0$, then F can be approximated by the Maclaurin polynomial,

$$F(t) = F(0) + F'(0)t + \frac{1}{2!}F''(0)t^2 + \cdots + \frac{1}{n!}F^{(n)}(0)t^n + R_{n+1}(\theta, t) \quad (2.9)$$

for all t in the interval I, and with (Lagrange) remainder,

$$R_{n+1}(\theta, t) = \frac{t^{n+1}}{(n+1)!} F^{(n+1)}(\theta t), \quad \text{for some } \theta \in (0, 1).$$

If F possesses derivatives of all orders at $t = 0$, then from Definition 2.10 we can define, in complete correspondence with the Taylor series, the *Maclaurin series* representation of F:

$$F(t) = \sum_{k=0}^{\infty} a_k t^k \text{ for } t \in I, \text{ with } 0 \in I, \text{ and } a_k = \frac{F^{(k)}(0)}{k!} \ \forall k.$$

For example, it is easy to verify by repeated differentiation and substitution that the Maclaurin series for the sine function is

$$\sin t = \sum_{k=0}^{\infty} \frac{(-1)^{k+1}}{(2k+1)!} t^{2k+1}.$$

The Taylor approximation for $f : \mathbb{R}^n \to \mathbb{R}$

From the single-variable case versions of Taylor and Maclaurin polynomials (and series) can be derived for functions of several variables. For the convenience of writing, the development below focuses on a function of two variables, $f(x, y)$. However, the derivation and discussion may easily be extended to functions of more variables.

The strategy that is followed begins with the construction of a particular function of one variable, $F(t)$, from a given function of two variables. From that construction one examines the value of $F(t)$ at $t = 1$.

Let f be a continuous function of two variables, $f : \mathbb{R}^2 \to \mathbb{R}$, and have continuous partial derivatives up to and including order n in a neighborhood $S_r(x_0, y_0) \subset D_f$ of a point (x_0, y_0). Moreover suppose f possesses $(n+1)$th order partial derivatives in the neighborhood of (x_0, y_0). Fix point (x, y) in $S_r(x_0, y_0)$ and define the single-valued function, $F(t)$, by

$$F(t) = f(x_0 + th, y_0 + tk), \qquad \text{for} \quad t \in [0, 1],$$

where, $h = x - x_0$ and $k = y - y_0$. Clearly then, at $t = 0$, $F(0) = f(x_0, y_0)$, while at $t = 1$, $F(1) = f(x_0 + h, y_0 + k) = f(x, y)$.

Since f has continuous partial derivatives up to and including order n, it follows that the single-variable function, $F(t)$, will have continuous (ordinary) derivatives of order up to and including n. In fact, by means of the multivariable chain rule the derivatives of F with respect to t, evaluated at $t = 0$, can be derived:

$$F(0) = f(x_0, y_0), \qquad F'(0) = \left(\left.\frac{\partial f}{\partial x}\right|_{(x_0,y_0)} h + \left.\frac{\partial f}{\partial y}\right|_{(x_0,y_0)} k \right),$$

$$F''(0) = \left(\left.\frac{\partial^2 f}{\partial x^2}\right|_{(x_0,y_0)} h^2 + 2\left.\frac{\partial^2 f}{\partial x \partial y}\right|_{(x_0,y_0)} hk + \left.\frac{\partial^2 f}{\partial y^2}\right|_{(x_0,y_0)} k^2 \right), \quad \text{etc.}.$$

Inserting these and higher order derivatives into the Maclaurin polynomial for $F(t)$, Eq (2.9), evaluated at $t = 1$, gives the *Taylor polynomial approximation to* $f(x, y)$ valid for (x, y) in a neighborhood of $(x_0, y_0) \in D_f$:

$$\begin{aligned} F(1) &= F(0) + F'(0) + \frac{1}{2!}F''(0) + \cdots + \frac{1}{n!}F^{(n)}(0) + R_{n+1}(\theta, 1) \\ &= f(x_0 + h, y_0 + k) \\ &= f(x_0, y_0) + \left.\frac{\partial f}{\partial x}\right|_0 h + \left.\frac{\partial f}{\partial y}\right|_0 k \\ &\quad + \frac{1}{2}\left(\left.\frac{\partial^2 f}{\partial x^2}\right|_0 h^2 + 2\left.\frac{\partial^2 f}{\partial x \partial y}\right|_0 hk + \left.\frac{\partial^2 f}{\partial y^2}\right|_0 k^2 \right) + \cdots \\ &\quad + \sum_{j=0}^{n} \frac{1}{j!(n-j)!} \left.\frac{\partial^n f}{\partial x^j \partial y^{n-j}}\right|_0 h^j k^{n-j} + R_{n+1}(\theta, 1), \end{aligned} \tag{2.10}$$

where the remainder $R_{n+1}(\theta, 1)$ stems directly from the (Lagrange) remainder valid for the Maclaurin polynomial approximation of a function of one variable. We note that based on its form as a sum of terms involving the $(n+1)$ partial derivatives of f (similar to the last term quoted in the polynomial approximation), the remainder, R_{n+1}, will be of the order $o\left(\left(\sqrt{h^2 + k^2}\right)^{n+1}\right)$.

Alternative derivation:
Suppose we can approximate $f(x, y)$ in a neighbourhood $S_r(x_0, y_0)$ of (x_0, y_0) by a general polynomial:

$$\begin{aligned} f(x, y) &= a_{00} + a_{10}(x - x_0) + a_{01}(y - y_0) \\ &\quad + a_{20}(x - x_0)^2 + a_{11}(x - x_0)(y - y_0) + a_{02}(y - y_0)^2 + \cdots \\ &\quad + a_{n0}(x - x_0)^n + \cdots + a_{0n}(y - y_0)^n + E_{n+1}(\boldsymbol{x}_0). \end{aligned}$$

(Approximation error will depend on $\boldsymbol{x}_0$ and n.)

If f is differentiable to order n, then taking partial derivatives of both sides and evaluating these results at (x_0, y_0) we identify

$$\left.\frac{\partial f}{\partial x}\right|_0 = a_{10} \qquad \left.\frac{\partial f}{\partial y}\right|_0 = a_{01}$$

$$\left.\frac{\partial^2 f}{\partial x^2}\right|_0 = 2a_{20} \qquad \left.\frac{\partial^2 f}{\partial y^2}\right|_0 = 2a_{02} \qquad \left.\frac{\partial^2 f}{\partial x \partial y}\right|_0 = a_{11} = \left.\frac{\partial^2 f}{\partial y \partial x}\right|_0$$

$$\text{and generally} \quad \left.\frac{\partial^{k+\ell} f}{\partial x^k \partial y^\ell}\right|_0 = k!\ell! a_{k\ell}.$$

Substitution will again give Eq (2.10).

We shall postpone until the next chapter a discussion and demonstration of the usefulness of Taylor approximations. For the present we provide a few appropriate remarks.

Remarks

* With the trivial step of setting $x_0 = y_0 = 0$ we get the 2D version of a Maclaurin polynomial approximation of order n.

* As in the single-variable case, if our multivariable function has partial derivatives of all orders, then the Taylor polynomial approximations of our $f(x, y)$ can be developed into a full Taylor series representation — provided it converges, of course.

* The Taylor polynomial and Taylor series for a function $f(x, y)$ developed about a specific point (x_0, y_0) is unique.

* A function of the form of a finite double sum $f(x, y) = \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij} x^i y^j$ is its own Maclaurin polynomial approximation (about the point $(0, 0)$).

* If we need the Taylor polynomial approximation to a function of the form of a finite double sum $f(x, y) = \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij} x^i y^j$, developed about some other point (x_0, y_0) then we could use algebra alone to reexpress $f(x, y)$ in the form $f(x, y) = \sum_{k=1}^{n} \sum_{l=1}^{m} b_{kl} (x - x_0)^k (y - y_0)^l$ (if simple enough).

* For some suitable composite multivariable functions, we can utilize known Taylor polynomials or Taylor series of (outer) functions of one variable as starting points.

* In Section 2.H we dealt with implicit functions and showed how one can calculate first derivatives of such functions even though the functions themselves could not be expressed explicitly. Now, with assistance from the Taylor and Maclaurin expansions, one can construct explicit polynomial or even full series representations of implicit functions by successively differentiating these first-order derivatives (with the help of the chain rule — Section 2.G). The following Mastery Check exercise explores this possibility.

We end this section with an Example, a Mastery Check involving Taylor polynomials and a final comment.

Example 2.24:

Determine Taylor's polynomial of order 2 to the function, $f(x, y) = \ln(2x^2 + y^2) - 2y$, about the point $(0, 1)$ and use the polynomial to determine an approximation to $f(0.1, 1.2)$.

Solution:

This exercise involves the straightforward procedure of differentiating and evaluating. We have firstly the partial derivatives at an arbitrary point:

$$\begin{aligned}
\frac{\partial f}{\partial x} &= \frac{1}{2x^2+y^2}.4x, \quad \frac{\partial f}{\partial y} = \frac{1}{2x^2+y^2}.2y - 2, \\
\frac{\partial^2 f}{\partial x^2} &= \frac{4}{2x^2+y^2} + 4x.\left(\frac{-1}{(2x^2+y^2)^2}.4x\right) = \frac{4(y^2-2x^2)}{(2x^2+y^2)^2}, \\
\frac{\partial^2 f}{\partial y \partial x} &= \frac{-4x}{(2x^2+y^2)^2}.2y = \frac{-8xy}{(2x^2+y^2)^2} = \frac{\partial^2 f}{\partial x \partial y}, \\
\frac{\partial^2 f}{\partial y^2} &= \frac{2}{2x^2+y^2} + \frac{2y}{(2x^2+y^2)^2}.(-2y) = \frac{4x^2-2y^2}{(2x^2+y^2)^2}.
\end{aligned}$$

These are then evaluated at the point $(x, y) = (0, 1)$:

$$f(0,1) = -2, \quad \frac{\partial f}{\partial x}\Big|_{(0,1)} = 0, \quad \frac{\partial f}{\partial y}\Big|_{(0,1)} = 0,$$

$$\frac{\partial^2 f}{\partial x^2}\Big|_{(0,1)} = 4, \quad \frac{\partial^2 f}{\partial x \partial y}\Big|_{(0,1)} = 0, \quad \frac{\partial^2 f}{\partial y^2}\Big|_{(0,1)} = -2,$$

and the values inserted into the formula for the Taylor polynomial of order 2:

$$f(0+h, 1+k) \approx -2 + 0 + 0 + \frac{1}{2}\left(4h^2 + 0 + (-2)k^2\right) = -2 + 2h^2 - k^2.$$

Choosing $h = 0.1$ and $k = 0.2$, we can get an estimate for $f(0.1, 1.2)$:

$$f(0.1, 1.2) \approx -2 + 2(0.01) - (0.04) = -2.02.$$

Note: A first-order (*i.e.*, linear) approximation would give $f(0.1, 1.2) \approx f(0, 1) = -2$.

■

Mastery Check 2.18:

Determine the Taylor polynomial of order 2 about the point $(0, 0)$ to the implicit function $z = f(x, y)$ defined by the equation

$$e^{x+y+z} - (x + y + z)^2 - 1 = 0.$$

Hint: see Section 2.H Problem 2.

The reader will have noted that the first order Taylor polynomial approximation to a function $f(x, y)$ in Equation (2.10), for domain points (x, y) in the vicinity of point (x_0, y_0), is none other than the tangent plane approximation to f. Including higher order terms, in particular the second order terms, improves on the linear approximation by adding crucial curvature information about the surface near the point $(x_0, y_0, f(x_0, y_0))$. We shall demonstrate in the next chapter just how useful these terms can be.

More generally, however, the Taylor (and Maclaurin) polynomial approximations and series representations play important roles in other applications such as the development of approximations and representations of implicit functions (as demonstrated by Mastery Check 2.18), the numerical solution of differential equations and the evaluation of multiple integrals (Chapter 4), as well as aiding in the development of theoretical analyses in more abstract settings. We shall not take up or demonstrate such applications in this book. The reader may review [15, 16] for discussions on the first two of these applications.

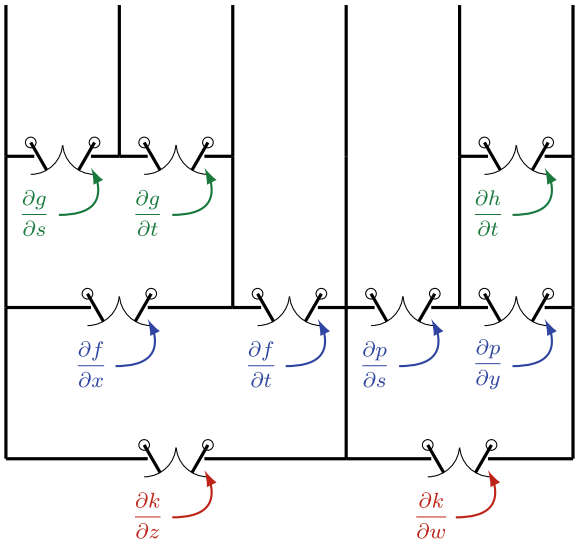


Figure 2.47 The floodgate diagram for partial derivatives of the composite function $F(s, t)$ in supplementary problem 23.

2.J Supplementary Problems

§2.B.1. Determine whether the following functions are continuous at $(0,0)$?

(a) $f(x,y) = \dfrac{xy}{x^2+y^2}$, $f(0,0) = 0$. (b) $f(x,y) = \dfrac{xy}{\sqrt{x^2+y^2}}$, $f(0,0) = 0$.

2. Establish whether the limits of the following functions exist at $(x,y) = (0,0)$, and if so determine their values.

(a) $f(x,y) = \dfrac{\tan(xy)}{x^2+y^2}$. (b) $f(x,y) = \dfrac{x^2-x}{y^2-y}$.

(c) $f(x,y) = \dfrac{x^4+y\sin(x^3)}{x^4+y^4+x^2y^2}$. (d) $f(x,y) = \dfrac{x^2\sin y}{x^2+y^2}$.

*3. Use the limit definition to show that

(a) $\lim_{(x,y)\to(1,1)} \left(x + \dfrac{1}{y}\right) = 2$. (b) $\lim_{(x,y)\to(1,2)} \left(x^2+2y\right) = 5$.

(c) $\lim_{(x,y)\to(0,0)} \left(\dfrac{\cos(2xy)}{1+x^2+y^2}\right) = 1$.

Repeat these limit calculations using the limit laws, where these are applicable.

§2.C.4. Determine all first partial derivatives of the following functions:

(a) $f(x,y) = \arctan(y/x)$. (b) $f(x,y) = \arctan(x^2+xy+y^2)$.

(c) $f(x,y) = \left(x^2y^3+1\right)^3$. (d) $f(x,y,z) = x^2\sqrt{y^2+xz}$.

(e) $f(x,y) = \exp\left(x^2\sin^2 y + 2xy\sin x\sin y + y^2\right)$.

(f) $f(x_1,x_2,x_3) = \ln|x_1x_2 + x_2x_3 + x_1x_3|$.

§2.D.5. Consider the function $f:\mathbb{R}^2\to\mathbb{R}$, $f(x,y) = \dfrac{x^2}{x^2+y^2}$, for $x,y\neq 0$, $f(0,y) = 0$, $f(x,0) = 1$. Establish whether or not f is differentiable at points along the y-axis and determine the first partial derivatives of f along this line if they exist.

6. Consider the function

$$f(x,y) = \frac{x^2y + \cos(xy)}{x^2+y^2}.$$

(a) Determine the domain and range of f.

(b) Using a first principles approach based on Definition 2.4 show that f is differentiable at $\boldsymbol{a} = (2,0)$.

(c) Determine the equation of the tangent plane and the normal to the surface $z = f(x, y)$ at $(2, 0, 1/4)$.

§2.E.7. Consider the function $f(x, y, z) = xz^3 + yx^3$. What is the directional derivative at the point $(2, 1, -1)$ in the direction $\boldsymbol{u} = 2\mathbf{e}_1 + \mathbf{e}_2 + 2\mathbf{e}_3$?

8. Consider the surface $xy^3z^2 = 8$. What is the unit normal to this surface at the point $(1, 2, -1)$?

9. Calculate the directional derivative of $f(x, y, z) = xy + \mathrm{e}^{yz} + z$ at the point $(1, 1, 0)$ in the direction $\boldsymbol{u} = (\alpha, \beta, \gamma)$, where $\alpha^2 + \beta^2 + \gamma^2 = 1$. When you have found your directional derivative, answer this question: How should α, β, γ be chosen so that this derivative should be maximal?

10. The air temperature (in degrees Celsius) at height z above the point $(x, y, 0)$ on the Earth surface is given by the function

$$T(x, y, z) = z \sin\left(\frac{\pi}{2}(x^2y + z^2)\right) \mathrm{e}^{-\left((x^2+y^2+1)z\right)}$$

Suppose P is the point $(1, 1, 1)$.

(a) Determine the temperature gradient vector at P.

(b) Determine the linear approximation and hence the tangent plane to T at P?

(c) A bee flies toward P with speed 0.5 $\mathrm{m.s}^{-1}$ in a straight line from the point $Q = (2, -1, 2)$. What rate of change of temperature does the bee experience upon reaching P?

(d) What direction should the bee fly emerging from P in order to experience the greatest rate of *increase* of temperature?

*11. Determine the points on the flattened ellipsoid

$$x^2 + 13y^2 + 7z^2 - 6\sqrt{3}zy = 16$$

where the tangent plane is parallel to one of the coordinate planes.

12. Determine all points on the surface

$$x^2 + 2y^2 + 3z^2 + 2xy + 2yz = 1$$

where the tangent plane is parallel to the plane $x + y + z = 0$.

§2.F.13. Find the first and second partial derivatives of the following functions:

(a) $f(x, y) = \big(\sin xy\big)^2$.

(b) $f(x, y) = \sin(xy)^2$.

(c) $f(x, y) = \ln\big(x^2 + 2y\big)$.

(d) $f(x, y) = \sqrt{1 + x^2 + y^3}$.

14. Suppose $f : \mathbb{R}^2 \to \mathbb{R}$ is a C^3 harmonic function of variables (x, y). That is, suppose f satisfies the 2D Laplace equation,

$$\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0$$

(see Section 3.E for more information on this topic). Show that the function $g = x\dfrac{\partial f}{\partial x} + y\dfrac{\partial f}{\partial y}$ is also a solution.

§2.G.15. Consider the functions $f : x \mapsto y = f(x)$, and $g : t \mapsto x = g(t)$.
In each example find the domain D_F of the composite function $F : t \mapsto y = \big(f \circ g\big)(t)$, and the derivative $\dfrac{\mathrm{d}F}{\mathrm{d}t}$.

(a) $f(x) = \dfrac{x^2}{1+x^2}$, $g(t) = \sinh t$. (b) $f(x) = \arcsin x^2$, $g(t) = 3\mathrm{e}^{-t}$.

(If possible, do this example in two ways: by determining $F(t)$ explicitly then differentiating, and by using the chain rule.)

16. Consider the functions $f : x \mapsto y = f(x)$, and $g : (s, t) \mapsto x = g(s, t)$.
In each example that follows, find the domain D_F of the composite function $F : (s, t) \mapsto y = \big(f \circ g\big)(s, t)$, and the derivatives $\dfrac{\partial F}{\partial s}$, $\dfrac{\partial F}{\partial t}$.

(a) $f(x) = \ln x$, $g(s, t) = s(1 - t^2)$.

(b) $f(x) = \arccos(x)$, $g(s, t) = \sqrt{s^2 - t^2}$.

17. Consider the function $z = f(x, y) = \mathrm{e}^{x^2 y} + xy$, and the composite function $z = F(t) = f(\cos t, \sin t)$. Determine where $F(t)$ makes sense and compute $\dfrac{\mathrm{d}F}{\mathrm{d}t}$.

18. Consider the function $z = f(x, y) = \arcsin xy$, where $x = s - 2t$ and $y = \dfrac{s}{t^2}$.
What is the domain of the composite function $z = F(s, t)$? Compute $\dfrac{\partial F}{\partial s}$ and $\dfrac{\partial F}{\partial t}$.

19. By introducing new variables $u = x^2 - y$ and $v = x + y^2$ transform the differential equation

$$(1 - 2y)\frac{\partial f}{\partial x} + (1 + 2x)\frac{\partial f}{\partial y} = 0.$$

20. Suppose $f : \mathbb{R}^2 \to \mathbb{R}$ is a C^2 function of variables (x, y). By introducing the change of variables $x = 2s + 3t$ and $y = 4s - 4t$ we define the C^2 function $F(s, t)$ from $f(x, y)$. Show that

$$\frac{\partial^2 F}{\partial t^2} = 9\frac{\partial^2 f}{\partial x^2} - 24\frac{\partial^2 f}{\partial y \partial x} + 16\frac{\partial^2 f}{\partial y^2}.$$

21. Use the Leibniz integral rule to determine the two first partial derivatives of the integral function

$$F(x, y) = \int_{y/x}^{\pi/2} \sin(xu) \exp\left(-(x^2 + y^2)u\right) \, \mathrm{d}u, \quad x \neq 0.$$

Then, determine the second order mixed partial derivative $\dfrac{\partial^2 F}{\partial x \partial y}$. (Aside: consider the alternative of first evaluating the integral w.r.t u, then taking derivatives. You may need to employ complex analysis methods.)

22. Suppose $f : \mathbb{R}^2 \to \mathbb{R}$ is a C^2 function of variables (x, y), by introducing the new variables $s = x^2 + y$ and $t = 2x$ transform the expression

$$\frac{\partial^2 f}{\partial x^2} + 2\frac{\partial^2 f}{\partial y \partial x} + \frac{\partial^2 f}{\partial y^2}$$

into a form involving a function $F(s, t)$.

23. *How well do you understand the floodgate model?*
Let F be a C^1 composite function of the variables s and t and assume its first derivatives can be described by the floodgate model shown in Figure 2.47. Sketch the branch diagram of F. Derive expressions for $\dfrac{\partial F}{\partial s}$ and $\dfrac{\partial F}{\partial t}$, and finally for $\dfrac{\partial^2 F}{\partial t \partial s}$.

§2.H.24. Establish whether the equation $f(x, y, z) = x^3 e^{y+z} - y \sin(x - z) = 0$ defines z implicitly as a function of x and y. If so, find $\dfrac{\partial z}{\partial x}$ and $\dfrac{\partial z}{\partial y}$ and provide their respective domains of definition.

25. Suppose the equation $z^3 + z(y^2 + 1) + x^3 - 3x + y^2 - 8 = 0$ defines z as a function f of x, y in the neighbourhood of the point $(2, -1, -1)$. Find the derivatives of $\dfrac{\partial f}{\partial x}$ and $\dfrac{\partial f}{\partial y}$ at this point.

*26. The equations $z\left(1 + x^2\right) + y^2 \ln|z| = 1$ and $u = xz + ye^z$ define a function $u = f(x, y)$ with continuous derivatives of order 1. Evaluate

$$\frac{\partial u}{\partial x}(0, 1) \quad \text{and} \quad \frac{\partial u}{\partial y}(0, 1).$$

*27. The C^2 function

$$F(x,y,z,w) = \frac{\pi^2 e^w \sin(\pi z)}{\sqrt{x^2+\pi^2}} + (2yz-1)^2 + w = \pi$$

defines w as the implicit function, $w = f(x,y,z)$. Determine values z_0 and w_0 that satisfy the level set equation $F(0,1,z_0,w_0) = \pi$. What is the maximum slope of the implicit function f at the point $(0,1,z_0)$ and in what direction, $\boldsymbol{u} = (\alpha,\beta,\gamma)$, is that slope found?

*28. (a) Assuming that $F(x,y,z) = 0$ defines z implicitly as a function of x and y, *i.e.* $z = f(x,y)$, derive the second order partial derivative, $\dfrac{\partial^2 f}{\partial y^2}$, in terms of derivatives of F.

(b) Show that the equation $x^2 + y^2 + z^2 + \sin z = 0$, defines $z = f(x,y)$ in the neighborhood of the point (0,0,0) and determine whether f has a local maximum or a local minimum at $(0,0)$.

*29. (a) Assuming that $F(x,y,z) = 0$ defines z implicitly as a function of x and y, *i.e.* $z = f(x,y)$, derive the mixed partial derivative, $\dfrac{\partial^2 f}{\partial x \partial y}$, in terms of derivatives of F.

(b) Show that the equation $\left(1 + x^2 + y^2\right) z^3 + z\mathrm{e}^{(x^2+y^2)} = 2$, defines z as a function $f(x,y)$, for all $(x,y) \in \mathbb{R}^2$, and determine if f has a local maximum or a local minimum at $(0,0)$.

*30. Consider the following system of equations.

$$\begin{aligned} F(x,y,z,u) &= x^2 + yx + z^3 - uxy = 5, \\ G(x,y,z,u) &= u^2 - xz - 3x^3y^2 = 0, \\ H(x,y,z,u) &= xuz + yz = -1. \end{aligned}$$

(a) Establish whether the equations define x, y, and z as functions of u at the 3D point $(x,y,z) = (1,1,1)$.

(b) Evaluate $\dfrac{\mathrm{d}x}{\mathrm{d}u}$, $\dfrac{\mathrm{d}y}{\mathrm{d}u}$, and $\dfrac{\mathrm{d}z}{\mathrm{d}u}$.

(c) Determine the equation of the plane that is orthogonal to this function and that passes through the point $(1,1,1)$.

*31. (a) Show that the equations

$$\begin{aligned} 2x + y + 2z + u - v &= 1, \\ xy + z - u + 2v &= 1, \\ yz + xz + u^2 + v &= 0, \end{aligned}$$

define x, y, and z as functions of u and v in the neighborhood of $(1,1,-1,1,1)$.

(b) Find the matrix of derivatives of the vector-valued function, $\boldsymbol{r} = \boldsymbol{F}(u, v)$ at $\boldsymbol{u}_0 = (1, 1)$.

(c) The vector-valued function describes a surface in 3D. Determine the equation of the tangent plane to this surface at $\boldsymbol{r}_0 = (1, 1, -1)$.

§2.I.32. Find the Taylor polynomial approximations of order 1, 2, ..., to the function $F(t) = \cos(t^{3/2})$ about the point $t = t_0 = 0$. Use a suitable low-order approximation to determine whether $t = 0$ is a maximum or minimum point of $F(t)$.

33. If a function may be approximated by a convergent Taylor series whose terms are alternating in sign, then the absolute value of the error term at finite n is bounded by the absolute value of the first omitted term in a finite polynomial approximation. Use this idea to decide how many terms are needed to find $\sin 3^\circ$ to ten decimal places.

34. Write down the Taylor series for $\cos t$ about $t_0 = \pi/3$, and use it to compute $\cos 55^\circ$ to seven decimal places. (First establish how many terms are needed.)

35. Write down all the terms up to order $n = 3$ in the Taylor series for $f(x, y) = \sin(x + y) + x^2$ about $(x_0, y_0) = (0, \pi/6)$.

*36. The function $z = f(x, y)$ satisfies $f(1, 1) = 0$ and $\mathrm{e}^{xz} + x^2y^3 + z = 2$. Establish that $z = f(x, y)$ indeed exists in a region near $(1, 1)$ and determine its Taylor series approximation up to order 2 valid near that point.

37. Determine the Taylor polynomial approximation up to and including second-order terms of $F(x, y) = \displaystyle\int_0^y \ln(1 + x + t)\mathrm{d}t$ about the point $(0, 0)$. Note that we assume $x + y > -1$.



Chapter 3

Applications of the Differential Calculus

The differential calculus of multivariable functions covered in the preceding chapter is applied in this chapter to problems arising in four contexts: finding function maxima and minima, analyzing numerical approximation errors, constructing function approximations, and solving partial differential equations. Although applications arise in other areas these are among the more common topics. Also, although all four are covered from a theoretical perspective, the emphasis of the supplementary problems, at least, is placed on the first and fourth topics.

3.A Extreme Values of $f : \mathbb{R}^n \longrightarrow \mathbb{R}$

Many applications of differential calculus fall under the banner of *optimization*. In essence, the objective of mathematical optimization is to determine those points in the domain of a scalar function, $f(\boldsymbol{x})$, that give rise to maximum or minimum values, so-called *extreme values* of $f(\boldsymbol{x})$. The points where these extreme values occur are appropriately called *extreme points*. There are three types of extreme points, which will be considered here. The first type, discussed in this section, are the so-called *critical points*, which are determined directly with the help of the differential calculus. The second and third types, taken up in the next section, are the so-called *singular points* and *boundary points* which are not directly accessible using derivative means.

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Identifying the critical points of a function is an important first step in optimization. However, equally important is the second, characterization step. That is, once *identified* these points need to be *characterized* according to whether they give rise to maximum values or minimum values of the function being considered, or possibly neither. Tackling these tasks successfully, which will require the use of mathematical tools from the previous chapter, can be assisted if one knows what to look for. Naturally, as with most things in mathematics, the task becomes easier when the type of points we seek can be defined within a concrete framework of fundamental principles.

Definition 3.1
Let $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ *be a continuous function.*
A point $\boldsymbol{a} \in D_f$ *is called a* **local**
(i) **minimum point** *if* $f(\boldsymbol{x}) \geq f(\boldsymbol{a}),\ \forall \boldsymbol{x} \in S_r(\boldsymbol{a}) \subset D_f,$
(ii) **maximum point** *if* $f(\boldsymbol{x}) \leq f(\boldsymbol{a}),\ \forall \boldsymbol{x} \in S_r(\boldsymbol{a}) \subset D_f.$

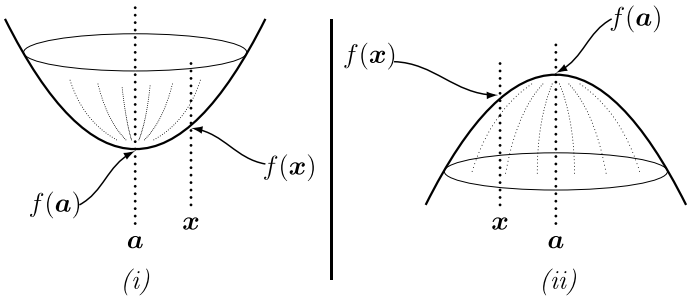


Figure 3.1 A function minimum and maximum.

One reason for invoking the open sphere, $S_r(\boldsymbol{a})$, in this definition, to represent the set of points $\boldsymbol{x}$ different from but near to the centre point $\boldsymbol{a}$ (with a radius $0 < r \ll 1$), is to emphasize the fact that *only* so-called *local* properties of f are of interest. This will be contrasted with so-called *global* properties to be discussed in the next section. Local minimum points (Figure 3.1(i)) and local maximum points (Figure 3.1(ii)) are examples of *critical points* which we now define.

Definition 3.2
A **critical point** *of a* C^1*-class, scalar function* $f(\boldsymbol{x})$ *is an interior point* $\boldsymbol{a}$ *in the domain* D_f *at which* $\boldsymbol{\nabla} f\Big|_{\boldsymbol{a}} = \boldsymbol{0}$.

While a point $\boldsymbol{a}$ that is a local maximum point or a local minimum point must satisfy the condition that $\boldsymbol{\nabla} f(\boldsymbol{a}) = \boldsymbol{0}$, the converse is not necessarily

true. That is, it is *not* assured that a critical point, for which $\boldsymbol{\nabla} f = \mathbf{0}$, will be either a point of local maximum or a point of local minimum; there is a third alternative.

Definition 3.3
A critical point which is neither a maximum nor a minimum is called a **saddle point**.

Figures 3.1(i) and (ii) in Definition 3.1 suggest that in the case of either a local minimum (left-hand figure) or a local maximum (right-hand figure) at $\boldsymbol{x} = \boldsymbol{a}$, the condition $\boldsymbol{\nabla} f = 0$ is tantamount to saying that the tangent plane is horizontal. Mathematically speaking, for the vector gradient of f to be zero, each of its contributing partial derivatives $(\partial f/\partial x, \partial f/\partial y, \ldots)$ must be zero at $\boldsymbol{a}$. But this implies that the slopes of the n-independent tangent lines in the n orthogonal directions in the function's domain, must be zero at that point. However, since all of these n tangent lines lie in the same plane, the tangent plane itself must have zero slope in every direction and hence be horizontal. As this geometric description is valid for any critical point, even a saddle point, saddle points too must then be characterized by horizontal tangent planes, even though neither of the figures in Definition 3.1 apply. Instead, around a saddle point a part of the function's graph lies below the tangent plane and a part lies above. An example of the graph of a function around a saddle point is shown in Figure 3.2.

The next two simple examples convey the ideas in Definitions 3.1-3.3.

Example 3.1:

Identify and characterize the critical points of $f(x, y) = x^2 + y^2 - 2x$.

Solution:

As suggested, the first step involves identifying the location of any critical points. To do this the gradient is determined and set to zero:

$$\boldsymbol{\nabla} f \;=\; \begin{pmatrix} 2x - 2 \\ 2y \end{pmatrix} \;=\; \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \Longrightarrow \quad (x, y) = (1, 0).$$

The two component equations, solved simultaneosly, identify only one critical point. The next step is to examine f in the neighbourhood of this critical point $(1, 0)$. Introducing small magnitude scalars, h and k, we consider the function's value at an arbitrary neighbouring point, $(1 + h, 0 + k)$, in the domain of f $(D_f = \mathbb{R}^2)$. We have

$$f(1 + h, 0 + k) \;=\; (1 + h)^2 + k^2 - 2(1 + h) \;=\; h^2 + k^2 - 1,$$

whereas $f(1,0) = 1+0-2 = -1$. Consequently, we confirm that $f(1+h,0+k) > f(1,0)$ for all $h,k \neq 0$, since

$$f(1+h,0+k) - f(1,0) = h^2 + k^2 > 0.$$

As this is true for all (h,k), *i.e.*, for all (x,y) in the neighbourhood of $(1,0)$, then according to Definition 3.1, the point $(1,0)$ is a minimum point. ■

■ Example 3.2:

Identify and characterize the critical points of $f(x,y) = 1 + x^2 - y^2$.

Solution:

Consider again the gradient of f, set to zero.

$$\boldsymbol{\nabla} f = \begin{pmatrix} \dfrac{\partial f}{\partial x} \\ \dfrac{\partial f}{\partial y} \end{pmatrix} = \begin{pmatrix} 2x \\ -2y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \implies (x,y) = (0,0).$$

Once again, solving the two component equations simultaneously leads to only one critical point. Next, the behaviour of f in a neighbourhood of this critical point is examined with help of small magnitude quantities, h and k. For arbitrary neighbouring points, $(0+h,0+k)$, the difference in function values becomes

$$f(0+h,0+k) - f(0,0) = h^2 - k^2,$$

which is *positive* along the line $k = 0$, but is *negative* along the line $h = 0$. Consequently, the critical point $(0,0)$ is neither a local maximum nor a local minimum. So, by Definition 3.3, the critical point $(0,0)$ is a *saddle point*.

■

The reader should now try their hand at a similar style problem.

✍ Mastery Check 3.1:

Consider the function $z = f(x,y) = x^2 - y^2 - 2x$. Find the point (a,b) at which $\boldsymbol{\nabla} f = \mathbf{0}$, and then find an expression for $f(a+h,b+k)$ for small $h,k \neq 0$. Use Definitions 3.1-3.3 to decide whether the point (a,b) is a maximum or a minimum (or neither).

✍

Extreme values in two dimensions—general procedure

The functions in Examples 3.1 and 3.2 and Mastery Check 3.1 were nice ones to work with. Only a few simple algebraic manipulations were required to determine if a point of interest was a maximum point or a minimum point or

neither, based on explicit calculations of Δf. The question naturally arises: how does one proceed with more complicated functions?

The answer relies on the fact that since interest lies only on *local* extreme points, use can be made of *local approximations* to functions. In fact, as the next theorem states, *all* that will usually ever be needed is Taylor's polynomial approximation of second order to represent a function locally. For convenience, the theorem explicitly refers to a function of two variables. However, the theorem and the analysis to follow generalizes in an obvious way to functions of n variables.

Theorem 3.1
Let $f : D_f \subset \mathbb{R}^2 \longrightarrow \mathbb{R}$ be a C^3 function in some neighbourhood of a point $\boldsymbol{a} \in D_f$. Then for $\boldsymbol{h} = (h, k)$ with $|\boldsymbol{h}| \ll 1$,

$$f(a+h, b+k) = f(a,b) + \frac{\partial f}{\partial x}(a,b).h + \frac{\partial f}{\partial y}(a,b).k + \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}(a,b).h^2 + 2\frac{\partial^2 f}{\partial x \partial y}(a,b).hk + \frac{\partial^2 f}{\partial y^2}(a,b).k^2\right) + (h^2+k^2)^{3/2}B(h,k),$$

where B is some bounded function of (h, k).

Using Taylor polynomials of order two results in a considerable simplification. The difficulties associated with the characterization of critical points of more complex functions are reduced to the level featured in Examples 3.1 and 3.2 since the function approximations are algebraic. Of course, the task of identifying the location of all critical points in the first place must still be conducted with the original function. These are the points that, in turn, become the centre point, $\boldsymbol{a} = (a, b)$, for the development of the Taylor polynomial approximation.

The Taylor polynomial approximation of order two can be written more succinctly in a vector-matrix product form,

$$f(\boldsymbol{a}+\boldsymbol{h}) = f(\boldsymbol{a}) + \boldsymbol{\nabla} f(\boldsymbol{a}) \cdot \boldsymbol{h} + \frac{1}{2}\boldsymbol{h}^T \cdot H_{\boldsymbol{a}} f \cdot \boldsymbol{h} + \text{small terms}, \tag{3.1}$$

where, for a C^2 function of two variables we introduce the symmetric matrix,

$$H_{\boldsymbol{a}} f = \begin{pmatrix} \dfrac{\partial^2 f}{\partial x^2}(a,b) & \dfrac{\partial^2 f}{\partial y \partial x}(a,b) \\ \dfrac{\partial^2 f}{\partial x \partial y}(a,b) & \dfrac{\partial^2 f}{\partial y^2}(a,b) \end{pmatrix} = \begin{pmatrix} f_{xx}(a,b) & f_{xy}(a,b) \\ f_{yx}(a,b) & f_{yy}(a,b) \end{pmatrix}$$

called *the Hessian matrix*, and

$$\boldsymbol{h} = \begin{pmatrix} h \\ k \end{pmatrix}, \quad \boldsymbol{h}^T = (h,k), \quad \boldsymbol{\nabla} f(\boldsymbol{a}) = \left(\frac{\partial f}{\partial x}(a,b), \frac{\partial f}{\partial y}(a,b) \right).$$

The form taken by Equation 3.1 as a vector-matrix equation is extremely convenient as it is straightforward to generalize to functions of n variables. For $n \geq 3$ only the dimensions of the vector $\boldsymbol{h}$ and of the Hessian matrix $H_{\boldsymbol{a}} f$ increase, while the structure of Equation 3.1 remains the same.

Within the second order Taylor polynomial approximation, developed about a critical point, the linear terms vanish since by construction the gradient of the function itself is zero at that critical point. Consequently, for points, $\boldsymbol{a} + \boldsymbol{h}$, in a neighborhood of a critical point, $\boldsymbol{a}$, Equation (3.1) for a function of two variables reduces to (ignoring small, higher order terms),

$$\begin{aligned} f(a+h, b+k) &\approx f(a,b) + \frac{1}{2}\left(f_{xx}(a,b).h^2 + 2f_{xy}(a,b).hk + f_{yy}(a,b).k^2 \right) \\ &= f(a,b) + \frac{1}{2} Q(h,k). \quad \text{— since the gradient term} = 0 \end{aligned}$$

Here, $Q(h,k)$ is called a *quadratic form* for this function of two variables. For a function of more than two variables, the quadratic form will clearly still be defined by the vector-matrix product,

$$Q(\boldsymbol{h}) = \boldsymbol{h}^T \cdot H_{\boldsymbol{a}} f \cdot \boldsymbol{h}$$

but will be a function of n scalar arguments, $\boldsymbol{h} = (h,k,l,\ldots)$, with terms involving these variables raised to the power of 2, at most.

The introduction of the quadratic form is a significant step in the analysis of critical points. For $|\boldsymbol{h}| \ll 1$, it is the *sign of* Q that will determine whether $\boldsymbol{a}$ is a maximum, a minimum, or a saddle point.

Again for illustrative purposes, consider $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$ which has continuous derivatives of at least order 2 and let $\boldsymbol{a} = (a,b) \in D_f$ be a critical point of f. It follows from the simple relation $2\Delta f = Q(h,k)$ that,

(1) if $Q(h,k)$ is *positive definite*, then f has a local *minimum* value at $\boldsymbol{a}$:
since $Q(h,k) > 0$ for all $0 < |\boldsymbol{h}| \ll 1 \implies f(a+h, b+k) > f(a,b)$,

(2) if $Q(h,k)$ is *negative definite*, then f has a local *maximum* value at $\boldsymbol{a}$:
since $Q(h,k) < 0$ for all $0 < |\boldsymbol{h}| \ll 1 \implies f(a+h, b+k) < f(a,b)$,

(3) if $Q(h,k)$ is *indefinite*, then f has neither a maximum nor a minimum value at $\boldsymbol{a}$, and $\boldsymbol{a}$ is a *saddle point*: Since, for all $0 < |\boldsymbol{h}| \ll 1$,
if $Q(h,k) < 0$ for some $\boldsymbol{h} \implies f(a+h, b+k) > f(a,b)$,
if $Q(h,k) > 0$ for other $\boldsymbol{h} \implies f(a+h, b+k) < f(a,b)$,

(4) if $Q(h,k)$ is *positive or negative semi-definite*:
i.e., $Q > 0$ or $Q < 0$ and $Q = 0$ for some $|\boldsymbol{h}| \neq 0$,
then we cannot say anything just using the quadratic form.

Before continuing, it is insightful to summarize the discussion so far and compare the situation with that of single variable theory. The reader should take note of the similarities at corresponding stages.

In the **one-dimensional case**, an investigation into critical points of a function of one variable can be summarized as follows.

Consider $y = f(x)$. Critical points are determined from solutions of the zero-derivative equation,

$$\frac{\mathrm{d}f}{\mathrm{d}x}\Big|_a = 0 \implies x = a$$

In some interval,

$$I_r = \{x : 0 < |x - a| < r\},$$

about an identified critical point, $x = a$, the Taylor polynomial approximation of order two becomes,

$$f(x) \approx f(a) + \cancelto{0}{\frac{\mathrm{d}f}{\mathrm{d}x}\Big|_a}(x-a) + \frac{1}{2}\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\Big|_a (x-a)^2.$$

Hence, for points $x = a + h$ near $x = a$, where $|h| \ll 1$, we have

$$f(a+h) - f(a) \approx \frac{1}{2}\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\Big|_a h^2 \quad \begin{cases} < 0, & \Rightarrow a \text{ is a maximum point,} \\ > 0, & \Rightarrow a \text{ is a minimum point,} \\ = 0, & \Rightarrow a \text{ is a stationary point.} \end{cases}$$

In the **n-dimensional case**, the study of critical points of a function of n variables is very similar.

Consider $z = f(x_1, x_2, \ldots, x_n)$. Critical points are determined by the simultaneous solution of the n equations,

$$\boldsymbol{\nabla} f\Big|_a = 0 \implies \left\{ \begin{array}{c} \dfrac{\partial f}{\partial x_1} = 0 \\ \vdots \\ \dfrac{\partial f}{\partial x_n} = 0 \end{array} \right\} \implies \boldsymbol{x} = \boldsymbol{a}.$$

In some neighbourhood of an identified critical point, $\boldsymbol{x} = \boldsymbol{a}$,

$$S_r(\boldsymbol{a}) = \{\boldsymbol{x} : 0 < |\boldsymbol{x} - \boldsymbol{a}| < r\},$$

the Taylor polynomial approximation of order two becomes,

$$f(\boldsymbol{x}) \approx f(\boldsymbol{a}) + \cancelto{0}{\boldsymbol{\nabla} f\Big|_a} \cdot \boldsymbol{h} + \frac{1}{2}\boldsymbol{h}^T \cdot H(\boldsymbol{a}) \cdot \boldsymbol{h}.$$

Hence, for points $\boldsymbol{x} = \boldsymbol{a} + \boldsymbol{h}$ near the critical point $\boldsymbol{x} = \boldsymbol{a}$, where $|\boldsymbol{h}| \ll 1$, we have

$$f(\boldsymbol{a}+\boldsymbol{h}) - f(\boldsymbol{a}) \approx \frac{1}{2}\boldsymbol{h}^T \cdot H(\boldsymbol{a}) \cdot \boldsymbol{h} = \frac{1}{2}Q(\boldsymbol{a}) \begin{cases} < 0, & \Rightarrow \boldsymbol{a} \text{ is a maximum point,} \\ > 0, & \Rightarrow \boldsymbol{a} \text{ is a minimum point,} \\ = 0, & \Rightarrow \boldsymbol{a} \text{ is a saddle point.} \end{cases}$$

The correspondence with the single variable case of critical points and critical point characterization is clear. The only complications in the n-dimensional case over the one dimensional case are, firstly, the simultaneous solution of n equations instead of one to identify the critical points and, secondly, the analysis of the quadratic form in n variables for each critical point as opposed to a simple evaluation of the 2nd order derivative. Little to no general guidance can be offered for the former problem, as the system of equations can only be solved on a case-by-case basis. In the case of the second issue, some assistance is available.

A useful and almost universal,"recipe" for critical point classification in the 2D case can be obtained readily from the quadratic form.

Let $f : \mathbb{R}^2 \to \mathbb{R}$ be a C^2 function with critical point $\boldsymbol{x}_0$. The quadratic form may be expressed as

$$Q(h,k) = Ah^2 + 2Bhk + Ck^2,$$

where it is customary to identify the coefficients as

$$A = f_{xx}(\boldsymbol{x}_0),\ B = f_{xy}(\boldsymbol{x}_0),\ \text{and } C = f_{yy}(\boldsymbol{x}_0).$$

Then, for $A \neq 0$, $Q(h,k)$ can be rewritten as

$$\begin{aligned} Q(h,k) &= A\left(h^2 + \frac{2B}{A}hk + \frac{C}{A}k^2\right), \\ &= A\left(\left(h + \frac{B}{A}k\right)^2 - \frac{k^2}{A^2}\left(B^2 - CA\right)\right), \end{aligned} \tag{3.2}$$

obtained upon completing the square on the first two terms in the first of the above two expressions for Q. Consequently, referring back to the numbered list on Page 172, we may now deduce the conditions:

(1) if $A > 0$ and $B^2 - AC < 0$, then $Q(h,k) > 0$ (*i.e.*, is *positive definite*) and $\boldsymbol{x}_0$ is a local *minimum point*

(2) if $A < 0$ and $B^2 - AC < 0$, then $Q(h,k) < 0$ (*i.e.*, is *negative definite*) and $\boldsymbol{x}_0$ is a local *maximum point*

(3) if $B^2 - AC > 0$, then independent of the sign of A, $Q(h,k)$ could be positive or negative, depending on $\boldsymbol{h}$ (*i.e.*, is *indefinite*), and $\boldsymbol{x}_0$ is a local *saddle point*.

Note that the formula in Eq (3.2) is not unique and there is no special reason to extract the nonzero coefficient A at the initial step. One could equally well have extracted the coefficient C, if also nonzero, and arrived at a similar result. The reader is invited to do precisely that and establish for themselves conditions analogous to (1)-(3) above.

Obviously, the higher the dimension, *i.e.*, the greater the number of variables, the more complicated is the problem. Even though the process is the same, the number of equations to solve simultaneously will be greater. Moreover, the quadratic form, while still a quadratic in the variables, may be more difficult to analyze. Some explicit assistance in the case of problems in $\mathbb{R}^3$ can be found in the Supplementary Problems at the conclusion of this chapter. In addition, it is possible to generalize the stated quadratic form conditions for $\mathbb{R}^2$ and $\mathbb{R}^3$ to any finite n. However, this will not be necessary for our purposes.

We conclude this section with two examples to demonstrate the general procedure. These are followed by a slightly more challenging Mastery Check exercise.

■ Example 3.3:

For $z = f(x,y) = \ln(2x^2 + y^2) - 2y$, verify that $\boldsymbol{\nabla} f\Big|_{(0,1)} = \mathbf{0}$ at the point $(0,1)$, but that the function is neither a maximum nor a minimum at this point.
The graph of $z = f(x,y)$ is shown in Figure 3.2.

Solution:

$$\boldsymbol{\nabla} f\Big|_{(0,1)} = \begin{pmatrix} \dfrac{\partial f}{\partial x} \\ \dfrac{\partial f}{\partial y} \end{pmatrix}\Bigg|_{(0,1)} = \begin{pmatrix} \dfrac{4x}{2x^2+y^2} \\ \dfrac{2y}{2x^2+y^2} - 2 \end{pmatrix}\Bigg|_{(0,1)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{as required.}$$

Thus $(0,1)$ is a critical point of f. In fact, $(0,1)$ a saddle point, for using the second-order Taylor approximation (see Mastery Check 2.24) we have

$$f(0+h, 1+k) - f(0,1) \approx 2h^2 - k^2,$$

which is $< 0 \;\forall\; k \neq 0$ when $h = 0$, and is $> 0 \;\forall\; h \neq 0$ when $k = 0$.

Alternatively, in the quadratic form, $A = f_{xx}(0,1) = 4 > 0$, $B = f_{xy}(0,1) = 0$, and $C = f_{yy}(0,1) = -2 < 0$. Consequently, as the discriminant $B^2 - AC = 8 > 0$, Option (3) in our recipe list of conditions applies confirming that $(0,1)$ is a saddle point. ■

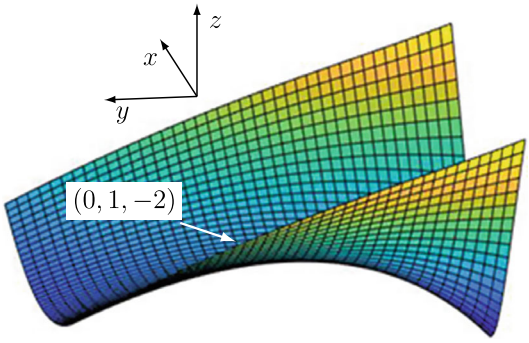


Figure 3.2 The graph of $z = \ln(2x^2 + y^2) - 2y$.

Example 3.4:

Determine and classify all critical points of the function

$$f(x, y) = x^2 + y^2 + 2\mathrm{e}^{xy+1}, \quad D_f = \mathbb{R}^2.$$

Solution:

Critical points are given by $\boldsymbol{\nabla} f = \mathbf{0}$:

$$\frac{\partial f}{\partial x} = 2x + 2\mathrm{e}^{xy+1}.y = 0 \ldots\ldots (1) \quad ; \quad \frac{\partial f}{\partial y} = 2y + 2\mathrm{e}^{xy+1}.x = 0 \ldots\ldots\ldots\ldots\ldots (2),$$

$$(1) \Rightarrow x = -y\mathrm{e}^{xy+1} \ldots\ldots\ldots (3) \quad ; \quad (3) \text{ in } (2) \Rightarrow y\big(1 - \mathrm{e}^{2(xy+1)}\big) = 0 \ldots\ldots (4).$$

Solutions to (4) are: (i) $y = 0$ and (ii) $\mathrm{e}^{2(xy+1)} = 1$.

Alternative (i) $\Longrightarrow x = 0 \quad \Longrightarrow$ point $(0, 0)$ is a critical point.

Alternative (ii) $\Longrightarrow xy + 1 = 0 \quad \Longrightarrow \quad y = -\dfrac{1}{x} \ldots\ldots$ (5).

(5)+(3) $\Longrightarrow \quad x = \dfrac{1}{x}.1 \quad \Longrightarrow \quad x^2 = 1 \quad \Longrightarrow \quad x = \pm 1.$

Consequently, points $(1, -1)$ and $(-1, 1)$ are also critical points. There are no others.

The next phase involves characterizing each of the three points.

The 2nd-order partial derivatives of f are

$$\frac{\partial^2 f}{\partial x^2} = 2 + 2y^2\mathrm{e}^{xy+1}, \quad \frac{\partial^2 f}{\partial y^2} = 2 + 2x^2\mathrm{e}^{xy+1}, \quad \frac{\partial^2 f}{\partial x \partial y} = 2xy\mathrm{e}^{xy+1} + 2\mathrm{e}^{xy+1}.$$

Consequently, the Hessian matrix at an arbitrary point (x, y) is,

$$H_{\boldsymbol{x}} f = \begin{pmatrix} 2 + 2y^2\mathrm{e}^{xy+1} & (2xy + 2)\mathrm{e}^{xy+1} \\ (2xy + 2)\mathrm{e}^{xy+1} & 2 + 2x^2\mathrm{e}^{xy+1} \end{pmatrix},$$

and evaluated at the critical points gives,

$$H_{(0,0)} f = \begin{pmatrix} 2 & 2\mathrm{e} \\ 2\mathrm{e} & 2 \end{pmatrix}, \quad H_{(1,-1)} f = H_{(-1,1)} f = \begin{pmatrix} 4 & 0 \\ 0 & 4 \end{pmatrix}.$$

Thus, at the critical point $(0, 0)$,

$$\begin{aligned}\Delta f_{(0,0)} &= f(0+h, 0+k) - f(0,0) \approx \frac{1}{2}Q(h,k) = \frac{1}{2}\boldsymbol{h}^T \cdot H_{(0,0)}f \cdot \boldsymbol{h} \\ &= \frac{1}{2}(h,k)\begin{pmatrix} 2 & 2\mathrm{e} \\ 2\mathrm{e} & 2 \end{pmatrix}\begin{pmatrix} h \\ k \end{pmatrix} = h^2 + 2\mathrm{e}hk + k^2 \\ &= \big(h^2 + 2\mathrm{e}hk + (\mathrm{e}k)^2\big) - (\mathrm{e}k)^2 + k^2 \;=\; (h + \mathrm{e}k)^2 - k^2(\mathrm{e}^2 - 1).\end{aligned}$$

The factor $(\mathrm{e}^2 - 1) > 0$. So,

$$\Delta f_{(0,0)} \quad \begin{cases} > 0 & \forall\ k \text{ when } h = 0, \\ > 0 & \forall\ h \text{ when } k = 0, \\ < 0 & \text{when } h = -\mathrm{e}k. \end{cases}$$

So, $\Delta f_{(0,0)}$ can be +ve or −ve $\implies$ $(0, 0)$ is a saddle point. Using the quadratic form conditions, $B^2 - AC = 4\mathrm{e}^2 - 4 > 0$, confirming $(0, 0)$ is a saddle point. Meanwhile,

$$\Delta f_{(1,-1)} = \Delta f_{(-1,1)} = \frac{1}{2}(h,k)\begin{pmatrix} 4 & 0 \\ 0 & 4 \end{pmatrix}\begin{pmatrix} h \\ k \end{pmatrix} \;=\; 2(h^2 + k^2) \;>\; 0.$$

The points $(1, -1)$, $(-1, 1)$ are therefore local minima. The quadratic form conditions give $A = C = 4 > 0$ and $B^2 - AC = -16 < 0$, again confirming that these points are points of local minima.
Figure 3.3 shows $z = f(x, y)$ for
$\{(x, y, z) : -1.5 \le x \le 1.5,\ -1.5 \le y \le 1.5,\ z \le 7.5\}$.

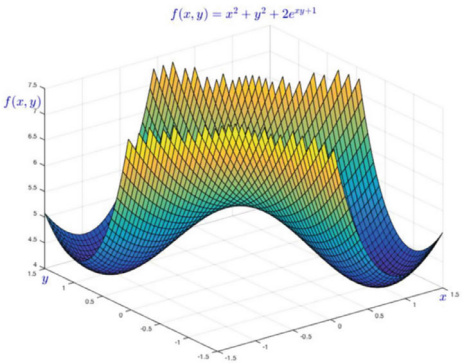


Figure 3.3 The graph of $z = x^2 + y^2 + 2\mathrm{e}^{xy+1}$.

■

✍ Mastery Check 3.2:

Determine and classify all critical points of the function

$$f(x, y, z) = 2xz^2 + z^2y - 2x^3 - 3y^2 + 6,\ D_f = \mathbb{R}^3.$$

Note and hint: This involves a function of three variables. Although the procedure to follow is identical to the above examples, three equations must be solved simultaneously to identify the critical points and no help can come from the quadratic form conditions listed on Page 174. On the other hand, as an alternative to manual manipulation of the resulting quadratic forms involving three factors, (h, k, l) say, the reader may find useful the recipe conditions listed in Supplementary Problems 3.3 and 3.4.

✍

3.B Extreme Points: The Complete Story

According to the discussion in the previous section, a critical point $\boldsymbol{a} \in D_f$ may be a point of *local* maximum if $f(\boldsymbol{a}) \geq f(\boldsymbol{a}+\boldsymbol{h})$ for $|\boldsymbol{h}| \ll \mathbf{1}$ or a point of *local* minimum if $f(\boldsymbol{a}) \leq f(\boldsymbol{a}+\boldsymbol{h})$ for $|\boldsymbol{h}| \ll \mathbf{1}$. Such critical points are also referred to as points of *relative* maximum or *relative* minimum, respectively.

We contrast these references to *local* and *relative* quantities, with the following definitions of *global* and *absolute* quantities.

Definition 3.4

A point $\boldsymbol{a} \in D_f$ *is called a point of* **global** *or* **absolute** $\left\{ \begin{array}{c} \textit{maximum} \\ \textit{minimum} \end{array} \right\}$ *if*

$$f(\boldsymbol{a}) \left\{ \begin{array}{lll} \geq & f(\boldsymbol{x}) & \textit{for all} \quad \boldsymbol{x} \in D_f \\ \leq & f(\boldsymbol{x}) & \textit{for all} \quad \boldsymbol{x} \in D_f. \end{array} \right.$$

Remarks

∗ The difference between Definition 3.1 and Definition 3.4 lies in the set of points being considered or compared with point $\boldsymbol{a}$. In Definition 3.1 only points in the immediate neighbourhood, $S_r(\boldsymbol{a})$, of $\boldsymbol{a}$ are considered, while in Definition 3.4 *all* points in the domain, D_f, of the function are involved.

∗ One consequence of Definition 3.4 is that a critical point, even if a point of local maximum or local minimum, need *not* be a point of *absolute* maximum or *absolute* minimum.

Earlier we said that critical points constitute only one of three types of extreme points. The other two types of extreme points, which are *not* found using the gradient, are introduced below. Invariably, so-called *singular* points and *boundary* points must be identified manually, either by inspection or by some restricted/limited differential analysis. Examples of such calculations will be given a little later in a more global context. For the present, the following descriptions should provide some insight into these two classes.

(i) *singular points of* f, points where ∇f does not exist (Figure 3.4):

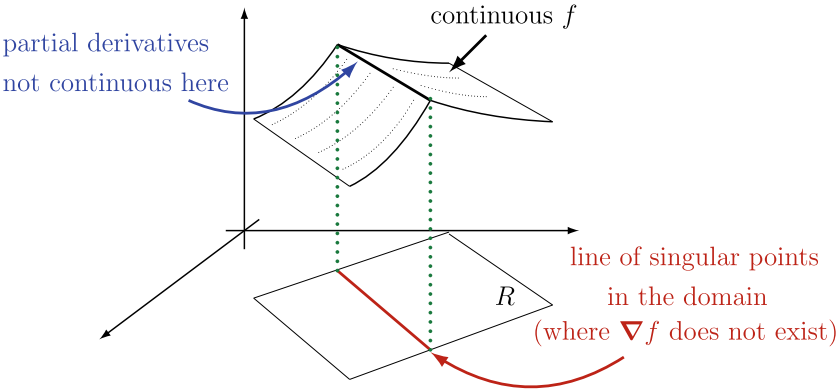


Figure 3.4 A function with singular points.

(ii) *boundary points of a restricted region* $R \subset D_f$ (Figure 3.5):

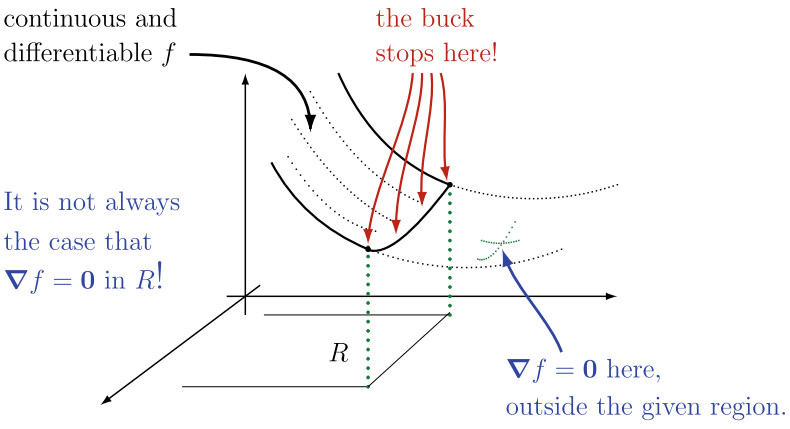


Figure 3.5 A function defined on a restricted region $R \subset D_f$.

In the preceding section, reference was made to the science of *optimization*, which has the goal of finding absolute maxima and minima of functions

$\mathbb{R}^n \longrightarrow \mathbb{R}$. It is not possible to achieve this goal generally by only looking for and characterizing local extreme points, even though these may turn out to be absolute extreme points. For a thorough optimization study it is necessary to include a consideration of the two other types, if the problem so demands. As such, now with the three classes of extreme points defined, we may focus on the types of optimization problems that can arise.

In general there are at least three categories of optimization problem:

(1) optimizing over a compact domain;

(2) optimizing completely free of restrictions;

(3) optimizing functions under one or more constraints.

We shall study these in turn. We begin with optimizing over compact domains, assuming throughout that the functions involved are differentiable.

Optimization over compact domains

Recall the definition of a *compact set* (Definition 1.8): a set $\Omega \subseteq \mathbb{R}^n$ is said to be compact if it is *closed* **and** *bounded*. From the perspective of optimization, the following theorem offers a particularly valuable guarantee for any function defined on a region $\Omega \subseteq D_f$ that is compact.

Theorem 3.2
A **continuous** *real-valued function,* $f : \mathbb{R}^n \to \mathbb{R}$*, defined on a* **compact** *region,* Ω*, attains an* **absolute maximum** *and an* **absolute minimum** *value.*

That is, there exist points $\boldsymbol{x}_m, \boldsymbol{x}_M \in \Omega$ such that $f(\boldsymbol{x}_m) \leq f(\boldsymbol{x}) \leq f(\boldsymbol{x}_M)$ for all $\boldsymbol{x} \in \Omega$.

A few comments on this theorem are warranted.

Firstly, it is not necessary for the region considered to be the function's entire domain of definition, D_f, but it might be. The problem statement will usually specify this. If no region is given then the reader should assume that the whole of D_f is implied.

Secondly, it follows from its definition that a continuous function defined on a closed and bounded region is necessarily bounded (Theorem 1.2). This means that a $K > 0$ can be found such that $|f(\boldsymbol{x})| < K$, for all $\boldsymbol{x}$ in that region.

This simple result implies that we should expect f to exhibit an absolute minimum and an absolute maximum. In fact, this is the only time we are *guaranteed* that *absolute* maximum and minimum points exist.

One should always bear in mind that a *continuous* function is *not* necessarily differentiable everywhere. A consequence of this is that singular points, points at which the function is not differentiable, can exist. Such points must then be inspected separately to any critical points. Finally, the assumption of a closed and finite domain means that the domain boundary (*i.e.*, the set of all boundary points) will also need to be considered separately. It is not to be expected that the gradient of f will identify points on the boundary (although it does happen). Instead, as the examples and Mastery Check below indicate, the boundary needs to be considered separately. This might simply involve evaluating f on the boundary, but may also involve considering a restricted derivative investigation.

We illustrate Theorem 3.2 in action with the following examples.

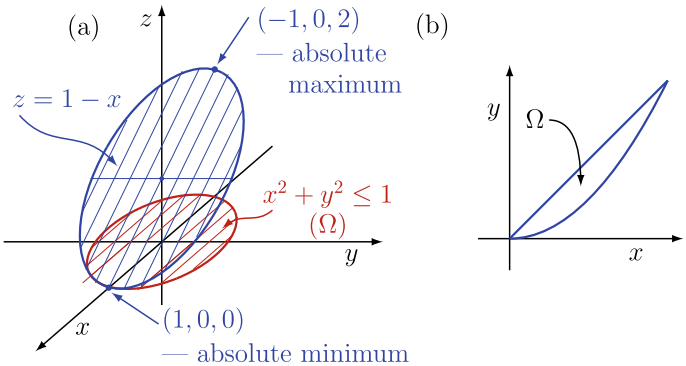


Figure 3.6 (a) The graph of $x + z = 1$ in Example 3.5; (b) The domain Ω in Example 3.6.

Example 3.5:

Determine the absolute maximum and minimum values of the function $f(x, y, z) = x + z = 1$, over the region $\Omega = \{(x, y) : x^2 + y^2 \leq 1\}$ (Figure 3.6(a)).

Solution:

In this example $\boldsymbol{\nabla} f \neq 0$ everywhere, so there are no critical points.

Moreover, the function and its gradient are well defined everywhere in the given domain, so there are no singular points.

Nevertheless, as demanded by Theorem 3.2, the function still attains an absolute maximum and an absolute minimum. These occur, respectively, at the points $(-1, 0)$ and $(1, 0)$ on the boundary.

■

Example 3.6:

Consider $f(x, y) = (y - x)\mathrm{e}^{x^2 - y}$ for $x^2 \leq y \leq x$. Where does f achieve its maximum and minimum values?

Solution:

We note that the domain, Ω, set by the above inequalities and shown in Figure 3.6(b), is non-empty provided $0 \leq x \leq 1$. Moreover, it is also compact, so we are sure that absolute extrema exist. The function is non-singular. Moreover, the gradient gives

$$\boldsymbol{\nabla} f = \begin{pmatrix} -1 + 2x(y - x) \\ 1 - (y - x) \end{pmatrix} \mathrm{e}^{x^2 - y} = \mathbf{0}, \text{ when } \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1/2 \\ 3/2 \end{pmatrix},$$

which is a point outside the compact region Ω. Hence, although the function has a critical point, it can be discounted as it does not belong to the given domain. Now all that remains is to inspect the boundaries.

On the boundary line $y = x$, the function $f(x, y) = 0$.
On the boundary curve $y = x^2$, $f(x, y) = x^2 - x$. Consequently, treating $f(x, x^2)$ as a function of one variable, we consider both internal points and end points. At the ends, $f(x, x^2) = 0$ at $x = 0$ and $x = 1$. As for interior points, we consider $\dfrac{\mathrm{d}f}{\mathrm{d}x} = 2x - 1 = 0 \Rightarrow x = \dfrac{1}{2} \Rightarrow y = \dfrac{1}{4}$.

Collating all findings, f has an absolute minimum of $f(\frac{1}{2}, \frac{1}{4}) = -1/4$ at $(\frac{1}{2}, \frac{1}{4})$, and an absolute maximum of $f(x, x) = 0$, along the line $y = x$ for $0 \leq x \leq 1$.

■

Using these examples as guidelines, the reader may now wish to pause and test their understanding by attempting the next, slightly more involved, Mastery Check.

Mastery Check 3.3:

Determine the greatest and least values of $f(x, y) = y\mathrm{e}^x - xy^2$ in the region

$$\Omega = \{(x, y) : 0 \leq x \leq 1,\ 0 \leq y \leq 2\},$$

the closed rectangle shown in Figure 3.8(a).

Hint: check for singular points, interior extreme points, and then check *all* boundary points.

✍

Optimization free of constraints

In relaxing the condition of compactness, either by allowing the region to be unbounded in one or more directions, or bounded but open, there is no longer any guarantee that points of finite maximum or minimum exist. For instance, a function might become infinite at one or more points on the boundary of a bounded open set. Consider for example the case

$$f(x,y) = \frac{xy}{\sqrt{1-x^2-y^2}}, \qquad D_f = \left\{(x,y) : x^2 + y^2 < 1\right\}.$$

The magnitude of this, otherwise continuous, function increases without bound as the independent variables approach the boundary of the unit disc: the function therefore attains neither an absolute maximum nor absolute minimum in D_f. In contrast, a continuous function on an unbounded domain may still attain a finite absolute maximum or minimum, as was the case of Example 1.10:

$$f(x,y) = \frac{4x}{1+x^2+y^2}, \qquad D_f = \mathbb{R}^2.$$

This function attains both an absolute maximum and an absolute minimum despite having an unbounded domain of definition.

So, how does one proceed? One possible answer is to *modify* the protocol for continuous functions on compact regions. This is described on the right-hand side of Flowchart 3.1, and explained stepwise below.

Step 1. First, one needs to ascertain if and where there are points on the edge of D_f, including on the edges of holes in domains, where the function f is discontinuous or not defined. Significantly, one must determine whether f diverges to positive or negative infinity at these points. This step will immediately answer the question of whether an absolute maximum or an absolute minimum exists at all.

Step 2. Based on the result of Step 1, one constructs a convenient closed and bounded subregion, $\Omega_n \subset D_f$, that not only avoids the singular points found, but over which f is continuous. Such are the black-shaded regions in Figure 3.7. The geometric extent of Ω_n should optimally be easily characterized in terms of one or a few parameters. Then, confining ourselves to Ω_n, one proceeds as before, identifying in Ω_n any critical points, points where the function's derivatives do not exist (singular points), and lastly f's behaviour on the boundary of Ω_n. Theorem 3.2 guarantees that f will have absolute extreme points in Ω_n.

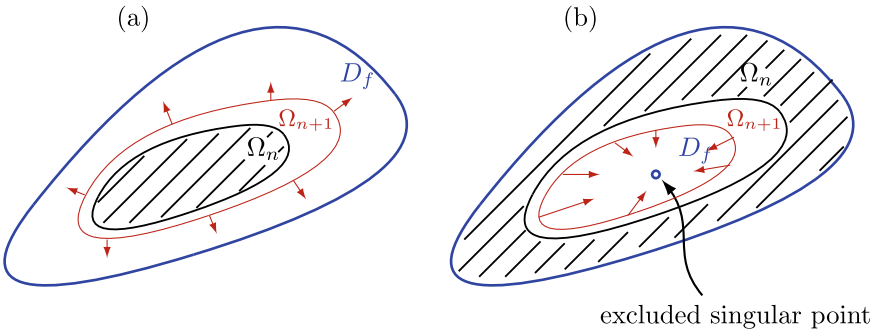
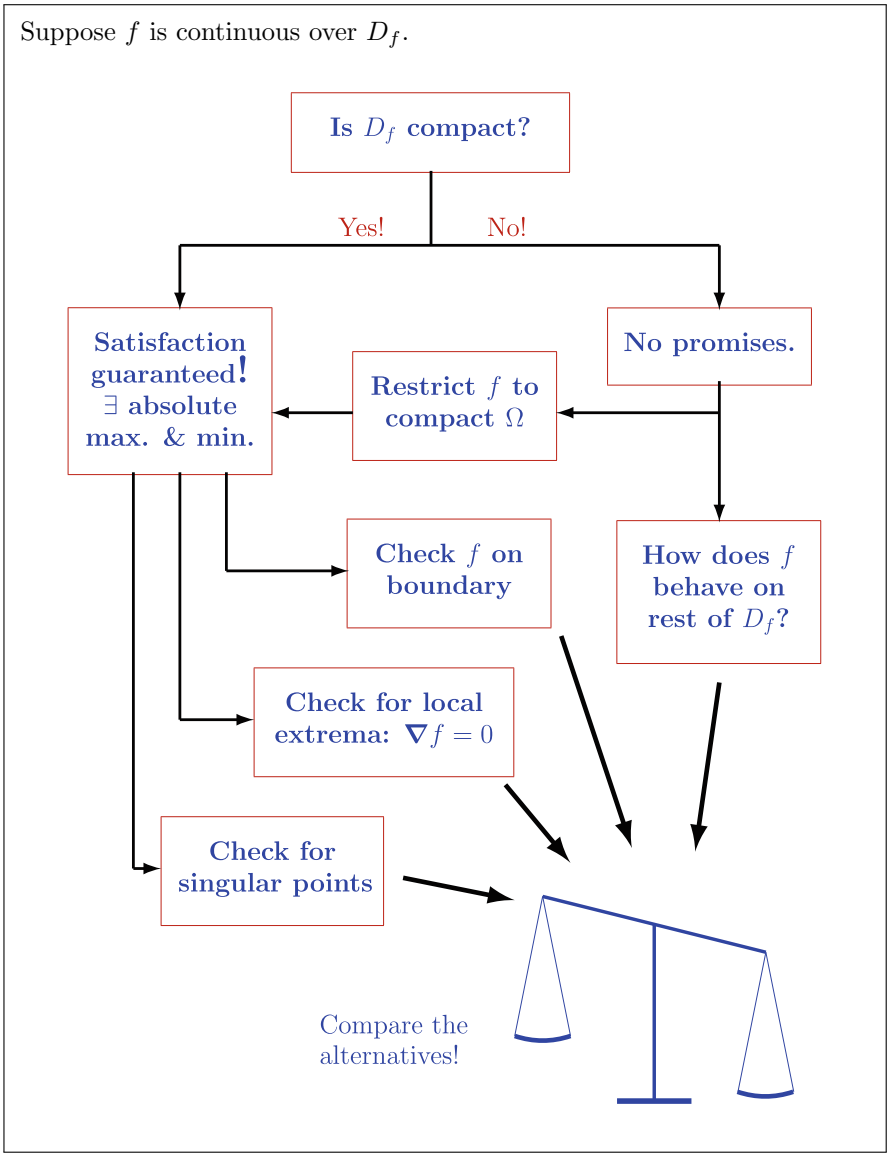


Figure 3.7 (a) Sequence of compact domains $\Omega_n \longrightarrow$ unbounded D_f;
(b) Sequence of compact domains $\Omega_n \longrightarrow$ singular D_f.

Step 3. Thirdly, the behavior of f in the region $D_f \cap \Omega_n^c$ must be examined. Presumably, D_f is unbounded ($\boldsymbol{x} \to \infty$ in at least one direction) or is open (with singular points on the boundary). If it is not feasible to conduct a individual investigation in this complementary space, then a limit of the results of Step 2 may be required. This limit may take the form of a limit of the absolute maximum and minimum values found in Ω_n, as Ω_n expands to encompass all of D_f (indicated by the red expanded set Ω_{n+1} and arrows in Figure 3.7). For example, supposing Ω_n is suitably characterized in terms of a finite set of parameters one takes appropriate limits of the absolute extreme values obtained in Step 2 with respect to these parameters. On the other hand, if the absolute values found within Ω_n do not depend on Ω_n's extent then an estimate of the bounds of f in the complementary space might be sufficient.

Step 4. The results of the first three steps are then compared to determine which, if any, of the points identified in D_f are points of absolute maximum and absolute minimum, and what values they produce.

Flowchart 3.1: Optimization — how to play the game



We demonstrate these calculation steps in an example.

Example 3.7:

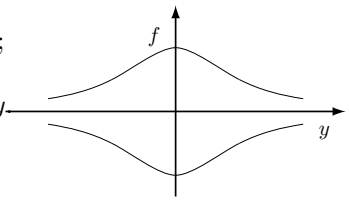
Determine the greatest and least values of

$$f(x,y) = \frac{4x}{1+x^2+y^2} \text{ for } (x,y) \in D_f = \mathbb{R}^2.$$

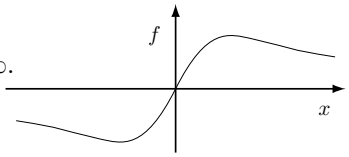
Solution:

This function was studied in Example 1.12. The picture that was compiled there is here completed with the identification of max and min points. Before we begin, note that

(i) for fixed $x > 0$,
f is a +ve even function of y;
for fixed $x < 0$,
f is a −ve even function of y.



(ii) for fixed y, $f = 0$ when $4x = 0$,
is −ve when $4x < 0$,
is +ve when $4x > 0$,
and $f \to 0$ as $x \to \pm\infty$.



$$\text{Thus} \quad |f(x,y)| = \frac{4|x|}{1+x^2+y^2} \qquad (\text{use } x = r\cos\theta,\ y = r\sin\theta)$$
$$= \frac{4|r\cos\theta|}{1+r^2} \le \frac{4r}{1+r^2} \sim \frac{4}{r} \to 0 \text{ as } r \to \infty.$$

From this we see that, quite arbitrarily, we can choose $R = 8$ so that $|f| \le \frac{1}{2}$ for $r \ge R$.
The inequality $|f| \le \frac{1}{2}$ sets an absolute bound on f over the unbounded region $r \ge R$.
To complement this we see that $r \le R$ then determines the compact subset in which we look for critical points, etc. The partial derivatives of f are:

$$\frac{\partial f}{\partial x} = \frac{4}{1+x^2+y^2} - \frac{4x(2x)}{(1+x^2+y^2)^2} = \frac{4(1+x^2+y^2)-8x^2}{(1+x^2+y^2)^2}$$

$$\frac{\partial f}{\partial x} = \frac{4-4x^2+4y^2}{(1+x^2+y^2)^2} \quad (3.1) \qquad \frac{\partial f}{\partial y} = \frac{4x(2y)}{(1+x^2+y^2)^2} = 0. \quad (3.2)$$

$$(3.1) \implies 4-4x^2+4y^2 = 0. \qquad (3.2) \implies 8xy = 0 \iff x = 0 \text{ or } y = 0.$$

If $x = 0$, then from (3.1) $4 + 4y^2 = 0$: *i.e.*, there is no solution.

If $y = 0$, then $4 - 4x^2 = 0 \iff x = \pm 1$. Thus, critical points are: $(1,0)$ and $(-1,0)$, while absolute max and min f values are, respectively, $f(1,0) = \dfrac{4}{1+1} = 2 > \frac{1}{2}$, $f(-1,0) = -2 < -\frac{1}{2}$. ■

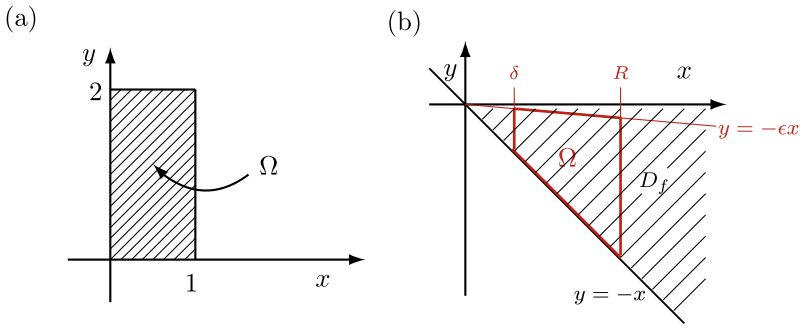


Figure 3.8 (a) Bounded domain, Ω, in Mastery Check 3.3; (b) Unbounded domain, D_f, in Mastery Check 3.4.

✍ Mastery Check 3.4:

Investigate whether the function $f(x,y) = 1 - xye^{(x^2/y)}$ attains finite absolute extreme values over the open unbounded domain (Figure 3.8(b))

$$D_f = \{(x,y) : -x \le y < 0, x > 0\}.$$

If so, determine the greatest and least value of f over D_f.

Suggestion: First determine the function's absolute extreme values over the closed and bounded domain,

$$\Omega = \{(x,y) : -x \le y \le -\epsilon x, \delta \le x \le R\},$$

then consider the limiting values of these as $R \to \infty$ and $\epsilon, \delta \to 0$.
(For convenience, δ could also be replaced by ϵ.)

✍

Optimization subject to constraints

Function optimization under one or more constraints is a fairly common type of problem. It involves maximizing or minimizing, generally expressed as optimizing, with respect to one or more variables, some quantity under special and restrictive conditions.

Such problems are generally expressed in a common way. For example, we:

maximize	volume	*subject to*	fixed surface area;
minimize	the physical dimensions of electronic circuitry	*subject to*	limited operating temperature;
optimize	work & train schedule	*subject to*	a fixed #trains & man hours per week.

Consequently, the generic model structure of such problems (with one constraint) can be expressed as follows:

optimize	$f(\boldsymbol{x})$	*subject to*	$g(\boldsymbol{x}) = 0$

In some applications f is called the *objective* function while g is the *constraint*. In the case where there are more than one constraint, the additional constraints would similarly be expressed as equations such as $h(\boldsymbol{x}) = 0$.

The conceptual picture I impart to students is this: Suppose f were a mountain, while g gives rise to a walking track on the mountain side (see Figure 3.9). The constraint g is *not* itself the walking track, but a set of points in the plane of the mountain's base (the domain) that gives rise to the walking track. The absolute unconstrained maximum of f would be the mountain's peak, but the maximum of f subject to constraint $g = 0$ would give only the highest point on the track.

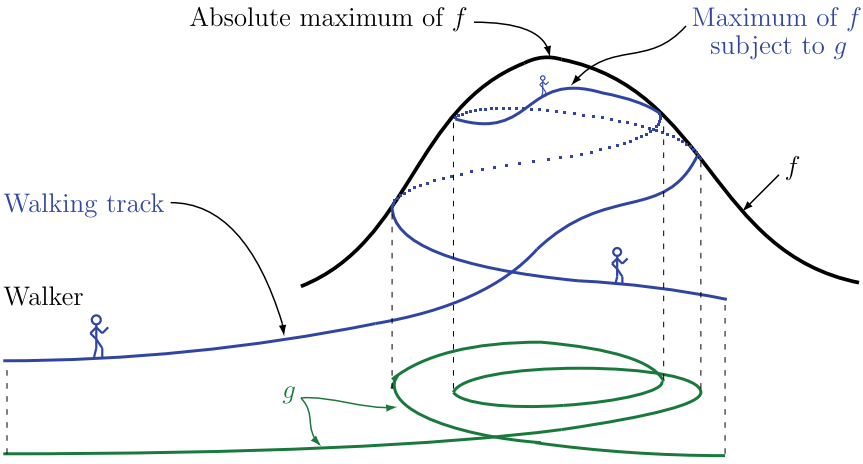


Figure 3.9 A constrained optimization problem.

In the following we will assume that both f and g have continuous partial derivatives of order 1 (at least). That is, f and g are of class C^1.

We must also assume that *the level set* of the function g,

$$L = \{\boldsymbol{x} : g(\boldsymbol{x}) = 0\}$$

is also a non-empty subset of D_f. That is, we assume that it lies inside D_f. Moreover, we assume that $L \subset D_g$, is a dense and connected set of points in common with D_f. This condition underpins the coming requirement that derivatives be defined at points in L.

Although the concepts are applicable to any $\mathbb{R}^n$ $(n < \infty)$, it is convenient for the discussion to restrict the analysis to $\mathbb{R}^2$.

Suppose

$$\begin{aligned} f : \mathbb{R}^2 &\longrightarrow \mathbb{R} \quad \text{and} \quad g : \mathbb{R}^2 \longrightarrow \mathbb{R} \\ (x, y) &\mapsto f(x, y) \qquad\quad (x, y) \mapsto g(x, y) \end{aligned}$$

In $\mathbb{R}^2$, the dense and connected level set L, with nonempty overlap with D_f, $L \cap D_f \neq \emptyset$, is a 1D curve lying across a 2D region in $\mathbb{R}^2$, as represented in Figure 3.10.

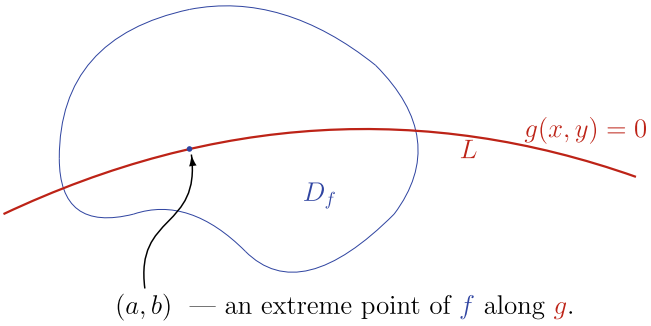


Figure 3.10 Domain D_f and the zero level set L of g.

In addition to the properties of L, the fact that g is a C^1 function means that there exists a continuous and differentiable parametrization of L in terms of a parameter t belonging to some interval, I. That is, there exist differentiable scalar functions $\phi, \psi : \mathbb{R} \to \mathbb{R}$ such that $x = \phi(t)$ and $y = \psi(t)$ for every point (x, y) on L corresponding to some $t \in I$. Now suppose (a, b) is an interior local maximum or local minimum point of f *when* f is restricted to points on L. By continuity of the parametrization map, there exists a $t_0 \in I$ such that $a = \phi(t_0),\ b = \psi(t_0)$. Moreover, the differentiability of the parametrization has the consequence that L has a *local tangent vector* at (a, b), or equivalently at $t = t_0$, given by $\big(\phi'(t_0), \psi'(t_0)\big)$.

Since (a, b) is a local extreme point of f along L, the single variable function of t, defined by $F(t) = f(\phi(t), \psi(t))$ must have a critical point at $t = t_0$. That is,

$$\left.\frac{\mathrm{d}F}{\mathrm{d}t}\right|_{t=t_0} = 0.$$

On the other hand, by the multivariable chain rule (Section 2.G) and the definition of the scalar product we find

$$\begin{aligned}
\left.\frac{\mathrm{d}F}{\mathrm{d}t}\right|_{t_0} &= \left.\frac{\partial f}{\partial x}\frac{\mathrm{d}\phi}{\mathrm{d}t}\right|_{t_0} + \left.\frac{\partial f}{\partial y}\frac{\mathrm{d}\psi}{\mathrm{d}t}\right|_{t_0} && \text{— by the chain rule} \\
&= \boldsymbol{\nabla} f(a,b)\cdot\big(\phi'(t_0),\psi'(t_0)\big) && \text{— by the scalar product} \\
&= 0.
\end{aligned}$$

The last equality implies the all-important fact that the plane vector $\boldsymbol{\nabla} f(a,b)$ at (a,b) and the tangent vector $\big(\phi'(t_0),\psi'(t_0)\big)$ at $t=t_0$, are orthogonal.

At the same time, in the discussion put forward in Section 2.E it was stated that the gradient of a scalar function, as a vector, is orthogonal to the level set of that function. In the present context, this means that $\boldsymbol{\nabla} g(a,b)$ is orthogonal to L at (a,b) and by implication is also orthogonal to the tangent vector $\big(\phi'(t_0),\psi'(t_0)\big)$ at $t=t_0$.

That both $\boldsymbol{\nabla} g(a,b)$ and $\boldsymbol{\nabla} f(a,b)$ are orthogonal to $\big(\phi'(t_0),\psi'(t_0)\big)$ must mean that the two gradient vectors are parallel. This reasoning underpins the following theorem.

Theorem 3.3
If (a,b) is a point which lies in both D_f and D_g, and which is an extreme point of $f:\mathbb{R}^2\longrightarrow\mathbb{R}$ under the constraint $g(x,y)=0$, then the vectors $\boldsymbol{\nabla} f(a,b)$ and $\boldsymbol{\nabla} g(a,b)$ are **parallel**.

As a corollary of the theorem, it follows that provided $\boldsymbol{\nabla} g$ is not identically zero, a scalar $\lambda_0\in\mathbb{R}$ can be found such that:

$$\boldsymbol{\nabla} f(a,b) = -\lambda_0\boldsymbol{\nabla} g(a,b) \iff \boldsymbol{\nabla}(f+\lambda g)\Big|_{a,b,\lambda_0} = 0.$$

Combining this result with the statement of the constraint itself, $g(x,y)=0$, which can be expressed equivalently in the form

$$g(x,y) = \frac{\partial}{\partial\lambda}\left(f(x,y)+\lambda g(x,y)\right)\Big|_{\lambda=\lambda_0} = 0,$$

we arrive at the summary situation that the 3D point $(a,b;\lambda_0)$ is a critical point of the new multivariable function of *three* variables,

$$L(x, y; \lambda) = f(x, y) + \lambda g(x, y).$$

This function is called the *Lagrangian function* and λ is called the *Lagrange multiplier*.

The geometrical situation showing the relationship between the gradients of f and g, and the curves of constant f and of constant g, is illustrated in Figure 3.11.

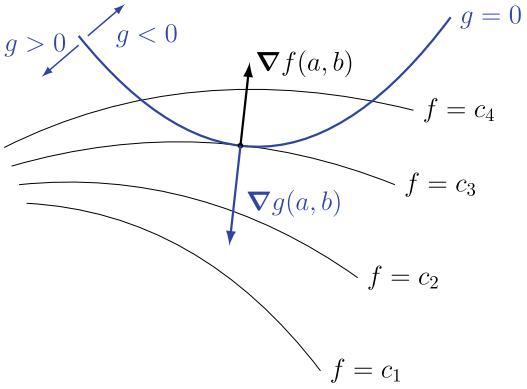


Figure 3.11 Level sets of f and g, and gradients ∇f and ∇g.

Remarks

* The reader should remember the following distinction concerning the point (a, b). It is a critical point of "f subject to g", but is *not* a critical point of f alone.

* The critical points of $L(x, y; \lambda)$ are found from the set of equations

$$\left.\begin{aligned} \frac{\partial L}{\partial x} &= \frac{\partial f}{\partial x} + \lambda \frac{\partial g}{\partial x} = 0 \\ \frac{\partial L}{\partial y} &= \frac{\partial f}{\partial y} + \lambda \frac{\partial g}{\partial y} = 0 \end{aligned}\right\} \text{— the condition } \nabla f \| \nabla g \text{ at } (a, b)$$

$$\left.\begin{aligned} \frac{\partial L}{\partial \lambda} &= g(x, y) = 0 \end{aligned}\right\} \text{— the constraint equation}$$

* In effect, what has occurred is that a restricted 2D optimization problem has been transformed into an *un*restricted 3D optimization problem. To completely solve the problem, one needs to determine a, b, *and* λ_0. Note that the actual value of λ_0 is not often needed, although it can be utilized in the numerical analysis of optimization problems.

* The preceding analysis takes for granted that $D_f \cap D_g \neq 0$ and moreover assumes that the critical points of $L(x, y; \lambda)$ or the critical points of the composite function, $F(t) = f(\phi(t), \psi(t))$, lie in the interior of $D_f \cap D_g$. However, as we noted earlier in this section, an extreme point of a function need not be a critical point. In fact, if the domain D_g extended beyond D_f as a subspace of $\mathbb{R}^n$, as suggested by Figure 3.10, *and* D_f was a closed subset, then it may be necessary to also consider the boundary points of $D_f \cap D_g$ as well as the interior critical points of $D_f \cap D_g$.

* The (differential) theory works beautifully for a general multivariable function $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ and multivariable constraint $g(x_1, \ldots, x_n) = 0$:

$$\boldsymbol{\nabla} f(\boldsymbol{a}) = -\lambda \boldsymbol{\nabla} g(\boldsymbol{a}) \quad \text{if} \quad \boldsymbol{\nabla} g \neq 0.$$

  This implies that the higher dimensional point $(\boldsymbol{a}; \lambda_0)$ is an extreme point in the $(n + 1)$-dimensional space on which the function $L : \mathbb{R}^{n+1} \longrightarrow \mathbb{R}$ is defined.

The theory leading to the Lagrangian function and the Lagrange multiplier also generalizes in the dimension of number of constraints. That is, the theory can be extended quite naturally to optimization problems involving two or more constraints. However, this is only feasible if the number of spatial dimensions exceeds the number of constraints.

For example, suppose we wish to optimize $f : \mathbb{R}^3 \longrightarrow \mathbb{R}$ subject to the two constraints $g_1(x, y, z) = 0$ and $g_2(x, y, z) = 0$. Then, the extension of the former 2D optimization problem has $\boldsymbol{\nabla} f(\boldsymbol{a})$, $\boldsymbol{\nabla} g_1(\boldsymbol{a})$, and $\boldsymbol{\nabla} g_2(\boldsymbol{a})$, as linearly dependent vectors, where $\boldsymbol{a}$ is the sought-after local extreme point. This means that for each extreme point, $\boldsymbol{a}$, there exist scalars $\lambda_0, \mu_0 \in \mathbb{R}$ such that

$$\boldsymbol{\nabla} f(\boldsymbol{a}) + \lambda_0 \boldsymbol{\nabla} g_1(\boldsymbol{a}) + \mu_0 \boldsymbol{\nabla} g_2(\boldsymbol{a}) = 0$$

provided also that $\boldsymbol{\nabla} g_1(\boldsymbol{a})$ and $\boldsymbol{\nabla} g_2(\boldsymbol{a})$ are *not* co-parallel, which can be checked easily by showing that $\boldsymbol{\nabla} g_1(\boldsymbol{a}) \times \boldsymbol{\nabla} g_2(\boldsymbol{a}) \neq 0$.

The linear dependency condition on the vectors, plus analogous λ-derivative and μ-derivative rewritten constraint conditions, means that the higher dimensional point $(\boldsymbol{a}; \lambda_0, \mu_0)$ is a critical point of the higher dimensional Lagrange function,

$$L(\boldsymbol{x}; \lambda, \mu) = f(\boldsymbol{x}) + \lambda g_1(\boldsymbol{x}) + \mu g_2(\boldsymbol{x}).$$

Both λ and μ are Lagrange multipliers.

Example 3.8:

Determine the maximum value of $f(x, y) = \mathrm{e}^{-(x^2+y^2)/2}$ subject to the constraint $g(x, y) = y - x^2 + 3 = 0$.

Solution:

We set up the Lagrangian $L(x, y; \lambda) = \mathrm{e}^{-(x^2+y^2)/2} + \lambda\big(y - x^2 + 3\big)$. Setting the higher dimensional gradient $\boldsymbol{\nabla}_3 = \left(\dfrac{\partial}{\partial x}, \dfrac{\partial}{\partial y}, \dfrac{\partial}{\partial \lambda}\right)$ of L to zero, we get

$$\boldsymbol{\nabla}_3 L = \begin{pmatrix} -x\mathrm{e}^{-(x^2+y^2)/2} - 2\lambda x \\ -y\mathrm{e}^{-(x^2+y^2)/2} + \lambda \\ y - x^2 + 3 \end{pmatrix} = \mathbf{0} \quad \text{when} \quad \begin{pmatrix} x \\ y \\ \lambda \end{pmatrix} = \begin{pmatrix} 0 \\ -3 \\ 3\mathrm{e}^{-9/2} \end{pmatrix}.$$

The maximum value of f found at point $(0, -3)$ on the parabola $y = x^2 - 3$ is $f(0, -3) = \mathrm{e}^{-9/2}$. Compare this with the unconstrained maximum of $f = 1$ that is found at the origin $(0, 0)$.

■

✍ Mastery Check 3.5:

Find the maximum and minimum of $f(x, y, z) = x + 2y - 3z$ over the ellipsoid $x^2 + 4y^2 + 9z^2 \leq 108$. Try these two methods of solution:

(1) Construct an argument that the maximum and minimum must both be on the surface of the ellipsoid. Then parameterize the ellipsoid in terms of the usual spherical coordinate angles (see Page 52ff) and look for critical points of f in terms of these angles.

(2) Set up the Lagrangian $L = f + \lambda g$ for suitable g and look for critical points of L.

Use MATLAB® to draw the graph of the ellipsoid and the maximal level set.

✍

3.C Differentials and Error Analysis

Definition 2.4 of a differentiable function allows the following interpretation:

$$f(\boldsymbol{x} + \Delta\boldsymbol{x}) - f(\boldsymbol{x}) \;=\; \operatorname{grad} f(\boldsymbol{x}) \cdot \Delta\boldsymbol{x} + |\Delta\boldsymbol{x}|\rho(\Delta\boldsymbol{x}),$$

or, more simply, that $\quad \Delta f(\boldsymbol{x}; \Delta\boldsymbol{x}) \approx \operatorname{grad} f(\boldsymbol{x}) \cdot \Delta\boldsymbol{x}$ for $|\Delta\boldsymbol{x}| \ll 1$.

This leads to the idea of constructing a new function of both

$$\boldsymbol{x} = (x_1, x_2, \ldots, x_n) \text{ and } \mathbf{d}\boldsymbol{x} = (\mathrm{d}x_1, \mathrm{d}x_2, \ldots, \mathrm{d}x_n).$$

That is, we may construct a function of $2n$ variables called the differential of f.

Definition 3.5
The differential of a function $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ *is defined as*

$$\begin{aligned} \mathrm{d}f(\boldsymbol{x}, \mathrm{d}\boldsymbol{x}) &= \boldsymbol{\nabla} f(\boldsymbol{x}) \cdot \mathrm{d}\boldsymbol{x} \\ &= \frac{\partial f}{\partial x_1}(\boldsymbol{x})\mathrm{d}x_1 + \cdots + \frac{\partial f}{\partial x_n}(\boldsymbol{x})\mathrm{d}x_n. \end{aligned}$$

The function $\mathrm{d}f$ has the following three features:

(1) It is an approximation to the change in f, Δf, coming from a change $\boldsymbol{x} \to \boldsymbol{x} + \mathrm{d}\boldsymbol{x}$;

(2) it is linear in $\mathrm{d}\boldsymbol{x}$; and

(3) it is a natural tool to use if considering overall error estimates when individual errors ($\mathrm{d}\boldsymbol{x}$) are known.

The last feature identifies the differential's most useful application.

Suppose we have a quantity f whose value depends on many parameters, say $x_1, \ldots, x_n$. Any errors incurred in measuring the x_i result in an error in the quantity f.

An estimate of the *maximum error* in f is thus given by

$$\left|\mathrm{d}f(\Delta\boldsymbol{x})\right| \leq \left|\frac{\partial f}{\partial x_1}\Big|_{\boldsymbol{x}}\right| |\Delta x_1| + \left|\frac{\partial f}{\partial x_2}\Big|_{\boldsymbol{x}}\right| |\Delta x_2| + \cdots + \left|\frac{\partial f}{\partial x_n}\Big|_{\boldsymbol{x}}\right| |\Delta x_n|, \tag{3.3}$$

by the triangle inequality (Section 1.B).

The right-hand side of Equation (3.3) gives the *maximum* possible error only if one knows the *maximum* uncertainty of the individual x_i. If one knows the *exact* values of the $\mathrm{d}x_i$ (or Δx_i) including their signs then we use the differential $\mathrm{d}f(\boldsymbol{x}, \mathrm{d}\boldsymbol{x})$ directly to give an approximate value to the change $\Delta f = f(\boldsymbol{x} + \Delta\boldsymbol{x}) - f(\boldsymbol{x})$.

3.D Method of Least Squares

In the year 1801 the world of astronomy was excited by the discovery of a new minor planet, Ceres, whose (rough) position in the night sky had been

noted a few times before it vanished from view. The young Carl Friedrich Gauss [22, 23] used a method — one he had worked out while still a student — to plot the orbit of the planet, and he was able to tell astronomers where in the sky to search for it. That method is the subject of this section.

In the first example that follows, we imagine the planet's orbit in the night sky to be a straight line which has to be fitted, in some optimal fashion, to a set of discrete observation points which are subject to errors. In the second example, the method is applied to discrete observations on a supposed planetary orbit. In the third example, the method is extended to continuous domains.

The field of statistics deals with the treatment of observations (*i.e.*, measurements) of variables that are known to be subject to random errors. When we observe two or more variables at once, it is often appropriate to ask what is the relationship between these two variables. This question is the basis of the study known as *regression analysis*. A detailed study of this lies outside the scope of this book, but at its core regression analysis is an application of the differential calculus called the method of least squares, invented independently by Gauss.

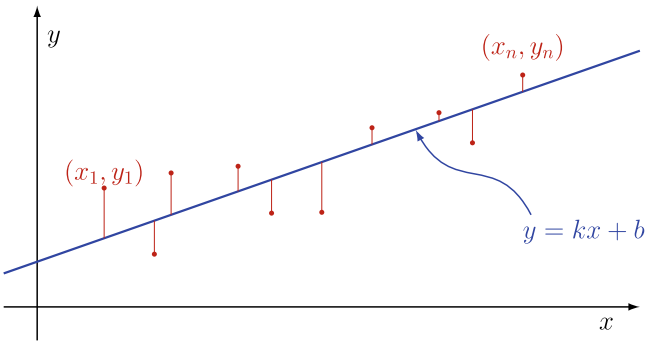


Figure 3.12 The line of best fit.

Fitting a straight line to observations

Suppose we believe that a variable y is in some way dependent on a variable x by the relation $y = kx + b$. In situations such as this it is implicitly assumed that the independent variable is *deterministic*, *i.e.*, it is given and not subject to error, while the dependent variable is subject to observation or measurement errors.

To find the dependency relationship, we select a sequence of values $\{x_1, x_2, \ldots, x_n\}$ of the independent variable, and measure the corresponding values $\{y_1, y_2, \ldots, y_n\}$ of the dependent variable.

Because observed measurements always have some error associated with them, the observations won't necessarily lie exactly on the straight line, but may fall above or below the line, as in Figure 3.12 above.

Problem: How to determine the "line of best fit" $y = k^*x + b^*$ through the "noisy" *discrete* experimental observations. (The values k^* and b^* become estimates of the true parameters k and b in the relation $y = kx + b$ which we believe connects x with y.)

Solution: We choose the line parameters k and b so as to make *the sum of the squares of the differences* between the observations and the fitted values a minimum.

That is, we construct the function $S(k, b) = \sum_{i=1}^{n}(y_i - kx_i - b)^2$ of k and b from the known data and the desired model and seek its minimum to give us the optimal k and b values. We apply the techniques of the preceding chapter to get the critical points of S by solving the two equations

$$\frac{\partial S}{\partial k} = 0 \quad \text{and} \quad \frac{\partial S}{\partial b} = 0.$$

Because of its form, S has no upper bound but does have a lower bound. Moreover, there will be only one critical point which will be the (k, b) point for which S has its minimum value. In fact, with the above explicit expression for S we get the equations

$$\sum_{i=1}^{n} 2(y_i - k^*x_i - b^*)(-x_i) = 0 \quad \text{and} \quad \sum_{i=1}^{n} 2(y_i - k^*x_i - b^*)(-1) = 0.$$

That is, $\sum_{i=1}^{n} x_i y_i - k^* \sum_{i=1}^{n} x_i^2 - b^* \sum_{i=1}^{n} x_i = 0$ and $\sum_{i=1}^{n} y_i - k^* \sum_{i=1}^{n} x_i - nb^* = 0.$

This pair of equations leads to the 2×2 matrix equation

$$\begin{pmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & n \end{pmatrix} \begin{pmatrix} k^* \\ b^* \end{pmatrix} = \begin{pmatrix} \sum x_i y_i \\ \sum y_i \end{pmatrix},$$

which can be solved to give the optimal k^* and b^*.

Mastery Check 3.6:

Invert this matrix equation to obtain explicit estimates of k^* and b^*.

Hint: First define symbols $\bar{x} = \sum x_i/n$, etc.

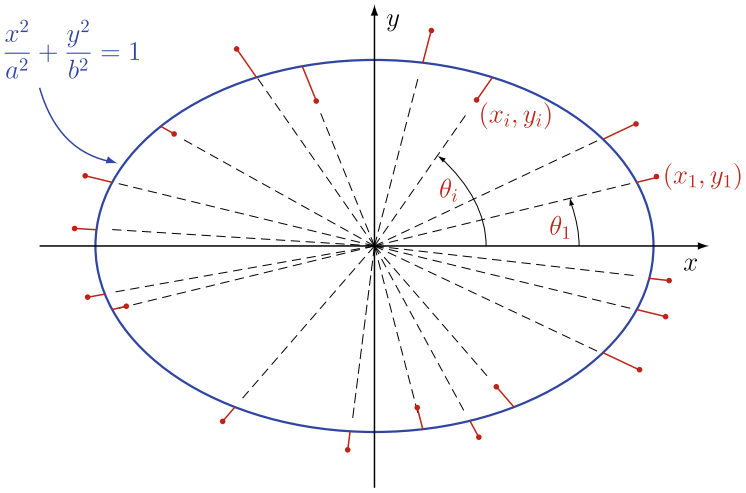


Figure 3.13 The ellipse of best fit.

Fitting a conic to observations

There is nothing unique about fitting straight lines: observations can follow other functional forms depending on the problem being considered.

Suppose, for example, the observations $\{(x_i, y_i)\}$ are scattered in the shape of an ellipse with the origin as centre. (Remember the case of the minor planet.) We want to determine that ellipse,

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1,$$

with optimal a and b that best represent the observations.

It is convenient at this point to convert to polar coordinates (Page 40)

$$(x_i, y_i) \longrightarrow (r_i, \theta_i) : \begin{cases} x_i &= r_i \cos\theta_i, \\ y_i &= r_i \sin\theta_i, \end{cases} \quad i = 1, 2, \ldots, n.$$

Choose as error function E the sum of squares of the distances of the observation pairs (x_i, y_i) from the corresponding points $\big(x(\theta_i), y(\theta_i)\big)$ on the ellipse along the rays at the given θ_i (the independent variables), as in Figure 3.13.

What we are doing from here on is assuming that the angles θ_i have no associated errors, but that the radial distances r_i *are* subject to error. Analogous to the straight line example we form the sum of squares of differences

$$\begin{aligned} E &= \sum_{i=1}^{n} \Big[\big(x(\theta_i) - x_i\big)^2 + \big(y(\theta_i) - y_i\big)^2 \Big] \\ &= \sum_{i=1}^{n} \Big[(a - r_i)^2 \cos^2\theta_i + (b - r_i)^2 \sin^2\theta_i \Big] \end{aligned}$$

As before, look for the critical points of $E(a, b)$ with respect to a and b.

$$\frac{\partial E}{\partial a} = 0 \qquad \text{and} \qquad \frac{\partial E}{\partial b} = 0.$$

The 2×2 system of equations can be solved to give the optimal ellipse parameters

$$a^* = \frac{\sum_{i=1}^{n} r_i \cos^2\theta_i}{\sum_{i=1}^{n} \cos^2\theta_i} \qquad \text{and} \qquad b^* = \frac{\sum_{i=1}^{n} r_i \sin^2\theta_i}{\sum_{i=1}^{n} \sin^2\theta_i}.$$

✍ Mastery Check 3.7:

Solve the equation pair, $\partial E/\partial a = 0$ and $\partial E/\partial b = 0$, where E is the above sum of squares, to verify the expressions for the optimum parameters a^* and b^*.

✍

Least-squares method and function approximations

The least-squares method admits a continuous version in which an integral replaces the discrete sum and a continuously varying function replaces the discrete observations. In truth, the function need not be continuous, only integrable. However, for this introduction it suffices to stay with the more restrictive but less complicated case. One motivation for approximating one function by another is if the original function, required as input into a complex series of subsequent calculations, is either only available as numerical data or is analytic but too complicated to work with. In either case it becomes more expedient to perform calculations on a simpler, approximating function at the expense of a manageable degree of error.

Obtaining the best approximation to a function f with an approximating function g within the context of simple least squares, is already the resolution of many deeper theoretical questions. Suffice it to say that some of the more fundamental questions that will be avoided here are: By what stan-

dard or "measure" does one determine what is the "best" approximation? Is the "measure" itself a reliable tool? What conditions do the approximating functions need to satisfy? How dependent on the choice of approximating function is the quality of the approximation? Since the interest here is on the application of differential calculus, we defer to dedicated texts for answers to these fundamental questions. For our purposes it is enough to focus on the particular and appropriate least squares "measure" and some simple g functions. Excellent texts on this subject are [12] and [13], which can be reviewed for more complete theoretical treatments.

Suppose $f : \mathbb{R} \longrightarrow \mathbb{R}$ is the given continuous function that is to be approximated on some interval $a \leq x \leq b$, which may be infinite. In addition, suppose $g(x; \lambda_1, \ldots, \lambda_n)$ is the "approximating" function, where $\{\lambda_i\}_{i=1}^n$ is a potential set of n parameters.

Appropriately for our least squares theme, the measure that is most often considered and one that is the most convenient to gauge best fit approximations is

$$I_2 = \left[\int_a^b \big(f(x) - g(x; \lambda_1, \ldots, \lambda_n) \big)^2 \, \mathrm{d}x \right]^{1/2},$$

which mathematicians refer to as the L_2 distance function, the L_2 measure, or the L_2 norm. Having defined the norm, it is common practice to use an even simpler version. Since the square root function is monotonic (*i.e.* if the argument increases, then so too does the square root) it suffices to simply seek the minimum of the square, I_2^2, of the L_2 norm, rather than the minimum of I_2 itself. For expedience then we shall continue this common practice in the following.

Clearly, the integral I_2 is an explicit function of the parameter set $\{\lambda_i\}$ (and an implicit functional of g). As in the discrete cases discussed earlier, the objective is to determine those parameters λ_i that minimize I_2. Obviously, I_2 cannot have an absolute upper bound as one can choose a g function that is arbitrarily far from f. On the other hand, the integral has a theoretical absolute lower bound of zero. The true value lies somewhere between these extremes: $0 \leq I_2 < \infty$. In the form taken by I_2, it is clearly a differentiable function of the λ_i variables. Consequently, its critical points are determined by setting all of its first partial derivatives (or those of I_2^2) to zero. For completely arbitrary $g(x; \lambda_1, \ldots, \lambda_n)$, the resulting n equations will generally be nonlinear which may indicate multiple solutions, *i.e.*, multiple critical points. If that were the case, then each critical point would need to be identified and corresponding values of the integral compared to ascertain which point is the global minimum.

Fortunately, this difficulty is eliminated with a suitable choice of approximating function g. This is usually a linear function of the λ_i. The general structure of such *linear approximating functions* is

$$g(x;\lambda_1,\ldots,\lambda_n)=\sum_{i=1}^{n}\lambda_i\phi_i(x),$$

where the individual functions $\phi_i(x)$ are independent in the sense that no one function can be written as a linear combination of the others. The ϕ_i may be chosen to satisfy some criteria specific to the problem being considered, such as satisfying the same conditions as f at the endpoints, $x=a$ and $x=b$. Or, if f is an even or odd function, then ϕ_i functions that mimic this behaviour may be chosen. The choice may also depend on the interval, [a,b]. If infinite, then ϕ_i functions that have appropriate decaying behaviour in the limit of $x\to\pm\infty$ would be chosen. Some simple examples of linear approximating functions (*i.e.*, the ϕ_i functions) are:

$$g(x;\lambda_0,\ldots,\lambda_n) = \lambda_0+\lambda_1x+\cdots+\lambda_nx^n \quad \text{—polynomial approximation}$$

$$g(x;\lambda_1,\ldots,\lambda_n) = \sum_{k=1}^{n}\lambda_n\sin kx \quad \text{—trigonometric (sine) approximation}$$

With the choices made of (a) a linear approximating function $g(x;\lambda_1,\ldots,\lambda_n)$ and (b) the $\phi_i(x)$, the zero partial derivatives of I_2^2 easily lead to the n equation set,

$$\frac{\partial I_2^2}{\partial\lambda_i}=0 \quad\Rightarrow\quad \int_a^b f(x)\phi_i(x)\mathrm{d}x=\sum_{j=1}^{n}\lambda_j\int_a^b\phi_j(x)\phi_i(x)\mathrm{d}x, \quad i=1,\ldots,n.$$

This is a system of linear equations, called the *normal equations*, for the n parameters λ_i, $i=1,\ldots,n$. It is clear that if a finite solution exists, it will be unique. Hence, there is at most one critical point $\{\lambda_i^*\}_{i=1}^n$ which, based on the above statements, must then be a minimum point of I_2.

A solution will exist provided the matrix of coefficient factors,

$$\left[\int_a^b\phi_j(x)\phi_i(x)\mathrm{d}x\right], \qquad i,j=1,2,\ldots,n,$$

is non-singular. This is readily proved if the ϕ_i functions are independent. However, a further simplifying condition makes this unnecessary.

A convenient and desirable property that is very often a factor in the choice or design of the ϕ_i functions, is that they be orthogonal over the interval $[a,b]$. That is, the ϕ_i functions are chosen or designed so that they satisfy the integral conditions,

$$\int_a^b\phi_i(x)\phi_j(x)\mathrm{d}x=0, \quad \text{for} \quad i\neq j.$$

Such functions are called *orthogonal functions* on the interval $[a, b]$. For orthogonal functions, the matrix of coefficients simplifies to a diagonal matrix of strictly positive diagonal elements and is then non-singular. With orthogonal functions, ϕ_i, the least squares problem is effectively solved to give the optimal parameters expressed in the form,

$$\lambda_i^* = \frac{\int_a^b f(x)\phi_i(x)\mathrm{d}x}{\int_a^b \left(\phi_i(x)\right)^2 \mathrm{d}x}, \quad i = 1, \ldots, n.$$

Moreover, with orthogonal functions it is easy to show, using the quadratic form criteria in Section 3.A, that the critical point is indeed a minimum point.

Example 3.9:

Determine constants $\{\lambda_k\}_{k=1}^n$ that give the best least squares approximation

$$f(x) = \frac{\pi}{4} \approx \sum_{k=1}^{n} \lambda_k \sin(kx), \qquad \text{for} \qquad x \in (0, \pi).$$

Solution:

This example demonstrates that the least square's method is useful even to approximate constants over some interval. We seek optimal values λ_k^* that minimize the integral

$$I_2^2 = \int_0^\pi \left(\frac{\pi}{4} - \sum_{k=1}^{n} \lambda_k \sin(kx) \right)^2 \mathrm{d}x.$$

Using Leibniz's integration rule, the partial derivatives of I_2^2 give

$$\frac{\partial I_2^2}{\partial \lambda_k} = \int_0^\pi 2 \left(\frac{\pi}{4} - \sum_{l=1}^{n} \lambda_l \sin(lx) \right) (-\sin(kx))\, \mathrm{d}x = 0, \qquad \text{for} \quad k = 1, \ldots, n.$$

For each index k we have,

$$\frac{\pi}{4} \int_0^\pi \sin(kx)\mathrm{d}x = \sum_{l=1}^{n} \lambda_l \int_0^\pi \sin(lx)\sin(kx)\mathrm{d}x.$$

The left hand side becomes,

$$\frac{\pi}{4\lambda_k}\left(1 - \cos(k\pi)\right) = \frac{\pi}{4\lambda_k}\left(1 - (-1)^k\right) = \begin{cases} 0, & k = 2j, \\ \dfrac{\pi}{2(2j-1)}, & k = 2j-1, \end{cases} \qquad j = 1, 2, \ldots$$

On the other hand, two cases arise for the integrals on the right hand side: when $k = l$ (diagonal cases) and when $k \neq l$ (off diagonal cases). In the latter case we have

$$\begin{aligned}\int_0^\pi \sin(lx)\sin(kx)\mathrm{d}x &= \frac{1}{2}\int_0^\pi [\cos((l-k)x) - \cos((l+k)x)]\,\mathrm{d}x,\\ &= \frac{1}{2}\left[\frac{\sin((l-k)x)}{(l-k)} - \frac{\sin((l+k)x)}{(l+k)}\right]_0^\pi,\\ &= 0, \quad \text{since } \sin(x) = 0 \text{ at } x = 0 \text{ and } m\pi, \text{ for } k \neq l.\end{aligned}$$

This zero result indicates that $\sin(kx)$ and $\sin(lx)$ are orthogonal over $0 \leq x \leq \pi$ for $k \neq l$.

Alternatively, when $k = l$ the right hand side reduces to

$$\int_0^\pi (\sin(kx))^2\,\mathrm{d}x = \frac{1}{2}\int_0^\pi [1 - \cos(2kx)]\,\mathrm{d}x = \frac{\pi}{2} - \frac{1}{2}\left[\frac{\sin(2kx)}{2k}\right]_0^\pi = \frac{\pi}{2}.$$

We are thus led to the approximation

$$\frac{\pi}{4} \approx \sum_{j=1}^{m} \frac{\sin((2j-1)x)}{2j-1}, \quad \text{for} \quad 0 < x < \pi.$$

It is clear that there is no equality when $x = 0$ or $x = \pi$. A demonstration of the accuracy of the calculation appears in Figure 3.14 showing the approximations based on 8 and 16 terms in the sum, respectively. At their respective peaks and troughs, well within the open interval $(0, \pi)$, the differences $|f(x) - g(x; \lambda_1, ..)|$ are demonstrably less in the case of $n = 16$ terms than in the case of $n = 8$ terms.

■

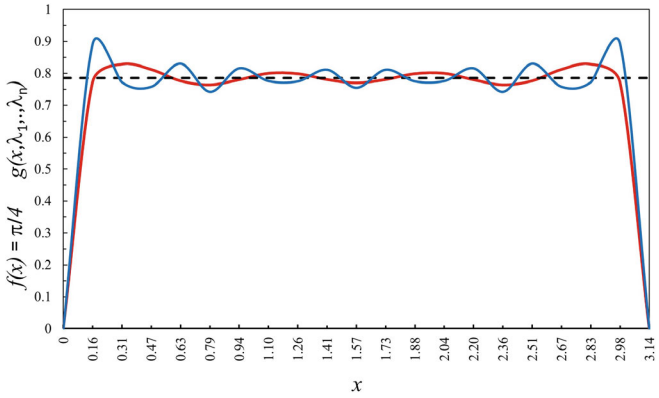


Figure 3.14 Best approximations of $\pi/4$ (black dashed line), by a sum of $n = 8$ (blue solid line) and $n = 16$ (red solid line) sine functions.

✍ Mastery Check 3.8:

Determine the best approximations for the function $f(x) = \frac{\pi}{4}$ under the following conditions

(i) $g(x; \lambda_1, ..\lambda_n) = \sum_{k=1}^{n} \lambda_k \cos(kx)$, over the interval $-\frac{\pi}{2} < x < \frac{\pi}{2}$.

(ii) $g(x; \lambda_1, ..\lambda_n) = \sum_{k=1}^{n} \lambda_k \sin(kx)$, over the interval $-\frac{\pi}{2} < x < \frac{\pi}{2}$.

(iii) $g(x; \lambda_1, ..\lambda_n) = \sum_{k=1}^{n} \lambda_k \cos(kx)$, over the interval $0 < x < \pi$.

Graph these best approximations for a number of n values. Compare the three results as well as the best approximation obtained in Example 3.9. What conclusions can be drawn about the appropriateness of the functions involved in relation to $f(x)$ and the interval?

✍

3.E Partial Derivatives in Equations: Partial Differential Equations

Although we treat the topic of partial differential equations (PDEs) as an application of differential calculus, the body of knowledge of PDEs is immense and can (and sometimes does) easily cover several thick volumes of dedicated texts. Our coverage keeps with the idea of giving only some basic practical information that students of engineering and science will find beneficial in their undergraduate studies, and possibly later.

While PDEs—which are simply scalar-valued equations that describe fixed relationships between the various partial derivatives of a scalar function—come in all shapes and sizes, the type that has been most thoroughly studied and on which we will focus is the *second-order, linear PDE*. The following definition features a scalar function u of two independent variables. However, second-order linear PDEs may depend on more than two variables.

Definition 3.6
A second-order, linear PDE with constant coefficients satisfied by a function $u \in C^2(\mathbb{R}^2)$ *on a domain* $D_u \subset \mathbb{R}^2$ *is an equation of the form*

$$Lu \;=\; Au_{xx} + 2Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu + G \;=\; 0,$$

where the constant real numbers A, B, C, D, E, F *satisfy the condition* $A^2 + B^2 + C^2 \neq 0$, *and* $G(x, y)$ *is a real-valued function defined on* D_u.

Even in this restrictive case there is a quite a lot known. Unfortunately, the following remarks and other comments made in this section do not do justice to the discipline or to the effort that has gone into accumulating all that is known. Nevertheless, it is hoped that the reader will become somewhat better oriented with the subject based on the salient terminology and information provided here.

Remarks

* In this section subscripts x, y, and t on the dependent variable u will denote partial derivatives w.r.t. those variables.

* The "L" as used here and in many texts will denote a "linear partial differential operator" with the property that $L(u + v) = Lu + Lv$.

* "Second order" refers to the highest *order* of partial derivative appearing in an equation.
— a *third order* PDE would have one or more of $u_{xxx}, u_{xxy}, \ldots, u_{yyy}$.

* "Linear" refers to PDEs containing terms which are *at most* proportional to u or one of its derivatives. — $G(x, y)$ *does not* involve u.

* The term "PDE" means an equation relating a function to its partial derivatives, or relating partial derivatives to one another.

* The function u is called a *solution* of the PDE.

* The PDE relationship applies locally in an open domain D_u but not on the boundary ∂D_u.

* A *time-dependent* PDE generalizes Definition 3.6 to include an explicit dependence on the time variable t through additional terms involving partial derivatives of u with respect to t.

Definition 3.7
The quantity $B^2 - AC$ is called the discriminant of the PDE.

The reader may speculate that this discriminant is somehow connected with the discriminant appearing in the solution of a quadratic equation. The connection *is* there and *is* important but would take us too far afield to explain what it is about. The curious reader might refer to the bibliography [14, 15, 16, 18] for more information. However, for our purposes it is sufficient to just state without proof some important facts.

Firstly, the value of the discriminant (more significantly its sign) determines the type or nature of the PDE. A PDE is said to be of

(a) hyperbolic type $\iff B^2 - AC > 0$;

(b) elliptic type $\iff B^2 - AC < 0$;

(c) parabolic type $\iff B^2 - AC = 0$.

These types of PDE exhibit distinctively different behaviour with regard to their properties and conditions. So too do their solutions.

Summary of some relevant facts

* Linearity
  - Adding any number of possible solutions leads to a new solution. Solutions $u_1(x, y)$, $u_2(x, y)$, and constants α and β, can be combined to give a new solution: $\alpha u_1(x, y) + \beta u_2(x, y)$
  - The solutions are not unique, since any scalar multiple of a solution is also a solution.
  - To get uniqueness we impose additional conditions, which are used to specify the scalar multipliers needed. These conditions are classed as either *initial* conditions (for PDEs involving time derivatives) or *boundary* conditions (for PDEs involving spatial derivatives).

* Initial conditions
  Initial conditions are needed for the solution of time-dependent PDEs and inform how the solution begins. They are of the form:
  - "initial displacement": $u(\cdot, t = 0) = u_0(\cdot)$, with $u_0(\cdot)$ specified;

- "initial velocity": $u_t(\cdot, t = 0) = v_0(\cdot)$, with $v_0(\cdot)$ specified;

where the "$\cdot$" indicates that other independent variables apply.

∗ Boundary conditions
Boundary conditions on the domain boundary ∂D_u relate to spatial-dependent PDEs.

These are of three forms:

- Dirichlet conditions
$u(\boldsymbol{r} = \boldsymbol{r}_b, t) = U_b(\boldsymbol{r}_b, t)$, with U_b specified at $\boldsymbol{r}_b \in \partial D_u$.
- Neumann conditions (Figure 3.15)
Let $\boldsymbol{N}(\boldsymbol{r}_b)$ be the outward normal to the boundary ∂D_u. Then the Neumann condition fixes the normal component of the solution gradient $\boldsymbol{\nabla} u(\boldsymbol{r} = \boldsymbol{r}_b, t) \cdot \boldsymbol{N}(\boldsymbol{r}_b) = V_b$, with V_b specified at $\boldsymbol{r}_b \in \partial D_u$.

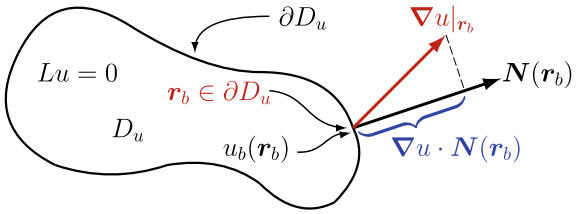


Figure 3.15 Neumann condition on the boundary of domain D_u.

- Cauchy conditions
These specify both the solution and the normal component of the solution gradient at the same point.

$$u(\boldsymbol{r} = \boldsymbol{r}_b, t) = U_b(\boldsymbol{r}_b, t), \boldsymbol{\nabla} u(\boldsymbol{r} = \boldsymbol{r}_b, t) \cdot \boldsymbol{N}(\boldsymbol{r}_b) = V_b(\boldsymbol{r}_b, t),$$

with U_b and V_b specified at $\boldsymbol{r}_b \in \partial D_u$.

∗ Mixed conditions
These are needed for solutions of PDEs that depend on both time and space in bounded spatial domains.

$$\text{For example,} \quad \begin{cases} u(\boldsymbol{r}, t = 0) = u_0(\boldsymbol{r}), \\ u(\boldsymbol{r} = \boldsymbol{r}_b, t) = U_b(\boldsymbol{r}_b), \\ \boldsymbol{\nabla} u(\boldsymbol{r} = \boldsymbol{r}_b, t) \cdot \boldsymbol{N}(\boldsymbol{r}_b) = V_b(\boldsymbol{r}_b). \end{cases}$$

(U_b, V_b are not time-dependent. Contrast this set with the boundary condition set on Page 217, Equation (3.7).)

∗ Rule of thumb for applying these conditions
- We need as many initial conditions as the order of the highest order time derivative;

- We need as many boundary conditions as the order of the highest order spatial derivative in *each independent* variable.

∗ Types of PDE

- The discriminant (Definition 3.7) indicates the type of PDE under consideration. In turn, the type dictates what additional conditions are needed and allowed in order to determine a unique solution to the problem.
- It is easily shown [15] that any second-order, linear PDE can be reduced to one of three forms in the respective classes of *hyperbolic*, *elliptic*, and *parabolic* PDE. We illustrate these forms by means of the most common example from each class.

Classic equations of mathematical physics

Heeding the last bullet point, we focus attention on three classic equations of mathematical physics: the Laplace equation (*elliptic*), the diffusion equation (*parabolic*) and the wave equation (*hyperbolic*). The applications in which they arise are mentioned in their respective sections below. Suffice to say that their solutions play central roles in describing a wide range of physical phenomena.

The Laplace equation

The Laplace equation is perhaps the PDE with the longest history, dating back to the late 18th century when it was introduced by Pierre-Simon Laplace [20] in the context of astronomy. Apart from being the equation satisfied by a free-space gravitational potential, the PDE also arises in the context of the steady dynamics of an incompressible fluid, and is satisfied by the electrostatic potential in electrostatic theory and the velocity potential in linear acoustic theory [16, 18]. Regardless of their different physical origins, the mathematical properties of the solutions are the same.

Definition 3.8
Suppose $u \in C^2(\mathbb{R}^3)$. *The equation*

$$u_{xx} + u_{yy} + u_{zz} = 0 \tag{3.4}$$

satisfied by u *in an open domain* $D_u \subset \mathbb{R}^3$ *is called the (three-dimensional)* **Laplace equation** *(***potential equation***).*

Remarks

∗ The Laplace equation is an example of an *elliptic* PDE.

* The appropriate boundary conditions to use to establish a unique solution of Laplace's equation are of Dirichlet type (Page 206).

Definition 3.9
The 2D Dirichlet Problem
Let D_u be a simply-connected bounded region in $\mathbb{R}^2$ and let ∂D_u be its boundary. Let $g(x, y)$ be a continuous function on ∂D_u. Then the Dirichlet problem is to find the (unique) function $u = f(x, y)$ such that

(a) u is defined and continuous on $\bar{D}_u$ (closure of D_u),

(b) u satisfies the 2D Laplace equation, $u_{xx} + u_{yy} = 0 \; \forall \; (x, y) \in D_u$,

(c) $u = g(x, y) \; \forall \; (x, y) \in \partial D_u$.

* There exists a branch of pure mathematics called *harmonic analysis* that specializes on analyzing the properties and behaviour of solutions of the 2D Laplace equation.

Definition 3.10
A function $u = f(x, y) \in C^2(\mathbb{R}^2)$ that is a solution of the 2D Laplace equation ($u_{xx} + u_{yy} = 0$) is called a **harmonic function**.

* Equation (3.4) is sometimes abbreviated $\Delta u \equiv \nabla^2 u \equiv \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} u = 0$, where $\boldsymbol{\nabla} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$ is the gradient operator, and $\Delta \equiv \nabla^2 \equiv \boldsymbol{\nabla} \cdot \boldsymbol{\nabla}$ — called the *Laplace operator* or *Laplacian operator*.

* All terms appearing in the Laplace equation involve the unknown function u. It is therefore said to be a *homogeneous* PDE. If a term not involving u were present it would then be an example of an *inhomogeneous* equation.

Definition 3.11
Suppose $u \in C^2(\mathbb{R}^3)$ and $g \in C(\mathbb{R}^3)$. The equation

$$\Delta u = u_{xx} + u_{yy} + u_{zz} = g(x, y, z)$$

satisfied by u in an open domain $D_u \cap D_g \subset \mathbb{R}^3$ is called a **Poisson equation** *(inhomogeneous version of the Laplace equation).*

∗ The Laplacian operator (appearing in 3D diffusion, potential, and wave problems) can be expressed in different forms depending on the problem geometry. The most common and the most studied forms are those shown in Figure 3.16 (see Section 1.D).

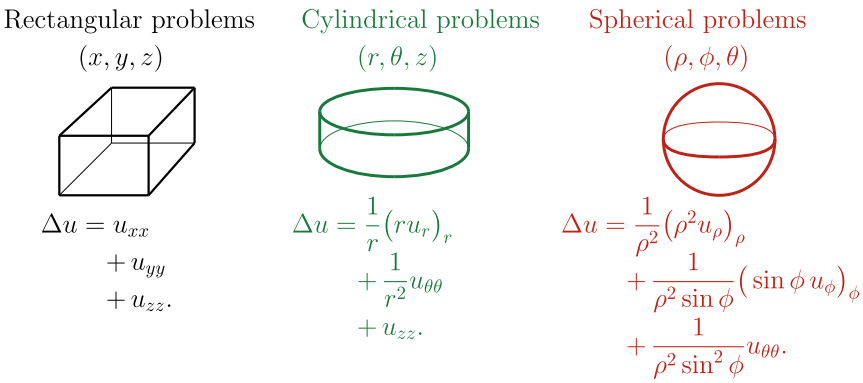


Figure 3.16 The Laplacian expressed in different curvilinear coordinates.

In Figure 3.16 we have used the notation introduced in the first remark immediately following Definition 2.3, where subscripts denote partial differentiation with respect to the variable featured in the subscript. For example,

$$(r u_r)_r \equiv \frac{\partial}{\partial r}\left(r \frac{\partial u}{\partial r}\right).$$

The diffusion equation

The diffusion equation is also commonly referred to as the equation of conduction of heat. The equation is satisfied by a function describing the temporal and spatial development of temperature in uniform medium. In the early 1800s Jean-Baptiste Joseph Fourier [20] provided the first in-depth study of this equation in the context of heat transfer, and of its solution by an innovative (for that time) solution method [16, 18]. The equation, with the same form and therefore with the same mathematical properties of its solution, is also satisfied by a function describing the concentration of material diffusing by random processes. The diffusion equation also arises in problems as diverse as radiative transfer, insect migration and the spread of infection.

Definition 3.12
Suppose $u \in C^2(\mathbb{R}^3 \times [0,\infty))$. *The equation*

$$\frac{\partial u}{\partial t} - k\Big(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\Big) = 0$$

satisfied by u *in the domain* $D_u \subset \mathbb{R}^3 \times [0,\infty)$ *is called the (three-dimensional)* **diffusion equation** *(***heat equation***).*

Remarks

* The diffusion equation is an example of a *parabolic* PDE.
* The appropriate supplementary conditions for the diffusion equation are of mixed type, with one initial condition and Dirichlet or Neumann boundary conditions.
* When u is the *temperature* at point $\boldsymbol{r}$ at time t the diffusion equation is called the *heat equation*.
* The constant k is called the thermal *diffusivity*: $k = \dfrac{K}{s\rho}$, where K is thermal *conductivity*, ρ is *mass* density, and s is *specific heat*.

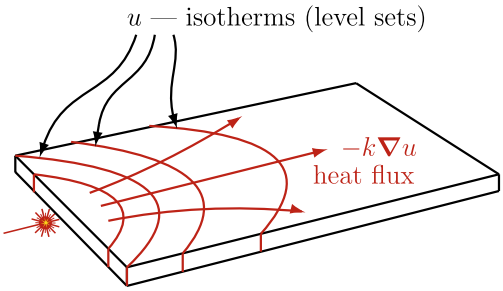


Figure 3.17 Illustration of heat diffusion in a slab.

The observant reader will have noticed our depiction in Figure 3.17 of the local heat flux being orthogonal to the isotherms. The gradient operator has that property, and moreover points in the direction of increasing scalar (isotherm) values. The negative sign inherent in the heat flux definition, shown in Figure 3.17, reverses that direction.

* The 3D diffusion (heat) equation can be abbreviated

$$\frac{\partial u}{\partial t} = k\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}u = k\Delta u$$

(Δ — the Laplacian operator.)

* In the limit $t \to \infty$, $\dfrac{\partial u}{\partial t} \to 0$, and $u(\boldsymbol{r}, t \to \infty) \to u_\infty(\boldsymbol{r})$,

  the steady-state solution of the Laplace equation: $\Delta u_\infty = 0$. Thus, the Laplace equation is the temporal limit of the diffusion equation.

The boundary-value problem for the diffusion equation

For some $b > 0$ consider $\bar{R}$ to be the closed set $\bar{R} = \{(x,t) : 0 \le x \le \pi,\ 0 \le t \le b\}$ with boundary $\partial R = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4$ where

$$\Gamma_1 = \{(0,t) : 0 \le t \le b\}, \quad \Gamma_2 = \{(x,0) : 0 \le x \le \pi\},$$
$$\Gamma_3 = \{(\pi,t) : 0 \le t \le b\}, \quad \Gamma_4 = \{(x,b) : 0 \le x \le \pi\}.$$

Definition 3.13
The boundary-value problem for the 1D heat-conduction problem is to find a function $u = f(x,t)$ such that

(a) f is continuous on $\bar{R}$,

(b) f satisfies the heat (diffusion) equation in R,

(c) f satisfies $f(0,t) = g_1$ on Γ_1; $f(\pi,t) = g_3$ on Γ_3; $f(x,0) = g_2$ on Γ_2.

Remarks

* Note that there is no explicit condition to be satisfied on Γ_4!

* The upper bound b could be taken as large as desired. The only restriction is that $b > 0$. That is, we *solve forward in time*. In fact, we often take $b = \infty$ so the time variable $t \in [0, \infty)$.

* The conditions to be applied on Γ_1 and Γ_3 are *boundary conditions*, while the condition on Γ_2 is an *initial condition*.

And, in terms of the time variable t and space variable x,

* The boundary conditions $u(0,t) = g_1(t)$ and $u(\pi,t) = g_3(t)$ describe the case of prescribed end temperatures, which may be time-dependent.

* The boundary conditions on Γ_1 and Γ_3 may instead be $u_x(0,t) = h_1(t)$ and $u_x(\pi,t) = h_3(t)$ which describe the case of *prescribed end heat fluxes*: rates at which heat is conducted across the ends.
  If $h_1 = h_3 = 0$, the ends are *insulating*. That is, there is no heat conduction.

The wave equation

The wave equation is the third classic equation of mathematical physics we discuss. As the name suggests it is an equation governing wave-like phenomena; not simply propagation, but oscillatory motion. Its discovery is associated with the names of the 18th-century mathematicians Jean-Baptiste d'Alembert (1D version) and Leonard Euler (3D version) [20]. The equation governs the linear dynamics of water waves, sound waves in linear acoustics, linear elastic vibrations in solid mechanics, and light waves in electromagnetism [16, 18].

Definition 3.14
Suppose $u \in C^2(\mathbb{R}^3 \times \mathbb{R})$. *The equation*

$$u_{tt} - c^2(u_{xx} + u_{yy} + u_{zz}) = G(x,y,z,t) \tag{3.5}$$

satisfied by u *in an open domain* $D_u \subset \mathbb{R}^3 \times \mathbb{R}$ *is called the (three-dimensional)* **wave equation**. *Here,* c *is called the* wave speed, *and* G *is defined on* D_u.

Remarks

* The wave equation is an example of a *hyperbolic* PDE.

* The appropriate supplementary conditions for a unique solution of the wave equation are either of Cauchy type for unbounded domains or of mixed type for bounded domains.

* Unlike the diffusion equation, the wave equation can be solved forwards or backwards in time.

* If $G(x,y,z,t) \equiv 0$ then Equation (3.5) is the *homogeneous* wave equation.

* The wave speed c is also called the phase speed of propagation of information.

* The general form of Equation (3.5) can be abbreviated

$$\frac{\partial^2 u}{\partial t^2} - c^2 \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} u = \frac{\partial^2 u}{\partial t^2} - c^2 \Delta u = G(x, y, z, t)$$

(Δ — the Laplacian operator.)

Having introduced a few classic equations, we now need to discuss ways in which their solutions can be obtained. Two ideas are presented below, with their potential scope for practical use explored further in the examples and supplementary exercises.

A PDE-specific method of solution: Change of variables

The following discussion is presented in terms of functions of only two variables. In theory, higher dimensional cases can be considered similarly but usually with increased practical difficulty.

In the study of composite functions and their derivatives (Section 2.G) a variety of relationships were revealed to exist between the derivatives of composite functions and the derivatives of their outer and inner functions. For example, consider again Case 3 (Page 115). A C^2 function $f : \mathbb{R}^2 \to \mathbb{R}$, $f(s,t)$, is composed with a C^2 vector function $\boldsymbol{g} : \mathbb{R}^2 \to \mathbb{R}^2$, $\boldsymbol{g}(x,y) = \big(g(x,y), h(x,y)\big)$, to define a composite function $F : \mathbb{R}^2 \to \mathbb{R}$,

$$F(x,y) = \big(f \circ \boldsymbol{g}\big)(x,y) = f\big(g(x,y), h(x,y)\big).$$

Applying the chain rule to the first and second order partial derivatives of F with respect to x and y, it has been shown that these can be related to partial derivatives of f with respect to s and t as follows,

$$\begin{aligned}
F_x &= f_s g_x + f_t h_x, \qquad F_y = f_s g_y + f_t h_y,\\
F_{xx} &= f_s g_{xx} + f_t h_{xx} + f_{ss}\big(g_x\big)^2 + 2 f_{st} g_x h_x + f_{tt}\big(h_x\big)^2,\\
F_{yy} &= f_s g_{yy} + f_t h_{yy} + f_{ss}\big(g_y\big)^2 + 2 f_{st} g_y h_y + f_{tt}\big(h_y\big)^2,\\
F_{xy} &= f_s g_{xy} + f_t h_{xy} + f_{ss} g_x g_y + f_{st}\left(g_x h_y + g_y h_x\right) + f_{tt} h_x h_y.
\end{aligned}$$

Based on these first and second order partial derivatives, it is theoretically possible, given a convenient choice of inner functions, $g(x,y)$ and $h(x,y)$, for the change of variables to assist in the solution of a second order PDE. The strategy involves transforming a given PDE in a function $F(x,y)$ to a simpler PDE in the function $f(s,t)$.

For example, using the above equations, a 2nd order linear PDE in the function $F(x,y)$ (combining zero and first order derivative terms into a single term H) transforms to,

$$\begin{aligned}
&A(x,y)F_{xx} + 2B(x,y)F_{xy} + C(x,y)F_{yy} + H\left(x, y, F_x, F_y, F\right)\\
&\qquad = f_{ss}\widetilde{A}(s,t) + 2 f_{st}\widetilde{B}(s,t) + f_{tt}\widetilde{C}(s,t) + \widetilde{H}\left(s, t, f_s, f_t, f\right),
\end{aligned} \tag{3.6}$$

where, for convenience, the f, f_s, and f_t are similarly clustered in the $\widetilde{H}$ term, and where the coefficients of the second order derivatives of f – *which theoretically are functions of* s *and* t – are given by,

$$\widetilde{A} = (g_x\,,\, g_y) \begin{pmatrix} A & B \\ B & C \end{pmatrix} \begin{pmatrix} g_x \\ g_y \end{pmatrix}, \quad \widetilde{C} = (h_x\,,\, h_y) \begin{pmatrix} A & B \\ B & C \end{pmatrix} \begin{pmatrix} h_x \\ h_y \end{pmatrix},$$

and

$$\widetilde{B} = (g_x\,,\, g_y) \begin{pmatrix} A & B \\ B & C \end{pmatrix} \begin{pmatrix} h_x \\ h_y \end{pmatrix}.$$

From the more important, second order terms on the right hand side of Eq (3.6), it is straightforward to verify that

$$\widetilde{B}^2 - \widetilde{A}\widetilde{C} = \left(B^2 - AC\right)\left(g_x h_y - g_y h_x\right)^2 = \left(B^2 - AC\right)\left[\frac{\partial(g,h)}{\partial(x,y)}\right]^2.$$

Hence, the sign of $B^2 - AC$ is invariant under a nonsingular transformation, $\frac{\partial(g,h)}{\partial(x,y)} \neq 0$. This means that the class in which a PDE falls (whether hyperbolic, elliptic or parabolic) does not change under an invertible transformation. It also follows that by means of a suitable transformation using functions g and h it is possible to convert a 2D linear PDE into one of the standard forms (such as the 2D Laplace equation, 1D wave equation, or 1D diffusion equation).

A thorough study of this approach lies outside the scope of this book, but briefly it amounts to solving equations such as $\widetilde{A} = 0$ for g and $\widetilde{C} = 0$ for h in the hyperbolic case; $\widetilde{C} = 0$ for h and $\widetilde{B} = 0$ in the parabolic case; and $\widetilde{A} = \widetilde{C}$ and $\widetilde{B} = 0$ in the elliptic case.

For instance, the hyperbolic case requires g to be the solution of the first order, nonlinear PDE,

$$A(x,y)\left(g_x\right)^2 + 2B(x,y)g_x g_y + C(x,y)\left(g_y\right)^2 = 0.$$

Similarly, for the function h. Solutions of this equation, and analogous equations in the other cases, are called *characteristics* of the PDE. It can be shown that for a hyperbolic PDE, there are two sets of real characteristics; for parabolic PDEs, there is one set of real characteristics; and for elliptic PDEs there are no real characteristics.

For a pursuit of a more complete study the reader is referred to more specialist texts such as [15, 18]. In line with this book's focus on multivariable calculus, on the other hand, we shall short circuit the analysis and simply suggest a change of variables in the exercises. By way of introduction, the simplest case of g and h, being linear functions of their independent variables, is taken up in Example 3.10.

Example 3.10:

Suppose $u : \mathbb{R}^2 \to \mathbb{R}$ is a C^2 function of variables (x, y). With the help of the change of variables $s = x + cy$ and $t = x - cy$, transform the hyperbolic, 1D wave equation

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial y^2} = 0$$

into a simpler form involving a function $U(s, t)$ and thereby determine all possible C^2 functions that solve the wave equation.

Solution:

We introduce the following change of variables

$$s = g(x, y) = x + cy, \qquad t = h(x, y) = x - cy,$$

where c is a constant - *the wave speed*. With these changes, the partial derivatives of the function

$$u(x, y) = u\left((s + t)/2, (s - t)/2c\right) = U(s, t),$$

become

$$\begin{aligned} \frac{\partial u}{\partial x} &= \frac{\partial U}{\partial s}\frac{\partial g}{\partial x} + \frac{\partial U}{\partial t}\frac{\partial h}{\partial x} = U_s.1 + U_t.1, \quad \text{and} \\ \frac{\partial u}{\partial y} &= \frac{\partial U}{\partial s}\frac{\partial g}{\partial y} + \frac{\partial U}{\partial t}\frac{\partial h}{\partial y} = U_s.c - U_t.c. \end{aligned}$$

The second derivatives are no more complicated, since the first derivatives only involve constant multiples of U_s and U_t:

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} &= \frac{\partial}{\partial x}\left(U_s + U_t\right) = U_{ss}.1 + U_{st}.1 + U_{ts}.1 + U_{tt}.1, \\ &= U_{ss} + 2U_{st} + U_{tt}, \end{aligned}$$

the last equality is valid since u is a C^2 function. Similarly,

$$\begin{aligned} \frac{\partial^2 u}{\partial y^2} &= \frac{\partial}{\partial y}\left(cU_s - cU_t\right) = c\left[\left(U_{ss}.c - U_{st}.c\right) - \left(U_{ts}.c - U_{tt}.c\right)\right], \\ &= c^2\left[U_{ss} - 2U_{st} + U_{tt}\right]. \end{aligned}$$

Combining these two pure second-order derivatives in the combination directed by the wave equation, we get some cancellation,

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial y^2} = 4U_{st} = 0.$$

The latter is itself a PDE, which is simple to integrate. Holding s fixed and integrating w.r.t. t we get (ignoring the inconsequential numerical multiplier)

$$\frac{\partial U}{\partial s} = f(s) \quad - \text{ an unknown function of the restrained variable, } s.$$

Integrating again, but this time w.r.t. s, we find

$$U(s,t) = \int^{s} f(s')\mathrm{d}s' + K(t).$$

At this last step we note that a partial integration w.r.t. s implies that t is held constant. That is, as in the first integration, the result can only be specified up to an arbitrary function of the variable we've held fixed, in this case t.

Rewriting the answer we have $U(s,t) = F(s) + K(t)$, and returning to the original variables we end with the most general solution of the wave equation,

$$u(x,y) = F(x+cy) + K(x-cy),$$

as required.

We conclude with two comments. Firstly the transformation variables, s and t are called *characteristic variables* and reflect lines in the xy-plane called *characteristics* along which their respective functions - *the contributions to the wave* - are constant, and orthogonal to which the wave motion propagates. In the case of $s = x + cy$ the wave propagates in the direction of negative x, while in the case of $t = x - cy$ the wave propagates in the positive x-direction. In the most general case both terms contribute to the wave motion. Secondly, the transformed equation

$$\frac{\partial U}{\partial s \partial t} = 0,$$

is called a *canonical form* of the hyperbolic wave PDE.

■

A general-purpose method of solution: Separation of variables

The method we shall now describe is based on the fact that the linear PDEs just described are *separable* in a number of coordinate systems. This means that their solutions can be expressed in terms of factors involving only one variable. A necessary assumption is that one of the coordinates of the system of choice is constant over a surface on which boundary conditions are prescribed. The method is actually applicable to a wider variety of linear PDEs than the ones that are here highlighted, defined on bounded or semi-bounded domains. Consequently, all students should be familiar with this method of

solution [15, 16, 18]. We illustrate the approach by applying it to a simple problem involving 1D wave propagation.

Consider the following *mixed boundary-value problem* on the space-time, semi-infinite strip $D_u = [a, b] \times [0, \infty)$ shown in Figure 3.18. Note that this problem involves one space dimension x and one time dimension t.

Definition 3.15
The 1D wave problem. *Find a function* $u(x, t)$ *on* $D_u \subset \mathbb{R} \times [0, \infty)$ *such that for functions* g_1 *and* g_2 *defined on* $[a, b]$ *and continuous functions* h_1 *and* h_2 *on* $[0, \infty)$, u *satisfies the homogeneous wave equation*

$$\left.\begin{array}{rl} & u_{tt} - c^2 u_{xx} = 0, \\ \textit{with } \textbf{initial conditions} & \left\{\begin{array}{lcl} u(x,0) & = & g_1(x) \\ u_t(x,0) & = & g_2(x) \end{array}\right\} a \le x \le b \\ \textit{and } \textbf{boundary conditions} & \left\{\begin{array}{lcl} u(a,t) & = & h_1(t) \\ u(b,t) & = & h_2(t) \end{array}\right\} t \ge 0. \end{array}\right\} \quad (3.7)$$

Remarks

* Equation (3.7) is a quite general form of a mixed b.v.p. for the wave equation in one space variable, but not the most general (see Supplementary problem 3.32).

* The smoothness (that is, degree of differentiability) of the boundary data, h_1 and h_2, and the initial data, g_1 and g_2, determine the smoothness of the solution $u(x, t)$.

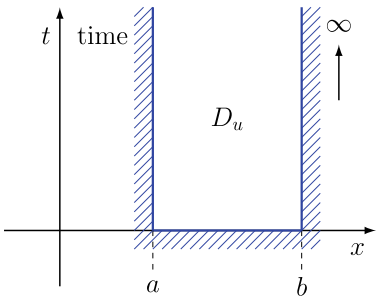


Figure 3.18 Domain D_u of the 1D wave problem.

To illustrate the separation of variables method we consider the special case:

$$(h_1, h_2, g_1, g_2) = (0, 0, g, 0).$$

Similar analyses apply in the other special cases: $(0, 0, 0, g)$, $(0, h, 0, 0)$, etc.

For the most general case of h_1, h_2, g_1, and g_2 all nonzero, we appeal to the *principle of superposition* (defined shortly). For the moment, we consider the simpler mixed b.v.p.

$$\left.\begin{array}{rcll} u_{tt} - c^2 u_{xx} & = & 0, & \\ u(x,0) & = & g(x), & 0 \le x \le L \\ u_t(x,0) & = & 0, & 0 \le x \le L \\ u(0,t) = u(L,t) & = & 0, & t \ge 0 \end{array}\right\} \tag{3.8}$$

Remarks

* Equation (3.8) is the mathematical model of a vibrating string of length L and density ρ under tension τ, fixed at its ends and subject to small displacements elsewhere along its length (Figure 3.19).

* $c = \sqrt{\dfrac{\tau}{\rho}}$; the *wave speed* is determined by the string properties.

* If $g \equiv 0$ then the unique solution would be $u \equiv 0$.
— a typical way of proving uniqueness

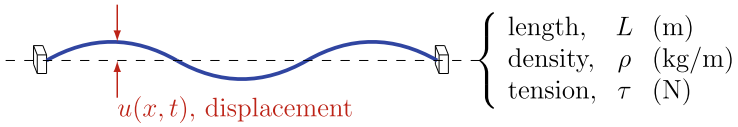
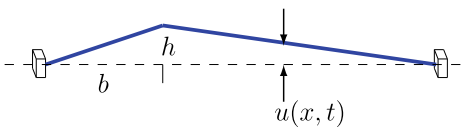


Figure 3.19 Schematic of a vibrating string.

For the vibrating string problem, u ($|u| \ll L$) is the local dynamic displacement of the stretched string at position x at time t. One sets the string vibrating either by "plucking" or "striking", or any linear combination of these. In our example we have chosen the first means. Suppose the string is pulled aside at $t = 0$ a distance h from equilibrium at $x = b$ (Figure 3.20) and released. This condition defines the function $g(x)$.



$$g(x) = \begin{cases} \dfrac{xh}{b} & \text{for } x \in [0, b] \\ \dfrac{(L-x)h}{L-b} & \text{for } x \in [b, L]. \end{cases}$$

Figure 3.20 Profile $g(x)$ of a string stretched a distance h at $x = b$.

We proceed in steps through the separation of variables method of solution of this problem.

Step 1:

The separation of variables method always begins by assuming a nontrivial solution in the form of a product of functions of the independent variables. In this case we assume the form

$$u(x,t) = X(x)T(t).$$

That is, the solution is a product of a function of x only (X) and a function of t only (T).

Substitution into Equation (3.8a) gives

$$X(x)\frac{\mathrm{d}^2T}{\mathrm{d}t^2} - c^2T(t)\frac{\mathrm{d}^2X}{\mathrm{d}x^2} = 0 \tag{3.9}$$

and assuming $X(x) \neq 0$ and $T(t) \neq 0$, Equation (3.9) implies

$$\begin{array}{ccccc} \dfrac{1}{X(x)}\dfrac{\mathrm{d}^2X}{\mathrm{d}x^2} & = & \dfrac{1}{c^2}\dfrac{1}{T(t)}\dfrac{\mathrm{d}^2T}{\mathrm{d}t^2} & = & \mu \\ \left\{\begin{array}{c}\text{function}\\ \text{of } x\text{–only}\end{array}\right\} & = & \left\{\begin{array}{c}\text{function}\\ \text{of } t\text{-only}\end{array}\right\} & = & \{\text{constant}\} \end{array} \tag{3.10}$$

The most critical element of the separation of variables method is the fact that the two expressions on the left of Equation (3.10) can be equal *only* if both equal the same constant! This allows the separation to occur. Equation (3.10) implies two equations

$$\left.\begin{array}{rcl} \dfrac{\mathrm{d}^2X}{\mathrm{d}x^2} & = & \mu X \\ \dfrac{\mathrm{d}^2T}{\mathrm{d}t^2} & = & \mu c^2 T \end{array}\right\} \left(\begin{array}{l}\text{Variables } x \text{ and } t\\ \text{have been separated}\end{array}\right) \tag{3.11}$$

and we have the critical simplifying step:

One PDE in two variables becomes *two ordinary differential equations (ODEs)* in single variables!

This separation is not always possible with other types of problems. Moreover, with some boundaries and some boundary conditions such a product form may not be possible either, even if the PDE allows it.

From this point on we need only to consider the solutions of the ordinary differential equations.

Step 2:

Consider possible values of μ. The boundary conditions (Equation (3.8d)) imply that

$$X(0) = X(L) = 0. \tag{3.12}$$

These are necessary for a unique solution.

- **Case 1:** $\mu = 0$
  Equation (3.11a) implies that $X'' = 0$, which is true if and only if $X(x) = c_1 x + c_2$. But the boundary conditions in Equation (3.12) imply $c_1 = c_2 = 0$.
  That is, $X(x) \equiv 0$

  — the trivial solution.

- **Case 2:** $\mu > 0$, that is, $\mu = k^2 > 0$.
  Equation (3.11a) implies that $X'' - k^2 X = 0 \iff X(x) = c_1 \mathrm{e}^{kx} + c_2 \mathrm{e}^{-kx}$. But the boundary conditions in Equation (3.12) imply

$$\left.\begin{array}{lrcl} x = 0: & c_1 + c_2 & = & 0 \\ x = L: & c_1 \mathrm{e}^{kL} + c_2 \mathrm{e}^{-kL} & = & 0 \end{array}\right\} \implies \begin{pmatrix} 1 & 1 \\ \mathrm{e}^{kL} & \mathrm{e}^{-kL} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0$$

$$\implies c_1 = c_2 = 0 \implies X(x) \equiv 0$$

  — the trivial solution again.

- **Case 3:** $\mu < 0$, that is $\mu = -k^2 < 0$.
  Equation (3.11a) implies that $X'' + k^2 X = 0$, which is true if and only if $X(x) = c_1 \cos kx + c_2 \sin kx$. And Equation (3.12) gives us

$$\begin{array}{lllll} X(0) = 0 & \implies & c_1 . 1 = 0 & \implies & c_1 = 0 \\ X(L) = 0 & \implies & c_2 \sin kL = 0 & \implies & c_2 = 0 \text{ or } \sin kL = 0 \end{array}$$

  A nontrivial solution is possible only if $kL = \pi, 2\pi, 3\pi, \ldots$, an integer multiple of π, and $c_2 \neq 0$.

The only nontrivial solutions are multiples of

$$X_n(x) = \sin\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, 3, \ldots .$$

Definition 3.16

$\mu = -k^2 = -\left(\frac{\pi}{L}\right)^2, -\left(\frac{2\pi}{L}\right)^2, -\left(\frac{3\pi}{L}\right)^2, \ldots$ *are called* **eigenvalues** *or* **characteristic values**.

$X_n(x) = \sin\left(\frac{n\pi x}{L}\right), \ n = 1, 2, 3, \ldots$ *are called* **eigenfunctions** *or* **characteristic functions**.

Step 3:

This choice of μ has implications for the solution of Equation (3.11b):

$$T''(t) + k^2c^2T(t) = 0, \quad k = \frac{\pi}{L}, \frac{2\pi}{L}, \frac{3\pi}{L}, \dots$$

means that for each possible k we get an independent solution. The coefficients of independent solutions will also depend on the values of k:

$$T_n(t) = A_n \cos\left(\frac{n\pi ct}{L}\right) + B_n \sin\left(\frac{n\pi ct}{L}\right), \ n = 1, 2, 3, \dots .$$

meaning that for each possible k we get a solution of (3.8a) satisfying (3.8d).

$$u_n(x,t) = \left(A_n \cos\left(\frac{n\pi ct}{L}\right) + B_n \sin\left(\frac{n\pi ct}{L}\right)\right)\sin\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, 3, \dots .$$

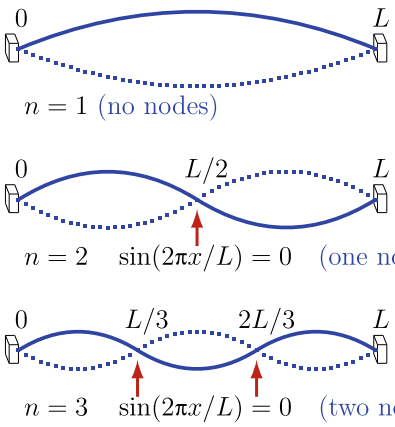
Since all the infinite n cases are possible solutions, called *harmonics*, the *principle of superposition* says that the most general solution is their linear combination. We have therefore an infinite series solution,

$$u(x,t) = \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right)\left(A_n \cos\omega_n t + B_n \sin\omega_n t\right),$$

which describes the most general vibration of the ideal string fixed at its ends.

Remarks

* The boundary conditions determine the *allowed* k's and ω's.
* $k_n = \dfrac{n\pi}{L} = \dfrac{2\pi}{\lambda_n}$, where the λ_n are the allowed *wavelengths*.
* $\omega_n = \dfrac{n\pi c}{L}$ are the allowed angular *frequencies* — *eigenfrequencies*.
* $\omega_n = \dfrac{n\pi c}{L} = n\omega$. That is, ω_n is an integer multiple of the *fundamental frequency* $\omega = \dfrac{\pi c}{L}$ — the nth *harmonic overtone.*
* $u_n(x,t) = \left(A_n \cos\omega_n t + B_n \sin\omega_n t\right) \sin\left(\dfrac{n\pi x}{L}\right)$ describe the nth *normal mode* of vibration, the first few examples of which are shown in Figure 3.21.



The *fundamental mode*
— greatest amplitude-
always set in motion?

The *first harmonic*
— lower amplitude
— twice fund. frequency
— not present when . . . ?

The *second harmonic*
— lower amplitude still
— thrice fund. frequency
— not present when . . . ?

Figure 3.21 The first few modes of vibration.

These are also some physical points to note at this stage.

* If the string is pulled aside (plucked) anywhere along its length then the fundamental mode, shown at the top of Figure 3.21, will be present in the solution, since the fundamental mode features displacement at all points.

* On the other hand, a given harmonic is not present in the solution when the plucked point coincides with any of that harmonic's nodes. For example, if the string were to be plucked at its centre, the implied displacement would be inconsistent with that point being a node—a point of no motion. Consequently, the first harmonic mode (and any others that feature a node at the centre) cannot be included in the series expansion.

* $\dfrac{\omega_n}{k_n} = \dfrac{n\pi c}{L} \cdot \dfrac{L}{n\pi} = c = \sqrt{\dfrac{\tau}{\rho}}$ — the same speed for all modes.

Step 4:

To determine the unknown constants, $\{A_n\}_{n=1,2,\ldots,\infty}$ and $\{B_n\}_{n=1,2,\ldots,\infty}$, we apply the initial conditions of Equations (3.8b) and (3.8c). These imply that

$$u(x,0) \;=\; \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi x}{L}\right) \;\equiv\; g(x), \tag{3.13}$$

and

$$u_t(x,0) \;=\; \sum_{n=1}^{\infty} B_n.\omega_n \sin\left(\frac{n\pi x}{L}\right) = 0. \tag{3.14}$$

Equation (3.14) tells us that

$$B_n = 0 \ \forall \ n,$$

and Equation (3.13) tells us that there exists a Fourier sine series for $g(x)$, with coefficients

$$A_n = \frac{2}{L}\int_0^L g(x)\sin\left(\frac{n\pi x}{L}\right)\mathrm{d}x.$$

Given an initial form such as that represented in Figure 3.20, the A_ns can be determined and inserted in the series solution.

More general initial conditions of either plucked or struck strings are described by functions such as

$$\begin{cases} u(x,0) &= u_0(x) &\text{—} & \text{string shape at } t=0, \\ u_t(x,0) &= v_0(x) &\text{—} & \text{string speed at } t=0. \end{cases}$$

These conditions, or any linear combination of these conditions, are invoked to give $\{A_n, B_n\}$ in the more general case:

$$\begin{cases} A_n &= \dfrac{2}{L}\displaystyle\int_0^L u_0(x)\sin\left(\frac{n\pi x}{L}\right)\mathrm{d}x \\ B_n &= \dfrac{2}{\omega_n L}\displaystyle\int_0^L v_0(x)\sin\left(\frac{n\pi x}{L}\right)\mathrm{d}x \end{cases}$$

With all unknowns determined, the problem is solved.

Remark

* The string system just considered is a good model for a string attached to an electric guitar. The electric guitar body is (usually) solid. It is therefore appropriate to assume the string ends are fixed. The body itself undergoes very little vibration of its own (if any) while the string is vibrating. Consequently, the notes registered by an electric guitar are almost as pure as those determined mathematically.

  This differs fundamentally from the case of an acoustic guitar. The body of an acoustic guitar is hollow with the strings attached at one end to its flexible top plate. The vibrations of the strings are therefore transferred in part to the vibrations of the top plate (the ensuing air vibrations in the body are in fact responsible for a large proportion of the sound produced).

  To describe the vibrations of a string on an acoustic guitar it is therefore more reasonable to adopt the model of one end of the string attached to a moveable mass which is subject to an elastic restoring force. However, even in this case it can be shown that discrete vibration modes arise. Although related by a mathematical formula, the

frequencies of the higher-order modes are not simple multiples of a fundamental frequency. (See Supplementary problem 3.32.)

✍ Mastery Check 3.9:

Redo the 1D wave vibrating string problem, Eq (3.7), for the initial and boundary condition set,

$$(h_1, h_2, g_1, g_2) = (0, 0, 0, g(x)), \quad \text{for } 0 \le x \le 2.$$

✍

3.F Supplementary Problems

§3.A.1. Use a Taylor series approximation to find the nature of any critical points for the function

$$f(x, y) = (x + y)\mathrm{e}^{-x^2-y^2}, \quad \text{for } \{(x, y) : x^2 + y^2 \le 1\}.$$

2. Locate and classify the critical points of the following functions:

   (a) $f(x, y) = \mathrm{e}^{-x^2}\left(2xy + y^2\right)$,
   (b) $f(x, y) = y^3 + 3x^2y - 3x^2 - 3y^2 + 2$,
   (c) $f(x, y) = x^2y - 5xy + 6y + z^2x + z^3$,
   (d) $f(x, y) = x^3 - y^3 - 2xy + 6$,
   (e) $f(x, y) = (y - 1)\left(x^2 - 2y - 2\right)$.

*3. (a) Working from first principles, show that the following are sufficient conditions for the critical point $\boldsymbol{x}_0 = (x_0, y_0, z_0)$ of the function $f(x, y, z)$ to be a local minimum:

   (i) $f_{zz}(\boldsymbol{x}_0) > 0$
   (ii) $f_{yy}(\boldsymbol{x}_0)f_{zz}(\boldsymbol{x}_0) - \left(f_{yz}(\boldsymbol{x}_0)\right)^2 > 0$
   (iii) $|H(\boldsymbol{x}_0)| > 0$,

   where $|H(\boldsymbol{x}_0)|$ is the determinant of the Hessian matrix of second derivatives evaluated at the critical point $\boldsymbol{x}_0$.

   (b) Based on your analysis state corresponding conditions for $\boldsymbol{x}_0$ to be a local maximum.

   (c) Determine and classify all the critical points of

$$f(x, y, z) = x^2 - 4y^2 + z^2 + y^3 + 2xy - 2yz.$$

   Hint: For part (a), consider the quadratic form $Q = \boldsymbol{h}^T H \boldsymbol{h}$, where H is the Hessian matrix of 2nd derivatives, $\boldsymbol{h}$ is a column vector with components, h, k and l, and $\boldsymbol{h}^T = (h, k, l)$ is a row vector.

*4. (a) Working from first principles, show that the following are sufficient conditions for the critical point $\boldsymbol{x}_0 = (x_0, y_0, z_0)$ of the function $f(x, y, z)$ to be a local minimum:

(i) $f_{xx}(\boldsymbol{x}_0) > 0$

(ii) $f_{xx}(\boldsymbol{x}_0) f_{zz}(\boldsymbol{x}_0) - (f_{xz}(\boldsymbol{x}_0))^2 > 0$

(iii) $|H(\boldsymbol{x}_0)| > 0$,

where $|H(\boldsymbol{x}_0)|$ is the determinant of the Hessian matrix evaluated at the critical point $\boldsymbol{x}_0$.

(b) Based on your analysis, state corresponding conditions for $\boldsymbol{x}_0$ to be a local maximum.

(c) Determine and classify all the critical points of

$$f(x, y, z) = x^3 + 3x^2 + 2y^2 + z^2 + 2xz - 2yz.$$

Hint: For part (a), consider the quadratic form $Q = \boldsymbol{h}^T H \boldsymbol{h}$, where H is the Hessian matrix of 2nd derivatives, $\boldsymbol{h}$ is a column vector with components, h, k and l, and $\boldsymbol{h}^T = (h, k, l)$ is a row vector.

§3.B.5. Show that in the region $\{(x, y); |x| \leq 1,\ |y| \leq 1\}$ the function $f(x, y) = \mathrm{e}^{x^4 - y^4}$ (Figure 3.22(a)) has a critical point which is a saddle point, then determine its maximum and minimum values in the region.

6. Determine the maximum and minimum values of the following functions over their respective regions.

(a) $f(x, y) = x^2 + y^2 - 3x$, over the region $\{(x, y) : |x| + |y| \leq 1\}$.

(b) $f(x, y) = \sin x \sin y \sin(x + y)$, over the region $\{(x, y) : 0 \leq x, y \leq \pi\}$.

(c) $f(x, y) = xy \ln(1 + x^2 + y^2)$, over the region $\{(x, y) : x^2 + y^2 \leq 1\}$.

(d) $f(x, y) = (x + y)\mathrm{e}^{-x^2 - y^2}$, over the region $\{(x, y) : x^2 + y^2 \leq 1\}$ (Figure 3.22(b)).

(e) $f(x, y) = (x + y)\mathrm{e}^{-x^2 - y^2}$, over the region $\{(x, y) : x, y \geq 0, x + y \leq 2\}$ (Figure 3.22(b)).

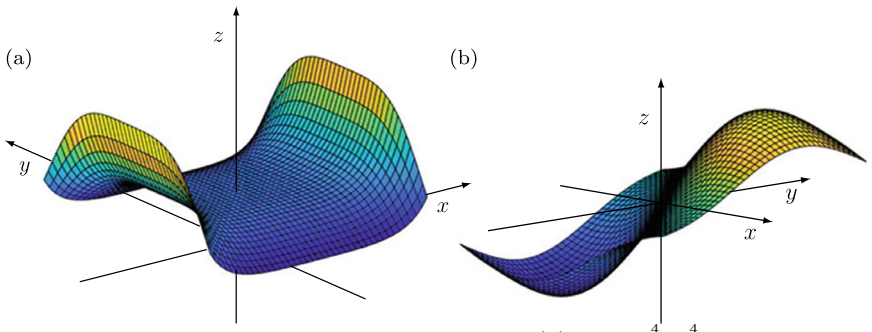


Figure 3.22 The graphs of (a) $z = \mathrm{e}^{x^4 - y^4}$ and (b) $z = (x + y)\mathrm{e}^{-x^2 - y^2}$.

7. Determine the largest and smallest values of the function

$$f(x, y) = \frac{x + 2y + 1}{x^2 + 4y^2 + 1},$$

such that $x^2 + 4y^2 \leq 1$ and $x, y \geq 0$.
Hint: For a useful simplification consider a change of variables $(u, v) = (x, 2y)$.

8. Determine the points of intersection of the two surfaces $x^2 - xy + y^2 - z^2 = 1$ and $x^2 + y^2 = 1$ in $\mathbb{R}^3$ that are closest to the origin, and those that are furthest from the origin.

9. (a) Determine the equation of the plane (P) that is tangent to the surface $z = x^2 + y^2$ (S) at the point $(1, 2, 5)$.

   (b) Determine the maximum distance between a point on S having coordinates (x, y, z_s), and a point on P with coordinates (x, y, z_p), where x and y satisfy the inequality $x^2 + y^2 \leq 0.2$.

*10. Determine the maximum of the function $f(x, y, z) = \log x + \log y + 3 \log z$, over that portion of the sphere $x^2 + y^2 + z^2 = 5r^2$ lying in the first octant. Deduce that

$$abc^3 \leq 27 \left(\frac{a + b + c}{5} \right)^5.$$

*11. Suppose C is the conic described by the equation

$$Ax^2 + 2Bxy + Cy^2 = 1,$$

where $A > 0$ and $B^2 < AC$. If we denote by p and P the distance from the origin to the closest and furthest point on the conic, respectively, show that

$$P^2 = \frac{A + C + \sqrt{(A - C)^2 + 4B^2}}{2(AC - B^2)},$$

with an analogous expression for p^2.

12. Determine the absolute maximum and minimum values of the function,

$$f(x,y) = xy^2 \exp(-xy), \quad \text{over the region } \{(x,y) : 0 \le x \le 2,\ 0 \le y \le b\},$$

where $1 < b < \infty$. Does the function possess a maximum value in the unbounded strip $\{0 \le x \le 2\} \times \{0 \le y < \infty\}$?

*13. (a) Determine the maximum value of $\Big|\sum_{k=1}^{n} a_k x_k\Big|$, if $\sum_{k=1}^{n} x_k^2 = 1$ and $a_k > 0$ for all $k \in \mathbb{N}$. Note that $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$.

(b) Determine the maximum of $(x_1 x_2 \ldots x_n)^2$ under the restriction $\sum_{k=1}^{n} x_k^2 = 1$.

Hint: These are Lagrange multiplier problems, but (a) can also be solved with help from the triangle and Cauchy-Schwarz inequalities.

14. Given that $a, b, c > 0$, determine the maximum of $f(x,y,z) = x^a y^b z^c$ subject to the condition that $x + y + z = 1$, and for $x, y, z \ge 0$.

§3.C.15. Surveyors have measured two sides and the angle between them of a triangular plot of land, for the purpose of finding the area of the plot. The area is given by $f = \frac{1}{2} ab \sin C$, where a and b are the lengths of the sides and C is the included angle. The measurements are all subject to error. The measured values for the sides were $a = 152.60 \pm 0.005$ m and $b = 163.81 \pm 0.005$ m, and for the included angle $\theta = 43°26' \pm 0.2'$.

What is the largest possible error in the computation of the area? What is the largest possible percentage error?

§3.D.16. Suppose we wish to represent the function $f(x) = x^2,\ -1 \le x \le 1$, by a combination of cosine functions of the form

$$g(x; a, b, c, d) = a + b\cos \pi x + c \cos 2\pi x + d \cos 3\pi x.$$

Find the least-squares values of a, b, c, d. Plot the two functions on the same graph to check the fit.

§3.E.17. Show that $u(x,t) = \exp(-x^2/4t)/\sqrt{t}$ is a solution to the parabolic, 1D diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}.$$

18. Show that $u(x, y, t) = t^{-1} \exp(-(x^2 + y^2)/4t)$ is a solution to the parabolic, 2D diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}.$$

19. Suppose $u : \mathbb{R}^3 \to \mathbb{R}$ is a C^2 function of variables (x, y, z). By introducing 3D cylindrical polar coordinates (Section 1.D) confirm the expression for the Laplacian shown in the centre of Figure 3.14, applied to $U(r, \theta, z) = u(r\cos\theta, r\sin\theta, z)$.

20. Suppose $u : \mathbb{R}^3 \to \mathbb{R}$ is a C^2 function of variables (x, y, z). By introducing 3D spherical polar coordinates (Section 1.D) confirm the expression for the Laplacian shown in the right-hand side of Figure 3.14, applied to $U(\rho, \phi, \theta) = u(\rho\sin\phi\cos\theta, \rho\sin\phi\sin\theta, \rho\cos\phi)$.

21. By introducing new variables $\xi = x + y$ and $\eta = \ln|x - y|$ and using the chain rule, determine all C^2 functions that solve the differential equation

$$(x - y)\left(\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2}\right) = 4(x + y)^2.$$

*22. (a) By introducing the change of variables $\xi = x + \mathrm{e}^y$ and $\eta = x - \mathrm{e}^y$, determine the most general solution to the partial differential equation

$$\mathrm{e}^{2y}\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} + \frac{\partial u}{\partial y} = 0.$$

(b) Determine *the unique* solution of the above equation that satisfies the two conditions:

$$u(x, y = 0) = 0, \qquad \frac{\partial u}{\partial y}(x, y = 0) = 1 + x.$$

*23. (a) By invoking the variable transformation $x = \mathrm{e}^u$ and $y = u + v$ transform the partial differential equation

$$x\frac{\partial^2 f}{\partial x \partial y} + \frac{\partial^2 f}{\partial y^2} = 0, \quad \text{for } x > 0,$$

and hence determine the most general solution of the given partial differential equation.

(b) Then, determine *the unique* solution that satisfies the two conditions:

$$f(x, y = 0) = x, \qquad \frac{\partial f}{\partial y}(x, y = 0) = 2\ln x.$$

*24. By introducing new variables, $u = \ln y + \ln x$ and $v = \ln y - \ln x$, for $x, y > 0$, find the unique solution to the partial differential equation

$$x^2 \frac{\partial^2 f}{\partial x^2} - y^2 \frac{\partial^2 f}{\partial y^2} = y \frac{\partial f}{\partial y} - x \frac{\partial f}{\partial x},$$

that satisfies the conditions, $f(1, y) = y^2$ and $f_x(1, y) = 1$.

*25. With help of the change of variables

$$u = g_1(x, y) = x - y \qquad \text{and} \qquad v = g_2(x, y) = \sin(x + y),$$

transform the differential equation,

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + 2 \frac{\partial^2 f}{\partial x \partial y} - 2 \tan(x + y) \left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} \right) = 0,$$

and determine its most general solution.

26. For any C^2 function, f, transform the partial differential equation,

$$x^2 \frac{\partial^2 f}{\partial x^2} - 2xy \frac{\partial^2 f}{\partial x \partial y} + y^2 \frac{\partial^2 f}{\partial y^2} + 3x \frac{\partial f}{\partial x} - y \frac{\partial f}{\partial y} = 1$$

into an equation for $F(u, v) = f\left(\sqrt{\frac{u}{v}}, \sqrt{uv} \right)$ in terms of the new variables u and v. Hence, find the most general solution to the equation for $f(x, y)$.

27. The composite function $z = f(x, y)$ is found to have the form

$$f(x, y) = F\big(h_1(x, y)\big) + G\big(h_2(x, y)\big),$$

where F and G are arbitrary, *single-variable* functions.

(a) Ignoring arbitrary integration constants, determine the functions $h_1(x, y)$ and $h_2(x, y)$ if it is known that f satisfies the equations

$$\begin{aligned} \mathrm{e}^{-x} \frac{\partial f}{\partial x} + y \frac{\partial f}{\partial y} &= 2F'\big(h_1(x, y)\big), \\ \mathrm{e}^{-x} \frac{\partial f}{\partial x} - y \frac{\partial f}{\partial y} &= 2G'\big(h_2(x, y)\big), \end{aligned}$$

where the primes denote differentiation with respect to the *respective* single-variable arguments of F and G.

(b) Show that $z = f(x, y)$ satisfies the differential equation

$$\mathrm{e}^{-2x} \left(\frac{\partial^2 f}{\partial x^2} - \frac{\partial f}{\partial x} \right) = y \left(y \frac{\partial^2 f}{\partial y^2} + \frac{\partial f}{\partial y} \right).$$

Note: This exercise essentially asks for you to determine the transformation necessary to obtain the most general solution of the pde of the form stated.

*28. Let D be a subset of the first octant $\{\boldsymbol{x} \in \mathbb{R}^3 : x, y, z > 0\}$ and suppose

$$F(x, y, z) = xy^2 z\mathrm{e}^z = 1$$

defines $z = f(x, y)$ implicitly as a C^2 function of x and y.
Determine functions $A(x, y)$, $B(x, y)$ and $C(x, y)$ such that $f(x, y)$ is a solution of the partial differential equation,

$$A(x, y)\frac{\partial^2 f}{\partial x^2} + B(x, y)\frac{\partial^2 f}{\partial x \partial y} + C(x, y)\frac{\partial^2 f}{\partial y^2} = 0.$$

Note: The choice of functions A, B, and C is not unique. However, a reasonably obvious and simple choice of A and C presents itself to enable a simple cancelation to occur. Following that, a choice of function B then becomes apparent. This exercise, which brings together implicit function theory and partial differential equations, illustrates that implicit solutions of partial differential equations are also possible.

29 Suppose $u : \mathbb{R}^2 \to \mathbb{R}$ is a C^2 function of time t and radial variable r. Use the method of separation of variables to find the unique solution, $u(r, t)$, of the partial differential equation

$$\frac{\partial u}{\partial t} = k\left(\frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r}\right), \quad \text{for} \quad 0 < r < a,\ t > 0,$$

subject to the initial and boundary conditions

$$\begin{cases} u(r, 0) = 0, & 0 < r < a, \\ u(a, t) = U_0, & t > 0, \\ \lim\limits_{r \to 0} \dfrac{\partial u}{\partial r}(r, t) = 0, & t > 0, \end{cases}$$

where a, k, U_0 are positive (dimensional) constants.
Hint: It may help to introduce a change of dependent variable $v = ru$. Note also that it is necessary to consider *all* cases of separation constant.

30 Use the method of separation of variables to find the general solution to the equation

$$x^2 u_{xx} + x u_x - u_y = 0.$$

Find the particular solution that satisfies the boundary conditions $u(1, 0) = 0,\ u(\mathrm{e}, 0) = 2$.
Hint: At some stage you will need to substitute $x = \mathrm{e}^v$.

31 For the problem defined by Equation (3.8) of a string of length L and density ρ under tension τ, fixed at its ends and pulled aside a distance h at $x = b$, derive a closed-form expression for the string's energy of vibration

$$E = \underbrace{\frac{1}{2}\rho \int_0^L \left(\frac{\partial u}{\partial t}\right)^2 \mathrm{d}x}_{\text{kinetic}} + \underbrace{\frac{1}{2}\tau \int_0^L \left(\frac{\partial u}{\partial x}\right)^2 \mathrm{d}x}_{\text{potential}},$$

using the separation of variables solution.

For the case $b = L/2$ show that the energy is conserved by comparing your result obtained above with the initial work done in pulling the string from its unstretched state.

*32 Redo the 1D wave (vibrating string) problem for initial conditions $(g_1, g_2) = (g(x), 0)$, and boundary conditions

$$\left(u(0,t) = 0, M\frac{\partial^2 u}{\partial t^2}(L,t) = -\tau\frac{\partial u}{\partial x}(L,t) - \kappa u(L,t)\right) \text{ for } M, \kappa > 0.$$

This models a string of length L under tension τ attached at $x = L$ to a mass M subject to an elastic restoring force of strength κ.

33 Using the separation of variables method, derive the unique solution to the mixed b.v.p. describing heat diffusion within a slab.

$$\begin{cases} \text{(a)} & u_t(x,t) = k u_{xx}(x,t) & 0 < x < a,\ t > 0 \\ \text{(b)} & u(0,t) = 0 & t \geq 0 \\ \text{(c)} & u(a,t) = 0 & t \geq 0 \\ \text{(d)} & u(x,0) = g(x) & 0 \leq x \leq a, \text{ where } g(0) = g(a) = 0. \end{cases}$$



Chapter 4

Integration of Multivariable Functions

We have seen that differentiation of a function is the result of a limit process. This process led to the definition of a tangent line to a curve in 2D and a tangent plane to a surface in 3D. In this chapter, we shall again consider limit processes but with the aim of establishing the reverse operation, that of integration of a scalar function of many variables.

The focus of attention will be on integration of scalar functions defined on subsets of $\mathbb{R}^n$. That is, the integrals we consider are taken over zero curvature regions in $\mathbb{R}^n$: a straight line segment in $\mathbb{R}$, a planar region in $\mathbb{R}^2$, a volume subset in $\mathbb{R}^3$, etc. The benefits are both practical and theoretical. Familiar geometric concepts, such as areas (under curves) and volumes (under surfaces) will not only assist theory development but also engender general understanding. In Chapter 5, in contrast, we will revisit 1D and 2D integration but in the sense of integrals over nonzero curvature geometries (curves in $\mathbb{R}^2$ and curved surfaces in $\mathbb{R}^3$). In that context, the geometric interpretations referred to in this chapter will be replaced with other physical properties.

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4.A Multiple Integrals

We set the stage with a brief review of the 1D theory of integration, limiting the discussion to the Riemann theory of integration for a function of one variable. Readers interested in the more general measure theory of Riemann-Stieltjes integration are referred to [1, 4, 6]. A comparison between the foundations of single-variable integration and multivariable integration is particularly fruitful, since the higher dimensional case is essentially a direct generalization of the former case.

Almost every idea introduced and theoretical consequence discussed in this chapter is applicable to functions of an arbitrary finite number of independent, orthogonal variables. However, to simplify the presentation, the theory will (mostly) be discussed with reference to functions of *two* variables. The more general case is briefly commented on at the end of the chapter. Any important practical differences will be highlighted in that discussion.

As already mentioned, the definition of the integral of a function f of $\boldsymbol{x} \in \mathbb{R}^n$ is based on a limit process. We illustrate the first steps of the process in Figure 4.1.

Integration of $f : I \subset \mathbb{R} \longrightarrow \mathbb{R}$

Suppose f is a continuous function of x and suppose that the interval I is closed and bounded and lying in the function domain, D_f. That is,

$$I = \{x : a \leq x \leq b\} \subset D_f.$$

The *graph* of f is a curve in $\mathbb{R} \times \mathbb{R} = \mathbb{R}^2$ as shown in Figure 4.1 below.

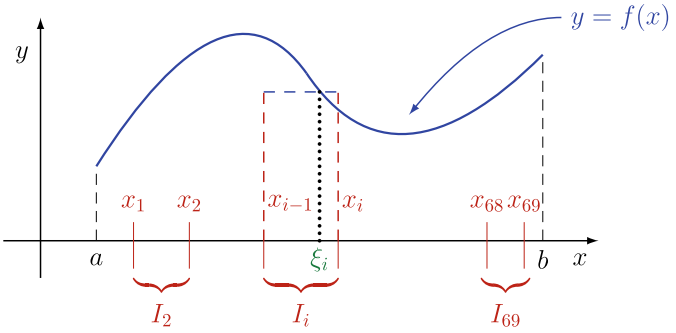

Figure 4.1 The graph of f and some subintervals of I.

A first step towards the goal of evaluating the area under the graph of f is to cut the interval I into small bits —this is called a *partition* of I:

$$a = x_0 < x_1 < x_2 < \ldots < x_{n-1} < x_n = b$$

with n *subintervals* $I_i = \{x : x_{i-1} \le x \le x_i\}$, of width $\Delta x_i = x_i - x_{i-1}$. A few of these subintervals are shown in Figure 4.1.

Then, choosing some real number ξ_i from each subinterval, I_i, we form the sum

$$\sigma_n = \sum_{i=1}^{n} f(\xi_i)\Delta x_i.$$

This is called the *Riemann sum of* f *over* I. So far in the development, the sum σ_n *must* clearly depend on the partition of n subintervals. A different subdivision of I and different choices of ξ_i will lead to a different value of σ_n. This dependence will be eliminated at the next step.

The geometric interpretation of σ_n for $f : I \longrightarrow \mathbb{R}$

If $f \ge 0$, then $f(\xi_i)\Delta x_i$ is the *area* of the rectangle of height $f(\xi_i)$ and width Δx_i as shown here in Figure 4.2.
Hence, the sum σ_n is an approximation to the area "under" the curve $y = f(x)$ and over I.

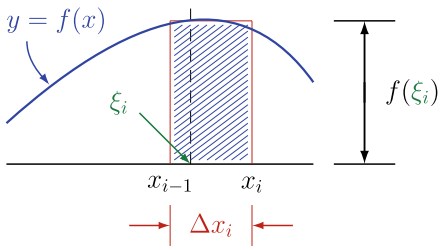

Figure 4.2 Rectangular area approximation.

To improve on this approximation we find numbers ℓ_i and m_i in each interval I_i such that $f(\ell_i) \le f(x) \le f(m_i)$ for all x in I_i. This will be possible because we have assumed f is continuous.

For a given partition we form the upper and lower sums

$$R_{\min} = \sum_{i=1}^{n} f(\ell_i)\Delta x_i \le \sum_{i=1}^{n} f(\xi_i)\Delta x_i \le \sum_{i=1}^{n} f(m_i)\Delta x_i = R_{\max}.$$

In this process, we have constructed upper and lower bounds on σ_n. That is,

$$R_{\min} \le \sigma_n \le R_{\max}.$$

We now take the simultaneous limit of the number of intervals $n \to \infty$ and the representative size of the intervals $\max(\Delta x_i) \to 0$. We find that, as $n \to \infty$, $R_{\min}$ increases and $R_{\max}$ decreases. If the dual limits exist and $\lim R_{min} = \lim R_{max}$, then an application of a squeeze theorem (Page 58) gives:

Definition 4.1
The integral of $f : \mathbb{R} \longrightarrow \mathbb{R}$ *over* I *is defined as the limit (if it exists)*

$$\lim_{\substack{n\to\infty \\ \max(\Delta x_i)\to 0}} \sigma_n = \int_a^b f(x)\,\mathrm{d}x.$$

Under the conditions of continuity of f and compactness of I this limit does exist. This is a unique number, called the *Riemann integral* [1, 4, 5, 6], which is now independent of how we set the partition originally.

Now let's see how things work for a function $f(x, y)$ of two variables.

Integration of $f : R \subset \mathbb{R}^2 \longrightarrow \mathbb{R}$

Suppose f is a continuous function of x and y and, to start with, we are given the closed and bounded rectangular region

$$R = \{(x, y) : a \leq x \leq b,\ c \leq y \leq d\}$$

which lies inside D_f, *i.e.*, $R \subset D_f$ and R is compact.

The *graph* of such a function f is a *surface* in $\mathbb{R}^2 \times \mathbb{R} = \mathbb{R}^3$ as shown in Figure 4.3 below.

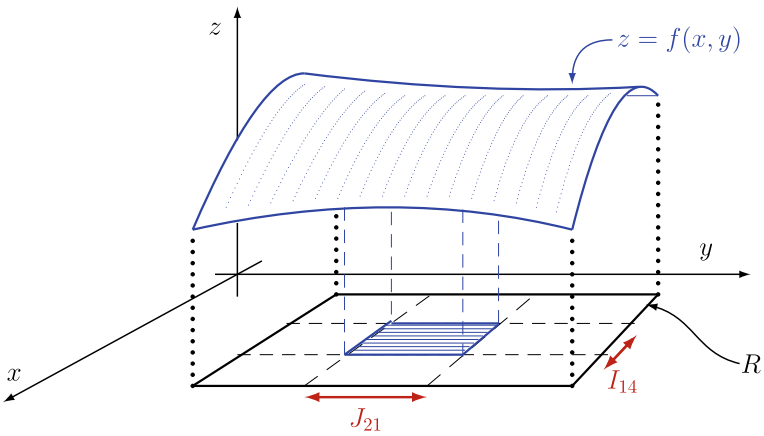

Figure 4.3 The graph of f over rectangle R, and subrectangle $I_{14} \times J_{21}$.

The construction of the integral of f over R is accomplished in perfect harmony with the 1D case except that rectangles replace intervals.

First, the rectangle R is partitioned into $n \times m$ rectangles $R_{ij} = I_i \times J_j$ of area $\Delta A_{ij},\ 1 \leq i \leq n, 1 \leq j \leq m$. We then choose some point (ξ_i, η_j) from each rectangle R_{ij} and form the sum

$$\sigma_{nm} = \sum_{i=1}^{n} \sum_{j=1}^{m} f(\xi_i, \eta_j) \Delta A_{ij}.$$

This is called the *Riemann sum of f over R*. From its construction this Riemann sum *must* therefore depend on the partition.

The geometric interpretation of σ_{nm} for $f : R \subset \mathbb{R}^2 \longrightarrow \mathbb{R}$

If $f \geq 0$, then $f(\xi_i, \eta_j)\Delta A_{ij}$ is the *volume* of the rectangular block of height $f(\xi_i, \eta_j)$ and base area $\Delta A_{ij} = \Delta x_i . \Delta y_j$ as shown in Figure 4.4 below.

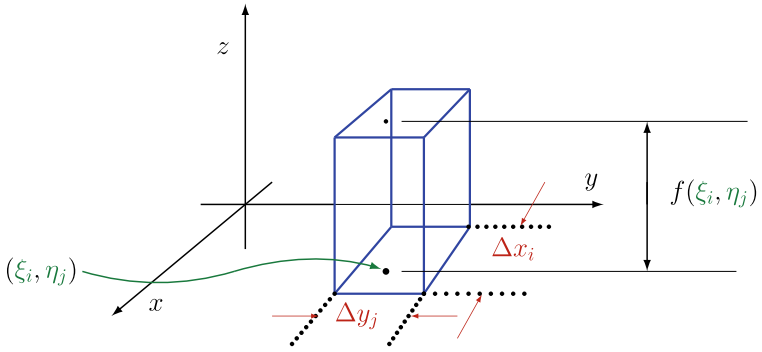

Figure 4.4 Rectangular block volume approximation.

Thus, the sum σ_{nm} is an approximation to the volume "under" the surface $z = f(x, y)$ and over R.

A completely analogous line of reasoning to the steps leading up to the definition of a 1D integral can now be applied as follows.

For a given partition we form upper and lower sums of the rectangular blocks. Between these two sums is the sum σ_{nm}. With each refinement of the partition, new upper and lower sums are determined with the new lower sum increased compared with its predecessor and the new upper sum decreased compared with its predecessor.

If in the dual limit process of $n, m \to \infty$ and $\max\left(\sqrt{(\Delta x_i)^2 + (\Delta y_j)^2}\right) \longrightarrow 0$ the limits of upper and lower sums exist and are equal, an application of the squeeze theorem leads to our next definition.

Definition 4.2
The **double integral** *of* $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$ *over* R *is defined as the limit (if it exists)*

$$\lim_{\substack{m,n\to\infty \\ \max\left(\sqrt{(\Delta x_i)^2+(\Delta y_j)^2}\right)\to 0}} \sigma_{nm} = \iint_R f(x)\,\mathrm{d}A.$$

An important theorem and some corollaries—1D version

Theorem 4.1 *All continuous functions are integrable on compact subsets of their domains of definition.*

Corollary 4.1.1 *If* $f \geq 0$, *then* $\int_I f(x)\,\mathrm{d}x$ *is the area under the curve* $y = f(x)$.

Corollary 4.1.2 *If* $f \geq g \geq 0$, *then* $\int_I \big(f(x) - g(x)\big)\,\mathrm{d}x \geq 0$ *is the area between the curves (Figure 4.5).*

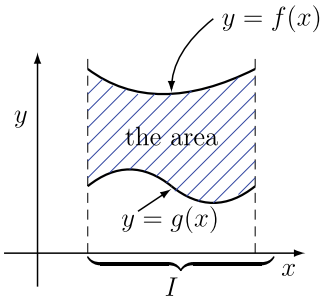

Figure 4.5 The area between two curves in 2D.

Corollary 4.1.3 $\int_I 1\,\mathrm{d}x$ *is the length of interval* I, *denoted* $|I|$.

Corollary 4.1.4 *For a continuous function* f *over compact* I, *there exists at least one point* $X \in I$ *such that*

$$|I|\, f(X) = \int_I f(x)\,\mathrm{d}x \quad - \textit{ 1st mean-value theorem for 1D integrals.}$$

Corollary 4.1.5 *Linearity: If $a, b \in \mathbb{R}$ then*

$$\int_I \big(af(x) + bg(x)\big)\,\mathrm{d}x \;=\; a\int_I f(x)\,\mathrm{d}x + b\int_I g(x)\,\mathrm{d}x.$$

Corollary 4.1.6 *Additivity: (very important)*
If $I \cap J = \{\} = \emptyset$, then $\displaystyle\int_{I\cup J} f(x)\,\mathrm{d}x \;=\; \int_I f(x)\,\mathrm{d}x + \int_J f(x)\,\mathrm{d}x.$

An important theorem and some corollaries—2D version

Theorem 4.1 *All continuous functions are integrable on compact subsets of their domains of definition.*

Corollary 4.1.1 *If $f \geq 0$, then* $\displaystyle\iint_R f(x,y)\,\mathrm{d}A$ *is the volume under the surface $z = f(x,y)$.*

Corollary 4.1.2 *If $f \geq g \geq 0$, then* $\displaystyle\iint_R \big(f(x,y) - g(x,y)\big)\,\mathrm{d}A \geq 0$ *is the volume of the body between the surfaces (Figure 4.6).*

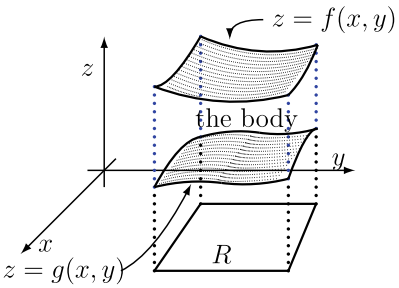

Figure 4.6 The volume between two surfaces in 3D.

Corollary 4.1.3 $\displaystyle\iint_R 1\,\mathrm{d}A$ *is the area of R, denoted $|R|$*

—true for any region!!

Corollary 4.1.4 *For a continuous function f over compact R, there exists at least one point $(X, Y) \in R$ such that*

$$|R|\,f(X,Y) = \iint_R f(x,y)\,\mathrm{d}A \;-\; \textit{1st mean-value theorem for 2D integrals.}$$

Corollary 4.1.5 *Linearity: If $a, b \in \mathbb{R}$ then*

$$\iint_R \big(af(x,y) + bg(x,y)\big)\,\mathrm{d}A \;=\; a\iint_R f(x,y)\,\mathrm{d}A + b\iint_R g(x,y)\,\mathrm{d}A.$$

Corollary 4.1.6 *Additivity: (very important)*
If $R_1 \cap R_2 = \{\} \equiv \emptyset$, then

$$\iint_{R_1 \cup R_2} f(x,y)\,\mathrm{d}A \;=\; \iint_{R_1} f(x,y)\,\mathrm{d}A + \iint_{R_2} f(x,y)\,\mathrm{d}A.$$

Some comments on Theorem 4.1 are warranted.

Theorem 3.2 says that all continuous functions on compact domains are bounded. So, these functions do not exhibit singular behaviour over closed and bounded integration regions. Consequently, all partitions lead to finite areas in the single-variable case and finite volumes in the two variable case. The unique limits in Definitions 4.1 and 4.2 therefore exist.

Corollary 4.1.3 may seem a trivial special case but proves to be particularly useful in some contexts. (See Example 5.23, Section 5.F.)

Corollary 4.1.4 is useful as a theoretical tool in proofs and for further analysis, but also as a means of estimating the numerical value of integrals.

Corollary 4.1.5 allows us to split complex functions into sums of simpler functions and to integrate them individually.

Corollary 4.1.6 is useful when an integration domain is or can be described piecewise, especially if the pieces warrant different techniques of integration.

4.B Iterated Integration in $\mathbb{R}^2$

Iterated integration is the workhorse of multiple integrals.

The definition of the multiple integral as the limit of a sum of rectangular prism volumes is not practical. Fortunately, there is an alternative. Underpinning *iterated integration* is the suggestion that we calculate our "volumes" by *slicing* rather than by *dicing*.

Consider the thin slice of the "body" under f shown in Figure 4.7. The area of the left-hand side face, *i.e.*, the area under the curve of constant y, $y = y_0$, is $A(y_0) = \int_a^b f(x, y_0)\,\mathrm{d}x$. Similarly, $A(y_0 + \Delta y) = \int_a^b f(x, y_0 + \Delta y)\,\mathrm{d}x$ is the area of the right-hand side face.

If $|\Delta y|$ is a small increment then $A(y_0) \approx A(y_0+\Delta y)$, which is easy to show by expanding $f(x, y_0 + \Delta y)$ in a Taylor series about (x, y_0) and keeping just the first two terms (for $\Delta y \ll 1$). Then, using the simple two-point trapezoidal rule approximation, the volume of the "slice" is approximately

$$V(y_0) = \frac{1}{2}\big(A(y_0) + A(y_0 + \Delta y)\big)\Delta y \;=\; A(y_0)\Delta y + O(\Delta y^2).$$

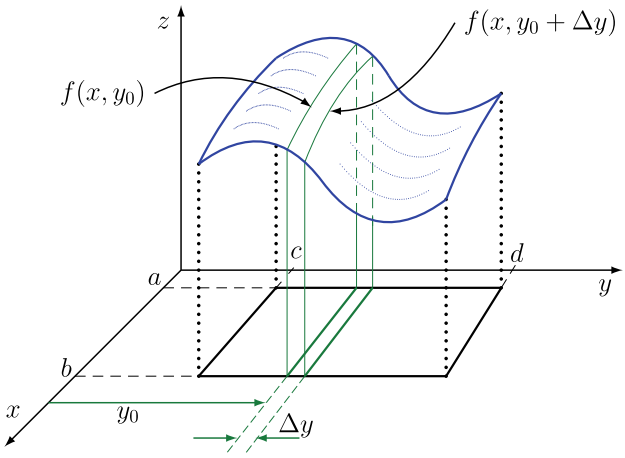

Figure 4.7 Adding slices to determine volumes.

The total volume of the "body" under $f(x, y)$ is then the limiting sum of these 1D volumes of slices (Definition 4.1) as $\Delta y \to 0$. That is, the volume under $f(x, y)$ over R is the Riemann integral of $A(y)$ over the interval $c \le y \le d$:

$$V = \int_c^d A(y)\,\mathrm{d}y = \int_c^d \left(\int_a^b f(x, y)\,\mathrm{d}x \right) \mathrm{d}y.$$

Alternatively, slicing first parallel to the y-axis instead of the x-axis, as we did above, would give

$$V = \int_a^b A(x)\,\mathrm{d}x = \int_a^b \left(\int_c^d f(x, y)\,\mathrm{d}y \right) \mathrm{d}x,$$

which must give the exact same value for the volume.

Hence, for integration of a continuous function over the bounded rectangle $[a,b]\times[c,d]$, we have the important result

$$\underbrace{\iint_R f(x,y)\,\mathrm{d}A}_{\text{double integral of } f \text{ over } R} \;=\; \underbrace{\int_a^b\left(\int_c^d f(x,y)\,\mathrm{d}y\right)\mathrm{d}x \;=\; \int_c^d\left(\int_a^b f(x,y)\,\mathrm{d}x\right)\mathrm{d}y}_{\text{iterated integrals of } f \text{ over } R}$$

The left-hand side is the definition of a double integral, while the two right-hand sides are the actual ways one can evaluate the double integral. These are called the *iterated* integrals of f. In each case of iterated integral, the *inner* integral within the parentheses is to be evaluated first, only then is the *outer* integral evaluated. Notice how in the above equation the integration limits follow the variable being integrated.

At a very practical level, when evaluating the inner integral we treat the *outer integral variable* as if it were a constant parameter. In each such calculation all single-variable techniques apply to each individual iterated integral. Example 4.1 illustrates this process.

Regarding notation, the above clearly specifies the order of operation. However, to skip the parentheses (and avoid the tedium of writing them), we have two alternative notations in common use:

$\displaystyle\int_a^b\int_c^d f(x,y)\,\mathrm{d}y\,\mathrm{d}x$ —this borders on the ambiguous; the user must not confuse the order.

$\displaystyle\int_a^b \mathrm{d}x\int_c^d f(x,y)\,\mathrm{d}y$ —this is somewhat better; it is easier to interpret and better for complex regions (next section). (For convenience we'll use this form in Sections 4.G–4.I).

■ Example 4.1:

Determine the volume under the surface $z=x^2+y^2$ (Figure 4.8) and over the rectangle,

$$R=\{(x,y): 0\le x\le 1,\ 0\le y\le 1\},\ \big(=[0,1]\times[0,1]\big).$$

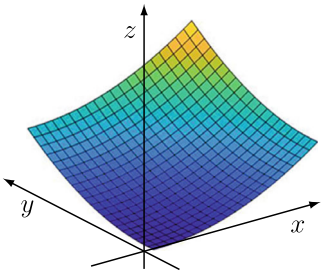

Figure 4.8 The graph of $z = x^2 + y^2$.

Solution:

$$\begin{aligned} V &= \iint_R (x^2+y^2)\,\mathrm{d}A \quad \text{— the double integral} \\ &= \int_0^1 \left(\int_0^1 (x^2+y^2)\,\mathrm{d}x \right) \mathrm{d}y \quad \text{— an iterated integral version} \\ &= \int_0^1 \left(\left[\frac{x^3}{3} + y^2 x \right]_{x=0}^{1} \right) \mathrm{d}y \quad \text{— } y \text{ is held "fixed" during the } x\text{-integration} \\ &= \int_0^1 \left(\frac{1}{3} + y^2 \right) \mathrm{d}y \quad \text{— } x \text{ limits are applied before the } y\text{-integration} \\ &= \left[\frac{y}{3} + \frac{y^3}{3} \right]_0^1 = \frac{2}{3} \text{ volume units.} \end{aligned}$$

In this iterated integral y is given the role of the *outer* integration variable, while x plays the role of *inner* variable. We could just as easily have reversed the roles to arrive at the same result. Notice the very important fact, which will be contrasted with later, that in this example the bounds on the x-integral are constants; they are *not* functions of y!

■

✍ Mastery Check 4.1:

Evaluate $\iint_R y\mathrm{e}^{xy}\,\mathrm{d}A$, where $R = \{(x,y) : 0 \le x \le 1, 0 \le y \le 2\}$.

✍

4.C Integration Over Complex Domains

In general practice a region of integration is more often *not* a rectangle. We therefore need a way to work with compact regions that are more complex. Luckily, we can treat this problem using our previous results, but after first rethinking the function, the domain, and the iteration definitions.

First, let's look at the function and its domain. Given a function f defined on a non-rectangular, compact domain D, we introduce a new function and new domain through the following definition.

Definition 4.3
Suppose $f(x,y)$ is continuous over a compact domain $D \subseteq D_f$. Let $\hat{f}$ be the **extension** *of f beyond D:*

$$\hat{f}(x,y) = \begin{cases} f(x,y), & \text{for} \quad (x,y) \in D, \\ 0, & \text{for} \quad (x,y) \notin D. \end{cases}$$

Since D is bounded there exists a rectangle R such that $D \subset R$. Thus, if $\hat{f}$ is integrable over R, then

$$\underbrace{\iint_D f(x,y)\,\mathrm{d}A}_{\text{definition}} = \underbrace{\iint_R \hat{f}(x,y)\,\mathrm{d}A}_{\text{calculable value}}$$

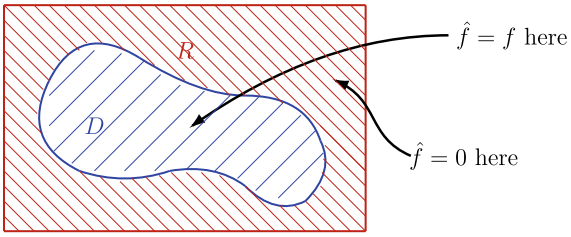

Figure 4.9 The extended function $\hat{f}$ and its domain R.

This last equation is true since all we have done is added zero to the original double integral. The picture we imagine is something like Figure 4.9.

Second, we examine the domain, D, a little further. What can these more complicated domains look like? In Figures 4.10–4.12 we define three main classes of regions into which the domain D, or a piece of D, may be placed.

Type I:
Suppose the domain D is of the kind shown in Figure 4.10(a) and defined as

$$D = \{(x,y) : a \le x \le b, g_1(x) \le y \le g_2(x)\}.$$

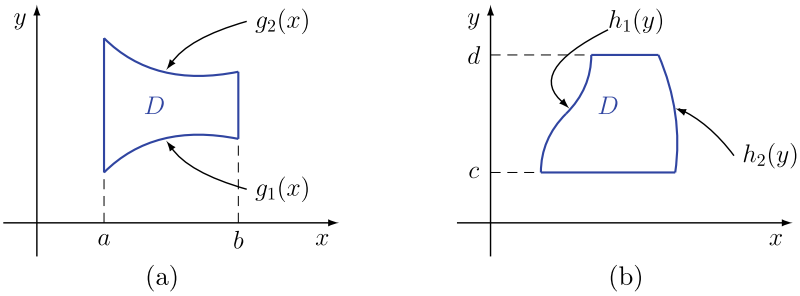

Figure 4.10 (a) A y-simple domain, and (b) an x-simple domain.

This is called a *y-simple domain*, with the variable y bounded by two functions of x.

Type II:
Suppose the domain D is of the kind shown in Figure 4.10(b) and defined as

$$D = \{(x, y) : c \le y \le d, h_1(y) \le x \le h_2(y)\}.$$

This is called a *x-simple domain*, with the variable x bounded by two functions of y.

Type III:
This is a domain D with an appearance like that shown in Figure 4.11 (*i.e.*, a convex domain so that any straight line intersects the boundary in at most two points), and with enough flexibility to have two interpretations. It could either be treated as a special case of **I** with $g_1(a) = g_2(a)$ and $g_1(b) = g_2(b)$, or as a special case of **II** with $h_1(c) = h_2(c)$ and $h_1(d) = h_2(d)$. That is, this sort of domain could be either x-simple or y-simple depending on how it is described.

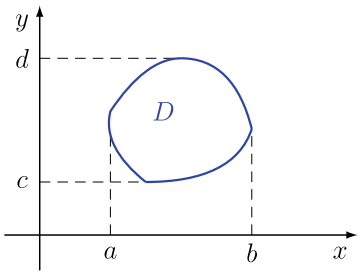

Figure 4.11 A domain that is both x-simple and y-simple.

Third, we bring these ideas together to arrive at a strategy for evaluating integrals over non-rectangular domains. We demonstrate this with a *y-simple domain* (Fig. 4.12).

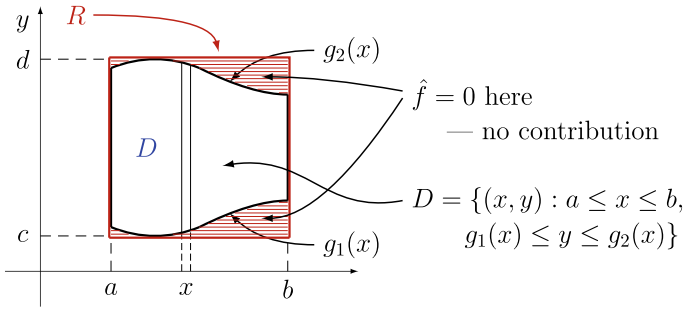

Figure 4.12 A y-simple domain in a rectangle R.

By construction, we have the iterated integral of $\hat{f}$ over $R = [a, b] \times [c, d] \supset D$,

$$\iint_D f(x, y)\,\mathrm{d}A = \iint_R \hat{f}(x, y)\,\mathrm{d}A = \int_a^b \left(\int_c^d \hat{f}(x, y)\,\mathrm{d}y \right) \mathrm{d}x$$

However, for every value of the outer integral variable x, $\hat{f} = 0$ outside the interval $g_1(x) \le y \le g_2(x)$, and $\hat{f} = f$ in the interior of that interval. Hence,

$$\begin{aligned} \int_a^b \left(\int_c^d \hat{f}(x, y)\mathrm{d}y \right) \mathrm{d}x &= \int_a^b \left(\int_c^{g_1(x)} \hat{f}\,\mathrm{d}y + \int_{g_1(x)}^{g_2(x)} \hat{f}\,\mathrm{d}y + \int_{g_2(x)}^d \hat{f}\,\mathrm{d}y \right) \mathrm{d}x, \\ &\qquad \text{—by Corollary 4.1.6} \\ &= \int_a^b \left(0 + \int_{g_1(x)}^{g_2(x)} f(x, y)\,\mathrm{d}y + 0 \right) \mathrm{d}x, \\ &= \underbrace{\int_a^b \left(\int_{g_1(x)}^{g_2(x)} f(x, y)\,\mathrm{d}y \right) \mathrm{d}x.}_{\text{iterated integral of } f \text{ over } y\text{-simple } D} \end{aligned}$$

We can now invoke the contrast alluded to earlier regarding the variable dependencies of the limits of the inner integral. For all cases of non-rectangular domains, the limits of the inner integral will be functions of the outer integral variable. In the above example, the limits on the inner integral depend on x and do *not* depend on y. Only in the case of rectangular domains will the limits of both the inner and outer integrals be constants!

For an *x-simple domain*, with $D = \{(x, y) : c \le y \le d,\ h_1(y) \le x \le h_2(y)\}$, we get the analogous result

$$\iint_D f(x,y)\,\mathrm{d}A = \underbrace{\int_c^d \left(\int_{h_1(y)}^{h_2(y)} f(x,y)\,\mathrm{d}x \right) \mathrm{d}y}_{\text{iterated integral of } f \text{ over } x\text{-simple } D}.$$

Once again, the limits of the inner integral depend on the outer integral variable; the limits of the inner integral here depend on y and do *not* depend on x.

Through a very simple development, we have arrived at very natural generalizations of iterated integrals over rectangles. Moreover, in the process, we have done away with function extensions and rectangular regions that we used in this development.

The reader should now bear two things in mind. First, the order in which the iterated integrals are to be performed must be strictly adhered to. Second, interchanging the order will *always* involve a change in the limits. This is illustrated in Example 4.2 wherein a double integral is evaluated in two ways. The reader should note the limits on the two inner integrals and how they come about (see the vertical and horizontal bars in Figure 4.13).

Example 4.2:

Let D be the region bounded by the lines $y = x$, $y = 2x$, and $x = 1$. Evaluate $\iint_D 1\,\mathrm{d}A$.

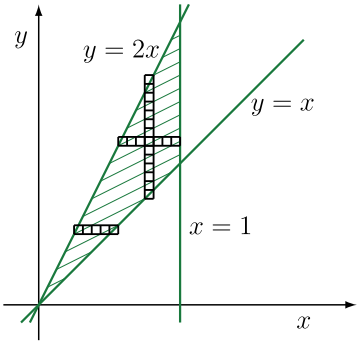

Figure 4.13 The y-simple domain D of Example 4.2.

It cannot be stressed enough that one should always start solving a multiple integral problem by drawing a picture of the *region* in question. Here it is the one shown in Figure 4.13. Sketching the region of integration, if it is possible, not only allows us to get some perspective on the task involved, it also allows us to determine the limits of the integration variables. More importantly, it can potentially identify difficulties with setting limits, which formulae themselves may not do. An example of such a complication arises when we treat D as an x-simple domain.

The domain in this example is both y-simple and *piecewise* x-simple. We first evaluate the double integral by treating D as a y-simple domain.

$$\begin{aligned}\text{Area of } D = \iint_D 1\,\mathrm{d}A &= \int_0^1 \left(\int_x^{2x} 1\,\mathrm{d}y\right)\mathrm{d}x \quad \text{—the outer variable is } x;\\ &\qquad\qquad \text{the limits on } y \text{ depend on } x.\\ = \int_0^1 \Big[y\Big]_x^{2x}\mathrm{d}x &= \int_0^1 x\;\mathrm{d}x = \left[\frac{x^2}{2}\right]_0^1 = \frac{1}{2} \text{ area units.}\end{aligned}$$

Now we treat D as x-simple. This is slightly more complex as Figure 4.13 suggests. We must break D up into two non-overlapping domains. One part of D is x-simple, bounded by the lines $y = 2x$ on the left and $y = x$ on the right. The other part of D is also x-simple but is bounded on the left by $y = 2x$, while on the right, it is bounded by the line $x = 1$. Corollary 4.1.6 allows us to split the double integral into a sum of two double integrals.

$$\begin{aligned}\text{Area of } D &= \iint_D 1\,\mathrm{d}A = \int_0^1 \left(\int_{y/2}^{y} 1\,\mathrm{d}x\right)\mathrm{d}y + \int_1^2 \left(\int_{y/2}^{1} 1\,\mathrm{d}x\right)\mathrm{d}y\\ &\qquad\qquad \text{—the outer variable is now } y; \text{ the limits on } x \text{ depend on } y.\\ &= \int_0^1 \Big[x\Big]_{y/2}^{y}\mathrm{d}y + \int_1^2 \Big[x\Big]_{y/2}^{1}\mathrm{d}y\\ &= \int_0^1 \frac{y}{2}\,\mathrm{d}y + \int_1^2 \left(1-\frac{y}{2}\right)\mathrm{d}y = \left[\frac{y^2}{4}\right]_0^1 + \left[y - \frac{y^2}{4}\right]_1^2\\ &= \frac{1}{4} + (2-1) - \left(1-\frac{1}{4}\right) = \frac{1}{2} \text{ area units.}\end{aligned}$$

Hence, we get the same answer after evaluating two iterated integrals instead of just one.

■

✍ Mastery Check 4.2:

Determine $\iint_D \left(xy + y^2\right) \mathrm{d}A$, over each of the following domains D.

(a) $D = \{(x, y) : 0 \le x \le 1,\ 0 \le y \le x^2\}$.

(b) $D = \{(x, y) : 0 \le x \le \sqrt{y},\ 0 \le y \le 1\}$.

✍

As suggested by the preceding example and Mastery Check, it is more usual to be given a domain and from it determine the limits on the iterated integral. Occasionally, however, a problem may be posed in the form of an iterated integral—often deliberately resulting in a difficult or intractable integral. In such an event, the solution requires the solver to use the given limits to determine the domain and possibly then re-express the multiple integral as an iterated integral with the order reversed. Supplementary problems 4.4, 4.18, 4.21, and 4.30 are of this kind.

4.D Generalized (Improper) Integrals in $\mathbb{R}^2$

The iterated integral approach only works if the corresponding multiple integral exists, *i.e.*, if the limit of the sum σ_{mn} exists. It is important to remember that thus far we have relied on the convenient assumptions of the function being continuous and the domain being compact. However, in other cases the Riemann theory of integration on which the double integral was founded can break down. In extreme cases, this leads to so-called *improper integrals*, of which there are two main types:

(a) One type involves *unbounded domains*, e.g.,
$D = \{(x, y) : x > 0,\ y > 0\}$.

(b) One type involves functions f, *not defined on part of the boundary.*
For example, $f(x, y) = 1/\left(x^2 + y^2\right)$ is not defined at $(0, 0)$.

Under these more general circumstances, to answer the question

$$\text{“Does } \iint_D f(x, y)\, \mathrm{d}A \text{ exist?”},$$

we can rely somewhat on the combined action of the following theorems.

Theorem 4.2

If ...

$$\left.\begin{array}{l} \displaystyle\int\left(\int |f(x,y)|\mathrm{d}y\right)\mathrm{d}x \\ \textit{and}\ \displaystyle\int\left(\int |f(x,y)|\mathrm{d}x\right)\mathrm{d}y \end{array}\right\} \quad \begin{array}{l}\textit{exist}\\ \textit{and are}\\ \textit{equal}\end{array}$$

then ...

$$\iint_D |f(x,y)|\,\mathrm{d}A \ \textit{exists.}$$

Theorem 4.3

$$\textit{If} \quad \iint_D |f(x,y)|\,\mathrm{d}A \quad \textit{exists, then} \quad \iint_D f(x,y)\,\mathrm{d}A \quad \textit{exists.}$$

These two theorems, considered sequentially, are informative and can be relied upon in the affirmative to guarantee the existence of a double integral. They are also useful in the negative when either (a) the two iterated integrals of $|f(x,y)|$ *do not* give the same result, or (b) if one iterated integral fails to converge; the double integral does *not* exist. However, the theorem is unhelpful in those cases when only *one* ordered iterated integral can be evaluated (and converges), while the other iterated integral cannot be evaluated. In such cases, there remains some doubt about the existence of the multiple integral overall.

Analysis of improper integrals

Despite the lack of uniformly valid conditions, we may still be guided by the above theorems and jump straight to the task of evaluating the *iterated* integral in the form of a generalized multiple integral. In tackling improper iterated integrals we take advantage of the wisdom of single-variable calculus.

In single-variable calculus, the improper definite integral $\displaystyle\int_I f(x)\,\mathrm{d}x$, for $f(x) > 0$ over the domain I, exists if

$\displaystyle\lim_{\epsilon\to 0^+} J(\epsilon) = \lim_{\epsilon\to 0^+}\int_{a+\epsilon}^{b} f(x)\,\mathrm{d}x,\ a < b$ *exists*, when f is a function which diverges at the integration limit $x = a \in \overline{I}$ (Figure 4.14(a)); or

$\displaystyle\lim_{R\to\infty} J(R) = \lim_{R\to\infty}\int_{a}^{R} f(x)\,\mathrm{d}x$ exists, when I is the unbounded domain, $I = [a,\infty)$ (Figure 4.14(b)).

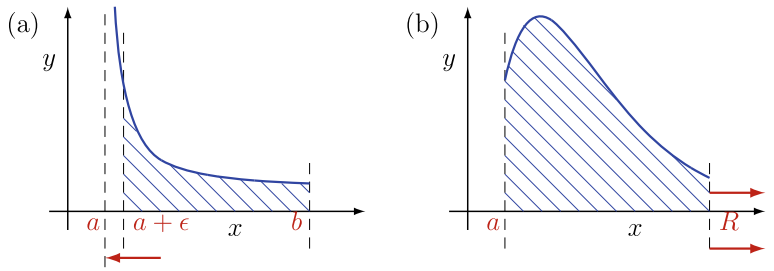

Figure 4.14 Two types of improper integral in single-variable calculus.

In Figure 4.14(a), the function f is singular at the lower limit $x = a$, while in Figure 4.14(b), the domain $I = [a, \infty)$ is unbounded to the right. Analogous limits can be constructed if instead of (a) f was singular at $x = b$ or, instead of (b), when $I = (-\infty, b]$ or $I = (-\infty, \infty)$.

Notice that both $J(\epsilon)$ and $J(R)$ rely on the Riemann theory of integration of a *continuous* function defined on a *bounded* subinterval to give a finite result, which then depends on ϵ or R, respectively. Moreover, after evaluating $J(\epsilon)$ or $J(R)$ for finite ϵ or R, we test for the convergence of their limits: the first being the limit $\epsilon \to 0$ as we approach the singular point; the second being the limit $R \to \infty$ as we infinitely extend the bounded domain. If the respective limits exist we define those limiting values as the values of the integrals.

In multivariable calculus, the existence of the improper multiple integral

$$\iint_D f(x, y)\, \mathrm{d}A$$

is similarly considered as a suitable limit. In practice it is more natural to work with the iterated integral version of a multiple integral. However, the principle involved is more easily explained and visualized using the multiple integral itself.

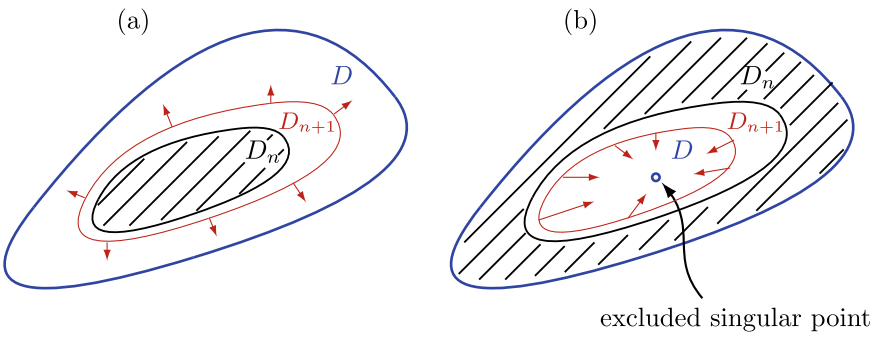

Figure 4.15 (a) Sequence of compact domains $D_n \longrightarrow$ unbounded D;
(b) Sequence of compact domains $D_n \longrightarrow$ singular D.

Just as in the single-variable case, two main scenarios are envisaged. In one, the integration region is unbounded in one or more directions, while the function is well behaved on bounded subsets. In the other, the integration region is bounded but contains isolated points, or lines of points, on which the function is not defined (these may be interior points or points on the region's boundary). In either scenario, progress can be made by introducing a suite of compact (or at least bounded) subsets, D_n, over which the function is at least bounded, if not continuous. The function would then attain an absolute maximum and an absolute minimum in D_n. Consequently, the integral of f over D_n would converge as a Riemann integral. The proposition then is to take the limit of the integration result as the subsets, D_n, converge to D, as $n \to \infty$. The process is indicated schematically in Figure 4.15. In either scenario, whether D is unbounded (Figure 4.15(a)) or D is a singular region (Figure 4.15(b)) the following useful result applies.

Theorem 4.4

Let f be a non-negative or non-positive function over a region, D, which may be unbounded or contain points on which f is undefined. For any sequence of bounded subsets, $\{D_n\}_{n=1}^{\infty}$, such that

$$D_1 \subset \cdots \subset D_n \subset D_{n+1} \subset \cdots \subset D \quad \text{and} \quad \lim_{N\to\infty} \bigcup_{n=1}^{N} D_n = D,$$

and with f integrable over D_n for all n, if

$$\lim_{n\to\infty} J(n) = \lim_{n\to\infty} \iint_{D_n} f(x,y)\,\mathrm{d}A$$

exists, then the improper integral $\displaystyle\iint_D f(x,y)dA$ exists and is equal to this limit.

An immediate corollary of the theorem is the following.

Corollary 4.4.1 *For the function and domain conditions of Theorem 4.4, if the improper integral $\displaystyle\iint_D f(x,y)\,\mathrm{d}A$ exists, then the iterated integrals*

$$\int \left(\int f(x,y)\,\mathrm{d}y \right) \mathrm{d}x \quad \text{and} \quad \int \left(\int f(x,y)\,\mathrm{d}x \right) \mathrm{d}y \quad \text{exist and are equal.}$$

Theorem 4.4 is limited to functions that are single signed (as does its proof). For more general cases in which the function changes sign over the integration region, the only assistance that can be offered is Theorem 4.3 (see Mastery Check 4.4).

As was said earlier, in practice we invariably work with iterated integral forms to evaluate the double integrals, $J(n)$, over bounded subsets, D_n, which can be characterized in terms of one or more parameters. The limit "$n \to \infty$" then manifests itself as a limit or limits of these parameters. This is illustrated by the next example.

■ Example 4.3:

Check whether the following integrals converge. If they do, compute them.

(a) $\displaystyle\iint_D \frac{\mathrm{d}x\,\mathrm{d}y}{1+(x+y)^2}$, $D = \{(x,y) : x > 0, y > 0\}$.

(b) $\displaystyle\iint_D \frac{\mathrm{d}x\,\mathrm{d}y}{\sqrt{xy}}$, $D = \{(x,y) : 0 < x < 1, 0 < y < 1\}$.

Solution:

(a) D is unbounded. So, we consider instead the x-simple integral over the finite subset $D_{AB} \subset D$,

$$D_{AB} = \{(x,y) : 0 < x < A, 0 < y < B\}.$$

$$J_{AB} = \iint_{D_{AB}} \frac{1}{1+(x+y)^2}\,\mathrm{d}x\,\mathrm{d}y = \int_0^B \left(\int_0^A \frac{1}{1+(x+y)^2}\,\mathrm{d}x\right)\mathrm{d}y$$

$$= \int_0^B \Big[\arctan(x+y)\Big]_{x=0}^{A}\,\mathrm{d}y = \int_0^B \big(\arctan(y+A) - \arctan y\big)\,\mathrm{d}y.$$

Now, it is sufficient to consider the limit,

$$\lim_{B\to\infty}\int_0^B \arctan y\,\mathrm{d}y = \lim_{B\to\infty}\left[y\arctan y - \frac{1}{2}\ln(1+y^2)\right]_0^B,$$

which evidently does not exist. Consequently, the integral of f over D does not exist.

(b) In this case, the integrand is undefined on the boundary of the finite region D: along $x = 0$ and along $y = 0$. So, instead we consider the integral over the region $D_\epsilon = \{(x,y) : \epsilon < x < 1, \epsilon < y < 1\}$. (Since the region and function are symmetric we may use the same ϵ parameter for both variables. The choice of integration order is also arbitrary as a result of symmetry.)

$$J_\epsilon = \iint_{D_\epsilon} \frac{1}{\sqrt{xy}}\,\mathrm{d}x\,\mathrm{d}y = \int_\epsilon^1 \left(\int_\epsilon^1 \frac{1}{\sqrt{xy}}\,\mathrm{d}x\right)\mathrm{d}y = \int_\epsilon^1 \left[2\sqrt{\frac{x}{y}}\right]_\epsilon^1 \mathrm{d}y$$

$$= \int_\epsilon^1 2\frac{1-\sqrt{\epsilon}}{\sqrt{y}}\,\mathrm{d}y = 4(1-\sqrt{\epsilon})^2.$$

Next, we consider the limit of J_ϵ as $\epsilon \to 0$. Clearly, we have $J_\epsilon \longrightarrow 4$.

The reader will confirm that since the integration limits are constants, the two iterated integrals (with opposite orders) give the same result. So, according to Theorems 4.3 and 4.4 the improper double integral exists with value equal to 4.

■

✍ Mastery Check 4.3:

Does the double integral $I = \iint_D f(x,y)\,\mathrm{d}A$ converge or diverge when

$$f(x,y) = \frac{1}{x^2+y^2} \quad \text{and} \quad D = \{(x,y) : x \geq 1,\ 0 \leq y \leq x\}?$$

Hint: Consider the subset $D_R = \{(x,y) : 1 \leq x \leq R,\ 0 \leq y \leq x\}$, and let $R \to \infty$.
Write out both iterated integral versions, and choose the simpler of the two for analysis.

✍

✍ Mastery Check 4.4:

Dangers in ∞!

Consider the two iterated integrals

$$I_1 = \int_0^1 \left(\int_1^\infty \left(\mathrm{e}^{-xy} - 2\mathrm{e}^{-2xy} \right) \mathrm{d}x \right) \mathrm{d}y, \quad \text{and} \quad I_2 = \int_1^\infty \left(\int_0^1 \left(\mathrm{e}^{-xy} - 2\mathrm{e}^{-2xy} \right) \mathrm{d}y \right) \mathrm{d}x.$$

Show that one of these must be < 0, while the other must be > 0, and ponder the implications in the context of Theorem 4.3.

✍

4.E Change of Variables in $\mathbb{R}^2$

In single-variable calculus, any practical difficulties encountered in evaluating an integral arise because of the function. In contrast, in multivariable calculus difficulties arise not only because of complicated functions but also from convoluted integration domains, as well as the combination of the two.

Among the many single-variable integration methods used to enable an integral calculation (which, as we said before, are legitimate to use for each individual one-variable iterated integration) we may highlight the method of substitution. The aim of this method is to simplify the integrand, hopefully

to reduce it to a form having a known antiderivative. In the multivariable case the difficulties encountered could possibly be circumvented by the related *method of a change of variables*. In this method, the original Cartesian variables, x and y, are converted to new integration variables, u and v, say.

In this section, we elaborate on the procedure for changing variables and along the way point out when it is possible to do so, and when it is not. As usual, the single-variable case provides an illuminating comparison.

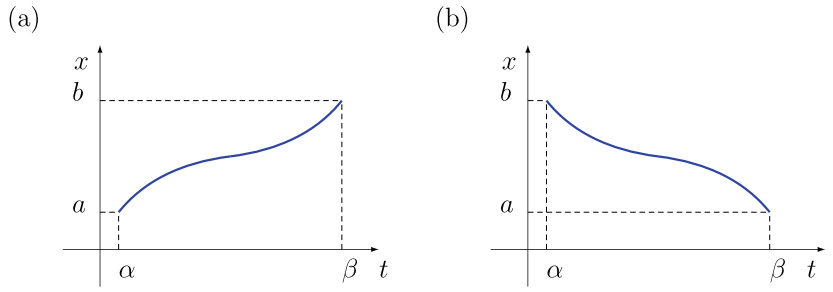

Figure 4.16 (a) $x(t)$ increasing; (b) $x(t)$ decreasing.

Change of variables in single integrals

Aim: We want to evaluate $\displaystyle\int_a^b f(x)\,\mathrm{d}x$ by invoking a transformation: $x \to t$.

Suppose $x = x(t)$ is a strictly *increasing* function of t, as in Figure 4.16(a), with end points $x(\alpha) = a$ and $x(\beta) = b$. Then, $x'(t) > 0$, $\forall\ t \in (\alpha, \beta)$. Suppose also that the antiderivative of f is F so that $\dfrac{\mathrm{d}F}{\mathrm{d}x} = f$. Then,

$$\begin{aligned}\int_\alpha^\beta f(x(t))x'(t)\,\mathrm{d}t &= \int_\alpha^\beta F'(x(t))x'(t)\,\mathrm{d}t \\ &= \int_\alpha^\beta \frac{\mathrm{d}}{\mathrm{d}t}F(x(t))\,\mathrm{d}t = F(x(\beta)) - F(x(\alpha)) \\ &= F(b) - F(a) = \int_a^b f(x)\,\mathrm{d}x.\end{aligned}$$

On the other hand, suppose $x(t)$ is strictly *decreasing* as in the case shown in Figure 4.16(b), now with end points $x(\alpha) = b$ and $x(\beta) = a$. Then, $x'(t) < 0,\ \forall\ t \in (\alpha, \beta)$. Again, the antiderivative F of f satisfies $\dfrac{\mathrm{d}F}{\mathrm{d}x} = f$. Then,

$$\begin{aligned}\int_\alpha^\beta f(x(t))\big(-x'(t)\big)\,\mathrm{d}t &= -\int_\alpha^\beta F'(x(t))x'(t)\,\mathrm{d}t \\ &= \int_\beta^\alpha \frac{\mathrm{d}}{\mathrm{d}t}F(x(t))\,\mathrm{d}t = F(x(\alpha)) - F(x(\beta)) \\ &= F(b) - F(a) = \int_a^b f(x)\,\mathrm{d}x.\end{aligned}$$

We see that in both cases, coincident with a change of integration variable and hence the interval of integration, a non-negative factor, $|x'(t)|$, is introduced in the integrand of the new integral. Combining these two results in the one summarizing statement, we have that

$$\int_a^b f(x)\,\mathrm{d}x = \int_\alpha^\beta f\left(x(t)\right)\left|\frac{\mathrm{d}x}{\mathrm{d}t}\right|\,\mathrm{d}t.$$

So, in either instance of $x(t)$ increasing or $x(t)$ decreasing, the integration interval length has changed, but this is accompanied by a non-negative, locally varying factor $|x'(t)|$ in the integrand. This factor is called a *scale factor* associated with the variable change x to t since it scales up or down the interval size. We should expect a similar factor to arise with a change of variables in a multiple integral.

Change of variables in double integrals

For convenience we shall consider only bijective transformations:

$$\tau : \boldsymbol{u} \mapsto \boldsymbol{x}(\boldsymbol{u}) = \left\{\begin{array}{rcl} x &=& x(u,v) \\ y &=& y(u,v)\end{array}\right. \qquad \text{such that} \quad \frac{\partial(x,y)}{\partial(u,v)} \neq 0.$$

We will soon see that Jacobian determinants (Definition 2.9) feature prominently in any transformation of multiple integrals. The double integral,

$$\iint_D f(x,y)\mathrm{d}A, \qquad \text{will transform to} \qquad \iint_E g(u,v)\mathrm{d}A',$$

where the original integration region D is replaced by (is transformed to) a new integration region E. Geometrically, the transformation $(x, y) \to (u, v)$ affects areas both globally and locally. To see this, consider in Figure 4.17 the (approximate) parallelogram $RSQP$ in the xy-plane. This parallelogram is the *image* under transformation τ of the rectangle $R'S'Q'P'$ bounded by lines of constant u and v in the uv-plane. Let this rectangle has side lengths given by the differential elements, $\mathrm{d}u$ and $\mathrm{d}v$.

For the infinitesimal differentials $\mathrm{d}u$ and $\mathrm{d}v$, the area of the parallelogram element in D is given by the vector product,

$$\begin{aligned} \mathrm{d}A &= \left|\overrightarrow{RP} \times \overrightarrow{RS}\right| \qquad \text{—geometric interpretation (see Page 4);} \\ &\qquad\qquad\qquad\qquad\qquad\qquad \text{absolute value signs enter here!} \\ &= \Big|\underbrace{\big(\mathrm{d}x_u\, \boldsymbol{e_1} + \mathrm{d}y_u\, \boldsymbol{e_2}\big)}_{\text{along a line of constant } v} \times \underbrace{\big(\mathrm{d}x_v\, \boldsymbol{e_1} + \mathrm{d}y_v\, \boldsymbol{e_2}\big)}_{\text{along a line of constant } u}\Big|. \end{aligned}$$

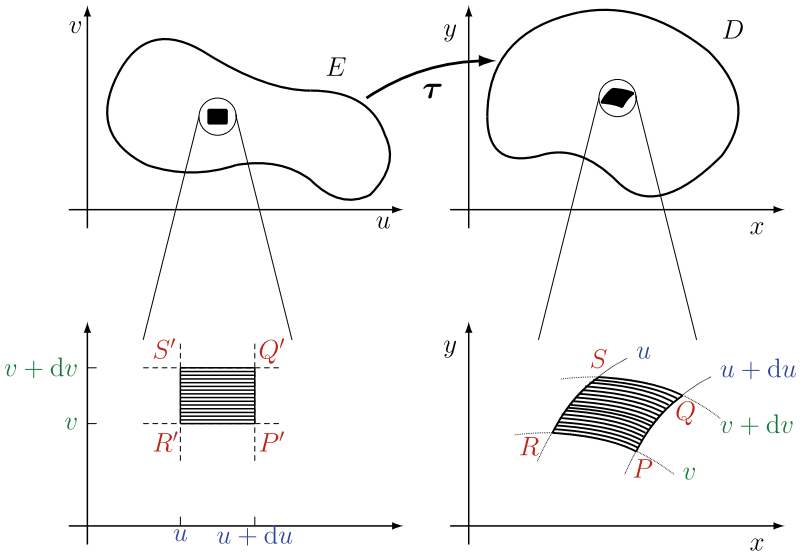

Figure 4.17 A geometrical view of a change of variables.

Thus,

$$\begin{aligned} \mathrm{d}A &= \left|\Big(\frac{\partial x}{\partial u}\,\mathrm{d}u\, \boldsymbol{e_1} + \frac{\partial y}{\partial u}\,\mathrm{d}u\, \boldsymbol{e_2}\Big) \times \Big(\frac{\partial x}{\partial v}\,\mathrm{d}v\, \boldsymbol{e_1} + \frac{\partial y}{\partial v}\,\mathrm{d}v\, \boldsymbol{e_2}\Big)\right| \\ &\qquad\qquad \text{— by the chain rule (Section 2.G)} \\ &= \left|\frac{\partial(x,y)}{\partial(u,v)}\right| \mathrm{d}u\,\mathrm{d}v \quad \text{— cross product gives the Jacobian determinant} \end{aligned}$$

The reader should note that it is the *absolute value* of the Jacobian determinant that appears here. This is reasonable since what we have done is transform one area element to another, preserving the positive sign.

And so we have the following important theorem.

Theorem 4.5
Let $x(u,v)$ and $y(u,v)$ be a bijective **[one-to-one and onto]** *and C^1 transformation of E in the uv-plane onto D in the xy-plane.*

If $f(x,y)$ is integrable in D then $f\big(x(u,v),y(u,v)\big) = F(u,v)$ is integrable in E and

$$\iint_D f(x,y)\,\mathrm{d}A = \iint_E F(u,v)\left|\frac{\partial(x,y)}{\partial(u,v)}\right|\mathrm{d}A'.$$

Remarks

* The *absolute value* of the Jacobian is the *scale factor* between the two area elements, $\mathrm{d}A$ in the xy-plane and $\mathrm{d}A'$ in the uv-plane; it takes the role played by $\left|\frac{\mathrm{d}x}{\mathrm{d}t}\right|$ in the single-variable case.

  In other words $\underbrace{\mathrm{d}A}_{\text{an area element in } (x,y)} = \left|\frac{\partial(x,y)}{\partial(u,v)}\right| \underbrace{\mathrm{d}A'}_{\text{an area element in } (u,v)}$.

* If $x(u,v)$ and $y(u,v)$ are bijective transformations, then $\dfrac{\partial(x,y)}{\partial(u,v)} \neq 0$.

* If $x(u,v)$ and $y(u,v)$ are C^1, then $F(u,v) = f(x(u,v),y(u,v))$ is integrable over E whenever f is integrable over D.

* Despite the analogy, a change of variables in a *double* integral is NOT the same as a substitution in an *iterated* integral. The latter might still be necessary when integrating with respect to each individual variable.

Before proceeding further it is worthwhile taking some time to reflect more on the Jacobian determinant. This is the aim of the next example and the follow-up Mastery Check.

Example 4.4:

Determine the Jacobian determinant for the change of variables $u = x + y, \quad v = \dfrac{x}{y}$. Assume $x, y > 0$ and hence that $u, v > 0$. Also, determine the Jacobian determinant for the inverse transformation. What do you notice about your two results?

Solution:

The Jacobian determinant (or just Jacobian) for this change of variables $((x,y) \to (u,v))$ is given by

$$\begin{aligned}\frac{\partial(u,v)}{\partial(x,y)} &= \begin{vmatrix} \dfrac{\partial u}{\partial x} & \dfrac{\partial u}{\partial y} \\ \dfrac{\partial v}{\partial x} & \dfrac{\partial v}{\partial y} \end{vmatrix} = \begin{vmatrix} 1 & 1 \\ \dfrac{1}{y} & -\dfrac{x}{y^2} \end{vmatrix}, \\ &= \left(-\frac{x}{y^2} - \frac{1}{y}\right) = \left(\frac{-x-y}{y^2}\right) = -\frac{x+y}{y^2} \quad \text{—negative since } x, y > 0.\end{aligned}$$

We note the single most important feature here; since $x, y > 0$, by assumption, the Jacobian determinant is nonzero. It is negative, which is another matter, but as long as we consider points x and y in the interior of the first quadrant, the Jacobian will be nonzero. Similarly, the inverse transformation $((u,v) \to (x,y))$,

$$x = \frac{uv}{1+v} \qquad y = \frac{u}{1+v},$$

elicits the Jacobian determinant

$$\begin{aligned}\frac{\partial(x,y)}{\partial(u,v)} &= \begin{vmatrix} \dfrac{\partial x}{\partial u} & \dfrac{\partial x}{\partial v} \\ \dfrac{\partial y}{\partial u} & \dfrac{\partial y}{\partial v} \end{vmatrix} = \begin{vmatrix} \dfrac{v}{1+v} & u\left(\dfrac{1}{1+v} - \dfrac{v}{(1+v)^2}\right) \\ \dfrac{1}{1+v} & -\dfrac{u}{(1+v)^2} < 0 \end{vmatrix}, \\ &= \left(-\frac{uv}{(1+v)^3} - \frac{u}{(1+v)^3}\right) = -\frac{u(1+v)}{(1+v)^3} = -\frac{u}{(1+v)^2} \quad \text{—negative}\end{aligned}$$

Utilizing either transformation we notice that

$$\begin{aligned}\frac{\partial(u,v)}{\partial(x,y)}\frac{\partial(x,y)}{\partial(u,v)} &= \left(-\frac{(x+y)}{y^2}\right)\left(-\frac{u}{(1+v)^2}\right), \\ &= \left(-\frac{(x+y)}{y^2}\right)\left(-\frac{x+y}{(1+x/y)^2}\right) = \left(-\frac{(x+y)}{y^2}\right)\left(-\frac{y^2}{(x+y)}\right), \\ &= 1.\end{aligned}$$

That is, the Jacobian determinant for an invertible transformation is the reciprocal of the Jacobian determinant for the inverse transformation. This is a very useful property of nonsingular Jacobian determinants; if the Jacobian of a complicated or implicit transformation is required but difficult to derive, one could *evaluate the Jacobian of the inverse transformation*, if it is possible and more practical, and then *take its reciprocal*.

In this example we also note that the two Jacobian determinants are in fact negative. In multiple integral applications, as argued above, it is the absolute value of the Jacobian determinant that is needed. Since $x, y, u, v > 0$, we would take the absolute value of the above results when determining the area element of a transformed region. For example,

$$\mathrm{d}u\mathrm{d}v = \left|\frac{\partial(u,v)}{\partial(x,y)}\right| \mathrm{d}x\mathrm{d}y = \frac{(x+y)}{y^2}\mathrm{d}x\mathrm{d}y.$$

■

Lastly, we encourage the reader to verify the following Jacobian determinants for some standard transformations.

✍ Mastery Check 4.5:

Show that in transforming from (Hint: See Section 1.D.)

(a) Cartesian to polar coordinates (r, θ), the Jacobian determinant is r;

(b) Cartesian to cylindrical coordinates (r, θ, z), the Jacobian determinant is r;

(c) Cartesian to spherical coordinates (ρ, ϕ, θ), the Jacobian determinant is $\rho^2 \sin\phi$.

✍

In the next example, we shall see the Jacobian determinant enter into an integral calculation.

■ Example 4.5:

Show that the volume of the right cone of Figure 4.18, of radius a and height h, is $V = \frac{1}{3}\pi a^2 h$.

Solution:

We do this by integrating a variable height function $z = \frac{h}{a}\left(a - \sqrt{x^2+y^2}\right)$ over the region $R : x^2 + y^2 \leq a^2$.

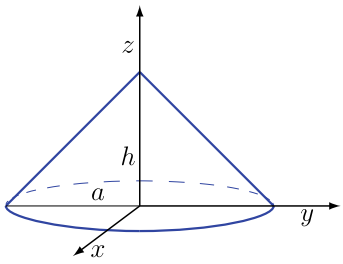

Figure 4.18 A right cone.

The volume is $V = \iint_R f(x,y)\,\mathrm{d}x\,\mathrm{d}y = \iint_R \frac{h}{a}\big(a - \sqrt{x^2+y^2}\big)\,\mathrm{d}x\,\mathrm{d}y.$

Change to polar coordinates:

$$R \to E = \{(r,\theta) : 0 \le r \le a,\ 0 \le \theta \le 2\pi\},$$
$$(x,y) \to (r,\theta),\ \ x = r\cos\theta,\ \ y = r\sin\theta,\ \ |J| = r.$$

$$V = \iint_E F(r,\theta)\left|\frac{\partial(x,y)}{\partial(r,\theta)}\right| dr\,\mathrm{d}\theta = \iint_E \frac{h}{a}(a-r)\,r\,dr\,\mathrm{d}\theta$$

Jacobian determinant, $|J|$ — area element, $\mathrm{d}A'$

$$= \int_0^a \left(\int_0^{2\pi} \frac{h}{a}(ar - r^2)\,\mathrm{d}\theta\right)\mathrm{d}r$$

$$= \frac{2\pi h}{a}\left[a\frac{r^2}{2} - \frac{r^3}{3}\right]_0^a = \frac{\pi h a^2}{3}, \text{ as required.}$$

■

✍ Mastery Check 4.6:

Does the integral $\iint_{\mathbb{R}^2} \frac{\mathrm{d}x\,\mathrm{d}y}{(1+x^2+y^2)^2}$ converge? If it does, find its value.

Hint: Find the integral over bounded $D = \{(x,y) : x^2 + y^2 < A^2\}$, using polar coordinates and then let $A \to \infty$.

✍

Philosophy of a change of variables

It is worthwhile pausing to reflect on the motivation behind a change of variables. This may help to guide the practitioner to choose the most suitable variables. Ultimately, of course, we invoke a change of variables to simplify the evaluation of a multiple integral. One therefore chooses a transformation

$$\big(x(u,v), y(u,v)\big) : \text{ from variables } (x,y) \text{ to variables } (u,v)$$

so as to *either*

(a) transform region D into a simpler region E (in Example 4.5 E was a simple rectangle); *or*

(b) transform the integrand $f(x,y)$ into some simpler $F(u,v)$.

Thus, in the case of (a), one might be guided by the shape of the given region D: consider what mathematical expressions determine the boundary, and reflect on whether these be used to define the new boundary.

In the case of (b), consider whether the form of $f(x, y)$ is suggestive of a suitable transformation. For example, the case $f(x, y) = g(x^2+y^2)$, a function of the combination $x^2 + y^2$, suggests the polar coordinate transformation $x = r\cos\theta$, $y = r\sin\theta$, so that $x^2 + y^2 = r^2$.

In either case one should always look for symmetry features. This having been said, there will always be consequences:

(c) The region can be transformed into a more complicated one, even if the integrand becomes simpler;

(d) The integrand may become more complex, even if the transformed region is simpler —*remember that a Jacobian determinant for the transformation must also be taken into account*;

(e) Sometimes, however, we get lucky and *both* the function *and* the region become simpler, as the next example demonstrates.

Example 4.6:

Evaluate the double integral

$$I = \iint_D \frac{1}{x\,(x^2 - y^2)}\,\mathrm{d}A,$$

where D is the first quadrant region bounded by the lines: $x+y = 1$, $x+y = 2$, $y = x/2$, and $y = x/4$.

Solution:

Although the region D is not overly complex (bounded by straight lines, it is piecewise x-simple and piecewise y-simple: Figure 4.19(a)), put in combination with the function to be integrated it is sufficiently inconvenient to make a direct evaluation of the double integral an unattractive prospect (three separate iterated integrals are required).

On the other hand, the boundaries of D motivate the following change of variables:

$$u = x + y,\ v = \frac{x}{y} \quad \Longleftrightarrow \quad x = \frac{uv}{1+v},\ y = \frac{u}{1+v},$$

transforming D into the rectangle, $E = \{(u, v) : 1 \le u \le 2,\ 2 \le v \le 4\}$: Figure 4.19(b).

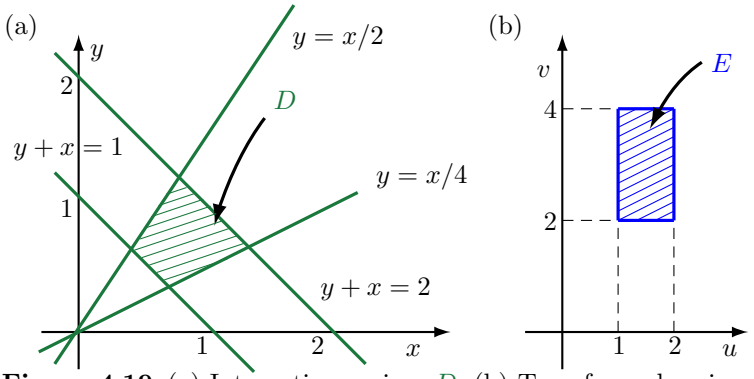

Figure 4.19 (a) Integration region, D; (b) Transformed region, E.

The Jacobian determinant − the scale factor, $|J|$ − becomes

$$\left|\frac{\partial(x,y)}{\partial(u,v)}\right| = \left(\left|\frac{\partial(u,v)}{\partial(x,y)}\right|\right)^{-1} = \left(\left\|\begin{array}{cc}\frac{\partial u}{\partial x} & \frac{\partial u}{\partial y}\\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y}\end{array}\right\|\right)^{-1} = \left(\left\|\begin{array}{cc}1 & 1\\ \frac{1}{y} & -\frac{x}{y^2}\end{array}\right\|\right)^{-1},$$

$$= \left(\left|-\frac{x}{y^2}-\frac{1}{y}\right|\right)^{-1} = \left(\left|-\frac{x+y}{y^2}\right|\right)^{-1} = \frac{y^2}{|x+y|} = \frac{|u|}{(1+v)^2}.$$

Thus, $|J| = \left|\frac{\partial(x,y)}{\partial(u,v)}\right| = \frac{u}{(1+v)^2} > 0$ in E. Meanwhile, the function $f(x,y)$ transforms as

$$f(x,y) = \frac{1}{x(x^2-y^2)} + \frac{1}{x}\frac{1}{(x-y)}\frac{1}{(x+y)} = \frac{1}{xy}\frac{1}{\left(\frac{x}{y}-1\right)}\frac{1}{(x+y)},$$

$$= \frac{(1+v)^2}{vu^2}\frac{1}{(v-1)}\frac{1}{u} = \frac{(1+v)^2}{vu^3(v-1)} = F(u,v).$$

Hence, the double integral over D transforms into the double integral over E,

$$I = \iint_E F(u,v)|J|\mathrm{d}u\mathrm{d}v = \iint_E \frac{(1+v)^2}{vu^3(v-1)}\frac{u}{(1+v)^2}\mathrm{d}u\mathrm{d}v = \iint_E \frac{1}{vu^2(v-1)}\mathrm{d}u\mathrm{d}v,$$

$$= \int_1^2 \frac{\mathrm{d}u}{u^2}\cdot\int_2^4 \frac{\mathrm{d}v}{v(v-1)} = \left[-\frac{1}{u}\right]_{u=1}^{u=2}\cdot\Big[\ln(v-1)-\ln(v)\Big]_{v=2}^{v=4} = \frac{1}{2}\ln\left(\frac{3}{2}\right).$$

The potential benefits of a change of variables are exhibited in this example:

(i) the simplification of region of integration, here to a rectangle,

(ii) the reduced number of iterated integrals to evaluate, here it is one instead of three,

(iii) the reduction of limits in the iterated integrals to constants, and as a bonus

(iv) the separation of variables in the integrand allowing them to be integrated individually.

■

✍ Mastery Check 4.7:

What is the image E of the region D bounded by the curves $x = y^2$, $y = \dfrac{1}{x}$, $y = \dfrac{2}{x}$, $x = \dfrac{y^2}{2}$, under the transformation $u = \dfrac{x}{y^2}$, $v = xy$?

Hint: Sketch region D in the xy-plane and its image E in the uv-plane. Then stop to think: Is this OK?

✍

4.F Triple Integrals

To cement the ideas just introduced we shall in the next few sections revisit the same terrain, this time for functions of *three* variables integrated over regions of $\mathbb{R}^3$.

Suppose $f : \mathbb{R}^3 \longrightarrow \mathbb{R}$ is a continuous function, defined (at least) over a rectangular box B:

$$B = \{(x, y, z) : a_1 \leq x \leq b_1,\ a_2 \leq y \leq b_2,\ a_3 \leq z \leq b_3\}.$$

—*i.e.*, we take B to be closed and bounded, $a_i \leq b_i < \infty$.

B is shown in Figure 4.20.

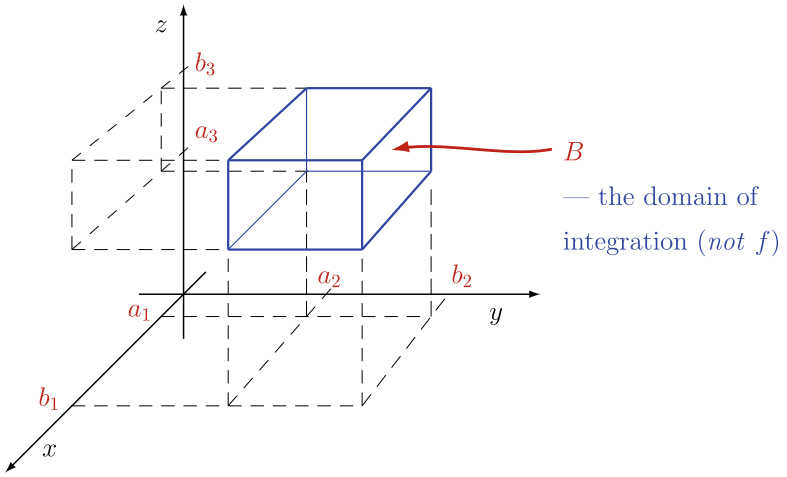

Figure 4.20 Box domain B in $\mathbb{R}^3$.

The definition of a triple integral follows analogously those of double and single integrals. We just outline the relevant steps leading to the definition.

- Partition B into small rectangular blocks B_{ijk} of volumes $\Delta V_{ijk} = \Delta x_i \Delta y_j \Delta z_k$
- If $f \geq 0$ for all $\boldsymbol{x} \in B$, then we interpret the quantity f as a *density* so that in choosing $(\xi_i, \eta_j, \zeta_k) \in B_{ijk}$, $f(\xi_i, \eta_j, \zeta_k)\Delta V_{ijk}$ will be an approximation to the mass of block B_{ijk}.
- The Riemann sum of all such masses in the partition,

$$\sigma_{nml} = \sum_{i=1}^{n} \sum_{j=1}^{m} \sum_{k=1}^{\ell} f(\xi_i, \eta_j, \zeta_k) \Delta V_{ijk},$$

  is an approximation to the total *mass* of the entire B.
- We then take the combined limits of the number of boxes to infinity with vanishing volumes. We therefore arrive at

Definition 4.4
The **triple integral** *of f over B is defined as the limit (if it exists)*

$$\lim_{\substack{n,m,\ell\to\infty \\ \max\sqrt{\Delta x_i^2+\Delta y_j^2+\Delta z_k^2}\to 0}} \sigma_{nml} = \iiint_B f(x,y,z)\,\mathrm{d}V.$$

For regions of more general shape, starting with bounded regions, S, we can extend the definition of the integral of f over $S \subset \mathbb{R}^3$ in analogy with the 2D version:

- we enclose S in a closed and bounded box B: $S \subset B \subset \mathbb{R}^3$, and
- define $\hat{f}(x,y,z) = \begin{cases} f(x,y,z), & \boldsymbol{x} \in S \\ 0, & \boldsymbol{x} \notin S \end{cases}$,

we then have

$$\iiint_S f(x,y,z)\,\mathrm{d}V \equiv \iiint_B \hat{f}(x,y,z)\,\mathrm{d}V.$$

This now sets the stage for Section 4.G where the practical evaluation of triple integrals over general regions is discussed. In the meantime, we have below the 3D version of Theorem 4.1 and its corollaries, the analogues of the 1D and 2D cases.

An important theorem and some corollaries—3D version

Theorem 4.1 *All continuous functions are integrable over compact subsets of their domains.*

Corollary 4.1.1
If $f \geq 0$ *is a* $\left.\begin{matrix} \textit{mass} \\ \textit{charge} \end{matrix}\right\}$ *density, then* $\iiint_B f\,\mathrm{d}V = \begin{cases} \textit{total mass} \\ \textit{total charge} \end{cases}$.
—a useful interpretation.

Corollary 4.1.2
If $f \geq g \geq 0$ *in* B, *then* $\iiint_B f(x,y,z)\,\mathrm{d}V \geq \iiint_B g(x,y,z)\,\mathrm{d}V \geq 0$.
—helpful for estimating integrals and resolving convergence issues.

Corollary 4.1.3 *If* $f = 1$, *then* $\iiint_B 1\,\mathrm{d}V =$ *volume of solid* B, *denoted* $|B|$.
—true even for more general regions.

Corollary 4.1.4 *For a continuous function* f *over compact* B, *there exists at least one point* $(X,Y,Z) \in B$ *such that*
$|B|\ f(X,Y,Z) = \iiint_B f(x,y,z)\,\mathrm{d}V$.
—1st mean-value theorem for 3D integrals.

Corollary 4.1.5 *Linearity: If $a, b \in \mathbb{R}$ then*

$$\iiint_B (af + bg)\,\mathrm{d}V \;=\; a \iiint_B f\,\mathrm{d}V + b \iiint_B g\,\mathrm{d}V.$$

Corollary 4.1.6 *Additivity: (very important)*
If $B_1 \cap B_2 = \{\} \equiv \emptyset$, then

$$\iiint_{B_1 \cup B_2} f\,\mathrm{d}V \;=\; \iiint_{B_1} f\,\mathrm{d}V + \iiint_{B_2} f\,\mathrm{d}V.$$

As for the actual calculation of triple integrals, Section 4.G extends the ideas outlined in Section 4.C.

4.G Iterated Integration in $\mathbb{R}^3$

In evaluating a triple integral, we again make use of the idea of "slicing". The combination of a 3D integration domain and a function $f(x, y, z)$ results in a 4D graph, but we can visualize only the 3D domain. Keep in mind therefore that the first slice through the domain actually results in a *projection* of the graph of f onto 3D space.

In Figure 4.21 we first take horizontal slices through the 3D integration domain (left panel) which results in 2D regions (right panel). We then take either constant x- or constant y-strips through the horizontal z-slice. The figure specifically shows the choice of taking constant x-strips after taking a constant z-slice through the region.

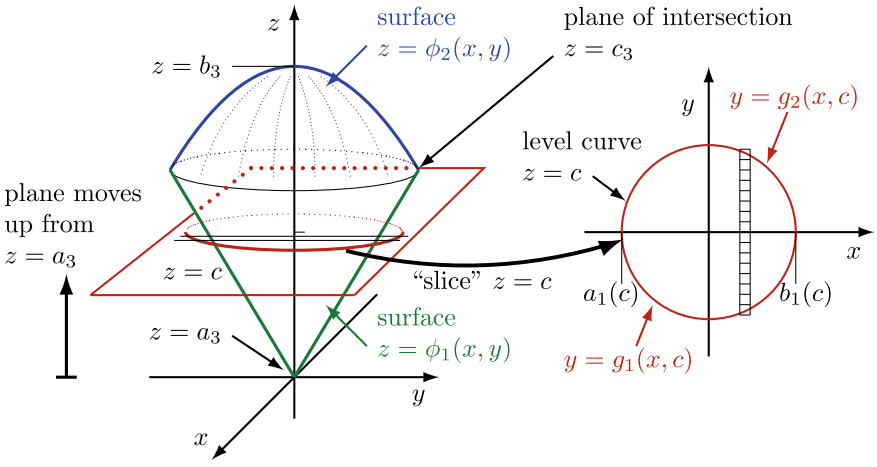

Figure 4.21 The process of domain slicing: first in z, then in x, last in y.

In choosing the order in which we take slices we also commit ourselves to the order in which we perform the iterated integrals, but in reverse order. For instance, for the region bounded by the cone and hemisphere surfaces shown in Figure 4.21 in choosing to integrate last with respect to z, the triple integral must be split into two: one extending from the cone surface to $z = c_3$ which defines the plane of intersection; and a triple integral from the intersection plane to the hemisphere surface. The first iterated integral is given by:

$$\iiint_S f \, \mathrm{d}V = \int_{a_3}^{c_3} \mathrm{d}z \int_{a_1(z)}^{b_1(z)} \mathrm{d}x \int_{g_1(x,z)}^{g_2(x,z)} f(x, y, z) \, \mathrm{d}y.$$

This is in reverse order to the choice of slicing in Figure 4.21: one integrates with respect to y first, between limits that depend on x and z. This gives a contribution along a single strip for given z and given x (right-hand panel of Figure 4.21). Then, one integrates with respect to x, between limits that depend on z. This step adds contributions from all such y-strips to make up a contribution for a single slice at a given z. Finally, one integrates with respect to z between two constant values, here from the very bottom of the cone at $z = a_3$ to the plane of intersection at $z = c_3$. This adds contributions from all such slices. A second integral, of the same form but extending from $z = c_3$ to $z = b_3$, accounts for the contribution from the hemisphere region above $z = c_3$.

For the exact same problem we can consider first taking vertical slices along the x-axis from a_1 to b_1. For each x value we can then take either y-strips or z-strips. Figure 4.22 shows the procedure corresponding to x-slices, then y-strips, and finally z-strips.

The iterated integral for the particular case shown in Figure 4.22 is then, in reverse order,

$$\iiint_S f \, \mathrm{d}V = \int_{a_1}^{b_1} \mathrm{d}x \int_{a_2(x)}^{b_2(x)} \mathrm{d}y \int_{\phi_1(x,y)}^{\phi_2(x,y)} f(x, y, z) \, \mathrm{d}z.$$

That is, one integrates with respect to z first, between limits that depend on x and y, then one integrates with respect to y, between limits that depend on x, and finally one integrates with respect to x between two constants.

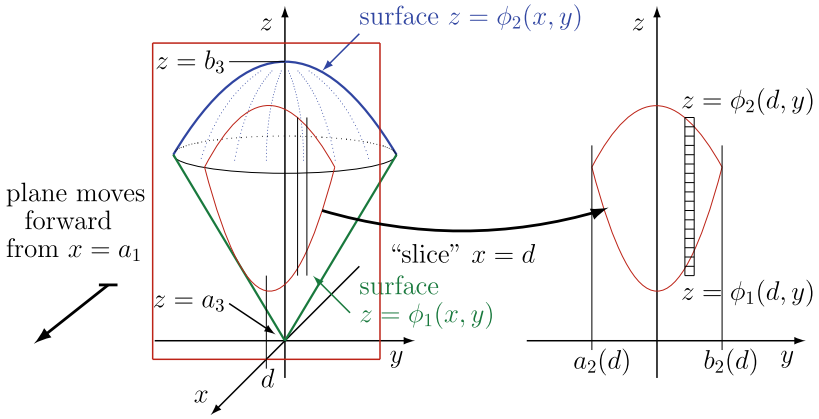

Figure 4.22 The process of domain slicing: first in x, then in y, last in z.

Notice that in contrast to the first choice represented by Figure 4.21 this second choice of integration order depicted in Figure 4.22 does not require a partitioning of the triple integral; the triple integral may be evaluated using a single iterated integral.

Generally, for any triple integral, the possible alternatives are these:

$$\iiint_S f\,\mathrm{d}V: \quad x\text{-slices} \quad \begin{cases} \displaystyle\int_{a_1}^{b_1} \mathrm{d}x \int_{a_2(x)}^{b_2(x)} \mathrm{d}y \int_{a_3(x,y)}^{b_3(x,y)} f\,\mathrm{d}z \\ \displaystyle\int_{a_1}^{b_1} \mathrm{d}x \int_{a_3(x)}^{b_3(x)} \mathrm{d}z \int_{a_2(x,z)}^{b_2(x,z)} f\,\mathrm{d}y \end{cases}$$

$$y\text{-slices} \quad \begin{cases} \displaystyle\int_{a_2}^{b_2} \mathrm{d}y \int_{a_1(y)}^{b_1(y)} \mathrm{d}x \int_{a_3(x,y)}^{b_3(x,y)} f\,\mathrm{d}z \\ \displaystyle\int_{a_2}^{b_2} \mathrm{d}y \int_{a_3(y)}^{b_3(y)} \mathrm{d}z \int_{a_1(y,z)}^{b_1(y,z)} f\,\mathrm{d}x \end{cases}$$

$$z\text{-slices} \quad \begin{cases} \displaystyle\int_{a_3}^{b_3} \mathrm{d}z \int_{a_1(z)}^{b_1(z)} \mathrm{d}x \int_{a_2(x,z)}^{b_2(x,z)} f\,\mathrm{d}y \\ \displaystyle\int_{a_3}^{b_3} \mathrm{d}z \int_{a_2(z)}^{b_2(z)} \mathrm{d}y \int_{a_1(y,z)}^{b_1(y,z)} f\,\mathrm{d}x \end{cases}$$

Thus, one triple integral gives rise to six possible iterated integrals. Note carefully the nature of the limits of each variable and how their dependencies vary from one integral to the next.

■ Example 4.7:

Evaluate the integral $\iiint_D xy\,\mathrm{d}V$, where D is the interior of the sphere $x^2 + y^2 + z^2 = 1$ in the first octant, $0 \le x, y, z \le 1$.

Solution:

As sketched in Figure 4.23, we will take horizontal slices, *i.e.*, hold z constant, for $0 \le z \le 1$, and (for fun) integrate first w.r.t. x before we integrate w.r.t. y, thereafter finally integrating w.r.t. z. The horizontal slices are quarter discs, $x^2 + y^2 \le 1 - z^2$, $x \ge 0,\ y \ge 0$, for a given z.

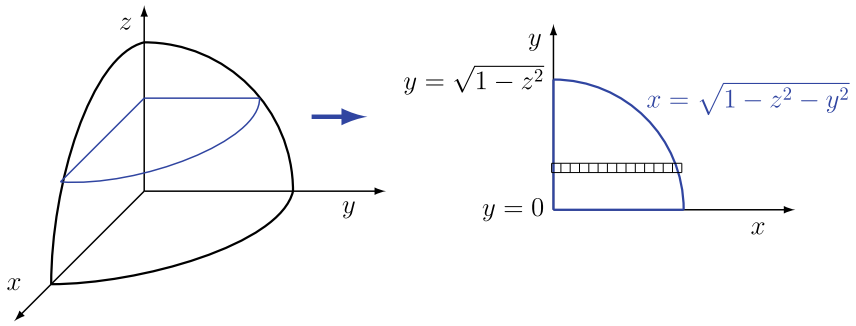

Figure 4.23 The domain D, and the projection of a z-slice onto the xy-plane.

We need to establish the bounds for the innermost, x-integration as functions of y and z. For arbitrary but allowed values of y and z, x will extend from its least value, which is $x = 0$ on the yz-plane to its largest value on the surface of the hemisphere: $x = \sqrt{1 - z^2 - y^2}$.

Next, are the limits on the y-integration, which will only depend on z. These are $y = 0$ on the x-axis, up to the circle limit $y = \sqrt{1 - z^2}$.

Finally, we have the limits on the outermost z-integration, which are the constants 0 and 1.

Consequently, the iterated integral becomes,

$$\begin{aligned}
\iiint_D xy\,\mathrm{d}V &= \int_0^1 \left[\int_0^{\sqrt{1-z^2}} \left(\int_0^{\sqrt{1-z^2-y^2}} xy\,\mathrm{d}x \right) \mathrm{d}y \right] \mathrm{d}z \\
&= \int_0^1 \left[\int_0^{\sqrt{1-z^2}} y \left[\frac{1}{2}x^2 \right]_{x=0}^{\sqrt{1-z^2-y^2}} \mathrm{d}y \right] \mathrm{d}z \\
&= \int_0^1 \left[\int_0^{\sqrt{1-z^2}} \frac{1}{2} y \left(1 - z^2 - y^2\right) \mathrm{d}y \right] \mathrm{d}z \\
&= -\int_0^1 \frac{1}{8} \left[\left(1 - z^2 - y^2\right)^2 \right]_{y=0}^{\sqrt{1-z^2}} \mathrm{d}z \\
&= -\int_0^1 \frac{1}{8} \left(0 - \left(1 - z^2\right)^2 \right) \mathrm{d}z \;=\; \frac{1}{15}.
\end{aligned}$$

■

Some practice is needed to become proficient in determining the limits for an iterated integral. This is particularly true of triple integrals, even when 3D regions are specified as these are potentially challenging to imagine, let alone draw, compared with regions in 2D. This is one of the reasons why the subject of visualizing 3D surfaces was raised in Chapter 1. A similar statement on the need to practice applies to the inverse operation of determining the region of integration if the limits are given. The next Mastery Check exercise explores both processes. Additional exercises can be found in Supplementary Problems 4.21 and 4.22.

Mastery Check 4.8:

Use the limits on the following iterated integral to determine the 3D region of integration,

$$I = \int_0^1 \mathrm{d}z \int_0^{1-z} \mathrm{d}x \int_{x+z}^1 f(x, y, z)\, \mathrm{d}y.$$

Based on this same 3D region, write the triple integral as an iterated integral where the outermost integration is taken w.r.t. x and the innermost integration is taken w.r.t. z.

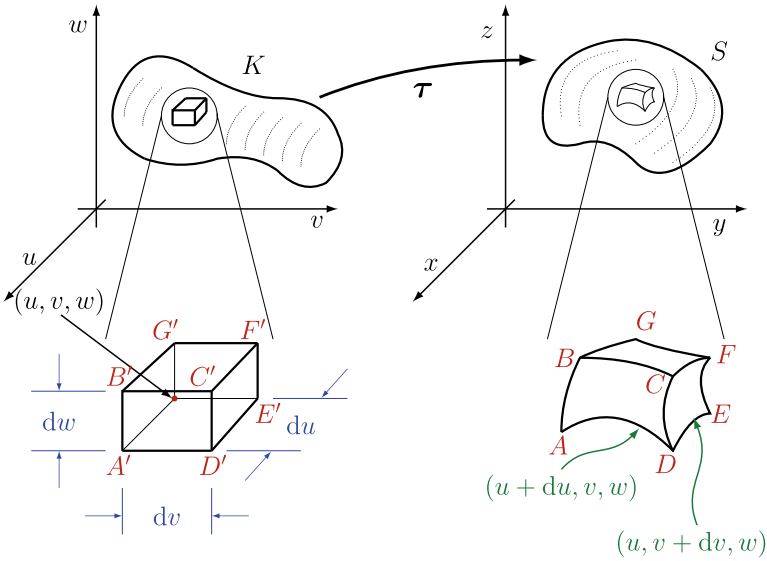

Figure 4.24 A geometrical view of a change of variables in a 3D domain.

4.H Change of Variables in $\mathbb{R}^3$

Consider the triple integral of a continuous function over a closed and bounded domain,

$$I = \iiint_S f(x,y,z)\,\mathrm{d}V,$$

and the bijective C^1-transformation:

$$\tau : \mathbb{R}^3 \longrightarrow \mathbb{R}^3; \quad \boldsymbol{u} \mapsto \boldsymbol{x} = \boldsymbol{g}(\boldsymbol{u}) = g(u,v,w)\mathbf{i} + h(u,v,w)\mathbf{j} + k(u,v,w)\mathbf{k}.$$

This mapping transforms an element of volume in the uvw-domain to a volume element in the xyz-domain, as suggested graphically in Figure 4.24.

If $\mathrm{d}u, \mathrm{d}v, \mathrm{d}w \ll 1$ then (according to Section 1.A) the volume element in S would be given by the absolute value of the scalar triple product

$$\begin{aligned} \mathrm{d}V &= \left|(\overrightarrow{BA} \times \overrightarrow{BC}) \cdot \overrightarrow{BG}\right| \\ &= \big|\big((\mathrm{d}x_u\mathbf{e}_1 + \mathrm{d}y_u\mathbf{e}_2 + \mathrm{d}z_u\mathbf{e}_3) \times (\mathrm{d}x_v\mathbf{e}_1 + \mathrm{d}y_v\mathbf{e}_2 + \mathrm{d}z_v\mathbf{e}_3)\big) \\ &\qquad \cdot(\mathrm{d}x_w\mathbf{e}_1 + \mathrm{d}y_u\mathbf{e}_2 + \mathrm{d}z_w\mathbf{e}_3)\big| \end{aligned}$$

Invoking the chain rule, the scalar triple product can be written in determinant form (Section 1.A, Page 13).

$$\mathrm{d}V = \left|\left| \begin{array}{ccc} \dfrac{\partial x}{\partial u}\mathrm{d}u & \dfrac{\partial y}{\partial u}\mathrm{d}u & \dfrac{\partial z}{\partial u}\mathrm{d}u \\ \dfrac{\partial x}{\partial v}\mathrm{d}v & \dfrac{\partial y}{\partial v}\mathrm{d}v & \dfrac{\partial z}{\partial v}\mathrm{d}v \\ \dfrac{\partial x}{\partial w}\mathrm{d}w & \dfrac{\partial y}{\partial w}\mathrm{d}w & \dfrac{\partial z}{\partial w}\mathrm{d}w \end{array} \right|\right| = \left|\frac{\partial(x,y,z)}{\partial(u,v,w)}\right| \mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w,$$

(derivatives are of course of functions g, h, and k.)

As was the case for a change of variables in a double integral, a change of variables in a triple integral involves the Jacobian determinant for that transformation. The *absolute value* of the Jacobian is the scaling factor between the volume elements $\mathrm{d}V = \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$ in xyz-space and $\mathrm{d}V' = \mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w$ in uvw-space.

Consequently, we have the end result that

$$\iiint_S f(x,y,z)\,\mathrm{d}V = \iiint_K F(u,v,w)\left|\frac{\partial(x,y,z)}{\partial(u,v,w)}\right| \mathrm{d}V',$$

where $F(u,v,w) = f(g(u,v,w), h(u,v,w), k(u,v,w))$, and S is the image of K under τ.

The next example is similar to the 2D example of a change of variables in a double integral in the sense that it is the integration domain that guides the choice of change of variables, but which has the additional benefit of simplifying the integrand. This will not always be the case.

Example 4.8:

Evaluate the triple integral

$$\iiint_V \frac{x+y}{(x+z)\,(y+z)}\mathrm{d}V,$$

where V is the 3D region confined between the six planes $x+z=1$, $x+z=2$, $x+y=0$, $x+y=2$, $y+z=1$, and $y+z=2$.

Solution:

The region V is a parallelepiped, bounded by three pairs of parallel planes. Conveniently, the linear combinations of Cartesian variables also appear in the integrand—the function to be integrated. Both the function and the region suggest the simple change of variables, and their respective range of values:

$$u = x+y \in [0,2] \quad ; \quad v = x+z \in [1,2] \quad ; \quad w = y+z \in [1,2].$$

Thus, the triple integral wrt x, y, z over V may be rewritten as the triple integral wrt u, v, w over the volume B in uvw-space:

$$\iiint_B \frac{u}{vw}\,|J|\,\mathrm{d}V_B,$$

where the Jacobian determinant, utilizing its reciprocal property, is

$$|J| = \left|\frac{\partial(x,y,z)}{\partial(u,v,w)}\right| = \left|\frac{\partial(u,v,w)}{\partial(x,y,z)}\right|^{-1}.$$

For this transformation, the Jacobian determinant evaluated becomes

$$\left|\frac{\partial(u,v,w)}{\partial(x,y,z)}\right|^{-1} = \left\|\begin{matrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{matrix}\right\|^{-1} = \left\|\begin{matrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{matrix}\right\|^{-1} = |-1-1+0|^{-1} = 2^{-1} = \frac{1}{2}.$$

Hence, the triple integral can be evaluated as the iterated integral,

$$\begin{aligned}\iiint_V \frac{x+y}{(x+z)(y+z)}\mathrm{d}V &= \frac{1}{2}\int_0^2 u\mathrm{d}u \int_1^2 \frac{1}{v}\mathrm{d}v \int_1^2 \frac{1}{w}\mathrm{d}w,\\ &= \frac{1}{2}\left[\frac{u^2}{2}\right]_0^2 . [\ln v]_1^2 . [\ln w]_1^2 = \frac{1}{2}.2.\ln 2.\ln 2,\\ &= (\ln 2)^2 .\end{aligned}$$

■

✍ Mastery Check 4.9:

Transform the iterated integral below into iterated integrals w.r.t. cylindrical coordinates, and w.r.t. spherical coordinates:

$$I = \int_0^1 \mathrm{d}x \int_0^{\sqrt{1-x^2}} \mathrm{d}y \int_0^{1+x+y} (x^2 - y^2)\,\mathrm{d}z.$$

(Do not proceed to evaluate the integrals. If you skip to the very last note in this chapter, you will see why!)

✍

4.I n-Tuple Integrals

As we did in going from double integrals to triple integrals, all the preceding ideas, concepts, and mathematical arguments can be generalized to n dimensions. Here, we provide only a skeletal analogue of our previous discussions.

n-tuple integrals

Let $S \subset \mathbb{R}^n$ be a compact set and let $f : S \longrightarrow \mathbb{R}$; the graph of $f \subset \mathbb{R}^{n+1}$.

Enclose S in an n-dimensional box

$$[a_1, b_1] \times [a_2, b_2] \times \ldots \times [a_n, b_n].$$

Partition the box into n-dimensional boxes of size

$$\Delta x_1 \times \Delta x_2 \times \Delta x_3 \times \ldots \times \Delta x_n.$$

Choose $\xi_i \in [x_i, x_i + \Delta x_i] \quad i = 1, 2, \ldots, n.$

Form the sum

$$\sum\sum \ldots \sum f(\xi_1, \xi_2, \ldots, \xi_n)\Delta x_1 \Delta x_2 \ldots \Delta x_n.$$

If the limit of this sum exists as $n \to \infty$ and $\max|\Delta \boldsymbol{x}| \to 0$, we call it the n-dimensional integral of f over S

$$\iint \dots \int_S f(x_1, x_2, \dots, x_n)\, \mathrm{d}V_n = I,$$

where $\mathrm{d}V_n$ is an n-dimensional volume element.

Iterated integrals

If S can be described as

$$\begin{aligned} S \quad &= \quad \big\{\boldsymbol{x} = (x_1, x_2, \dots, x_n) : (x_1, x_2, \dots, x_{n-1}) \in W \subset \mathbb{R}^{n-1} \\ \text{and} \quad &\phi_1(x_1, x_2, \dots, x_{n-1}) \le x_n \le \phi_2(x_1, x_2, \dots, x_{n-1})\big\} \end{aligned}$$

$$\text{then} \quad I \;=\; \iint \dots \int_W \mathrm{d}x_1 \dots \mathrm{d}x_{n-1} \int_{\phi_1}^{\phi_2} f(\boldsymbol{x})\, \mathrm{d}x_n \;=\; \dots$$

and, in fact,

$$I \;=\; \int_{\alpha_1}^{\alpha_2} \mathrm{d}x_1 \int_{\beta_1(x_1)}^{\beta_2(x_1)} \mathrm{d}x_2 \int_{\gamma_1(x_1,x_2)}^{\gamma_2(x_1,x_2)} \mathrm{d}x_3 \dots \int_{\phi_1(x_1,\dots,x_{n-1})}^{\phi_2(x_1,\dots,x_{n-1})} f(\boldsymbol{x})\, \mathrm{d}x_n,$$

which is just one of $n!$ alternative iterated integrals.

Change of variables

Consider a bijective C^1 transformation: $\tau : \boldsymbol{u} \longmapsto \boldsymbol{x} = \boldsymbol{g}(\boldsymbol{u})$, where the functions
$x_i = g_i(u_1, u_2, \dots, u_n),\ i = 1, 2, \dots, n$, are such that the Jacobian determinant (Section 2.H)

$$J = \frac{\partial(g_1, \dots, g_n)}{\partial(u_1, \dots, u_n)} \neq 0.$$

The n-tuple integral I of $f(x_1, \dots, x_n)$ over S is equal to the n-tuple integral of the product of $|J|$ and

$$F(u_1, \dots, u_n) = f\big(x_1(u_1, u_2, \dots, u_n), \dots, x_n(u_1, u_2, \dots, u_n)\big)$$

over the pre-image E of S under τ:

$$I = \iint \dots \int_S f(\boldsymbol{x}) \mathrm{d}V_n = \iint \dots \int_E F(\boldsymbol{u})|J| \mathrm{d}V'_n.$$

See Section 5.A for a more expansive discussion of J in this abstract case.

4.J Epilogue: Some Practical Tips for Evaluating Integrals

On the subject of symmetry

Recall that ...

* If $f(-x) = -f(x)$, then f is *odd*, and $\displaystyle\int_{-a}^{a} f(x)\,\mathrm{d}x = 0$.
—for example: $\sin(x)$, x^3, x^7, $\arctan(x)$

* If $f(-x) = f(x)$, then f is *even*, and $\displaystyle\int_{-a}^{a} f(x)\,\mathrm{d}x = 2\int_{0}^{a} f(x)\,\mathrm{d}x$.
—for example: $\cos(x)$, x^2, $\sin^2(x)$

Did you know that for functions of $n \geq 2$ variables there are other possible symmetry features?

* If $f(-x, y) = -f(x, y)$, then f is *odd with respect to* x, which means that
$$\int_c^d \left(\int_{-a}^{a} f(x,y)\,\mathrm{d}x \right) \mathrm{d}y = 0.$$
—for example: xy^2, $\sin(x).y$, $\arctan(xy)$

* If $f(-x, y) = f(x, y)$, then f is *even with respect to* x, which means that
$$\int_c^d \left(\int_{-a}^{a} f(x,y)\,\mathrm{d}x \right) \mathrm{d}y = 2\int_c^d \left(\int_{0}^{a} f(x,y)\,\mathrm{d}x \right) \mathrm{d}y.$$
—for example: x^2y, $\cos(x).y^3$, $\arctan(x^2y)$

* Similarly, we may have functions $f(x, y)$ which are *odd or even with respect to* y.

* Now, for $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$, we have a *new* possibility, indicated in Figure 4.25:

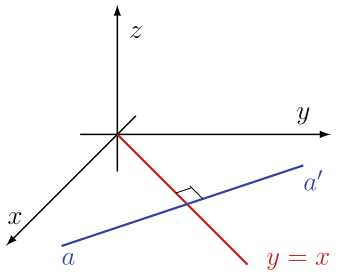

Figure 4.25 The oblique symmetry line $y = x$.

If $f(x, y) = f(y, x)$, then f is *symmetric* across $y = x$.
If $f(x, y) = -f(y, x)$, then f is *antisymmetric* across $y = x$.

Some examples of functions *symmetric* from point a to point a' are
$f(x, y) = x + y$,
$f(x, y) = x^2 + y^2$,
$f(x, y) = 1/\sqrt{x^2 + y^2}$,
$f(x, y) = b + (y - x)^2$ (Figure 4.26(a)).

Some examples of functions *antisymmetric* from point a to point a' are $f(x, y) = x - y$,
$f(x, y) = x^2 - y^2$,
$f(x, y) = \sin(y - x)$ (Figure 4.26(b)).

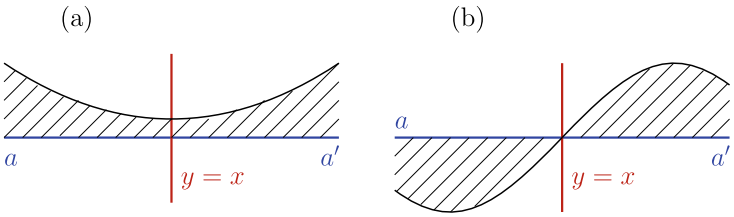

Figure 4.26 (a) Cross-section through $f(x, y) = b + (y - x)^2$;
(b) Cross-section through $f(x, y) = \sin(y - x)$.

Reduction formulae for trigonometric functions

Many of the Mastery Check exercises and Supplementary Problems in both this and the next chapter require the evaluation of integrals of products of positive powers of trigonometric functions, particularly sine and cosine functions. Integrals such as

$$\int_0^{\pi/2} \sin^7 x \, dx, \quad \int_{-\pi/2}^{\pi/2} \cos^8 x \, \sin^3 x \, dx, \quad \text{etc.},$$

may be calculated, without too much stress, with help from the following reduction formulae.

$$I_n = \int_0^{\pi/2} \sin^n x \, \mathrm{d}x \; = \; \int_0^{\pi/2} \cos^n x \, \mathrm{d}x \; = \; \frac{(n-1)}{n} \, I_{n-2}, \;\; \text{for} \;\; n \geq 2,$$

and

$$I_{m,n} = \int_0^{\pi/2} \sin^m x \, \cos^n x \, \mathrm{d}x \; = \; \begin{cases} \dfrac{(m-1)}{m+n} \, I_{m-2,n}, & \text{for} \;\; m \geq 2, n \geq 0, \\ \dfrac{(n-1)}{m+n} \, I_{m,n-2}, & \text{for} \;\; m \geq 0, n \geq 2, \end{cases}$$

complemented by the explicit values

$$I_0 = \int_0^{\pi/2} 1 \, \mathrm{d}x = \frac{\pi}{2}; \quad I_1 = \int_0^{\pi/2} \sin x \, \mathrm{d}x = \int_0^{\pi/2} \cos x \, \mathrm{d}x \; = \; 1,$$

and

$$I_{0,0} = \frac{\pi}{2}; \qquad I_{1,0} = I_{0,1} = 1; \qquad I_{1,1} = \frac{1}{2};$$
$$I_{m,1} = \frac{1}{m+1}, \quad m \geq 0; \qquad I_{1,n} = \frac{1}{n+1}, \quad n \geq 0.$$

These explicit complementary values are easy to verify. As for the reduction formulae, they too are readily proved. For example, using the integration-by-parts technique on I_n for $n \geq 2$ and invoking the trigonometric identity $\cos^2 x + \sin^2 x = 1$, we easily find that

$$n \int \sin^n x \, \mathrm{d}x = -\cos x \sin^{(n-1)} x + (n-1) \int \sin^{(n-2)} x \, \mathrm{d}x.$$

Inserting the limits $x = 0$ and $x = \pi/2$ we arrive at the first of our reduction formulae.

One may also infer from the above integration-by-parts expression (and its analogues) the handy fact that the reduction formulae remain valid when the limits 0 and $\pi/2$ are replaced by any integer multiple of $\pi/2$, although the explicit values of I_0, I_1, etc., may be different to the above quoted values.

By repeated application of the reduction formulae we rapidly reduce the calculation of I_n to either I_0 or I_1, depending on whether n is even or odd. Analogous statements hold for $I_{m,n}$.

As an example calculation, consider $I_8 = \int_0^{\pi/2} \sin^8 x \, \mathrm{d}x$. Using the formula for I_n, we have

$$I_8 = \frac{8-1}{8} I_6 = \frac{7}{8}\frac{6-1}{6} I_4 = \frac{7}{8}\frac{5}{6}\frac{3}{4} I_2 = \frac{7}{8}\frac{5}{6}\frac{3}{4}\frac{1}{2} I_0 = \frac{7}{8}\frac{5}{6}\frac{3}{4}\frac{1}{2}\frac{\pi}{2} = \frac{105\pi}{768}.$$

Similarly, consider the integral $I_{6,7} = \int_0^{\pi/2} \sin^6 x \cos^7 x \, \mathrm{d}x$. This evaluates to

$$\begin{aligned} I_{6,7} &= \frac{6-1}{6+7} I_{4,7} = \frac{5}{13} \cdot \frac{3}{11} I_{2,7} = \frac{5}{13} \cdot \frac{3}{11} \cdot \frac{1}{9} I_{0,7}, \\ &= \frac{5}{13} \cdot \frac{3}{11} \cdot \frac{1}{9} \cdot \frac{6}{7} I_{0,5} = \frac{5}{13} \cdot \frac{3}{11} \cdot \frac{1}{9} \cdot \frac{6}{7} \cdot \frac{4}{5} I_{0,3}, \\ &= \frac{5}{13} \cdot \frac{3}{11} \cdot \frac{1}{9} \cdot \frac{6}{7} \cdot \frac{4}{5} \cdot \frac{2}{3} I_{0,1}, \\ &= \frac{5}{13} \cdot \frac{3}{11} \cdot \frac{1}{9} \cdot \frac{6}{7} \cdot \frac{4}{5} \cdot \frac{2}{3} \cdot 1 = \frac{16}{3003}. \end{aligned}$$

Gamma and beta functions

In certain integration problems included in this and the next chapter, improper single-variable integrals of the form

$$\int_0^\infty \mathrm{e}^{-x} \, x^{a-1} \mathrm{d}x,$$

arise. Such integrals cannot be reduced to simpler expressions involving more elementary (transcendental) functions (such as trigonometric, exponential or logarithmic functions). However, based on ideas used to investigate the convergence of single-variable, improper integrals described in Section 4.D, it can be shown that such integrals converge for all $a > 0$. So, although the above integral cannot be written in closed form (*i.e.*, not as an integral), the fact that the integral converges underpins its consideration as a function (of a) in its own right. Thus, we define the so-called *gamma function*,

$$\Gamma(a) = \int_0^\infty \mathrm{e}^{-x} \, x^{a-1} \mathrm{d}x, \qquad a > 0.$$

From its integral definition, it is clear that $\Gamma(1) = \int_0^\infty \mathrm{e}^{-x} \, \mathrm{d}x = 1$. Moreover, and more importantly, integrating $\Gamma(a)$ by parts it is readily found that,

$$\Gamma(a+1) = \int_0^\infty \mathrm{e}^{-x} \, x^a \mathrm{d}x = -\Big[x^a \mathrm{e}^{-x}\Big]_0^\infty + a \int_0^\infty \mathrm{e}^{-x} \, x^{a-1} \mathrm{d}x.$$

Setting in the limits on the first term on the right-hand side, assuming that $a > 0$, we are led to the so-called recurrence relation:

$$\Gamma(a+1) = a\Gamma(a), \qquad \text{for all} \quad a > 0.$$

In particular, if $a = n$, a positive integer, we deduce that

$$\begin{aligned} \Gamma(n+1) &= n\Gamma(n) = n(n-1)\Gamma(n-1) = n(n-1)(n-2)\Gamma(n-2) \\ &= \cdots = n(n-1)(n-2)\ldots 3.2.1 = n!. \end{aligned}$$

For non-integer $a > 0$, the recurrence relation allows integrals involving fractional powers of x to be evaluated. For example,

$$\Gamma\left(\frac{3}{2}\right) = \frac{1}{2}\Gamma\left(\frac{1}{2}\right),$$

where

$$\Gamma\left(\frac{1}{2}\right) = \int_0^\infty \mathrm{e}^{-x}\, x^{-\frac{1}{2}}\mathrm{d}x = \left\{ \begin{array}{c} x = u^2 \\ \mathrm{d}x = 2u\mathrm{d}u \end{array} \right\} = 2\int_0^\infty \mathrm{e}^{-u^2}\mathrm{d}u = \sqrt{\pi}$$

—see Supplementary Problem 4.10

In the same vein as the gamma function, we introduce the well-known *beta function*, $\beta(m,n)$, defined as the integral

$$\beta(m,n) = \int_0^1 x^{m-1}\,(1-x)^{n-1}\,\mathrm{d}x, \qquad m,n > 0.$$

The beta function is a function of two variables, m and n. By a simple substitution, $x = 1-u$ the beta function takes exactly the same form, but with the roles of m and n switched. That is, the substitution leads to the symmetry property,

$$\beta(m,n) = \beta(n,m).$$

With various other substitutions, one can derive other expressions for $\beta(m,n)$. For example,

$$\beta(m,n) = \left\{ \begin{array}{c} x = \sin^2\theta \\ \\ x = \dfrac{u}{1+u} \end{array} \right\} = \left\{ \begin{array}{c} 2\displaystyle\int_0^{\pi/2} \sin^{2m-1}\theta\, \cos^{2n-1}\theta\, \mathrm{d}\theta \\ \\ \displaystyle\int_0^\infty \frac{u^m}{(1+u)^{m+n}}\, \mathrm{d}u \end{array} \right\},$$

whose forms appear on occasion in the exercises. Finally, the improper double integral,

$$4\int_0^\infty \int_0^\infty \mathrm{e}^{-x^2-y^2}\, x^{2m-1}\, y^{2n-1}\, \mathrm{d}x\mathrm{d}y,$$

defined on the first quadrant in the xy-plane, can be shown to converge for $m,n > 0$ to reveal an important connection between the gamma and beta functions:

$$\Gamma(m)\Gamma(n) = \beta(m,n)\Gamma(m+n) \Longrightarrow \beta(m,n) = \frac{\Gamma(m)\Gamma(n)}{\Gamma(m+n)}.$$

Of the many important relations that can be derived from this one equation, we may highlight the following useful result,

$$\Gamma(p)\Gamma(1-p) = \frac{\pi}{\sin(p\pi)}.$$

4.K Supplementary Problems

§4.B.1. Evaluate the following double integrals over the given rectangular domains.

(a) $\displaystyle\iint_D x\cos xy\,\mathrm{d}x\,\mathrm{d}y, \quad D=\{(x,y): 0\le x\le \pi/2,\ 0\le y\le 1\},$

(b) $\displaystyle\iint_D 2xy\sec^2(x^2y)\,\mathrm{d}x\,\mathrm{d}y,\ D=\{(x,y): 0\le x\le 1,\ 0\le y\le \pi/4\},$

(c) $\displaystyle\iint_D \frac{x\mathrm{e}^{x\sqrt{y}}}{\sqrt{y}}\,\mathrm{d}A \quad D=\{(x,y): 0<x<1,\ 0<y<1\}.$

Hint: Consider the two alternatives of iterated integral. Successful evaluation may depend on the choice of order of integration.

§4.C.2. Evaluate the following double integrals over the given closed convex domains.

(a) $\displaystyle\iint_D \sqrt{xy}\,\mathrm{d}x\,\mathrm{d}y, \quad D=\{(x,y): 0\le x\le 1,\ x^3\le y\le x^2\}.$

(b) $\displaystyle\iint_D xy\,\mathrm{d}x\,\mathrm{d}y, \quad D=\{(x,y): \cos y\le x\le \sin y,\ \frac{\pi}{4}\le y\le \frac{5\pi}{4}\}$

3. Determine the volume bounded by the surfaces: $z=4-x^2-y^2$, $z=0$, and $y=\pm\cos x$, for $-\pi/2\le x\le \pi/2$.

4. Evaluate the iterated integral $I=\displaystyle\int_0^1 \mathrm{d}x\int_{\sqrt{x}}^1 \mathrm{e}^{y^3}\,\mathrm{d}y.$

Hint: First rewrite as a double integral over an appropriate domain D.

§4.D.5. Determine whether the following integrals on open domains converge and if so evaluate them.

(a) $\displaystyle\iint_D \frac{\mathrm{d}x\,\mathrm{d}y}{1+(x+y)^2}, \quad D=\{(x,y): x>0,\ y>0\}.$

(b) $\displaystyle\iint_D \frac{\mathrm{d}x\,\mathrm{d}y}{\sqrt{xy}}, \quad D=\{(x,y): 0<x<1,\ 0<y<1\}.$

(c) $\displaystyle\iint_D x\mathrm{e}^{-(y+x^2/y)}\,\mathrm{d}x\,\mathrm{d}y$, where D is the first quadrant.

Hint: Consider $\{(x,y): 0<x<A,\ 0<y<B\}$, and let $A\to\infty,\ B\to\infty$.

6. Show that the integral $\iint_D \dfrac{(x-y)}{(x+y)^3}\,\mathrm{d}A$, where $D = \{(x,y) : 0 \le x, y \le 1\}$, does not converge.
Hint: Exclude a small rectangle $0 \le x \le \mu < 1$ and $0 \le y \le \nu < 1$ and consider the limits $\mu, \nu \to 0$.

7. Corollary 4.1.2 makes it possible to determine whether a generalized integral converges without undertaking an explicit calculation. Re-expressed as a *comparison criterion* it may be applied to prove convergence as well to provide an upper bound on the value of a given improper integral. Suppose a function $g(x,y)$ can be found such that

$$0 \le f(x,y) \le g(x,y) \ \text{ for all } \ (x,y) \in D.$$

If the double integral $\iint_D g(x,y)\,\mathrm{d}A < \infty$,
then the generalized integral $\iint_D f((x,y)\,\mathrm{d}A < \infty$. (An analogous comparison criterion – with inequality signs reversed – can also assist in determining whether an improper integral is divergent.)

Use the comparison criterion to determine whether the generalized integral

$$\iint_D \frac{\ln\left(1+\sqrt{x^2+y^2}\right)}{\left(x^2+y^2\right)^2}\mathrm{d}A, \quad D = \left\{(x,y) : x^2+y^2 > 1\right\},$$

converges. If so, provide an upper estimate of the integral.
Hint: Refer back to the squeeze relations in Chapter 1.

§4.E.8. Consider the transformation $x = \mathrm{e}^u, \quad y = u + v$. Determine the inverse transformation, specifying the condition under which it exists. For points where the transformation is invertible, confirm the Jacobian property that

$$\frac{\partial(x,y)}{\partial(u,v)}\frac{\partial(u,v)}{\partial(x,y)} = 1.$$

9. Determine $\iint_D y\mathrm{e}^{-(x^2+y^2)}\,\mathrm{d}x\,\mathrm{d}y$, where $D = \{(x,y) \in \mathbb{R}^2 : x^2+y^2 \le 1,\ y > 0\}$.

10. One can determine $I = \displaystyle\int_{-\infty}^{\infty} \mathrm{e}^{-x^2/2}\,\mathrm{d}x$ by considering the symmetry arrangement

$$I^2 = 4\left(\int_0^\infty \mathrm{e}^{-x^2/2}\,\mathrm{d}x\right)\left(\int_0^\infty \mathrm{e}^{-y^2/2}\,\mathrm{d}y\right)$$
$$= \iint_R \mathrm{e}^{-(x^2+y^2)/2}\,\mathrm{d}x\,\mathrm{d}y,$$

where R is the first quadrant on the Cartesian plane (see Section 4.J).

Use a polar coordinate transformation to evaluate this integral.

11. Calculate the volume of the solid defined by the intersection of the surfaces

$$x \geq 0, \quad z \geq 0, \quad z \leq x^2 + y^2, \quad 1 \leq x^2 + y^2 \leq 4.$$

Hint: Sketch the region of integration in the xy-plane and think of a suitable change of variables based on this.

12. Evaluate the double integral $\quad I = \iint_T \mathrm{e}^{(y-x)/(y+x)}\,\mathrm{d}A$
where T is the triangle with corners at the points $(0,0)$, $(a,0)$, $(0,a)$.
Hint: An attempt to integrate in the xy-plane is likely to fail. Apply the simplest and most obvious transformation based on the form of the function.
Try the "not-so-obvious" transformation: polar coordinates. Surprisingly, this works, too. You may need a few trigonometric relations:

$$\tan(\theta - \pi/4) = \frac{\tan\theta - 1}{1 + \tan\theta}, \quad \cos(\theta - \pi/4) = \frac{\cos\theta + \sin\theta}{\sqrt{2}}.$$

13. By introducing a change of variables $(x, y) \to (u = x^3, v = y^3)$ evaluate the double integral

$$\iint_D x^2 y^3 \sqrt{1 - x^3 - y^3}\,\mathrm{d}A,$$

where $D = \{(x, y) : x \geq 0, y \geq 0, x^3 + y^3 \leq 1\}$. You may need $\Gamma(1/3)$ and $\Gamma(1/6)$.

*14. Sketch the first quadrant region $D \subset \mathbb{R}^2$ bounded by the curves $2x^2 + y^2 = 8$ and $2x^2 + y^2 = 16$, and the lines $y = 2x$ and $y = 4x$. Express the double integral

$$I = \iint_D \frac{1}{x}\,\mathrm{d}A$$

as an iterated integral where one integrates *first* with respect to x and *then* with respect to y. From this, or otherwise, evaluate the double integral.

15. Determine the volume of the larger portion of the unit ball $x^2 + y^2 + z^2 \leq 1$ that is cut off by the plane $ax + by + cz = d$, where $a, b, c, d > 0$.
Express your answer in terms of the factor $\mathcal{D} = \dfrac{|d|}{\sqrt{a^2 + b^2 + c^2}}$.
This is an exercise in setting up integration limits. Do not assume a simplified orientation.
Hints: (i) First consider the simpler 2D problem of the unit disc $x^2 + y^2 \leq 1$ and the line $ax + by = d$.
(ii) For the 3D problem consider the relationship between the normal vectors to the two surfaces.

*16. Consider the region R bounded by the circles $x^2 + y^2 = Ax$, $x^2 + y^2 = Bx$, $x^2 + y^2 = Cy$, and $x^2 + y^2 = Dy$, where $B > A > 0, D > C > 0$. Using an appropriate change of variables, evaluate the integral

$$\iint_R \frac{dA}{(x^2 + y^2)^3}.$$

17. (i) Determine the Jacobian determinant for the mapping $x = u(1 + v),\ y = v(1 + u)$.
(ii) For region $D = \{(x, y) : 0 \leq y \leq x,\ 0 \leq x \leq 2\}$, evaluate the double integral

$$I = \iint_D \frac{\mathrm{d}A}{\sqrt{(x - y)^2 + 2(x + y) + 1}}.$$

Hint: For part (ii), consider the inverse of the transformation in (i).

*18. Consider the iterated integral

$$I = \int_0^{c\sqrt{h/k}} \left(\int_{kx^2/(c^2+x^2)}^{hc^2/(c^2+x^2)} f(x, y)\mathrm{d}y \right) \mathrm{d}x,$$

where h, k, and c are positive constants, with $h > k$.

(a) Sketch the domain of integration, D, and then rewrite I as an iterated integral with the order of integration reversed.

(b) Show that the change of variables

$$u = h_1(x, y) = y(c^2 + x^2) \quad ; \quad v = h_2(x, y) = \sqrt{\frac{k}{c}}x,$$

is a one-to-one and onto transformation.

(c) If S is the image of D under this transformation, express the transformed double integral over S as an iterated integral with respect to u and v.

19. For region $D = \{(x, y) : x \geq 0, \quad 1 \leq x + y \leq 2, \quad 1 \leq x^2 + (y-2)^2 \leq 4\}$, evaluate

$$I = \iint_D (y - x - 2)\mathrm{e}^{x^2+y^2-4y}\mathrm{d}A.$$

§4.F.20. Interpret the integral $\iiint_V f(x, y, z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$ if

(i) $f(x, y, z) = 1$.

(ii) $f(x, y, z)$ is the material density at point (x, y, z).

(iii) $f(x, y, z) = \sqrt{x^2 + y^2}\times$ the material density at point (x, y, z).

(iv) $f(x, y, z) = (x^2 + y^2)\times$ the material density at point (x, y, z).

§4.G.21. For each of the following, sketch the region and evaluate the integral

(i) $\displaystyle\int_0^1 \mathrm{d}z \int_0^z \mathrm{d}y \int_0^y \mathrm{d}x$ (ii) $\displaystyle\int_0^2 \mathrm{d}x \int_1^x \mathrm{d}y \int_2^{x+y-1} y\mathrm{d}z$

(iii) $\displaystyle\int_0^1 \mathrm{d}x \int_x^{\sqrt{x}} \mathrm{d}y \int_{1-x-y}^{1+x+y} xy\mathrm{d}z$

*22. Let S be the closed, first octant solid bounded by the coordinate planes
$(x = y = z = 0)$, the plane $y = 1 + 2x$ and the sphere
$x^2 + y^2 + z^2 = 4$.
For any integrable function f defined on S write the triple integral $\iiint_S f\mathrm{d}V$ as an iterated integral with respect to x, y, z in six different ways. That is, determine the respective limits depicted in the iterated integral formulae on Page 269.

23. Determine the volume of the region enclosed by the two surfaces $z = 8 - x^2 - y^2$ and $z = x^2 + 3y^2$ (Figure 4.27(a)). Hint: Take horizontal z-slices.

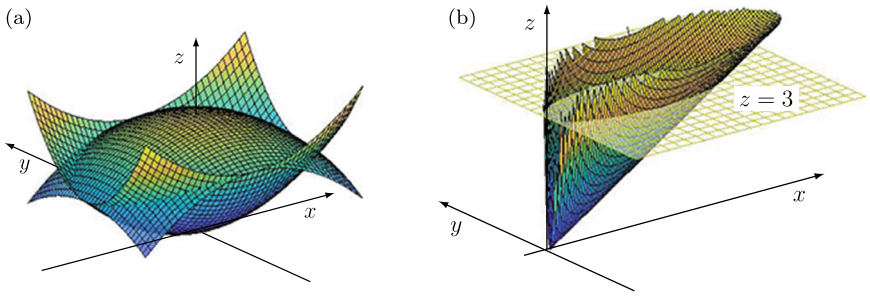

Figure 4.27 (a) Two intersecting paraboloids in Problem 23; (b) The graph of $x^2 + y^2 = xz$ intersected by $z = 3$ in Problem 26.

24. Let S be the body bounded by the planes $x = 0$, $y = 0$, and $z = 4$, and the surface $z = x^2 + y^2$. Calculate $I = \iiint_S x \, \mathrm{d}V$ by
(a) first taking z-slices, and (b) first taking x-slices.

25. Compute the volume of the finite region confined between the cylinder $x^2 - 2x + y^2 = 0$ and the cylinder $z^2 - 2x = 0$. The region defined by this intersection is shown in Figure 4.28. (See also Figure 1.35 on Page 60.)

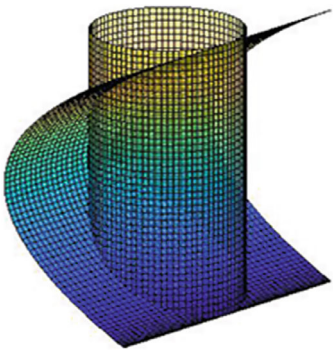

Figure 4.28 Two intersecting cylinders in Problem 25.

§4.H.26. Evaluate the triple integral of the function $f(x, y, z) = x^2 y^2 z$ over the region R bounded by the cone $x^2 + y^2 = xz$ and the planes $z = 0$ and $z = c$ (Figure 4.27(b)).

27. Determine the volume of the body defined by the inequalities,

$$z \leq 4 - x^2 - y^2 \quad ; \quad z \geq 3x^2 + y^2 \quad ; \quad y \geq \sqrt{2}\,|x|\,.$$

28. Determine the volume of the body defined by the inequality

$$x^2 + 2y^2 + 2xy + |z| \leq 4.$$

29. Show that for any $\alpha \in (0, \pi)$

$$\int_0^\infty \left(\int_0^\infty xy \mathrm{e}^{-(x^2+y^2+2xy\cos\alpha)} \mathrm{d}y \right) \mathrm{d}x = \frac{\sin\alpha - \alpha\cos\alpha}{4\sin^3\alpha}.$$

30. Transform each of the following two iterated integrals into iterated integrals with respect to both cylindrical and spherical coordinates.

*(i) $\displaystyle\int_0^{1/\sqrt{2}} \mathrm{d}x \int_0^{\sqrt{1-x^2}} \mathrm{d}y \int_0^{x+y} \mathrm{d}z$ (ii) $\displaystyle\int_{-1}^{1} \mathrm{d}x \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} \mathrm{d}y \int_{\sqrt{x^2+y^2}}^{1} \mathrm{d}z$

31. Determine the volume of the region lying within the two cylinders $x^2 + y^2 = 1$ and $y^2 + z^2 = 1$.

*32. Determine the volume of the region in the first octant bounded by the surface $x^4 + y^4 + z^4 = c^4$ and the coordinate planes. Express your answer in terms of a gamma function.

*33. Let T be the tetrahedron with vertices $(a, 0, 0)$, $(0, a, 0)$, $(0, 0, a)$, and $(0, 0, 0)$. Show that

$$\iiint_T \frac{x^{1/2}y^{3/2}z^{5/2}}{(x+y+z)^{13/2}} \mathrm{d}V = \frac{2\pi a}{3003}.$$

Hint: Find a transformation that maps T to the unit cube. You may need to utilize the integral and numerical properties of gamma functions.

*34. Evaluate the triple integral

$$I = \iiint_\Omega \frac{\mathrm{d}V}{\sqrt{x^2+y^2}},$$

where Ω is bounded by the surfaces $x^2 + y^2 = 2az$ and $z^2 = 2ax$ for $a \geq 0$.

*35 Suppose $a > 0$ is a constant. For what values of $m \in \mathbb{Z}$ is the improper integral

$$I = \int_0^\infty \int_0^\infty \int_0^\infty \frac{\left(x^2+y^2+z^2\right)^{m/2}}{\left(x^2+y^2+z^2+a^2\right)^{(m+5)/2}} \mathrm{d}x\mathrm{d}y\mathrm{d}z$$

convergent? For the convergent cases show that

$$I = \frac{\pi}{2(m+3)a^2}.$$

§4.I.36. Suppose $f(x, y, z, t)$ describes the rate of change of electric charge density at point (x, y, z) at time t throughout a volume V. Give meaning to the integral

$$I = \iiiint_D f(x, y, z, t)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}t$$

where $D = \{(x, y, z, t) : x^2 + y^2 + z^2 \le a^2,\ 0 \le t \le T\}$. Indicate how the integration might be carried out and evaluate I in the case $f(x, y, z, t) = c$, a constant.

*37. Show that

$$\int_0^x \mathrm{d}x_1 \int_0^{x_1} \mathrm{d}x_2 \int_0^{x_2} \mathrm{d}x_3 \cdots \int_0^{x_{n-1}} f(x_n)\mathrm{d}x_n = \frac{1}{(n-1)!}\int_0^x (x-t)^{n-1} f(t)dt.$$

*38. Devise suitable n-dimensional spherical polar coordinates to satisfy

$$x_1^2 + x_2^2 + \cdots + x_n^2 = a^2$$

and, using integral properties of gamma functions, derive the volume of the n-ball.

*39. Using the results of Supplementary Problem 38 determine the volume of the n-D ellipsoid:

$$\frac{(x_1 - b_1)^2}{a_1^2} + \frac{(x_2 - b_2)^2}{a_2^2} + \cdots + \frac{(x_n - b_n)^2}{a_n^2} \le 1.$$

§4.J.40. Let S be the unit ball in $\mathbb{R}^3$. Show that $\iiint_S f(x, y, z)\mathrm{d}V = -4\pi$, where

$$f(x, y, z) = -3 + 2y + (x^4 + y^6 + z^8)\sin x^3.$$

41. Give reasons why you may decide whether the following integrals are zero or not by inspection only (*i.e.*, without any computation).

(a) $\iint_D x\mathrm{e}^{-x^2-y^2}\,\mathrm{d}x\,\mathrm{d}y$, where $D = \{(x, y) : |x| \le 1,\ |y| \le 1\}$.

(b) $\iint_D x\mathrm{e}^{-x^2-y^2}\,\mathrm{d}x\,\mathrm{d}y$, where $D = \{(x, y) : |x| \le 1,\ 0 \le y \le 1\}$.

(c) $\iint_D y\mathrm{e}^{-x^2-y^2}\,\mathrm{d}x\,\mathrm{d}y$, where $D = \{(x, y) : |x| \le 1,\ 0 \le y \le 1\}$.

(d) $\iint_D (x - y)\mathrm{e}^{-x^2-y^2}\,\mathrm{d}x\,\mathrm{d}y$, where $D = \{(x, y) : |x| \le 1,\ |y| \le 1\}$.

(e) $\iint_D (x-y)\mathrm{e}^{-x^2-y^2}\,\mathrm{d}x\,\mathrm{d}y$, where $D = \{(x,y) : |x| \le 1,\ 0 \le y \le 1\}$.

(f) $\iint_D (x-y)^2\mathrm{e}^{-x^2-y^2}\,\mathrm{d}x\,\mathrm{d}y$, where $D = \{(x,y) : |x| \le 1,\ |y| \le 1\}$.

(g) $\iint_D (x-y)^2 \sin(x-y)\,\mathrm{d}x\,\mathrm{d}y$, where $D = \{(x,y) : |x| \le 1,\ |y| \le 1\}$.

(h) $\iint_D (x-y)\sin(x-y)\,\mathrm{d}x\,\mathrm{d}y$, where $D = \{(x,y) : |x| \le 1,\ |y| \le 1\}$.

(i) $\iint_D (x-y)\sin(x+y)\,\mathrm{d}x\,\mathrm{d}y$, where $D = \{(x,y) : |x| \le 1,\ |y| \le 1\}$.

42. Evaluate the following one-dimensional integrals using the methods of Section 4.J.

(a) (i) $\int_0^{\pi/2} \sin^7 x\ \mathrm{d}x$, (ii) $\int_0^{\pi} \sin^{10} x\ \mathrm{d}x$, (iii) $\int_0^{\pi/6} \cos^9 3x\ \mathrm{d}x$.

(b) (i) $\int_0^{\pi} \sin^8 x \cos^6 x\ \mathrm{d}x$, (ii) $\int_{-\pi}^{\pi} \sin^6 x \cos^4 x\ \mathrm{d}x$, (iii) $\int_{-\pi/4}^{\pi/4} \sin^4 2x \cos^9 2x\ \mathrm{d}x$.

43. Evaluate: (i) $\Gamma(\frac{7}{2})$, (ii) $\Gamma(\frac{1}{6})\Gamma(\frac{5}{6})$, (iii) $\beta(2, \frac{3}{2})$, (iv) $\Gamma(\frac{10}{3})\Gamma(\frac{11}{3})$.

44. Show that $\beta(p,p) = 2^{(1-2p)}\beta(p, \frac{1}{2})$.

45. Express $\int_0^1 \int_0^{(1-x)} (xy)^{-3/4}\ \mathrm{d}y\mathrm{d}x$ in terms of a single gamma function.



Chapter 5

Vector Calculus

The majority of systems that arise in engineering and in the physical sciences fall into one of three camps: kinematic, dynamic, and static systems. In all three categories, a system is only partially described by magnitudes of quantities. Whether a system is in a state of motion or in a state of equilibrium, it can only be completely characterized when directional dependencies are considered. The complete characterization of a system is therefore achieved by quantities that describe both *direction and magnitude*. These are vector-valued functions which may vary with respect to specified independent variables, *e.g.*, position $\boldsymbol{x}$ and time t. A force acting on an object is an example of such a *vector-valued function*, as is the object's response in terms of its velocity of motion. Another example, this time of a distributed character, is the flow field of a fluid continuum.

This chapter brings together concepts that were introduced in Chapters 2 and 4 for scalar-valued functions, and extends their applications to functions that are themselves vectors. However, the outcomes of those applications are not always simple generalizations of scalar-valued results. We will discover that by including a directional attribute a range of new results, new concepts, and new features emerge that hold specifically for vector-valued functions.

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5.A Vector-Valued Functions

Force and velocity are two common-place examples of vector-valued functions. While it helps to keep such physical quantities in mind in a study of vector functions, it is also helpful to be familiar with a more general definition that is not tied to a specific application.

Definition 5.1
A vector, $\boldsymbol{f}$, is called a vector-valued (m-dimensional) function of the vector variable $\boldsymbol{x} \in \mathbb{R}^n$ if each of its m components, f_i, for $i = 1, \ldots m$, are real-valued functions of $\boldsymbol{x}$:

$$f_i = f_i(\boldsymbol{x}); \quad f_i : \mathbb{R}^n \longrightarrow \mathbb{R},\ i = 1, 2, \ldots, m$$

and

$$\boldsymbol{f}(\boldsymbol{x}) = \big(f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \ldots, f_m(\boldsymbol{x})\big).$$

We may say that $\boldsymbol{f} : \mathbb{R}^n \longrightarrow \mathbb{R}^m$ defines a transformation $\boldsymbol{x} \longmapsto \boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x})$:

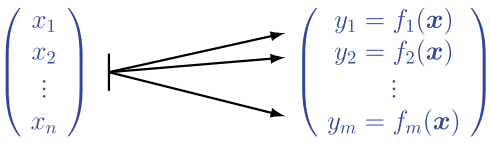


Figure 5.1 The vector mapping $\boldsymbol{x} \longmapsto \boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x})$.

The f_i, $i = 1, 2, ..., m$, in Figure 5.1 are the components of $\boldsymbol{f}$ in the corresponding mutually orthogonal directions $\mathbf{e}_i$, $i = 1, 2, ..., m$ in $\mathbb{R}^m$ (in $\mathbb{R}^3$ these would be $\mathbf{i}, \mathbf{j}, \mathbf{k}$).

From this most general form we now consider three important, specific classes of vector-valued functions.

I. Curves $\boldsymbol{f} : \mathbb{R} \to \mathbb{R}^m$

The dependence here is on a single variable. For applications in physics where (x, y, z) denotes position of an object in $\mathbb{R}^3$, it is customary to denote the independent variable by t, alluding to time. $\boldsymbol{f}(t) = (x(t), y(t), z(t))$ then describes the position of the point at time t. From a mathematical perspective, the vector function $\boldsymbol{f}$ here defines a transformation $t \longmapsto \boldsymbol{f}(t)$ for a point in $\mathbb{R}^m$. As the independent variable varies over some interval domain I in $\mathbb{R}$, the point traces out a *curve* in $\mathbb{R}^m$. This is illustrated in Figure 5.2 for the case $m = 2$.

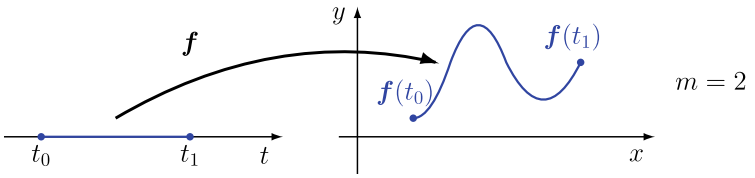


Figure 5.2 A curve in 2-space.

From the point of view of physics, the vector function describes the *path* or *trajectory* of an object in motion. It is the foundation stone of the field of kinematics.

Example 5.1:

Consider a ball rolling down a funnel at uniform vertical speed, such as that shown Figure 5.3. The position (x, y, z) of the ball is time-dependent (t-dependent), with coordinate dependencies.

$$\begin{cases} x = \left(1 - \dfrac{t}{4\pi}\right)^2 \cos t, \\ y = \left(1 - \dfrac{t}{4\pi}\right)^2 \sin t, \qquad t \in [0, 4\pi]. \\ z = 1 - \dfrac{t}{4\pi}, \end{cases}$$

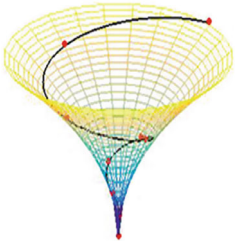


Figure 5.3 A trajectory in $\mathbb{R}^3$ described in Example 5.1.

From both a mathematical perspective on the subject of curves and a physics perspective on applications to particle trajectories, it is common practice use $\boldsymbol{r}$ in place of $\boldsymbol{f}$ to reflect spatial position. Generalizing to higher dimension systems, we are thus motivated to write

$$\boldsymbol{r}(t) = \big(x_1(t), x_2(t), \ldots, x_m(t)\big),$$

to represent a curve in m-space. However, limiting ourselves to the real-world case of $\mathbb{R}^3$, as indicated earlier, we use the more familiar notation

$$\boldsymbol{r}(t) = \big(x(t), y(t), z(t)\big),$$

although even in this low-dimensional case there are advantages to using the index notation (see Section 5.G).

The physical world places some restrictions on the types of vector functions that can be used to describe trajectories or curves in 3D space. The primary restrictions relate to continuity and differentiability, *i.e.*, smoothness of the curves.

Theorem 5.1
Suppose I is an open connected interval in $\mathbb{R}$. The vector $\boldsymbol{r}(t)$ is a continuous vector function of $t \in I$, with continuous first derivatives (i.e., is a C^1 function of t) if each of its component functions are C^1 functions of $t \in I$.

As with all derivatives, the derivative of the vector-valued function $\boldsymbol{r}(t)$ is based on a converged limit process. This limit is defined in much the same way as it appeared in Chapter 1, but now is applied to *each* component of $\boldsymbol{r}(t)$, with the results combined to produce a new vector quantity.

The theorem implies that the limit $\lim\limits_{\Delta t \to 0} \dfrac{\boldsymbol{r}(t+\Delta t) - \boldsymbol{r}(t)}{\Delta t}$ exists if corresponding limits of all components exist.

That is,

$$\begin{aligned}
&\lim_{\Delta t \to 0} \frac{\boldsymbol{r}(t+\Delta t) - \boldsymbol{r}(t)}{\Delta t} \\
&\quad = \left(\lim_{\Delta t \to 0} \frac{x_1(t+\Delta t) - x_1(t)}{\Delta t}, \ldots, \lim_{\Delta t \to 0} \frac{x_m(t+\Delta t) - x_m(t)}{\Delta t} \right) \\
&\qquad\qquad \text{—the limit process applied to each component} \\
&\quad = \left(\frac{\mathrm{d}x_1}{\mathrm{d}t}(t), \ldots, \frac{\mathrm{d}x_m}{\mathrm{d}t}(t) \right) \qquad \text{—valid if all } x_i \text{ are } C^1 \text{ functions} \\
&\quad \equiv \underbrace{\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}(t)}_{\text{definition}} \quad = \quad \underbrace{\boldsymbol{v}(t)}_{\text{connection to physics, the velocity of an object in motion}} \quad = \quad \boldsymbol{r}'(t).
\end{aligned}$$

Some discrete steps in this limit process are depicted in Figure 5.4.

Assuming the derivative function $\boldsymbol{r}'(t)$ is similarly differentiable, then the limit process can be repeated to define the second derivative function $\boldsymbol{r}''(t)$.

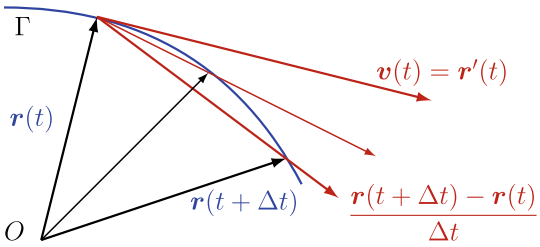


Figure 5.4 The limit process for defining the vector $\boldsymbol{r}'(t)$ for curve Γ.

Rules for differentiating curve vectors

As the definition of the derivative of a vector-valued function of one variable is a straightforward generalization of the derivative definition for a scalar function of one variable, it is natural to expect that the rules for differentiating scalar functions also generalize. These can be proved by breaking the vector functions down into their components and applying concepts from single-variable calculus to each component. The results are then combined to form corresponding vector versions.

For differentiable vector and scalar functions

$$\boldsymbol{u}, \boldsymbol{v} : \mathbb{R} \longrightarrow \mathbb{R}^n, \quad \phi : \mathbb{R} \longrightarrow \mathbb{R}, \quad f : \mathbb{R}^n \longrightarrow \mathbb{R},$$

it can be shown that

(a) $\dfrac{\mathrm{d}}{\mathrm{d}t}\Big(\boldsymbol{u}(t) + \boldsymbol{v}(t)\Big) = \boldsymbol{u}'(t) + \boldsymbol{v}'(t)$

(b) $\begin{aligned} \dfrac{\mathrm{d}}{\mathrm{d}t}\Big(\phi(t)\boldsymbol{u}(t)\Big) &= \dfrac{\mathrm{d}}{\mathrm{d}t}\Big(\phi(t)u_1(t) + \cdots + \phi(t)u_m(t)\Big) \\ &= \phi'(t)\boldsymbol{u}(t) + \phi(t)\boldsymbol{u}'(t) \end{aligned}$

(c) $\dfrac{\mathrm{d}}{\mathrm{d}t}\Big(\boldsymbol{u}(t) \cdot \boldsymbol{v}(t)\Big) = \boldsymbol{u}'(t) \cdot \boldsymbol{v}(t) + \boldsymbol{u}(t) \cdot \boldsymbol{v}'(t)$ —the scalar product rule

(d) $\dfrac{\mathrm{d}}{\mathrm{d}t}\Big(f\big(\boldsymbol{u}(t)\big)\Big) = \boldsymbol{\nabla} f\big(\boldsymbol{u}(t)\big) \cdot \boldsymbol{u}'(t)$ —the chain rule

(e) $\dfrac{\mathrm{d}}{\mathrm{d}t}\Big(\boldsymbol{u}\big(\phi(t)\big)\Big) = \boldsymbol{u}'\big(\phi(t)\big)\phi'(t)$ —another chain rule application

and, for $n = 3$, we also have

$$\text{(f)}\quad \frac{\mathrm{d}}{\mathrm{d}t}\Big(\boldsymbol{u}(t)\times\boldsymbol{v}(t)\Big) \;=\; \boldsymbol{u}'(t)\times\boldsymbol{v}(t)+\boldsymbol{u}(t)\times\boldsymbol{v}'(t)$$

—the vector product rule—the order of the vectors is important

✍ Mastery Check 5.1:

Prove the derivative laws (c)–(f) by breaking down the vectors into component parts.

✍

Remark

* Within the context of particle mechanics one can make a number of physical associations, this time for the derivatives of $\boldsymbol{r}(t)$:

$\boldsymbol{r}(t)$	—	particle position at time t
$\boldsymbol{r}'(t)=\boldsymbol{v}(t)$	—	particle velocity at time t
$\boldsymbol{r}''(t)=\boldsymbol{a}(t)$	—	particle acceleration at t
$\lvert\boldsymbol{v}(t)\rvert = v(t) = \sqrt{v_1^2(t)+\cdots+v_m^2(t)}$	—	particle speed at time t

Elementary differential properties of curves

Describing trajectories, which are fundamental to particle mechanics, is one application of a vector-valued function of one variable. In that case, the physical interest is divided between determining where the particle is at any point in time and computing the particle's position history, *i.e.*, the entire path the particle took leading up to that point in time. Another area of interest focuses on the local properties of the path itself, as a turning and twisting curve in space. While this perspective can potentially increase our understanding of particle dynamics, its real value lies in its application to differential geometry, continuum dynamics of materials (fluid and solid) and general relativity. The fundamental property on which this latter perspective is based is that of the *tangent vector*.

In order for the tangent vector to be well defined at any point along the curve, the curve must be such that the limit process defining the derivative can be executed (*the condition of continuity*) and then for that limit to exist (*the condition of differentiability*). In addition to these conditions, which apply even in single-variable calculus, we have the further condition that the derivative of the vector *must be nonzero*. This leads to the concept of curve *smoothness*.

Definition 5.2
Suppose I is an open connected interval in $\mathbb{R}$. A curve Γ, described by a vector function $\boldsymbol{r}(t)$ for $t \in I$, is called **smooth** *if $\boldsymbol{r}(t)$ is a C^1-function* $\left(\dfrac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} \text{ exists}\right)$ *and* $\dfrac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}$ **never** *vanishes* $\left(\dfrac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} = \boldsymbol{v} \neq 0.\right)$ *for any $t \in I$.*

Remarks

* In many texts, points $\boldsymbol{r}(t)$ for $t \in I$ at which $\boldsymbol{r}'(t)$ exists and is nonzero are called *regular points*. A curve possessing only regular points is therefore also called *regular*.

* The condition $\boldsymbol{r}'(t) \neq 0$ means that not all components of the vector $\boldsymbol{r}'(t)$ can vanish simultaneously. It may still arise that one or more components vanish, but not all n at the same t value.

  The reason why the nonzero derivative condition is essential for smoothness is demonstrated in the 2D example cases below.

  Let $\boldsymbol{r}(t) = (x(t), y(t))$ describe a curve or trajectory in the xy-plane for t in some interval I. Suppose the component functions of time, $x(t)$ and $y(t)$, exhibit either of the two behaviours depicted in Figure 5.5 in which $x(t)$ and $y(t)$ simultaneously possess extreme points as functions of t.

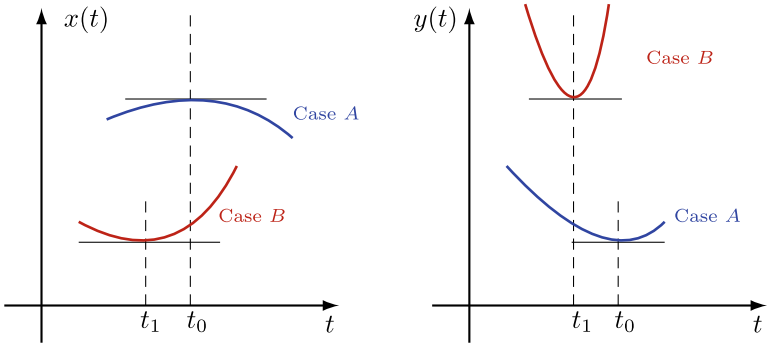


Figure 5.5 Two cases of $x(t)$ and $y(t)$ extreme points at common t values.

In Case A, $x(t)$ exhibits a maximum at $t = t_0$, while $y(t)$ exhibits a minimum at $t = t_0$. In Case B, both $x(t)$ and $y(t)$ have a minimum at $t = t_1$. In both cases, both functions have zero derivatives at the respective t points: $t = t_0$ and $t = t_1$. The corresponding trajectories

in the xy-plane that are consistent with these extremum conditions are shown in Figure 5.6. The arrows indicate the path taken as t increases.

In both (and all similar) cases the curve derivative

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{\mathrm{d}y/\mathrm{d}t}{\mathrm{d}x/\mathrm{d}t} = \begin{pmatrix} 0 \\ \overline{0} \end{pmatrix},$$

is not defined at the point where the derivatives of the t-dependent functions $x(t)$ and $y(t)$ are both zero. This occurs at t_0 in Case A and t_1 in Case B. Correspondingly, a kink singularity appears in the respective trajectories in the xy-plane, as displayed in Figure 5.6. Hence the curves are not smooth at those points. The reader may wish to work out what situation corresponds to Case C included in Figure 5.6.

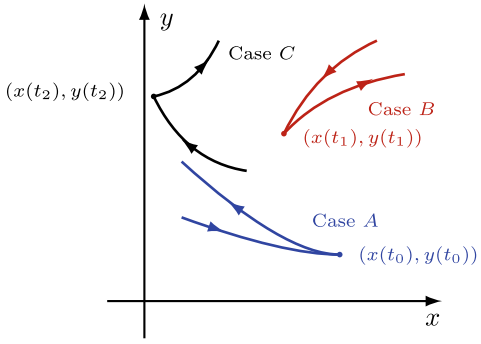


Figure 5.6 Curve trajectories possessing singular points.

Definition 5.3
Suppose I is an open connected interval in $\mathbb{R}$. For a smooth curve Γ defined by $\boldsymbol{r}(t)$ for $t \in I$, the vector function $\boldsymbol{v}(t) = \boldsymbol{r}'(t)$ is a **tangent vector** *to Γ at the point $\boldsymbol{r}(t)$.*

The tangent vector is the end result of the limit process illustrated schematically in Figure 5.4. While that specific vector already provides new information about the curve, *e.g.*, indicating the direction in which the curve continues with increasing t, much more can be derived from it.

Definition 5.4
For a smooth curve Γ *described by a vector function* $\boldsymbol{r}(t)$ *defined on an open connected interval* I, *let* $\boldsymbol{T}(t) = \dfrac{\boldsymbol{r}'(t)}{|\boldsymbol{r}'(t)|}$ *be the unit vector in the direction of the tangent vector* $\boldsymbol{r}'(t)$.

Then at those points of Γ *for which* $\boldsymbol{T}'(t) \neq 0$ *we define the* **unit principal normal vector to** Γ *as* $\boldsymbol{N}(t) = \dfrac{\boldsymbol{T}'(t)}{|\boldsymbol{T}'(t)|}$, *and we define the* **binormal vector to** Γ *as* $\boldsymbol{B}(t) = \boldsymbol{T}(t) \times \boldsymbol{N}(t)$.

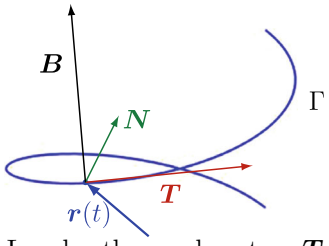


Figure 5.7 Local orthogonal vectors $\boldsymbol{T}$, $\boldsymbol{N}$, and $\boldsymbol{B}$.

Some elementary but general properties of $\boldsymbol{T}$, $\boldsymbol{N}$, and $\boldsymbol{B}$ can be derived from their respective definitions, *e.g.*, those in the next Mastery Check exercise.

✍ Mastery Check 5.2:

Show that for any smooth curve in 3D, $\boldsymbol{T}(t)$ and $\boldsymbol{T}'(t)$ are orthogonal.

Hint: Differentiate $\boldsymbol{T} \cdot \boldsymbol{T}$ with respect to t (see Rule (c) on Page 295). What conclusions can you then draw about $\boldsymbol{N}(t)$ and $\boldsymbol{N}'(t)$, and $\boldsymbol{B}(t)$ and $\boldsymbol{B}'(t)$? ✍

Remarks

* For each t, the orthogonal vectors $\boldsymbol{T}(t)$ and $\boldsymbol{N}(t)$ define the so-called *osculating plane* whose orientation (in 3D) changes with t. The binormal vector $\boldsymbol{B}(t)$ is orthogonal to the osculating plane.

* The vectors $\boldsymbol{T}$, $\boldsymbol{N}$, and $\boldsymbol{B}$, shown in Figure 5.7, define a local orthonormal set of vectors, much the same as the vectors $\mathbf{i}, \mathbf{j}, \mathbf{k}$. That is, they define a right-handed coordinate system. However, in contrast to the Cartesian unit vector set, this coordinate system moves and changes

direction as t increases. The system is appropriately called a *moving trihedral*. The vectors $\{\boldsymbol{T}, \boldsymbol{N}, \boldsymbol{B}\}$ establish what is called the *Frenet* framework.

* As a consequence of the foregoing remark, any 3D vector that is a function of $\boldsymbol{r}(t)$ and therefore relevant to the curve, can be expressed in terms of the moving trihedral system. That is, for any vector function of the curve coordinates, $\boldsymbol{u}(\boldsymbol{r}(t))$, scalar functions $\alpha(t)$, $\beta(t)$, and $\gamma(t)$ can be found so that

$$\boldsymbol{u}(\boldsymbol{r}(t)) = \alpha(t)\boldsymbol{T}(t) + \beta(t)\boldsymbol{N}(t) + \gamma(t)\boldsymbol{B}(t).$$

In particular, such constructions can be derived for the derivatives $\boldsymbol{T}'(t)$, $\boldsymbol{N}'(t)$, and $\boldsymbol{B}'(t)$, as is revealed by Definition 5.5 and Supplementary Problem 5.3.

Definition 5.5
Let Γ *be a smooth curve described by* $\boldsymbol{r}(t)$ *defined on an open connected interval* I*. At any point* $\boldsymbol{r}(t)$ *on* Γ *the non-negative function* $\kappa(t) = \dfrac{|\boldsymbol{T}'(t)|}{|\boldsymbol{r}'(t)|}$ *is called the* **curvature** *of* Γ *at that point, and the real-valued function* $\tau(t)$*, defined such that* $\boldsymbol{B}'(t) = -\tau(t)\,|\boldsymbol{r}'(t)|\,\boldsymbol{N}(t)$*, is called the* **torsion** *of* Γ *at that point.*

The function $\tau(t)$ gives a measure of the tendency of the curve to twist out of the osculating plane. It can be positive, zero, or negative. On the other hand, the curvature κ, which measures the extent to which the curve bends at a point, is always non-negative ($\kappa(t) \geq 0$).

Example 5.2:

A straight line, $\boldsymbol{r}(t) = \boldsymbol{r_0} + t\boldsymbol{u}$, in the direction $\boldsymbol{u}$ has a constant tangent vector, $\boldsymbol{T}(t) = \boldsymbol{u}/|\boldsymbol{u}|$, and therefore has zero curvature, *i.e.*, $\kappa(t) = 0$.

A circle in 2D, $\boldsymbol{r}(\theta) = \boldsymbol{r_0} + a(\cos\theta, \sin\theta)$, or a circle in 3D,
$\boldsymbol{r}(\theta) = \boldsymbol{r_0} + a(\sin\phi\cos\theta, \sin\phi\sin\theta, \cos\phi)$ with $\phi = f(\theta)$, has constant curvature, $\kappa(\theta) = 1/a$, equal to the reciprocal of the circle radius.
The torsion also reduces to $\tau(\theta) = 0$ since the circle remains in the same plane. (For example, set $b = 0$ in Mastery Check 5.3. See also Supplementary Problem 5.5.)

✍ Mastery Check 5.3:

Consider the helical curve in 3D described by the vector function

$$\boldsymbol{r}(t) = (a\cos t, a\sin t, bt),\ 0 \le t \le 2\pi.$$

Compute $\boldsymbol{r}'(t)$, $\boldsymbol{r}''(t)$, $\boldsymbol{T}(t)$, $\boldsymbol{N}(t)$, and $\boldsymbol{B}(t)$.

Verify that $\kappa^2 = \dfrac{a^2}{(a^2+b^2)^2}$, and that $\boldsymbol{\tau}(t) = \dfrac{b}{a^2+b^2}$ for all t.

✍

II. Surfaces $\boldsymbol{r} : \mathbb{R}^2 \longrightarrow \mathbb{R}^3$

Another important class of vector-valued functions comprises those that depend on *two* independent variables, which we denote generically by u and v. That is, we consider the class of vector-valued functions $\boldsymbol{f} : \mathbb{R}^2 \longrightarrow \mathbb{R}^m$, which map points (u, v) in the plane to points in m-space:

$$(u, v) \longmapsto \boldsymbol{f}(u, v) = \big(f_1(u, v), f_2(u, v), ..., f_m(u, v)\big).$$

Since functions from $\mathbb{R}^2$ to $\mathbb{R}^3$ have great physical significance and are most readily illustrated, we limit the following discussion to these. As in **I**, we present the function as a point in $\mathbb{R}^3$, $\boldsymbol{r} = (x, y, z)$, all components of which depend on the two variables (u, v):

$$\boldsymbol{r}(u, v) = \big(x(u, v), y(u, v), z(u, v)\big).$$

This vector function maps points in the uv-plane to points in 3-space and thereby traces out a *surface* as shown in Figure 5.8.

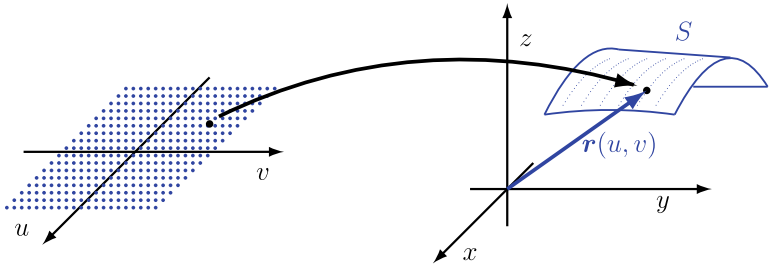


Figure 5.8 A surface in $\mathbb{R}^3$.

It is worth reinforcing here that in **I** we saw that a curve $\boldsymbol{r}(t)$ in 3D depends on *one* variable (Example 5.2). Here we see that a surface $\boldsymbol{r}(u, v)$ in 3D depends on *two* variables. The distinction is worth remembering as we shall have occasion to invoke a dimensional reduction (see the Remarks immediately following). Incidentally, the expression above, as well as most of the analysis to follow, supposes that x, y, z are *explicit* functions of u & v. However, in practice this may not always be the case; a surface may be defined *implicitly* in terms of two variables (see the discussion on implicit

functions in Section 2.H). Nevertheless, the ideas developed below remain valid even for implicitly defined surfaces.

Example 5.3:

The set of parametric equations

$$\left.\begin{array}{rcl} x &=& a\cos u\sin v \\ y &=& a\sin u\sin v \\ z &=& a\cos v \end{array}\right\} \quad \text{satisfies} \quad x^2+y^2+z^2=a^2.$$

That is, this set of functions is a parametric representation of a sphere of radius a centred at the origin.

■

Remarks

* Before continuing, the reader might find it useful to revisit the discussions on coordinate systems and visualization of surfaces in Sections 1.D and 1.E.

* If we keep $u=u_0$ fixed we get $\boldsymbol{r}=\boldsymbol{r}(u_0,v)$, which is a vector function of the one variable v (Figure 5.9). That is, restricting the variable u results in a curve on S called the constant u curve. Based on what was said in the preceding section, this curve has a *tangent vector* given by

$$\boldsymbol{r}'_v(u_0,v)=\frac{\partial \boldsymbol{r}}{\partial v}(u_0,v)=\left(\frac{\partial x}{\partial v}(u_0,v),\frac{\partial y}{\partial v}(u_0,v),\frac{\partial z}{\partial v}(u_0,v)\right).$$

* Similarly, if we keep $v=v_0$ fixed we get $\boldsymbol{r}=\boldsymbol{r}(u,v_0)$, a vector function of the single variable u. This too represents a curve on S, called the constant v curve. Analogously, this curve has a tangent vector given by

$$\boldsymbol{r}'_u(u,v_0)=\frac{\partial \boldsymbol{r}}{\partial u}(u,v_0)=\left(\frac{\partial x}{\partial u}(u,v_0),\frac{\partial y}{\partial u}(u,v_0),\frac{\partial z}{\partial u}(u,v_0)\right).$$

* The independent variables u and v take the place of the variables x and y in Section 2.C in forming the vector normal $\boldsymbol{r}'_u(u_0,v_0)\times\boldsymbol{r}'_v(u_0,v_0)\neq 0$. This vector is orthogonal to the aforementioned tangent vectors $\boldsymbol{r}'_u(u_0,v_0)$ and $\boldsymbol{r}'_u(u_0,v_0)$ at the point $\boldsymbol{r}(u_0,v_0)$ as well as orthogonal to the plane spanned by these vectors and hence orthogonal (*i.e.*, normal) to the surface S at the point $\boldsymbol{r}(u_0,v_0)$. The analogy to the argument employed in Section 2.C becomes an identity once again with the choice x and y as the independent variables to describe the surface.

This more general definition of the vector normal to a surface, for arbitrary variables u and v, will be exploited in Section 5.D for the evaluation of surface integrals.

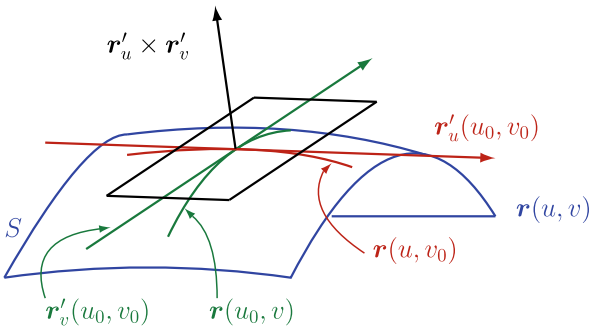


Figure 5.9 The tangent plane to S spanned by tangent vectors $\boldsymbol{r}'_u$ and $\boldsymbol{r}'_v$.

III. The most general vector-valued function $\boldsymbol{f} : \mathbb{R}^n \longrightarrow \mathbb{R}^m$

Three-dimensional vector-valued functions, $\boldsymbol{f} : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$, play an important role in the analysis of the real world and will be considered in depth in the next and subsequent sections. As for higher dimensional cases, although applications arise in even more general cases of $\boldsymbol{f} : \mathbb{R}^n \longrightarrow \mathbb{R}^m$ we derive no benefit by specializing any further. We can instead reflect on the parallels that may be drawn between "projections" of the more general scenario and the special cases we have already discussed.

A differentiable vector function $\boldsymbol{f} : \mathbb{R}^n \longrightarrow \mathbb{R}^m$ with components $f_i,\ i = 1, 2, 3, \ldots, m$, which are real-valued functions of $\boldsymbol{x}$, is a vector-valued function

$$\boldsymbol{f}(\boldsymbol{x}) = \big(f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), f_3(\boldsymbol{x}), \ldots, f_m(\boldsymbol{x})\big).$$

When we say that $\boldsymbol{x} \in \mathbb{R}^n$ is in the domain of $\boldsymbol{f}$ we mean that $\boldsymbol{x}$ is in the domain of each of the m component, scalar functions, $f_i,\ i = 1, 2, ..., m$. Then, if each of the f_i is continuous and has continuous partial derivatives, the gradient for each component

$$\boldsymbol{\nabla} f_i(\boldsymbol{x}) = \left(\frac{\partial f_i}{\partial x_1}, \ldots, \frac{\partial f_i}{\partial x_n}\right),\ i = 1, 2, ..., m,$$

may be computed.

The gradient was introduced in Section 2.E, where it was used to determine, among other things, the rate of change of a scalar function in a specified direction. Indeed, for the special case of $n = 2$ and $m = 1$, with $z = f(x, y)$ describing a surface in 3D space, the rate of change of z at a point (x_0, y_0) in the direction of unit vector $\boldsymbol{u} = (u, v)$ was given by

$$D_{\boldsymbol{u}} f(x_0, y_0) = \boldsymbol{\nabla} f\big|_0 \cdot \boldsymbol{u} = \left(\frac{\partial f}{\partial x}\Big|_0 \mathbf{i} + \frac{\partial f}{\partial y}\Big|_0 \mathbf{j} \right) \cdot (u\mathbf{i} + v\mathbf{j}).$$

However, instead of a scalar product, the directional derivative may be rewritten in the form of a matrix multiplication,

$$D_{\boldsymbol{u}} f(x_0, y_0) = \begin{bmatrix} \dfrac{\partial f}{\partial x}\Big|_0 & \dfrac{\partial f}{\partial y}\Big|_0 \end{bmatrix} \begin{pmatrix} u \\ v \end{pmatrix}.$$

Expressed as a matrix product it is easy to see how this directional derivative might be generalized to determine the rate of change of more general vector-valued functions, $\boldsymbol{f}(\boldsymbol{x})$. One simply adds a row of first partial derivatives for each component function, f_i. For instance, for the case $n = 2$ and $m = 3$ we would have

$$D_{\boldsymbol{u}} \boldsymbol{f}(x_0, y_0) = \begin{bmatrix} \dfrac{\partial f_1}{\partial x}\Big|_0 & \dfrac{\partial f_1}{\partial y}\Big|_0 \\ \dfrac{\partial f_2}{\partial x}\Big|_0 & \dfrac{\partial f_2}{\partial y}\Big|_0 \\ \dfrac{\partial f_3}{\partial x}\Big|_0 & \dfrac{\partial f_3}{\partial y}\Big|_0 \end{bmatrix} \begin{pmatrix} u \\ v \end{pmatrix}.$$

The 3×2 matrix on the right is an example of a *Jacobian matrix*. The Jacobian matrix lies at the heart of every generalization of single-variable differential calculus to higher dimensions.

Definition 5.6
Let $\boldsymbol{f} : \mathbb{R}^n \longrightarrow \mathbb{R}^m$ be a C^1 vector-valued function. The $m \times n$ matrix of first derivatives of $\boldsymbol{f}$ is called the **Jacobian matrix**.

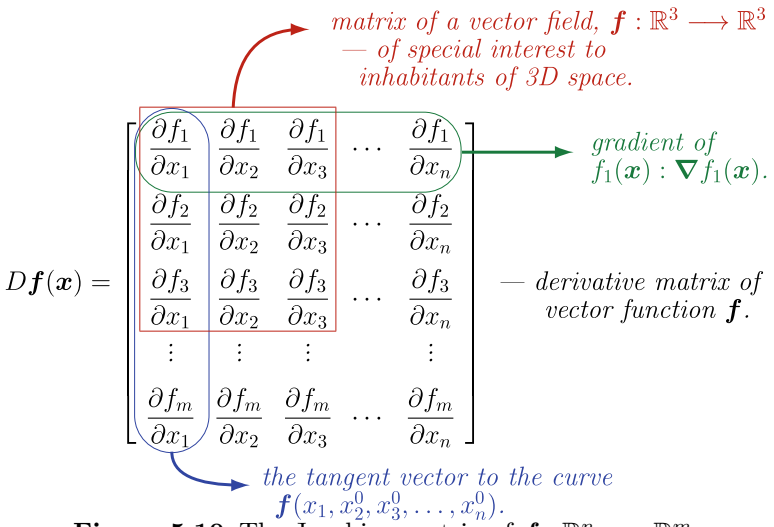


Figure 5.10 The Jacobian matrix of $\boldsymbol{f} : \mathbb{R}^n \longrightarrow \mathbb{R}^m$.

Remarks

* The jth row of the Jacobian in Figure 5.10 is the *gradient* of a scalar function $f_j(\boldsymbol{x})$, and there are m of them.

* The ith column of the Jacobian in Figure 5.10 is a *tangent vector* to a curve in $\mathbb{R}^m$, and there are n of them.

* The first three rows and first three columns correspond to the derivative matrix of a 3D vector field. (See Section 5.B.)

* In Section 2.E, we declared the gradient to be the generalization to a scalar function of n variables of the ordinary derivative of a function of one variable. It is now natural to expand further on this generalization to explicitly call the Jacobian matrix *the derivative of a vector-valued multivariable function.*

Example 5.4:

For a scalar function $f : \mathbb{R}^n \longrightarrow \mathbb{R},\ \boldsymbol{x} \longmapsto f(\boldsymbol{x})$, the differential is

$$\mathrm{d}f = \frac{\partial f}{\partial x_1}\mathrm{d}x_1 + \frac{\partial f}{\partial x_2}\mathrm{d}x_2 + \cdots + \frac{\partial f}{\partial x_n}\mathrm{d}x_n \;=\; \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n}\right) \begin{pmatrix} \mathrm{d}x_1 \\ \mathrm{d}x_2 \\ \vdots \\ \mathrm{d}x_n \end{pmatrix}.$$

In the case of a vector function $\boldsymbol{f} : \mathbb{R}^n \longrightarrow \mathbb{R}^m,\ \boldsymbol{x} \longmapsto \boldsymbol{f}(\boldsymbol{x})$, the differential generalizes to this:

$$\mathrm{d}\boldsymbol{f} \;=\; \begin{pmatrix} \dfrac{\partial f_1}{\partial x_1} & \cdots & \dfrac{\partial f_1}{\partial x_n} \\ \vdots & & \vdots \\ \dfrac{\partial f_m}{\partial x_1} & \cdots & \dfrac{\partial f_m}{\partial x_n} \end{pmatrix} \begin{pmatrix} \mathrm{d}x_1 \\ \mathrm{d}x_2 \\ \vdots \\ \mathrm{d}x_n \end{pmatrix},$$

—a matrix-vector product giving a vector.

■

Example 5.5:

For a scalar function $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ mapping $\boldsymbol{x}$ to $f(\boldsymbol{x})$, where, in turn, the x_i are functions of the scalar variable u_j, the chain rule (Section 2.G) may also be expressed as a multiplication of a row matrix with a column matrix:

$$\frac{\partial f}{\partial u_i} = \frac{\partial f}{\partial x_1}\frac{\mathrm{d}x_1}{\mathrm{d}u_i} + \frac{\partial f}{\partial x_2}\frac{\mathrm{d}x_2}{\mathrm{d}u_i} + \cdots + \frac{\partial f}{\partial x_n}\frac{\mathrm{d}x_n}{\mathrm{d}u_i} = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n}\right) \begin{pmatrix} \dfrac{\mathrm{d}x_1}{\mathrm{d}u_i} \\ \vdots \\ \dfrac{\mathrm{d}x_n}{\mathrm{d}u_i} \end{pmatrix}.$$

Moreover, in the case of a vector function $\boldsymbol{f} : \mathbb{R}^n \longrightarrow \mathbb{R}^m,\ \boldsymbol{x} \longmapsto \boldsymbol{f}(\boldsymbol{x})$, where each of the x_i are functions of the k variables, u_j, for $j = 1, \ldots, k$, the chain rule generalizes to a product of an $m \times n$ matrix of derivatives with respect to x_i with an $n \times k$ matrix of derivatives with respect to u_j, to result in an $m \times k$ matrix:

$$
\begin{aligned}
D\big(\boldsymbol{f}\circ\boldsymbol{x}\big)(\boldsymbol{u}) &= \begin{pmatrix} \dfrac{\partial f_1}{\partial x_1} & \cdots & \dfrac{\partial f_1}{\partial x_n} \\ \vdots & & \vdots \\ \dfrac{\partial f_m}{\partial x_1} & \cdots & \dfrac{\partial f_m}{\partial x_n} \end{pmatrix} \begin{pmatrix} \dfrac{\partial x_1}{\partial u_1} & \cdots & \dfrac{\partial x_1}{\partial u_k} \\ \vdots & & \vdots \\ \dfrac{\partial x_n}{\partial u_1} & \cdots & \dfrac{\partial x_n}{\partial u_k} \end{pmatrix} \\
&= D\boldsymbol{f}(\boldsymbol{x})\cdot D\boldsymbol{x}(\boldsymbol{u})
\end{aligned}
$$

—a matrix product giving a matrix. ■

5.B Vector Fields

A 3D vector-valued function of a 3D vector variable,

$$\boldsymbol{f} : D_f \subseteq \mathbb{R}^3 \longrightarrow \mathbb{R}^3,\ \boldsymbol{x} \longmapsto \boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}),$$

defined on an open connected domain, D_f has special significance in physics and engineering, and other applications in the real world. Hence, it is given a special name: a *vector field*. To be explicit, written in the three ways we first introduced vectors, an arbitrary vector field has the form

$$
\begin{aligned}
\boldsymbol{f}(\boldsymbol{x}) &= \big(f_1(x,y,z), f_2(x,y,z), f_3(x,y,z)\big) \\
&= f_1(x,y,z)\mathbf{i} + f_2(x,y,z)\mathbf{j} + f_3(x,y,z)\mathbf{k} \\
&= f_1(x,y,z)\mathbf{e}_1 + f_2(x,y,z)\mathbf{e}_2 + f_3(x,y,z)\mathbf{e}_3
\end{aligned}
$$

where the f_1, f_2, and f_3 are scalar functions of the three variables x, y, z.

Note that the subscripts "1", "2", and "3" on f do *not* here refer to partial derivatives, they refer to the respective components of the vector field.

Unless otherwise stated, the vector fields discussed herein will be assumed to have *continuous partial derivatives of order* $m \geq 2$. We will often refer to these as *smooth* vector fields and presume their component functions to be C^2 functions, if not of higher differentiability.

Some examples from physics

(i) **Gravitational field**
The gravitational force per unit mass, with G as the gravitational constant and $\boldsymbol{r} = (x, y, z)$, is a 3D vector field (Figure 5.11).

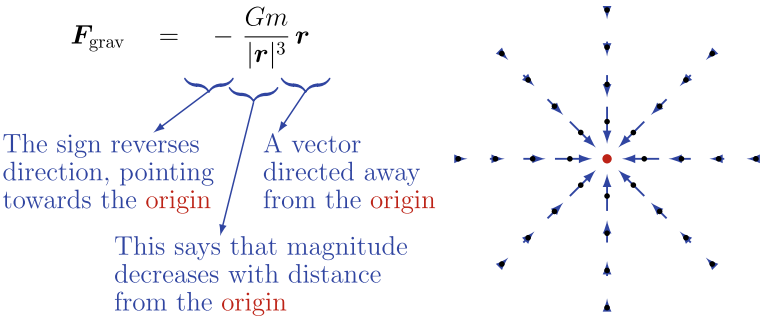


Figure 5.11 The gravitational field of a point mass.

(ii) **Electrostatic fields**

(a) The 3D electrostatic field intensity − the force per unit charge − is expressed in SI units by

$$\boldsymbol{E} = \frac{q}{4\pi\epsilon_0|\boldsymbol{r}|^3}\boldsymbol{r} \quad \text{—due to a point charge } q \text{ at the origin.}$$

The direction depends on the sign of q. The constant ϵ_0 is the "permittivity" of free space. Again, the position vector $\boldsymbol{r} = (x, y, z)$.

(b) The corresponding 2D version, with $\boldsymbol{r} = (x, y)$, has the form,

$$\boldsymbol{E} = \frac{\rho}{2\pi\epsilon_0|\boldsymbol{r}|^2}\boldsymbol{r}.$$

The latter case can be thought of as a field in 3D free space that is independent of (the same for all) z values. It can be found in situations involving uniformly charged wires of infinite length (Figure 5.12), with the quantity ρ being the charge per unit length of the wire.

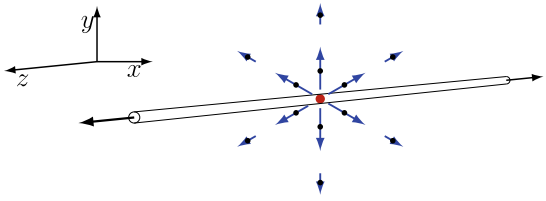


Figure 5.12 The electrostatic field near a charged wire.

(iii) **Gradient field**

A vector field can also be derived from any spatially dependent scalar function by taking its gradient. For example, if $T = T(\boldsymbol{r})$ is a spatially varying temperature field, then $\boldsymbol{\nabla} T$ is a vector field derived from the scalar field. This is obviously called the *temperature gradient*.

Gradient fields were discussed at some length in Section 2.E. They will recur often in this chapter, in both the differential and the integral contexts (see also page 325 *et. seq.*).

Remarks

* By now the reader will appreciate that both the magnitude and direction of a vector field will depend on position. This is exaggeratingly depicted in Figure 5.13, but is more accurately suggested by the arrow directions and lengths shown in Figures 5.11 and 5.12.

* As mentioned, Examples (i) and (ii)(a) are examples of 3D vector fields $\mathbb{R}^3 \longrightarrow \mathbb{R}^3$.

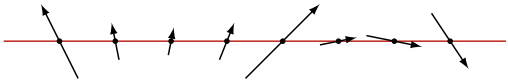


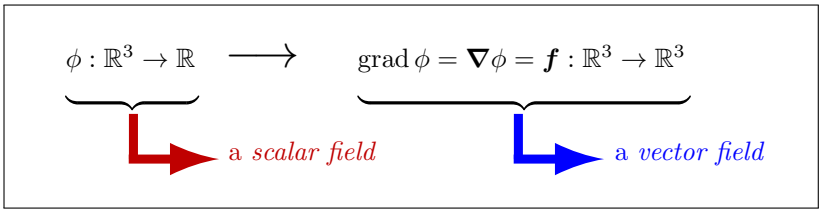
Figure 5.13 A field varying in direction and magnitude with position.

* In Example (ii)(b), there are just *two* components to $\boldsymbol{E}$: $E_1 = E_1(x, y)$ and $E_2 = E_2(x, y)$. This is an example of a *plane vector field*

$$\boldsymbol{E} = E_1(x, y)\mathbf{i} + E_2(x, y)\mathbf{j}.$$

These will feature from time to time and specifically in Section 5.F.

* Example (iii) shows that a vector field can be obtained by taking the gradient of a real-valued, scalar function, $\phi \in C^1(\mathbb{R}^3)$.



More information about vector fields

- **Divergence and curl**

  The physical significance of the gradient was explained on Pages 96–99. However, there are two siblings of the gradient that are worth defining now in an operational sense as they too have physical

meaning and mathematical utility. These are the *divergence* and *curl* of a vector field.

Definition 5.7
Let $\boldsymbol{f} : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ *be a* C^1 *(at least) vector field defined on an open and connected domain,* D_f*. Denote and define the* **divergence of** $\boldsymbol{f}$ *by*

$$\text{div}\boldsymbol{f} \;=\; \frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} + \frac{\partial f_3}{\partial z} \equiv \boldsymbol{\nabla} \cdot \boldsymbol{f}.$$

The divergence thus operates on a vector field to give a *scalar* property of the field that applies locally. That is:

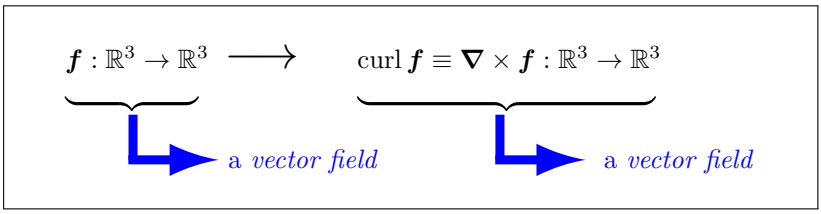
$$\underbrace{\boldsymbol{f} : \mathbb{R}^3 \to \mathbb{R}^3}_{\text{a } \textit{vector field}} \longrightarrow \underbrace{\text{div}\, \boldsymbol{f} \equiv \boldsymbol{\nabla} \cdot \boldsymbol{f} : \mathbb{R}^3 \to \mathbb{R}}_{\text{a } \textit{scalar field}}$$

The notation employed in Definition 5.7 involving the gradient operator is standard and is used as a mnemonic to remind us of how the divergence is calculated, which is the expression shown in the central equality. The operator $\boldsymbol{\nabla}$ is treated as a vector in executing the scalar product with $\boldsymbol{f}$ although no actual component-wise multiplication is performed; instead, the components of $\boldsymbol{f}$ are partially differentiated with respect to the position variable corresponding to that component.

Definition 5.8
Let $\boldsymbol{f} : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ *be a* C^1 *(at least) vector field. Denote and define the* **curl of** $\boldsymbol{f}$ *by*

$$\begin{aligned} \textit{curl}\,\boldsymbol{f} \;&=\; \Big(\frac{\partial f_3}{\partial y} - \frac{\partial f_2}{\partial z}\Big)\mathbf{i} + \Big(\frac{\partial f_1}{\partial z} - \frac{\partial f_3}{\partial x}\Big)\mathbf{j} + \Big(\frac{\partial f_2}{\partial x} - \frac{\partial f_1}{\partial y}\Big)\mathbf{k} \\ &=\; \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ f_1 & f_2 & f_3 \end{vmatrix} \equiv \boldsymbol{\nabla} \times \boldsymbol{f}. \end{aligned}$$

In contrast to the divergence, the curl operates on a vector field to give a *vector* property of the field, also applied locally. That is:



As with the divergence operation, the notation employed in Definition 5.8 is standard form to help us remember how the curl is calculated, which is that shown on the right-hand side of the first equality. The operator $\boldsymbol{\nabla}$ is treated as a vector in the vector product with $\boldsymbol{f}$. Again, however, instead of pairwise multiplication, the components of $\boldsymbol{f}$ are partially differentiated with respect to the scalar variable corresponding to that location in the vector product.

Later, we shall see that the *divergence* of a vector field is a measure of how much the field spreads out locally, while the *curl* of a vector field is a measure of how much the vector field turns or twists locally around an axis parallel to the direction of the vector $\boldsymbol{\nabla} \times \boldsymbol{f}$.

Along with these physical interpretations, we may also document here that a field that has zero divergence in a finite domain is said to be *solenoidal*, while a field with zero curl is said to be *irrotational*.

Note that in the case of two real vectors, switching the order of the vectors in the scalar product doesn't change the result of that product, while switching the orders of the vectors in the vector product results only in a vector pointing in the opposite direction. In the case of the divergence and curl, switching the order of $\boldsymbol{\nabla}$ and $\boldsymbol{f}$, *i.e.*, writing $\boldsymbol{f} \cdot \boldsymbol{\nabla}$ and $\boldsymbol{f} \times \boldsymbol{\nabla}$ makes no sense, as stand-alone quantities. On the other hand, either expression may be legitimate if used in the context of an operation on another scalar field or another vector field, the latter in the case of another scalar or vector product, say. For example, the following makes perfect sense:

$$(\boldsymbol{f} \cdot \boldsymbol{\nabla})\phi = \left(f_1 \frac{\partial}{\partial x} + f_2 \frac{\partial}{\partial y} + f_3 \frac{\partial}{\partial z} \right) \phi = f_1 \frac{\partial \phi}{\partial x} + f_2 \frac{\partial \phi}{\partial y} + f_3 \frac{\partial \phi}{\partial x}$$

Analogous meanings can be ascribed to expressions such as $(\boldsymbol{f} \times \boldsymbol{\nabla}) \cdot \boldsymbol{g}$ and $(\boldsymbol{f} \times \boldsymbol{\nabla}) \times \boldsymbol{g}$. Remember, though, that the operations must be carried out in the correct order.

A large number of general and specific results of applications of the gradient, the divergence, the curl, and their combinations have been established. Some of these are listed in the next bullet point. The reader is invited in Mastery Check 5.4 to prove some of these by direct application of the definitions.

Example 5.6:

Evaluate the divergence and curl of the following vector fields

(a) $\boldsymbol{f}(x,y,z) = xyz\mathbf{i} + \sin(z)\sin(y)\mathbf{j} + \cos y \cos z\mathbf{k}$,

(b) $\boldsymbol{g}(x,y,z) = \dfrac{\boldsymbol{r}}{|\boldsymbol{r}|}$ for $\boldsymbol{r} \neq 0$,

(c) $\boldsymbol{h}(x,y,z) = \alpha(x)\mathbf{i} + \beta(y)\mathbf{j} + \gamma(z)\mathbf{k} = x^n\mathbf{i} + y^n\mathbf{j} + z^n\mathbf{k}$, for $n \in \mathbb{N}$.

Solution:

(a) With this C^∞ vector we demonstrate evaluating divergence and curl.

div $\boldsymbol{f}$:

$$\begin{aligned}\boldsymbol{\nabla}\cdot\boldsymbol{f} &= \frac{\partial}{\partial x}(f_1) + \frac{\partial}{\partial y}(f_2) + \frac{\partial}{\partial z}(f_3),\\ &= \frac{\partial}{\partial x}(xyz) + \frac{\partial}{\partial y}(\sin z \sin y) + \frac{\partial}{\partial z}(\cos y \cos z)\\ &= yz + \sin z\cos y + \cos y(-\sin z) = yz.\end{aligned}$$

curl $\boldsymbol{f}$:

$$\begin{aligned}\boldsymbol{\nabla}\times\boldsymbol{f} &= \begin{vmatrix}\mathbf{i} & \mathbf{j} & \mathbf{k}\\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z}\\ f_1 & f_2 & f_3\end{vmatrix} = \begin{vmatrix}\mathbf{i} & \mathbf{j} & \mathbf{k}\\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z}\\ xyz & \sin y\sin z & \cos y\cos z\end{vmatrix}.\\ &= \mathbf{i}\left(\frac{\partial}{\partial y}(\cos y\cos z) - \frac{\partial}{\partial z}(\sin y\sin z)\right)\\ &\qquad -\mathbf{j}\left(\frac{\partial}{\partial x}(\cos y\cos z) - \frac{\partial}{\partial z}(xyz)\right)\\ &\qquad +\mathbf{k}\left(\frac{\partial}{\partial x}(\sin y\sin z) - \frac{\partial}{\partial y}(xyz)\right)\\ &= (-\sin y\cos z - \sin y\cos z)\mathbf{i} - (0-xy)\mathbf{j} + (0-xz)\mathbf{k}\\ &= 2\sin y\cos z\mathbf{i} + xy\mathbf{j} - xz\mathbf{k}.\end{aligned}$$

(b) The vector field $\boldsymbol{g}$ is, firstly, a unit vector field (it has magnitude 1 for all points $\boldsymbol{r}$). Secondly, $\boldsymbol{g}$, irrespective of $\boldsymbol{r}$ is directed in straight lines away from a single point, the origin. The directions are opposite to the field vectors depicted in Figure 5.11. Given that the curl is a measure of the degree to which the field "turns" it should be expected that our calculations will prove that $\boldsymbol{g}$ is irrotational. The divergence on the other hand, which measures the degree to which a field spreads out, will be nonzero.

For convenience we write $r = |\boldsymbol{r}| = \sqrt{x^2 + y^2 + z^2}$.

div $\boldsymbol{g}$:

$$\boldsymbol{\nabla} \cdot \boldsymbol{g} \quad = \quad \frac{\partial}{\partial x}\left(\frac{x}{r}\right) + \frac{\partial}{\partial y}\left(\frac{y}{r}\right) + \frac{\partial}{\partial z}\left(\frac{z}{r}\right).$$

Considering just the derivative with respect to x, we get

$$\frac{\partial}{\partial x}\left(\frac{x}{r}\right) = \frac{1}{r} - x\frac{1}{2}(x^2 + y^2 + z^2)^{-3/2}.2x = \frac{1}{r} - \frac{x^2}{r^3},$$

and similarly for the derivatives with respect to y and z. Adding all three contributions we get

$$\boldsymbol{\nabla} \cdot \boldsymbol{g} \quad = \quad \frac{3}{r} - \frac{x^2 + y^2 + z^2}{r^3} = \frac{2}{r} \equiv \frac{2}{|\boldsymbol{r}|}.$$

Hence, the spread of the field decreases the further away the point is from the origin. (See identity 12 in the following list of useful vector identities.)

curl $\boldsymbol{g}$:

$$\boldsymbol{\nabla} \times \boldsymbol{g} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ \frac{x}{r} & \frac{y}{r} & \frac{z}{r} \end{vmatrix},$$

$$= \mathbf{i}\left(z\frac{\partial}{\partial y}(\tfrac{1}{r}) - y\frac{\partial}{\partial z}(\tfrac{1}{r})\right) - \mathbf{j}\left(z\frac{\partial}{\partial x}(\tfrac{1}{r}) - x\frac{\partial}{\partial z}(\tfrac{1}{r})\right) + \mathbf{k}\left(y\frac{\partial}{\partial x}(\tfrac{1}{r}) - x\frac{\partial}{\partial y}(\tfrac{1}{r})\right).$$

Considering again just the first term, the component in direction $\mathbf{i}$, we find,

$$\begin{aligned} z\frac{\partial}{\partial y}(\frac{1}{r}) \quad - \quad & y\frac{\partial}{\partial z}(\frac{1}{r}) \\ = \quad & z\frac{1}{2}(x^2 + y^2 + z^2)^{-3/2}.2y - y\frac{1}{2}(x^2 + y^2 + z^2)^{-3/2}.2z, \\ = \quad & 0. \end{aligned}$$

A similar outcome is found for the components in the $\mathbf{j}$ and $\mathbf{k}$ directions. Combining these contributions we find

$$\boldsymbol{\nabla} \times \boldsymbol{g} = 0\mathbf{i} + 0\mathbf{j} + 0\mathbf{k} = \mathbf{0},$$

confirming that $\boldsymbol{g}$ is an irrotational field. (See identity 13 in the following list of useful vector identities.)

(c) The vector field $\boldsymbol{h}$ has been written deliberately first in a nonspecific way with components that are functions respectively of the one variable that is associated with the orthogonal direction in which the function appears. Specifically, $\alpha(x)$, etc. The second expression for $\boldsymbol{h}$ is a particular case of the former. The calculation proceeds with this particular case, but the reader should be able to draw conclusions with the more general setting.

div $\boldsymbol{h}$:

$$\begin{aligned}\boldsymbol{\nabla}\cdot\boldsymbol{h} &= \frac{\partial}{\partial x}\left(x^n\right)+\frac{\partial}{\partial y}\left(y^n\right)+\frac{\partial}{\partial z}\left(x^n\right)\\ &= nx^{n-1}+ny^{n-1}+nz^{n-1}=n\left(x^{n-1}+y^{n-1}+z^{n-1}\right).\end{aligned}$$

The power $n = 1$ implies that $\boldsymbol{h}(\boldsymbol{r})$ is the radial vector $\boldsymbol{r}$, giving a constant divergence of 3 indicating a uniform "spread" of the vector field. (See identity 10 in the following list of useful vector identities.)

curl $\boldsymbol{h}$:

$$\boldsymbol{\nabla}\times\boldsymbol{h}=\begin{vmatrix}\mathbf{i} & \mathbf{j} & \mathbf{k}\\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z}\\ x^n & y^n & z^n\end{vmatrix},$$

$$\begin{aligned}&= \mathbf{i}\left(\frac{\partial}{\partial y}(z^n)-\frac{\partial}{\partial z}(y^n)\right)-\mathbf{j}\left(\frac{\partial}{\partial x}(z^n)-\frac{\partial}{\partial z}(x^n)\right)+\mathbf{k}\left(\frac{\partial}{\partial x}(y^n)-\frac{\partial}{\partial y}(x^n)\right)\\ &= 0\mathbf{i}+0\mathbf{j}+0\mathbf{k}=\mathbf{0}.\end{aligned}$$

Consequently, the vector field $\boldsymbol{h}$ is also irrotational independent of the power n.
Note also that the same conclusion follows in the slightly more general case $\boldsymbol{h}(\boldsymbol{r})=\alpha(x)\mathbf{i}+\beta(y)\mathbf{j}+\gamma(z)\mathbf{k}$.

■

- **Some useful vector identities**

  Apart from the simple linear identities
  (*e.g.*, $\boldsymbol{\nabla}(\phi+\psi)=\boldsymbol{\nabla}\phi+\boldsymbol{\nabla}\psi$), the operations of gradient, divergence, and curl obey a number of standard relations when applied to differentiable fields.

  Suppose vector fields $\boldsymbol{f},\boldsymbol{g}:\mathbb{R}^3\longrightarrow\mathbb{R}^3$ are C^2; vector $\boldsymbol{r}=(x,y,z)$; scalar functions $\phi,\psi:\mathbb{R}^3\longrightarrow\mathbb{R}$ are C^2; scalar function $h:\mathbb{R}\longrightarrow\mathbb{R}$ is C^1; and $\boldsymbol{c}\in\mathbb{R}^3$ is a constant vector. Then the following identities can be readily derived:

1. $\boldsymbol{\nabla}(\phi\psi) = \psi\boldsymbol{\nabla}\phi + \phi\boldsymbol{\nabla}\psi$
2. $\boldsymbol{\nabla}\cdot(\phi\boldsymbol{f}) = \phi\boldsymbol{\nabla}\cdot\boldsymbol{f} + \boldsymbol{f}\cdot\boldsymbol{\nabla}\phi$
3. $\boldsymbol{\nabla}\times(\phi\boldsymbol{f}) = \phi\boldsymbol{\nabla}\times\boldsymbol{f} + \boldsymbol{\nabla}\phi\times\boldsymbol{f}$
4. $\boldsymbol{\nabla}(\boldsymbol{f}\cdot\boldsymbol{g}) = (\boldsymbol{f}\cdot\boldsymbol{\nabla})\,\boldsymbol{g} + (\boldsymbol{g}\cdot\boldsymbol{\nabla})\,\boldsymbol{f} + \boldsymbol{f}\times(\boldsymbol{\nabla}\times\boldsymbol{g}) + \boldsymbol{g}\times(\boldsymbol{\nabla}\times\boldsymbol{f})$
5. $\boldsymbol{\nabla}\cdot(\boldsymbol{f}\times\boldsymbol{g}) = \boldsymbol{g}\cdot(\boldsymbol{\nabla}\times\boldsymbol{f}) - \boldsymbol{f}\cdot(\boldsymbol{\nabla}\times\boldsymbol{g})$
6. $\boldsymbol{\nabla}\times(\boldsymbol{f}\times\boldsymbol{g}) = \boldsymbol{f}\,(\boldsymbol{\nabla}\cdot\boldsymbol{g}) - \boldsymbol{g}\,(\boldsymbol{\nabla}\cdot\boldsymbol{f}) + (\boldsymbol{g}\cdot\boldsymbol{\nabla})\,\boldsymbol{f} - (\boldsymbol{f}\cdot\boldsymbol{\nabla})\,\boldsymbol{g}$
7. $\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\phi) = \boldsymbol{0}$
8. $\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\times\boldsymbol{f}) = 0$
9. $\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{f}) = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{f}) - \boldsymbol{\nabla}^2\boldsymbol{f}$
10. $\boldsymbol{\nabla}\cdot\boldsymbol{r} = 3$
11. $\boldsymbol{\nabla}h(r) = \dfrac{\mathrm{d}h}{\mathrm{d}r}\dfrac{\boldsymbol{r}}{r}$
12. $\boldsymbol{\nabla}\cdot(h(r)\boldsymbol{r}) = 3h(r) + r\dfrac{\mathrm{d}h}{\mathrm{d}r}$
13. $\boldsymbol{\nabla}\times(h(r)\boldsymbol{r}) = \boldsymbol{0}$
14. $\boldsymbol{\nabla}(\boldsymbol{c}\cdot\boldsymbol{r}) = \boldsymbol{c}$
15. $\boldsymbol{\nabla}\cdot(\boldsymbol{c}\times\boldsymbol{r}) = 0$
16. $\boldsymbol{\nabla}\times(\boldsymbol{c}\times\boldsymbol{r}) = 2\boldsymbol{c}$

✍ Mastery Check 5.4:

By direct calculation confirm vector identities 5, 7, 8, 12, and 13.
Hint: Section 5.G contains a discussion of the so-called *summation convention* which is a concise, index-based, calculation methodology that simplifies the type of calculations suggested in this Mastery Check.

✍

- **Field lines**

  A useful concept particularly in fluid dynamics is that of field lines, also called *stream lines*. These are lines (actually *curves*) whose tangent vectors are parallel to the field vector at those points. That is, given that $\boldsymbol{r} : \mathbb{R} \longrightarrow \mathbb{R}^3, t \longmapsto \boldsymbol{r}(t)$ describes a curve in $\mathbb{R}^3$ (see page 292), then the field lines of a vector field $\boldsymbol{f}$ are defined by the equality:

$$\underbrace{\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}}_{\text{tangent vector}} = \underbrace{\lambda(t)}_{\substack{\text{proportionality constant that is a function of position}\\ \text{(not usually of interest)}}}\ \underbrace{\boldsymbol{f}\big(\boldsymbol{r}(t)\big)}_{\text{vector field}}$$

This vector equation hides three equations that must be solved simultaneously. If we assume the conditions of a smooth curve ($|\boldsymbol{r}'(t)| \neq 0$) then we deduce that $\lambda \neq 0$. Hence, we can solve the three component equations for λ to get

$$\begin{aligned} \frac{1}{f_1(x,y,z)}\frac{\mathrm{d}x}{\mathrm{d}t} &= \frac{1}{f_2(x,y,z)}\frac{\mathrm{d}y}{\mathrm{d}t} = \frac{1}{f_3(x,y,z)}\frac{\mathrm{d}z}{\mathrm{d}t} \\ \Longrightarrow \qquad \frac{\mathrm{d}x}{f_1(x,y,z)} &= \frac{\mathrm{d}y}{f_2(x,y,z)} = \frac{\mathrm{d}z}{f_3(x,y,z)}, \quad f_i \neq 0 \end{aligned}$$

Solving these three simultaneous differential equations, if possible, gives the curve described by $\boldsymbol{r}(t)$.

Even though the concept of field lines applies to vector-valued functions of any dimension, it is usually difficult to obtain closed-form expressions in dimensions greater than two. Even then it may be difficult to interpret or visualize without numerical assistance. The next example, in which the field is chosen simply to illustrate the process of calculation, supports this statement. The example also illustrates the fact that the restrictions $f_i \neq 0$ are not to be overlooked, as they determine, from the start, the valid domain(s) over which the field line solution is viable.

■ Example 5.7:

For the 3D vector

$$\boldsymbol{f}(x,y,z) = x^2 \sin y\ \mathbf{i} - x^3 \cos y\ \mathbf{j} + x^3 \tan z\ \mathbf{k}.$$

show that the field lines are a two-parameter family of curves generated as functions of one spatial variable.

Solution:

The equations for the field lines are

$$\begin{aligned} \frac{\mathrm{d}x}{f_1(x,y,z)} = \frac{\mathrm{d}y}{f_2(x,y,z)} = \frac{\mathrm{d}z}{f_3(x,y,z)}, &\qquad f_i \neq 0, \\ \Longrightarrow \qquad \frac{\mathrm{d}x}{x^2 \sin y} = \frac{-\mathrm{d}y}{x^3 \cos y} + \frac{\mathrm{d}z}{x^3 \tan z}, & \end{aligned}$$

Note that the condition $f_i \neq 0$ here implies that $x, \sin y, \cos y$ and $\tan z \neq 0$, which is quite restrictive and partitions 3D space into disjoint, periodic subsets of $\mathbb{R}^3$.

Choosing the first two of the above set of equations, and the last two, and simplifying we get

$$x\ \mathrm{d}x = -\tan y\, \mathrm{d}y \qquad ; \qquad -\sec y\, \mathrm{d}y = \cot z\, \mathrm{d}z. \tag{5.1}$$

These are separable, first-order equations that may be integrated directly to give, respectively,

$$\frac{x^2}{2} = \ln|\cos y| + \text{constant} = \ln|\cos y| - \ln H,$$

where H is a true constant, and

$$\ln|\sec y + \tan y| = -\ln|\sin z| + \text{constant} = -\ln|\sin z| + \ln K,$$

with K being another true constant. Taking exponentials of both sides of both equations and assuming that K and H are strictly positive constants we obtain

$$|\sin z| = \frac{K}{|\sec y + \tan y|} \quad \text{and} \quad \mathrm{e}^{x^2/2} = \frac{|\cos y|}{H}.$$

Removing the absolute value signs is feasible provided one is consistent with signs of both sides of the two equations.

For fixed H and K these equations, along with $y = y$, describe, in principle, a curve in $\mathbb{R}^3$, $\boldsymbol{r} = (x(y), y, z(y))$, with y as the variable generating the curve. Different curves are generated for different (permissable) values of H and K. We thus have a two-parameter family of curves in $\mathbb{R}^3$. Admittedly, without computational assistance it is difficult to follow the behaviour of the curve(s). We leave to the reader the task of numerically producing curves for allowed values of K and H, bearing in mind the original restriction on allowed values of x, y, and z.

An alternative description of the curve, introducing a new curve variable t, is

$$\boldsymbol{r}(t) = (x(t), y(t), z(t)) \Longrightarrow \begin{cases} \mathrm{e}^{-x^2/2} & = & \dfrac{H}{2K}\, t, \\[2ex] |\cos y| & = & \dfrac{2K}{t}, \\[2ex] |\sin z| \left(\dfrac{K^2}{|\sin z|^2} + 1 \right) & = & t. \end{cases}$$

This description is also subject to permissible values of constants H and K, with additional constraints on $|t| \geq 2K$ (not explored further here).

■

- **Conservative fields**

  From the perspectives of physical significance and mathematical simplicity, one of the most important classes of vector fields is the class of so-called *conservative fields*.

Definition 5.9
A vector field $\boldsymbol{f}: D \subseteq \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ *is called a* **conservative vector field** *if there exists a* C^1 *scalar function* $\phi: D \subseteq \mathbb{R}^3 \longrightarrow \mathbb{R}$ *such that*

$$\boldsymbol{f}(x, y, z) = \boldsymbol{\nabla}\phi(x, y, z).$$

The function $\phi(x, y, z)$ *is called a* **scalar potential** *of* $\boldsymbol{f}$.

Although scalar potentials and conservative fields arise in many areas of physics, it is far from true that all vector fields are conservative. That is, it is not generally true that all vector fields can be derived from scalar fields. However, when one encounters a conservative field, one can exploit many of its important properties. In the next section, we will discover one such important and appealing mathematical property of conservative fields. But first we must address the question whether a vector field is conservative and if so determine its scalar potential.

Consider some of the properties of the scalar potential itself as outlined in Definition 5.9. Firstly, for $\phi : D \longrightarrow \mathbb{R}$ to be a scalar potential it must be at least C^1. So, as a C^1 function the differential of ϕ can be defined but as a scalar potential this differential can be reexpressed:

$$\begin{aligned} \mathrm{d}\phi &= \frac{\partial\phi}{\partial x}\,\mathrm{d}x + \frac{\partial\phi}{\partial y}\,\mathrm{d}y + \frac{\partial\phi}{\partial z}\,\mathrm{d}z \\ &\Longrightarrow \qquad \mathrm{d}\phi = f_1\,\mathrm{d}x + f_2\,\mathrm{d}y + f_3\,\mathrm{d}z. \end{aligned}$$

The replacement of $\boldsymbol{\nabla}\phi$ with $\boldsymbol{f}$ in the last equation is valid since $\boldsymbol{f} = \boldsymbol{\nabla}\phi$ by assumption. The right-hand side of this last equation, expressed only in terms of $\boldsymbol{f}$, is thus an *exact differential* since it equals $\mathrm{d}\phi$. Conversely, the conclusion that may be drawn is that for f to be conservative, $f_1\,\mathrm{d}x + f_2\,\mathrm{d}y + f_3\,\mathrm{d}z$ should be an exact differential.

A much more practical criterion to use as a test for a conservative field follows if ϕ were a C^2 function and not just a C^1 function, *i.e.*, if ϕ were to possess continuous second-order partial derivatives. Then, according to Definition 2.8 (Page 106), these partial derivatives would satisfy the symmetry conditions

$$\frac{\partial^2\phi}{\partial x\partial y} = \frac{\partial^2\phi}{\partial y\partial x}, \qquad \frac{\partial^2\phi}{\partial x\partial z} = \frac{\partial^2\phi}{\partial z\partial x}, \qquad \frac{\partial^2\phi}{\partial y\partial z} = \frac{\partial^2\phi}{\partial z\partial y}.$$

In the context of ϕ being a scalar potential, these conditions have important consequences for the field.

Substituting $\boldsymbol{f}$ in place of $\boldsymbol{\nabla}\phi$ in these equalities we find that for $\boldsymbol{f}$ to be a conservative field, its components must satisfy the following three equations:

$$\frac{\partial f_1}{\partial y} = \frac{\partial f_2}{\partial x}, \qquad \frac{\partial f_3}{\partial x} = \frac{\partial f_1}{\partial z}, \qquad \frac{\partial f_3}{\partial y} = \frac{\partial f_2}{\partial z}.$$

These equations represent necessary conditions for the identification $\boldsymbol{f} = \boldsymbol{\nabla}\phi$ to be true and thus for $\boldsymbol{f}$ to be a conservative field. Despite their practical appeal, which will nevertheless be utilized in the following example, the conditions alone are not sufficient until they are complemented by the requirement that the domain in which they apply is open and connected, see Pages 341–344 and 381.

■ Example 5.8:

Show that the 3D vector field

$$\boldsymbol{F}((x, y, z) = \left(6x^2 + 1\right)\mathbf{i} + 2yz\mathbf{j} + y^2\mathbf{k}.$$

is a conservative field and determine its scalar potential.

Solution:

The vector field $\boldsymbol{F}$ is a C^∞ field. To show that it is conservative we begin by verifying that $\boldsymbol{F}$ satisfies the necessary conditions involving the partial derivatives of its components.

$$\begin{cases} \dfrac{\partial F_1}{\partial y} = \dfrac{\partial}{\partial y}\left(6x^2 + 1\right) = 0 = \dfrac{\partial}{\partial x}\left(2yz\right) = \dfrac{\partial F_2}{\partial x}, \\ \dfrac{\partial F_3}{\partial x} = \dfrac{\partial}{\partial x}\left(y^2\right) = 0 = \dfrac{\partial}{\partial z}\left(6x^2 + 1\right) = \dfrac{\partial F_1}{\partial z}, \\ \dfrac{\partial F_3}{\partial y} = \dfrac{\partial}{\partial y}\left(y^2\right) = 2y = \dfrac{\partial}{\partial z}\left(2yz\right) = \dfrac{\partial F_2}{\partial z}. \end{cases}$$

Consequently, all three necessary conditional equations are satisfied. This gives us reason to suppose that a scalar potential exists. To be certain, all that is required is to determine the potential.

We assume there exists a scalar potential ϕ that satisfies $\boldsymbol{\nabla}\phi = \boldsymbol{F}$. We determine this scalar potential by solving, sequentially, the three differential equations:

$$\frac{\partial \phi}{\partial x} = 6x^2 + 1, \quad \frac{\partial \phi}{\partial y} = 2yz, \quad \frac{\partial \phi}{\partial z} = y^2.$$

Step 1. Taking the first of these equations and integrating with respect to x we get

$$\phi(x, y, z) = 2x^3 + x + f(y, z),$$

where f is as yet an undetermined function of y and z.

Notice the important feature (repeated in subsequent steps) that, by integrating a multivariable function with respect to one variable, we pick up an unknown function of the other variables—NOT just a constant.

Step 2. Substituting this expression into the second differential equation we find $\dfrac{\partial f}{\partial y} = 2yz$. Integrating this equation with respect to y

– knowing that we are now working with a function of two variables

we find that $f(y, z) = y^2 z + g(z)$, for some unknown function g.

Step 3. Inserting this result into our expression for ϕ and substituting *that* result into the third differential equation leads to $\dfrac{\mathrm{d}g}{\mathrm{d}z} = 0$. Finally, integrating this last equation with respect to z we get $g(z) = C$, a true constant.

We thus finally arrive at a scalar potential of

$$\phi(x, y, z) = 2x^3 + x + y^2 z + C.$$

That this scalar potential, determined up to an arbitrary constant C, does indeed satisfy $\boldsymbol{F} = \boldsymbol{\nabla}\phi$ is readily verified by evaluating its gradient.

■

With the process of determining whether a field is conservative and then deriving its scalar potential outlined in the above example, the reader may wish to test their understanding with the following Mastery Check, which, in principle, requires taking the same steps.

✍ Mastery Check 5.5:

Determine whether the vector field $\boldsymbol{f} = \left(xy - \sin z, \dfrac{x^2}{2} - \dfrac{\mathrm{e}^y}{z}, \dfrac{\mathrm{e}^y}{z^2} - x\cos z\right)$ is conservative, and if so, determine a potential to $\boldsymbol{f}$.

Hints:

(1) For what values of (x, y, z) is $\boldsymbol{f}$ C^1?
(2) For those points (x, y, z) confirm the necessary conditions for $\boldsymbol{f} = \boldsymbol{\nabla}\phi$.
(3) If possible, solve $\boldsymbol{\nabla}\phi = \boldsymbol{f}$ for a possible scalar potential ϕ.
(4) Does ϕ exist? Everywhere? Does ϕ have any arbitrary constants? Are they unique?

✍

A scalar potential to a vector field $\boldsymbol{f}$ is also a real-valued scalar function and as we have seen in Section 2.E, the *level surfaces* of ϕ : $\phi(x, y, z) = c$, have normal vectors given by $\boldsymbol{\nabla}\phi$. This means that for a conservative field, $\boldsymbol{f} = \boldsymbol{\nabla}\phi$ is a vector that is normal to the surface $\phi = c$ at $\boldsymbol{r}$. The field lines of $\boldsymbol{f}$, given by $\dfrac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} = \lambda(t)\boldsymbol{f}(\boldsymbol{r}(t))$, are thus also perpendicular to the surface $\phi = c$. The level surfaces of ϕ (defined in Section 1.F) are called *equipotential* surfaces of $\boldsymbol{f}$. See Figure 5.14.

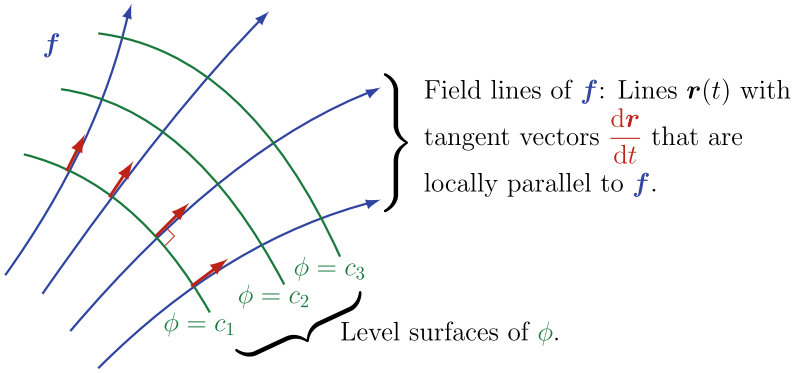


Figure 5.14 Conservative field lines and level surfaces of a scalar potential.

We leave differential vector calculus for the moment and consider some elements of the integral vector calculus, specifically so-called *curve* and *surface* integrals.

5.C Line Integrals

In both a theoretical and practical sense, line integrals can be thought of as somewhat more elaborate versions of one-dimensional integrals. As we alluded to in Chapter 4, one obvious generalization of scalar integration of a function of one variable involves replacing the straight-line *interval*, over which an integral is evaluated, with a one-variable parameterized curve in $\mathbb{R}^n$. Consequently, the intuitive view of a 1D integral as an area under a curve that was taught to us in our single-variable calculus courses is no longer applicable. Instead, one must refer to different and more physical ideas. Given their respective physical applications, line integrals can be divided into two classes: line integrals of scalar-valued functions (I) and line integrals of vector-valued functions (II). Within each class it is possible to refer to a specific physical picture to appreciate that class of integral.

Much if not all of what will be discussed in this section will be applicable to $\mathbb{R}^n$ for general n. However, because of obvious interest in the physical world, the discussion will be expressed in terms of points, curves, functions, and fields in $\mathbb{R}^3$.

I. Line integrals of real-valued functions

Physical motivation

In the simplest of terms, these are concerned with one-dimensional integrals of scalar functions that give the total measure of some quantity that is distributed along a curve.

As mentioned above, and outlined in detail in Chapter 4.A, in single-variable calculus the integral

$$\int_a^b f(x)\,\mathrm{d}x$$

is motivated as giving the area "under" f and "over" straight-line interval $[a, b]$

—this is a geometric interpretation

Suppose instead that we interpret $f(x)$ as a variable linear density of some quantity (*e.g.*, a mass/unit length or a charge/unit length) that is defined along the interval $I = [a, b]$. Then

$$\int_I f(x)\,\mathrm{d}x$$

would give the total amount of that quantity, say the total mass or the total charge, "borne" by I

—this is a physical interpretation

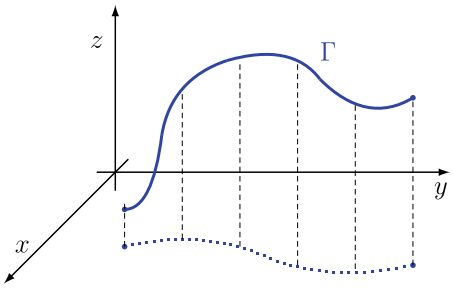


Figure 5.15 The curve Γ in 3D and its projection onto the 2D plane.

Both interpretations are physically valid and meaningful.

Now let's extend the latter idea to 1D structures sitting in higher dimensions. Suppose we were interested in evaluating the total mass or total charge carried by a nonlinear, one-dimensional object in 3D, say an object that is represented by the curve $\Gamma \subset \mathbb{R}^3$ in Figure 5.15.

What is needed is an expression for the total mass or total charge of the curved object which would correspond to the integral $\int_I f(x)\,\mathrm{d}x$ in the case of a straight-line interval.

Mathematical construction

Suppose Γ is a finite *smooth* curve in $\mathbb{R}^3$. Then, as discussed in Section 5.A.I, there exists a (non-unique) one-to-one parametrization of Γ,

$$\boldsymbol{r}(t) = \big(x(t), y(t), z(t)\big), \quad t \in [a, b],$$

such that $\boldsymbol{r}(t)$ is continuously defined on the finite connected interval $[a, b]$, and such that $|\boldsymbol{r}'(t)| \neq 0$.

Consider a partition of $[a, b]$, $a = t_0 < t_1 < t_2 < \cdots < t_{n-1} < t_n = b$, which leads to a set of discrete and sequential points on Γ: $\{\boldsymbol{r}(t_0), \boldsymbol{r}(t_1), \ldots, \boldsymbol{r}(t_n)\}$, as indicated in Figure 5.16.

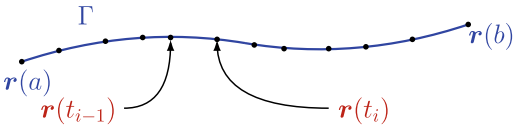


Figure 5.16 A parametrization of Γ.

The leading-order distance between nearest neighbour (in t) points on Γ is $|\Delta \boldsymbol{r}_i| = \big|\boldsymbol{r}(t_i) - \boldsymbol{r}(t_{i-1})\big|$. Adding all n such contributing line segment lengths gives

$$\sigma_n = \sum_{i=1}^{n} |\Delta \boldsymbol{r}_i| = \sum_{i=1}^{n} \big|\boldsymbol{r}(t_i) - \boldsymbol{r}(t_{i-1})\big|$$

as an approximation to the total length of Γ. Since the curve is smooth with respect to t, we can apply the mean value theorem (w.r.t. t) to each contributing difference in $\boldsymbol{r}$ values to give

$$|\Delta \boldsymbol{r}_i| = \big|\boldsymbol{r}(t_i) - \boldsymbol{r}(t_{i-1})\big| = \big|\,(x'(\zeta_i), y'(\eta_i), z'(\xi_i))\,\big|\Delta t_i$$

where $\{\zeta_i, \eta_i, \xi_i\}$ are some values of t, not necessarily the same, in the interval (t_{i-1}, t_i). We then have

$$\sigma_n = \sum_{i=1}^{n} \big|\,(x'(\zeta_i), y'(\eta_i), z'(\xi_i))\,\big|\Delta t_i.$$

Now, taking the dual limit of an infinite number of partition intervals ($n \to \infty$) and of vanishing partition size ($\max\{\Delta t_i\} \to 0$) we obtain the total length of the curve Γ:

$$\big|\Gamma\big| = \lim_{\substack{n\to\infty \\ \max|\Delta t_i|\to 0}} \sum_{i=1}^{n} |\Delta \boldsymbol{r}_i| = \int_a^b \Big|\boldsymbol{r}'(t)\Big|\,\mathrm{d}t$$

—provided the limit exists, which it should. (Why?)

This, the total length, is the most fundamental integral property of a curve.

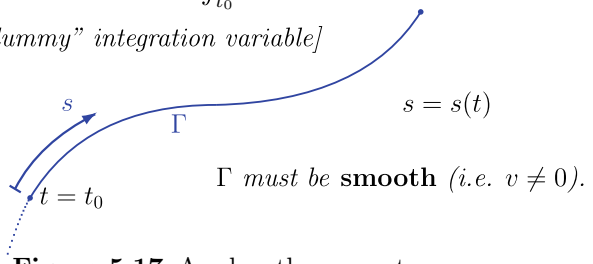
If we consider the curve to be the trajectory of a moving object, then physically the curve length will also be the total n-dimensional distance (in $\mathbb{R}^n$) travelled by the object. So, intuitively, this distance will be a function of the speed of the object and the duration of its travel. The derivation above shows us precisely this relation between curve length $|\Gamma|$ and speed $v(t) = |\boldsymbol{r}'(t)|$.

If, instead of a fixed terminal value, $t_n = b$, we consider a variable end point t (but keeping with the initial value t_0), the above derivation leads us to define a progressive, curve integral quantity called *arc length*.

Definition 5.10
The **arc length** *of a smooth curve* Γ *described by* $\boldsymbol{r}(t)$ *defined on an open connected interval* I *measured from* $t = t_0 \in I$ *to an arbitrary* $t \in I$ *is*

$$s = \int_{t_0}^{t} v(\tau)\mathrm{d}\tau. \tag{5.2}$$

[τ is a "dummy" integration variable]



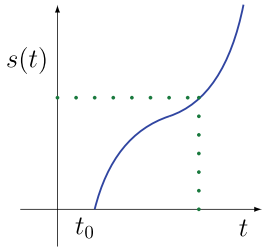
Γ *must be* **smooth** *(i.e.* $v \neq 0$*).*

Figure 5.17 Arc length parameter, s.

By differentiating both sides of Equation (5.2) with respect to t, using Leibniz's rule (Page 132), we verify the fundamental theorem of calculus

$$\mathrm{d}s/\mathrm{d}t = |\boldsymbol{r}'(t)| = v(t) > 0.$$

This formula confirms, firstly, that length is an increasing function of t and secondly that s is a bijective function of t. This means that t may equivalently be considered a function of s.



s — a one-to-one and onto function of t, which means that t is a function of s, that is, $t = t(s)$

Figure 5.18 Arc length is a one-to-one function of t.

Given the one-to-one relationship between t and s (Figures 5.17 and 5.18), we may equally well parameterize Γ with respect to the arc length s instead of the original variable t. Applying the chain rule, we find that

$$\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}s} = \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}\frac{\mathrm{d}t}{\mathrm{d}s} = \frac{\boldsymbol{r}'(t)}{|\boldsymbol{r}'(t)|}$$

—*the unit tangent vector* to Γ (a normalized velocity)

which, by construction, satisfies the condition that

$$\left|\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}s}\right| = 1.$$

—the "speed" of travel as measured by arc length is constant

Example 5.9 and Mastery Check 5.6 serve only to illustrate the technical side of arc length calculations, albeit in the case of simple curves.

Example 5.9:

Calculate the length of the 3D helical curve described by the vector function,

$$\boldsymbol{r}(t) = \cos t\,\mathbf{i} + \sin t\,\mathbf{j} + t/\pi\,\mathbf{k}, \qquad 0 \le t \le 2\pi.$$

Solution:

As t increases from 0 to 2π we are effectively calculating the length of one loop of the helix. To determine the length of multiple loops we simply multiply our result with that multiple of 2π.

Assuming a point on the curve is represented by $\boldsymbol{r}(t) = \cos t\,\mathbf{i} + \sin t\,\mathbf{j} + t/\pi\,\mathbf{k}$, tangent or velocity vector is given by $\boldsymbol{r}'(t) = -\sin t\mathbf{i} + \cos t\mathbf{j} + \frac{1}{\pi}\mathbf{k}$. The magnitude of this vector, the speed, is then $|\boldsymbol{r}'(t)| = \sqrt{\sin^2 t + \cos^2 t + \frac{1}{\pi^2}}$.

So, the length of the curve is

$$\begin{aligned} s &= \int_0^{2\pi} |\boldsymbol{r}'(t)|\,\mathrm{d}t = \int_0^{2\pi} \sqrt{\sin^2 t + \cos^2 t + \frac{1}{\pi^2}}\,\mathrm{d}t \\ &= \int_0^{2\pi} \sqrt{1 + \frac{1}{\pi^2}}\,\mathrm{d}t = 2\sqrt{1+\pi^2}. \end{aligned}$$

For comparison we may cite the circumference 2π of a circle of radius 1, which is what the helix would be were it to collapse onto the xy-plane.

■

Since curve length is a physical quantity its mathematical calculation is always possible in principle, even when a curve is piecewise smooth. However, calculations of curve length are not always so easily achieved in practice. Excluding the possibility of numerical evaluations, curve length calculations will depend ultimately on the existence of known, closed-form single-variable integrals.

✍ Mastery Check 5.6:

Using a suitable parametrization, calculate the distance travelled by an object traversing the path described by $y = \left(x + \frac{1}{2}\right)^2 + \frac{3}{4}$ in the xy-plane from $\left(-\frac{3}{2}, \frac{7}{4}\right)$ to $(0, 1)$.

✍

While the above Mastery Check problem is not too difficult to work through, it does demonstrate that the degree of difficulty is not always commensurate with the simplicity of the given curve.

Total curve length and arc length are the most basic properties of a curve, but by no means the only properties. The analytical argument underpinning their definitions can be generalized to also include a position-dependent scalar function.

Let $f : \mathbb{R}^3 \longrightarrow \mathbb{R}$ be a continuous scalar function defined on some domain in $\mathbb{R}^3$. When restricted to Γ in that domain it becomes, in effect, a composite function of one variable: $f(x(t), y(t), z(t)) = f(\boldsymbol{r}(t))$.

With this restriction f can be thought of as a *local linear density* of some property of Γ (again, *e.g.*, mass or charge per unit length). Multiplying f by a segment length $|\Delta \boldsymbol{r}|$ then gives the total amount of that property (mass or charge) possessed by that segment.

By an argument analogous to that used to define curve length, but applied to $f(\boldsymbol{r})|\Delta \boldsymbol{r}|$, we find that the integral measure of the property represented by f is given by ($t_i^* \in [t_{i-1}, t_i]$),

$$\lim_{\substack{n\to\infty \\ \max(|\Delta t_i|)\to 0}} \sum_{i=1}^{n} f(x(t_i^*), y(t_i^*), z(t_i^*))|\Delta \boldsymbol{r}_i|$$

$$= \lim_{\substack{n\to\infty \\ \max(|\Delta t_i|)\to 0}} \sum_{i=1}^{n} f(x(t_i^*), y(t_i^*), z(t_i^*))\left|\left(x'(\zeta_i), y'(\eta_i), z'(\xi_i)\right)\right| \Delta t_i$$

$$= \int_a^b f(x(t), y(t), z(t))\left|\boldsymbol{r}'(t)\right| \mathrm{d}t$$

—provided the limit exists, which it will if f is continuous and $[a, b]$ is bounded (Theorem 3.2).

Remarks

* It may be obvious from our derivation of curve length and its extension to the total mass, that integrals along a given curve of *scalar* functions have *no dependence* on the *direction* taken along the curve. We could have started at either end and arrived at the same result provided the parametrization is defined in a one-to-one manner, increasing from the start position to the end position. This is true of all curve integrals of scalar functions.

* Setting $f = 1$ in the above argument would have led to the total length of the curve, $|\Gamma|$, and, by restriction, Definition 5.10 for the arc length.

* In the above limit definitions we may identify the *differential arc length*

$$\mathrm{d}s = |\mathrm{d}\boldsymbol{r}| = \left|\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}\right| \mathrm{d}t,$$

Consequently, in terms of this differential arc length (and its equivalence to a parametric integral), the total length of Γ is

$$|\Gamma| = \int_\Gamma \mathrm{d}s \quad = s(b) = \int_a^b \left|\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}\right| \mathrm{d}t,$$

while the integral of $f(\boldsymbol{r})$ over Γ becomes

$$\int_\Gamma f(\boldsymbol{r}(s))\mathrm{d}s \quad = \int_a^b f\big(\boldsymbol{r}(t)\big)\left|\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}\right| \mathrm{d}t.$$

In practice, the left-hand sides of these definitions are considered more theoretical expressions, whereas the right-hand sides, expressed in terms of integrals with respect to a parameter t, are the working definitions to be used in actual calculations. See Example 5.10 below.

* Neither integral can depend on how we define Γ. That is, they cannot depend on what parametrization we choose to represent Γ whether in terms of t or s or in terms of any other parametrization.

Example 5.10:

Determine the integral $\displaystyle\int_\Gamma (xy + y)\,\mathrm{d}s$ where Γ is the path along the 2D curve $y = \sqrt{x}$ from the point $(4, 2)$ to the point $(9, 3)$.

Solution:

Let $\boldsymbol{r}(x, y)$ define a point on Γ. We parameterize $\boldsymbol{r} = (x, y)$ as $(t, \sqrt{t})$, with $t : 4 \to 9$, and $\dfrac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} = \left(1, \dfrac{1}{2\sqrt{t}}\right)$.

Then $\left|\dfrac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}\right| = \sqrt{1+\dfrac{1}{4t}}$ and

$$\begin{aligned}\int_\Gamma (xy+y)\,\mathrm{d}s &= \int_4^9 \left(t^{3/2}+t^{1/2}\right)\sqrt{1+\frac{1}{4t}}\,\mathrm{d}t = \frac{1}{2}\int_4^9 (t+1)\sqrt{4t+1}\,\mathrm{d}t\\ &= \left[(t+1)\frac{1}{6}(4t+1)^{3/2}\right]_4^9 - \int_4^9 \frac{1}{6}(4t+1)^{3/2}\,\mathrm{d}t\\ &= \left[(t+1)\frac{1}{6}(4t+1)^{3/2} - \frac{1}{60}(4t+1)^{5/2}\right]_4^9\\ &= \left[\frac{1}{20}(2t+3)(4t+1)^{3/2}\right]_4^9 = \frac{1}{20}(777\sqrt{37}-187\sqrt{17}).\end{aligned}$$

■

✍ Mastery Check 5.7:

Evaluate $\displaystyle\int_\Gamma x^2y^2\,\mathrm{d}s$ where Γ is the full circle $x^2+y^2=2$ in $\mathbb{R}^2$.

Hint: A suitable parametrization for a circle is with polar coordinates. In this case $\boldsymbol{r}(t) = \sqrt{2}\cos t\mathbf{e}_1 + \sqrt{2}\sin t\mathbf{e}_2,\ t:0\to 2\pi$.

✍

II. Line integrals of vector-valued functions

Line integrals in this class differ from those in Class I, firstly in the fact that Class II integrals involve vector fields (vector-valued functions in general) comprising several component functions, not just one. Secondly, the values of these line integrals will depend explicitly on the direction of the integration path relative to the direction of the vector field.

Physical motivation

Imagine a block of mass m that is stationary on a horizontal table and subject only to (a) the force of gravity which acts in the vertical direction (downward), $\boldsymbol{F}_g = -mg\mathbf{k}$ and (b) a balancing force exerted by the table, also in the vertical direction (upward), as shown in Figure 5.19(a). If the table is frictionless then despite the action of these two forces no effort is required to slide the block along the table since no resistance is offered by the table. We say that no work is done − no energy has been expended − in displacing the block in a direction perpendicular to the forces acting.

On the other hand, if we wished to lift the block directly upwards a distance h, Figure 5.19(b), then an upward force of $\boldsymbol{F} = mg\mathbf{k} + \boldsymbol{F}_v$, of magnitude exceeding the gravitational force would be needed to achieve this. It is the net upward force $\boldsymbol{F}_v = \boldsymbol{F} + (-mg\mathbf{k}) = \boldsymbol{F} + \boldsymbol{F}_g$ (we add vectors), that is responsible for this vertical displacement. The effort required – the work done by this force – is proportional to the magnitude of this excess force $|\boldsymbol{F}_v| = F_v > 0$ and the upward distance moved $h > 0$. That is, the work done is $W = F_v h$. Moreover, since the force acts in the same direction as the displacement, the work done *by* $\boldsymbol{F}_v$ is positive.

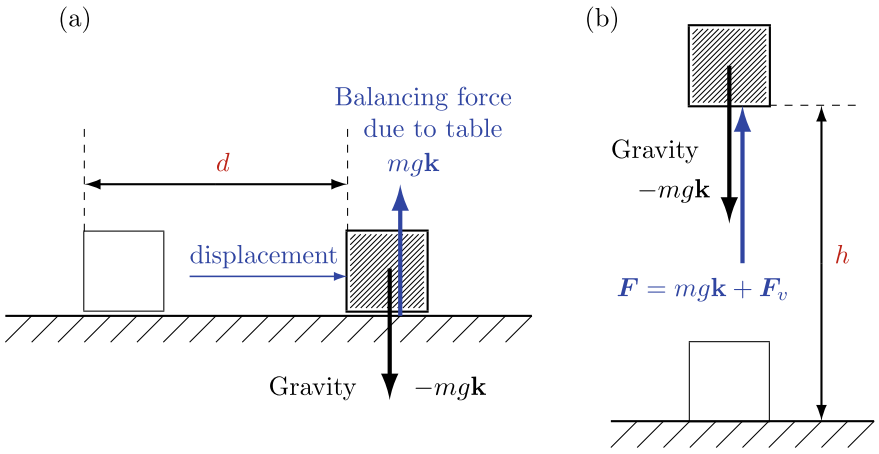


Figure 5.19 (a) Horizontal displacement on a frictionless table; (b) Vertical displacement opposing gravity.

Suppose now we apply the same upward force, $\boldsymbol{F} = mg\mathbf{k} + \boldsymbol{F}_v = mg\mathbf{k} + F_v\mathbf{k}$, opposing gravity, but instead move the block a distance d in the plane of the page at an arbitrary angle ϕ to the horizontal, and thus an angle $\theta = \pi/2 - \phi$ to the vertical (Figure 5.20). The displacement results in a change of height, $h = d\sin\phi = d\sin(\pi/2 - \theta) = d\cos\theta$. Given the conclusions of the two previous scenarios as well as the fact that all forces still act only in the vertical direction, we see that the work done by the net force is $W = F_v h = F_v d\cos\theta$. If the displacement were again upward then ϕ is positive and so $\cos\theta > 0$. Hence, positive work, $W > 0$, is again done *by* the force but is reduced in magnitude compared with a strictly upward vertical displacement. On the other hand, if the displacement were to be downward, in the direction opposite to the net force, then ϕ would be negative and so $\cos\theta < 0$. Consequently, the work done *by* $\boldsymbol{F}_v$ would then also be negative ($\theta > \phi/2$).

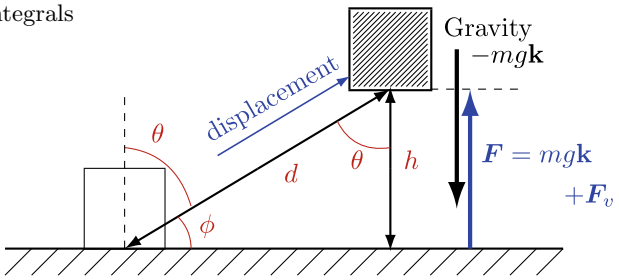


Figure 5.20 Displacement in an oblique direction.

This relationship between work, force, and displacement, $W = F_v d \cos\theta$, also accounts for the special case when force and displacement were at right angles: $W = 0$ since $\theta = \pi/2$, and so no work is done.

Notice that the angle θ is not only the angle to the vertical, it is also the angle between the displacement and force directions!

In full 3D, the act of displacing the block from a point A to a point B in Figure 5.21, again with the *net* force directed upwards, $\boldsymbol{F}_v = F_v\mathbf{k}$, the work done by the force is

$$\begin{aligned} W &= F_v.(h_b - h_A) = F_v.d.\sin\phi = F_v.d.\sin(\pi/2 - \theta) \\ &= F_v.d.\cos\theta = F_v.|\boldsymbol{r}_B - \boldsymbol{r}_A|\,.\cos\theta = \boldsymbol{F}_v \cdot (\boldsymbol{r}_B - \boldsymbol{r}_A). \end{aligned}$$

That is, the work done by $\boldsymbol{F}_v$ is simply but significantly given by the scalar product of the *net* vector force, $\boldsymbol{F}_v$ (in excess of gravity), and the vector displacement, $\boldsymbol{r}_B - \boldsymbol{r}_A$.

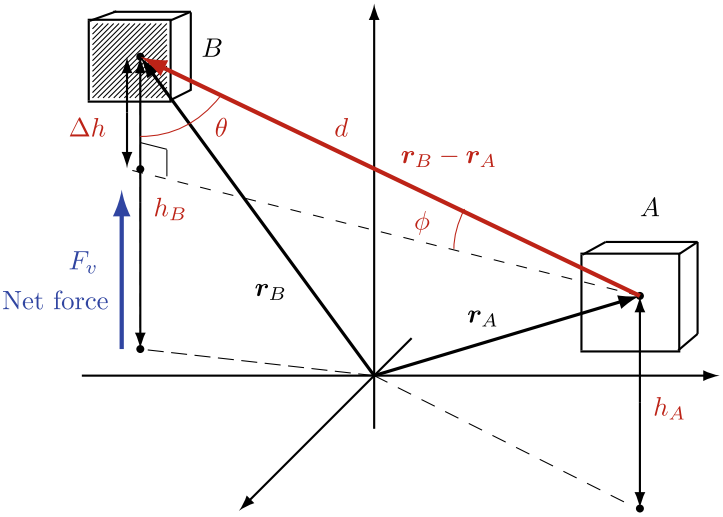


Figure 5.21 Displacement in 3D space.

Disconnected from our specific physical example of displacing a block, we have the general finding that the work done by a force, $\boldsymbol{F}$, is given by the component of the force acting in the direction of a vector displacement, $\boldsymbol{d}$, multiplied by the magnitude of that displacement. That is,

$$W = \boldsymbol{F} \cdot \boldsymbol{d} = Fd\cos\theta.$$

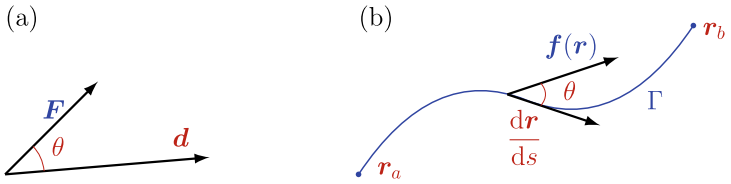


Figure 5.22 Constant (a) and variable (b) force and displacement.

Mathematical construction

In the above description we assumed that both force and displacement were constant in terms of both direction and magnitude, as in Figure 5.22(a). What is now needed is an expression for work when the force $\boldsymbol{f}$ is not constant, but whose magnitude and direction are functions of position, $\boldsymbol{f} = \boldsymbol{f}(\boldsymbol{r})$, and when the displacement is not a straight line but instead is taken along a more variable path.

Suppose $\boldsymbol{r} = \boldsymbol{r}(s)$ defines pointwise the *smooth* path Γ to be taken (Figure 5.22(b)) and consider a small segment of this curve, specifically given by the arc length differential $\mathrm{d}s$ at $\boldsymbol{r}(s)$. Lastly, suppose the path Γ lies in a locally varying vector field $\boldsymbol{f} = \boldsymbol{f}(\boldsymbol{r})$.

As we've done in considering line integrals of scalar fields (Class I), we can break Γ up into n finite segments of length Δs_i, which are sufficiently short so that over their respective extents the field $\boldsymbol{f}$ is approximately constant, while $\Delta\boldsymbol{r}(s_i)$ is approximately straight in the direction $\boldsymbol{r}(s_i + \Delta s_i) - \boldsymbol{r}(s_i)$. Hence, for $|\Delta s_i| \ll 1$ the incremental work done by the vector field in the course of the displacement $|\Delta\boldsymbol{r}(s_i)|$ will be

$$\begin{aligned}
\Delta W(s_i) &= |\boldsymbol{f}(\boldsymbol{r}(s_i)| \cos\theta(\boldsymbol{r}(s_i)) \, |\Delta\boldsymbol{r}(s_i)| \\
&= |\boldsymbol{f}(\boldsymbol{r}(s_i))| \cos\theta(\boldsymbol{r}(s_i)) \left|\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}s}(s_i^*)\right| \Delta s_i \\
&\qquad\qquad \text{—by the mean value theorem} \\
&= \boldsymbol{f}(\boldsymbol{r}(s_i)) \cdot \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}s}(s_i^*) \, \Delta s_i,
\end{aligned}$$

where s_i^* is some s value in the interval $[s_i, s_i + \Delta s_i]$. Summing all such incremental contributions and taking the dual limit of $n \to \infty$ and $\max |\Delta s_i| \to 0$, we get

$$W = \lim_{\substack{n\to\infty \\ \max(|\Delta s_i|)\to 0}} \sum_{i=1}^{n} \boldsymbol{f}(\boldsymbol{r}(s_i)) \cdot \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}s}(s_i^*)\, \Delta s_i,$$
$$= \int_\Gamma \Big(\boldsymbol{f}(\boldsymbol{r}) \cdot \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}s} \Big) \mathrm{d}s = \int_\Gamma \boldsymbol{f}(\boldsymbol{r}) \cdot \mathrm{d}\boldsymbol{r},$$

as the total work done by $\boldsymbol{f}$ in moving from start to finish along Γ.

Remarks

* $\displaystyle\int_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}$ is called the line integral of the vector field $\boldsymbol{f}$ along Γ.

* Since $\left|\dfrac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}s}\right| = 1$ (Page 326), then $\boldsymbol{f}(\boldsymbol{r}) \cdot \dfrac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}s} = |\boldsymbol{f}| \cos\theta$.

  —the tangential component of $\boldsymbol{f}$ along Γ

  So the line integral of *vector* field, $\boldsymbol{f}$, along Γ is identical to the line integral of the *scalar* field, $|\boldsymbol{f}| \cos\theta$, which is the locally varying tangential component of $\boldsymbol{f}$.

* With the derivation of the line integral complete we may now reflect on its evaluation. Neither form

  $$\int_\Gamma \boldsymbol{f}(\boldsymbol{r}(s)) \cdot \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}s} \mathrm{d}s \qquad \text{or} \qquad \int_\Gamma \boldsymbol{f}(\boldsymbol{r}) \cdot \mathrm{d}\boldsymbol{r},$$

  is immediately practical. Arc length parameterizations are not usually convenient so other means are necessary. Here, we present two useful versions.

  (a) Interpreting the second form literally in terms of a scalar product of Cartesian differentials and Cartesian field components we have

  $$\int_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = \int_\Gamma \Big(f_1(x,y,z)\mathrm{d}x + f_2(x,y,z)\mathrm{d}y + f_3(x,y,z)\mathrm{d}z \Big).$$

  —this is often a possible approach if the path is specified in x, y, and z as in Example 5.11

  (b) Most often, a curve is expressed in terms of some parameter t, *e.g.*, $\boldsymbol{r} = \boldsymbol{r}(t)$, where $t \in [a, b]$, $\boldsymbol{r}_a = \boldsymbol{r}(a)$, and $\boldsymbol{r}_b = \boldsymbol{r}(b)$. Then, assuming a bijective change of variable, $t = t(s) \Leftrightarrow s = s(t)$, the integral in terms of arc length may be reexpressed in the very useful form,

$$\int_\Gamma \boldsymbol{f}(\boldsymbol{r}(s)) \cdot \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}s}\mathrm{d}s = \int_a^b \boldsymbol{f}\big(\boldsymbol{r}(t)\big) \cdot \frac{\mathrm{d}\boldsymbol{r}(t)}{\mathrm{d}t}\mathrm{d}t,$$

i.e., as a one-dimensional integral over t. Note that even the Cartesian case can be converted into this form.

∗ On this last note, we emphasize the uniqueness of the line integral: $\int_\Gamma \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{r}$ is independent of the choice of parametrization, *as long as we go in the same direction*. The following argument demonstrates this.

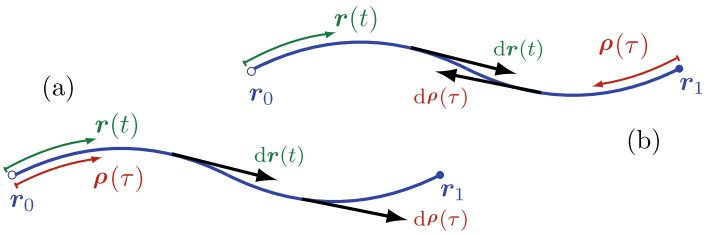


Figure 5.23 Traversing a curve (a) in the same, and (b) in the opposite direction.

Suppose $\boldsymbol{r}(t)$ and $\boldsymbol{\rho}(\tau)$ are two smooth parametrizations of the same curve, Γ, joining end points $\boldsymbol{r}_0$ and $\boldsymbol{r}_1$. Then, for any point P with coordinate vector $\boldsymbol{r}$ on the curve, unique t and τ values can be found such that $\boldsymbol{r} = \boldsymbol{r}(t) = \boldsymbol{\rho}(\tau)$. Moreover, a bijective relationship exists identifying a unique τ to every t: $\tau = g(t) \Leftrightarrow t = g^{-1}(\tau)$.

If the parametrizations trace Γ in the same direction (Figure 5.23(a)) then

$$\begin{cases} \boldsymbol{r}_0 = \boldsymbol{r}(a) = \boldsymbol{\rho}(\alpha) & \alpha = g(a), \\ \boldsymbol{r}_1 = \boldsymbol{r}(b) = \boldsymbol{\rho}(\beta) & \beta = g(b), \end{cases}$$

with $\dfrac{\mathrm{d}g}{\mathrm{d}t} > 0$, *i.e.*, t increases as τ increases. Consequently,

$$\begin{aligned} \int_{\Gamma(t)} \boldsymbol{f} \bullet \mathrm{d}\boldsymbol{r} &= \int_a^b \boldsymbol{f}(\boldsymbol{r}(t)) \bullet \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}\mathrm{d}t = \left\{ \begin{array}{c} t = g^{-1}(\tau) \\ \mathrm{d}t = \dfrac{\mathrm{d}t}{\mathrm{d}\tau}\mathrm{d}\tau \end{array} \right\} = \\ &= \int_\alpha^\beta \boldsymbol{f}(\boldsymbol{r}(g^{-1}(\tau))) \bullet \frac{\mathrm{d}\boldsymbol{r}(g^{-1}(\tau))}{\mathrm{d}\tau}\frac{\mathrm{d}\tau}{\mathrm{d}t}\cdot\frac{\mathrm{d}t}{\mathrm{d}\tau}\mathrm{d}\tau, \\ &= \int_\alpha^\beta \boldsymbol{f}(\boldsymbol{\rho}(\tau)) \bullet \frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}\tau}\mathrm{d}\tau = \int_{\Gamma(\tau)} \boldsymbol{f} \bullet \mathrm{d}\boldsymbol{\rho}, \end{aligned}$$

and we have an identical result.

If the parametrizations trace Γ in the opposite directions (Figure 5.23(b)) then

$$\begin{cases} \boldsymbol{r}_0 = \boldsymbol{r}(a) = \boldsymbol{\rho}(\beta) & \beta = g(a), \\ \boldsymbol{r}_1 = \boldsymbol{r}(b) = \boldsymbol{\rho}(\alpha) & \alpha = g(b), \end{cases}$$

with $\dfrac{\mathrm{d}g}{\mathrm{d}t} < 0$. That is, t decreases as τ increases. Consequently,

$$\begin{aligned} \int_{\Gamma(t)} \boldsymbol{f} \bullet \mathrm{d}\boldsymbol{r} &= \int_a^b \boldsymbol{f}(\boldsymbol{r}(t)) \bullet \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}\mathrm{d}t = \left\{ \begin{array}{c} t = g^{-1}(\tau) \\ \mathrm{d}t = \dfrac{\mathrm{d}t}{\mathrm{d}\tau}\mathrm{d}\tau \end{array} \right\} = \\ &= \int_\beta^\alpha \boldsymbol{f}(\boldsymbol{r}(g^{-1}(\tau))) \bullet \frac{\mathrm{d}\boldsymbol{r}(g^{-1}(\tau))}{\mathrm{d}\tau}\frac{\mathrm{d}\tau}{\mathrm{d}t}.\frac{\mathrm{d}t}{\mathrm{d}\tau}\mathrm{d}\tau, \\ &= -\int_\alpha^\beta \boldsymbol{f}(\boldsymbol{\rho}(\tau)) \bullet \frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}\tau}\mathrm{d}\tau = -\int_{\Gamma(\tau)} \boldsymbol{f} \bullet \mathrm{d}\boldsymbol{\rho}. \end{aligned}$$

This last result is consistent with the physical interpretation that the work done in traversing a given direction is the negative of the work found in traversing in the opposite direction. We may conveniently denote the latter course: $\Gamma(\tau)$ as $-\Gamma(t)$. We therefore conclude that

$$\int_{\Gamma(\tau)} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{\rho} = -\int_{\Gamma(t)} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = \int_{-\Gamma(t)} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}.$$

In other words, a line integral in which a curve is traversed in one direction is the negative of a line integral in which the curve is traversed in the opposite direction. A curve with a specified direction is called *oriented*. –this is important to remember in calculations.

* As mentioned earlier, the total or net work done by vector field (or force) can be positive or negative (or zero) depending on the direction of the displacement relative to the direction of the vector field acting. The sign indicates whether energy is gained in a displacement going with the field (work is positive) or energy is lost in a displacement going against the field (work is negative). This physical interpretation is made from the perspective of the energy state of the object being displaced. In general, this interpretation explains why, in contrast to line integrals of scalar functions, the direction of a displacement must always be specified when evaluating line integrals of vector fields.

* If $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \cdots \cup \Gamma_n$, as in Figure 5.24, then

$$\int_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = \int_{\Gamma_1} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} + \int_{\Gamma_2} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} + \int_{\Gamma_3} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} + \cdots + \int_{\Gamma_n} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}.$$

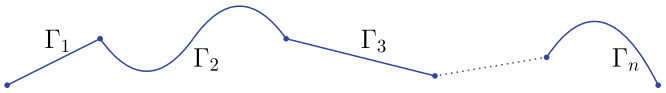


Figure 5.24 A connected, piecewise smooth, curve.

The total line integral over Γ is the sum of the line integrals over the *connected* pieces Γ_i that link the start (of Γ) to the end (of Γ).

∗ If Γ is a closed curve (Figure 5.25), that is if $\boldsymbol{r}_a = \boldsymbol{r}_b$, then the line integral of $\boldsymbol{f}$ along Γ is called the *circulation* of $\boldsymbol{f}$ around Γ:

Circulation of $\boldsymbol{f}$ around Γ is denoted $\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}$.

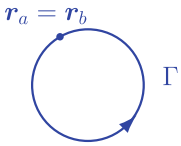


Figure 5.25 The circle: a simple closed curve.

In the next three examples we demonstrate the different ways of evaluating line integrals of vector fields.

Example 5.11:

Examples of evaluating line integrals using Cartesian coordinates (x, y, z).

Evaluate the line integral $\int_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}$ where $\boldsymbol{f} = (x + y, y - x)$ and Γ is a curve with endpoints $(1, 1)$ and $(4, 2)$. Suppose,

(a) $\Gamma = \{(x, y) : x = y^2\}$ (Figure 5.26(a)), and

(b) $\Gamma = \Gamma_1 \cup \Gamma_2$, where Γ_1 and Γ_2 are the straight-line segments of constant y and constant x, respectively, as shown in Figure 5.26(b).

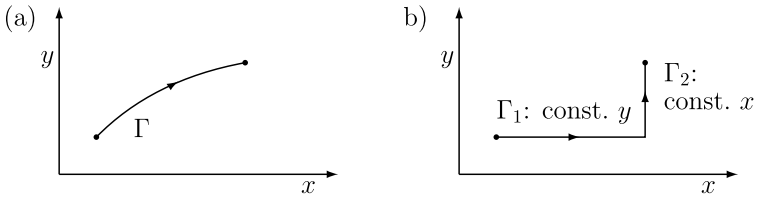


Figure 5.26 The paths (a) $x = y^2$, and (b) $\Gamma = \Gamma_1 \cup \Gamma_2$.

Solution:

(a) In this case we may consider y to be the active parameter with $y \in [1,2]$.
The 2D vector field $\boldsymbol{f} = (f_1, f_2) = (y^2+y, y-y^2)$, and since $\boldsymbol{r} = (y^2, y)$ we have $\mathrm{d}\boldsymbol{r} = (2y\mathrm{d}y, \mathrm{d}y)$.
Hence,

$$\int_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = \int_1^2 (y^2+y, y-y^2) \cdot (2y, 1)\, \mathrm{d}y \;=\; \frac{34}{3}.$$

(b) In this problem we invoke the addition property (the 6th bullet point above)

$$\int_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} \;=\; \int_{\Gamma_1} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} \;+\; \int_{\Gamma_2} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r},$$

and consider separately each leg of the total path.

On Γ_1, x is the active variable with $x \in [1,4]$ whereas y is a constant, $y = 1$.
So, $\mathrm{d}\boldsymbol{r} = (\mathrm{d}x, 0)$ and $\boldsymbol{f} = (f_1, f_2) = (x+1, 1-x)$.
On Γ_2, $x = 4$ is constant, while $y \in [1,2]$ is the active variable.
Then, $\mathrm{d}\boldsymbol{r} = (0, \mathrm{d}y)$ and $\boldsymbol{f} = (f_1, f_2) = (4+y, y-4)$.

Consequently,

$$\begin{aligned}
\int_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} \;&=\; \int_{\Gamma_1} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} + \int_{\Gamma_2} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}, \\
&=\; \int_1^4 (x+1, 1-x, 0) \cdot (1,0)\, \mathrm{d}x + \int_1^2 (4+y, y-4) \cdot (0,1)\, \mathrm{d}y \\
&=\; \int_1^4 (x+1)\, \mathrm{d}x + \int_1^2 (y-4)\, \mathrm{d}y \;=\; 8.
\end{aligned}$$

■

■ Example 5.12:

Examples of evaluating line integrals using curve parametrization $\big(x(t), y(t), z(t)\big)$.

Evaluate $\displaystyle\int_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = \int_\Gamma \big(xz\,\mathrm{d}x + y^2\,\mathrm{d}y + x^2\,\mathrm{d}z\big)$ from $(0,0,0)$ to $(1,1,1)$. along the curves (a) $\boldsymbol{r}(t) = (t, t, t^2)$, and (b) $\boldsymbol{r}(t) = (t^2, t, t^2)$ (Figure 5.27).

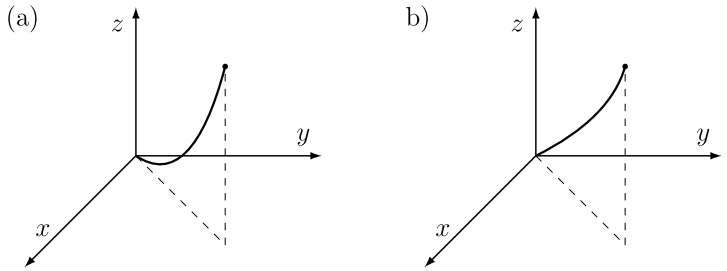


Figure 5.27 The paths (a) $\boldsymbol{r}(t) = (t, t, t^2)$, and (b) $\boldsymbol{r}(t) = (t^2, t, t^2)$.

Solution:

In both cases $t \in [0, 1]$ will work.

(a) We have $x = t,\ y = t,\ z = t^2$, so $\boldsymbol{f} = (t^3, t^2, t^2)$, $\dfrac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} = (1, 1, 2t)$, and

$$\int_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} \;=\; \int_0^1 (t^3, t^2, t^2) \cdot (1, 1, 2t)\, \mathrm{d}t \;=\; \int_0^1 (t^3 + t^2 + 2t^3)\, \mathrm{d}t \;=\; \frac{13}{12}.$$

(b) We have $x = t^2,\ y = t,\ z = t^2$, so $\boldsymbol{f} = (t^4, t^2, t^4)$, $\dfrac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} = (2t, 1, 2t)$, and

$$\int_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} \;=\; \int_0^1 (t^4, t^2, t^4) \cdot (2t, 1, 2t)\, \mathrm{d}t \;=\; \int_0^1 (2t^5 + t^2 + 2t^5)\, \mathrm{d}t \;=\; 1.$$

■

Readers may now wish to try their hand at a similar calculation involving a curve parameterization $(x(t), y(t), z(t))$.

✍ Mastery Check 5.8:

Calculate the work done by a force $\boldsymbol{f}(\boldsymbol{r}) = y\,\mathbf{e}_1 + 2x\,\mathbf{e}_2 - z\,\mathbf{e}_3$ along a helical curve Γ defined by $\boldsymbol{r}(t) = \cos t\,\mathbf{e}_1 + \sin t\,\mathbf{e}_2 + t\,\mathbf{e}_3,\ t : 0 \to 2\pi$.

✍

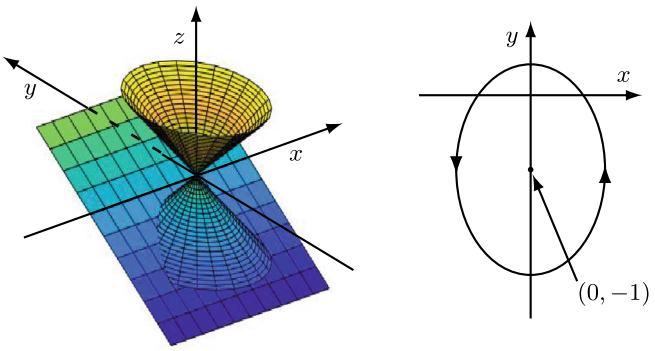
There is yet a third type of line integral where a parametrization of a curve is not specified, and the curve itself may not be explicitly defined. This case is covered in this third example. The strategies followed are typically used in such cases.

■ Example 5.13:

Example of evaluating a line integral when a curve needs identifying.

Evaluate $\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}$ where $\boldsymbol{f} = y\mathbf{i} + \mathbf{k}$ and Γ is the curve of intersection of the cone $z^2 = 2x^2 + 2y^2$ and the plane $y = z + 1$. See Figure 5.28(a).

Orientation is counterclockwise seen from $(0, 0, 117)$.



(a) (b)

Figure 5.28 Intersection of a plane and a cone. (a) The 3D graphs. (b) The 2D projection of the curve of intersection.

Solution:

The curve along which we need to integrate must be identified mathematically before proceeding.

Method 1. Utilize the equations for the surfaces: three variables appear in the cone equation, while two appear in the plane equation. Use the plane equation to reduce the number of variables in the cone equation. Thus,

$$z = y - 1 \Longrightarrow (y-1)^2 = 2x^2 + 2y^2, \quad \text{or} \quad x^2 + \frac{(y+1)^2}{2} = 1.$$

This is an equation for a 2D ellipse, but *not* the 3D curve of intersection itself. This ellipse is the *projection* of the curve of intersection onto the xy-plane (Figure 5.28(b)).

From the ellipse projection, with centre at $(0, -1)$ and semi-axes 1 and $\sqrt{2}$, we introduce the standard parametrization:

$$x = \cos t, \;\; y = -1 + \sqrt{2}\sin t, \;\; t \in [0, 2\pi].$$

Use this also in the plane equation: $z = -2 + \sqrt{2}\sin t$.

The final 3D parametrization of the curve of intersection is then,

$$x(t) = \cos t, \quad y(t) = -1 + \sqrt{2}\sin t \quad z(t) = -2 + \sqrt{2}\sin t, \ t \in [0, 2\pi].$$

Note that the parameter range, from $t = 0$ to $t = 2\pi$, is consistent with the stipulated orientation of the curve of intersection, being counterclockwise as viewed from high on the z axis (see the arrows shown in Figure 5.28(b)).

Now we follow the steps of Example 5.12. That is,

$$\boldsymbol{f}(\boldsymbol{r}(t)) = (f_1(t), f_2(t), f_3(t)) = (-1 + \sqrt{2}\sin t, 0, 1), \quad \text{and}$$
$$\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} = (-\sin t, \sqrt{2}\cos t, \sqrt{2}\cos t).$$

Thus

$$\begin{aligned}
\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} &= \int_0^{2\pi} \big(-1 + \sqrt{2}\sin t, 0, 1\big) \cdot \big(-\sin t, \sqrt{2}\cos t, \sqrt{2}\cos t\big)\, \mathrm{d}t \\
&= \int_0^{2\pi} \big(\sin t - \sqrt{2}\sin^2 t + \sqrt{2}\cos t\big)\, \mathrm{d}t \\
&= \int_0^{2\pi} \big(\sin t - \frac{1}{\sqrt{2}}(1 - \cos 2t) + \sqrt{2}\cos t\big)\, \mathrm{d}t \\
&= \Big[-\cos t - \frac{t}{\sqrt{2}} + \frac{1}{2\sqrt{2}}\sin 2t + \sqrt{2}\sin t\Big]_0^{2\pi} = -\pi\sqrt{2}.
\end{aligned}$$

Notice that in this example the curve of intersection was a closed curve. Hence, this example illustrates the calculation of a *circulation*.

Method 2. The cone has circular symmetry so use standard polar coordinates: $x = r\cos\theta$ and $y = r\sin\theta$:

$$z^2 = 2x^2 + 2y^2 \Longrightarrow z^2 = 2r^2 \Longrightarrow z = \pm\sqrt{2}r.$$

The plus/minus signs on z refer to the upper/lower branches of the cone. Only the minus branch is relevant (why?). The plane equation becomes

$$y = z + 1 \Longrightarrow y = r\sin\theta = -\sqrt{2}r + 1.$$

Also

$$x = r\cos\theta = \pm\sqrt{r^2 - r^2\sin^2\theta} = \pm\sqrt{2\sqrt{2}r - 1 - r^2}.$$

All three variables are parameterized: $(x(r), y(r), z(r))$. r has limiting values when $\theta = \mp\pi/2$, *i.e.*, $r_{max/min} = \sqrt{2} \pm 1$.
Note that both signs on the x parametrization are required. Two integrals need to be evaluated and added in order to complete the closed curve *with the correct orientation*:

$$\text{for } x > 0 \Rightarrow \int_{\sqrt{2}+1}^{\sqrt{2}-1} \boldsymbol{f} \cdot \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}r}\mathrm{d}r, \quad \text{and for } x < 0 \Rightarrow \int_{\sqrt{2}-1}^{\sqrt{2}+1} \boldsymbol{f} \cdot \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}r}\mathrm{d}r.$$

The remainder of the example is left for the reader to complete.

■

Remarks

* Each of the line integrals in Examples 5.11 and 5.12 and Mastery Check 5.8 involved some form of curve parametrization which resulted in the line integrals being reduced to one-dimensional integrals of functions of one variable, the parameter.

* In the (a) and (b) parts of Examples 5.11 and 5.12 the line integrals involved the same field and the same endpoints, but *different* curves. They gave *different* results!

  To help understand why this might happen we defer to a physical motivation. In the respective (a) and (b) cases, the work done in going from point $\boldsymbol{r}_a$ to point $\boldsymbol{r}_b$ depended on the path taken. If the fields involved were the actions of the force of *friction*, then taking different routes with different path lengths (and possibly with different character—sandy as opposed to paved, say) would naturally result in different degrees of energy expenditure, *i.e.*, different amounts of work done.

The last remark raises an important point and an important question. What conditions do we need to impose on a vector field to get the same result for the line integral, independent of path?

The very satisfactory answer to this question is that the field must be *conservative*!

Theorem 5.2
Suppose $\boldsymbol{f}(\boldsymbol{x}) = \big(f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), f_3(\boldsymbol{x})\big)$ *is a conservative field with potential* $\phi(\boldsymbol{x})$ *defined on an open connected domain,* D*. Then*

$$\int_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = \phi(\boldsymbol{r}_b) - \phi(\boldsymbol{r}_a)$$

for **every** *curve* Γ *lying entirely in* D *which joins the points* $\boldsymbol{r}_a \longrightarrow \boldsymbol{r}_b$*.*

Theorem 5.2 states that the line integral $\int_\Gamma \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{r}$ is independent of the choice of Γ if $\boldsymbol{f}$ *is conservative* and is dependent only on the endpoints, $\boldsymbol{r}_a$ and $\boldsymbol{r}_b$. To be precise, the integral is determined by, and dependent only on, the values of the scalar potential, ϕ, at these points.

A proof of the theorem, and our consequential statements, follows readily from our earlier finding that for a conservative field $\boldsymbol{f}\cdot\mathrm{d}\boldsymbol{r}$ is a perfect differential, $\mathrm{d}\phi$. The integral of this perfect differential results in the difference in the values of the potential at the terminal points of the curve Γ.

Example 5.14:

Evaluate the line integral $\int_\Gamma \boldsymbol{F}\cdot\mathrm{d}\boldsymbol{r}$ by direct calculation using a suitable parametrization of the curve, Γ, and verify your answer using the scalar potential to the conservative field $\boldsymbol{F}$.
Here Γ is that part of the piecewise smooth curve of intersection of the right circular cylinder $x^2+y^2=1$ and the plane $x+y+z=1$, extending from the point $(1,0,0)$ to the point $(-1,0,0)$ in a counterclockwise direction as seen from the perspective of the point $(0,0,10)$,
and

$$\boldsymbol{F}=(6x^2+1)\mathbf{i}+2yz\mathbf{j}+y^2\mathbf{k}.$$

Solution:

That this vector field is conservative was already confirmed in Example 5.8 with its scalar potential determined there. Hence, the focus of the present example is on determining the line integral by direct means and then verifying the result based on Theorem 5.2.

The curve of intersection is readily parameterized after recognizing that one of the surfaces is the cylinder, $x^2+y^2=1$, with polar coordinates as its natural parametrization. We then solve the equation of the plane for z to get the 3D parametrization of Γ:

$$\Gamma=\left\{\boldsymbol{r}\in\mathbb{R}^3 : x=\cos\theta, y=\sin\theta, z=1-\cos\theta-\sin\theta, \quad 0\le\theta\le\pi\right\}.$$

From this we deduce

$$\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}\theta}=-\sin\theta\mathbf{i}+\cos\theta\mathbf{j}+(\sin\theta-\cos\theta)\mathbf{k}, \quad \theta\in[0,\pi].$$

The line integral now becomes

$$\begin{aligned}
&\int_\Gamma \boldsymbol{F}\cdot \mathrm{d}\boldsymbol{r} = \int_0^\pi \boldsymbol{F}\left(\boldsymbol{r}(\theta)\right)\cdot\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}\theta}\mathrm{d}\theta,\\
=\ &\int_0^\pi \left(1+6\cos^2\theta, 2\sin\theta(1-\cos\theta-\sin\theta), \sin^2\theta\right)\cdot(-\sin\theta, \cos\theta\sin\theta-\cos\theta)\,\mathrm{d}\theta,\\
=\ &\int_0^\pi \left(-\sin\theta-8\cos^2\theta\sin\theta-3\sin^2\theta\cos\theta+\sin^3\theta+2\sin\theta\cos\theta\right)\mathrm{d}\theta,\\
=\ &\left[\cos\theta+\frac{8}{3}\cos^3\theta-\sin^3\theta+(-\cos\theta+\frac{1}{3}\cos^3\theta)+\sin^2\theta\right]_0^\pi,\\
=\ &(-1-\frac{8}{3}-0+(1-\frac{1}{3})+0)-(1+\frac{8}{3}-0+(-1+\frac{1}{3})+0)=-\frac{18}{3}=-6.
\end{aligned}$$

The scalar potential to the conservative field $\boldsymbol{F}$ was determined in Example 5.8 to be

$$\phi(x,y,z)=2x^3+x+y^2z+C.$$

With this scalar function in Theorem 5.2 we find

$$\begin{aligned}
\int_\Gamma \boldsymbol{F}\cdot\mathrm{d}\boldsymbol{r} &= \phi(-1,0,0)-\phi(1,0,0)\\
&= \left(2(-1)^3+0+(-1)\right)-\left(2(1)^3+0+(1)\right)=-6,
\end{aligned}$$

in agreement with the direct calculation above. ■

Corollary 5.2.1 *For the conditions of Theorem 5.2, let Γ_1 and Γ_2 be two curves in D that join $\boldsymbol{r}_a$ and $\boldsymbol{r}_b$ (Figure 5.29). Then*

$$\begin{aligned}
&\int_{\Gamma_1}\boldsymbol{f}\cdot\mathrm{d}\boldsymbol{r} = \int_{\Gamma_2}\boldsymbol{f}\cdot\mathrm{d}\boldsymbol{r}\\
\Longrightarrow\quad &\int_{\Gamma_1}\boldsymbol{f}\cdot\mathrm{d}\boldsymbol{r}-\int_{\Gamma_2}\boldsymbol{f}\cdot\mathrm{d}\boldsymbol{r}=0\\
\Longrightarrow\quad &\int_{\Gamma_1}\boldsymbol{f}\cdot\mathrm{d}\boldsymbol{r}+\int_{-\Gamma_2}\boldsymbol{f}\cdot\mathrm{d}\boldsymbol{r}=0\\
\Longrightarrow\quad &\int_{\Gamma_1\cup(-\Gamma_2)}\boldsymbol{f}\cdot\mathrm{d}\boldsymbol{r}=\oint_\Gamma\boldsymbol{f}\cdot\mathrm{d}\boldsymbol{r}=0.
\end{aligned}$$

That is, the circulation of conservative field $\boldsymbol{f}$ is zero: $\displaystyle\oint_\Gamma \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{r}=0.$

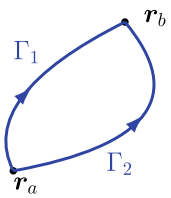


Figure 5.29 Two curves joining the same end points.

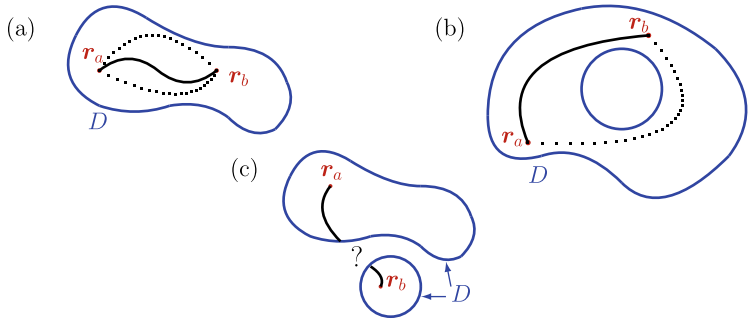


Figure 5.30 Connected domains (a) and (b), (c) is a disjoint or disconnected domain.

In the statement of Theorem 5.2 we imposed the condition that D must be a *connected domain*. Connected sets were first introduced in Definition 1.11. Of direct relevance here is the reference to a set D being connected meaning that any pair of points $\boldsymbol{r}_a$ and $\boldsymbol{r}_b$ in D can be joined by a piecewise smooth curve which lies *entirely* inside D. Two examples of a connected domain, and a counterexample, are shown in Figure 5.30.

Remark

∗ Theorem 5.2 and Corollary 5.2.1 are useful even for non-conservative fields—especially for *nearly* conservative fields. See, for example, Supplementary Problems 5.20 and 5.24.

We conclude this section with another opportunity for the reader to hone their line integration skills. At the same time the exercise aims to demonstrate again the power of Theorem 5.2.

✍ Mastery Check 5.9:

Evaluate the line integral of $\boldsymbol{f}(\boldsymbol{r}) = x\mathbf{e}_1 + \mathrm{e}^y\mathbf{e}_2$ along a curve Γ where Γ is
(a) a circular arc from $(0, 2)$ to $(2, 0)$, and
(b) a straight line connecting $(0, 2)$ to $(2, 0)$.
Is $\boldsymbol{f}$ conservative? If so, determine its scalar potential and verify the results of the above calculations.

✍

5.D Surface Integrals

Surface integrals are to double integrals what line integrals are to single-variable integrals. They are generalizations of double integrals to integration over surfaces (in $\mathbb{R}^3$) that are not planar. In complete correspondence with line integrals, surface integrals fall into one of two classes dictated by the function being integrated. In the first class (I) the integrals involve scalar-valued functions defined over a non-planar surface. In the second class (II) the integrations are performed on vector-valued functions. As with Class II line integrals, additional considerations of direction become important when dealing with surface integrals of vector fields. As in Section 5.C particular attention is paid to functions, fields, and surfaces defined in $\mathbb{R}^3$. Generalizations to higher dimensions may be possible in some cases although these are less easy to conceptualize.

In contrast to a double integral where the integration is performed over a planar domain, and where the interpretation is of a volume under the graph of a function, a surface integral in either class I or II is effectively a sum of some quantity that is distributed over the surface itself. In the respective sections below, we shall elaborate on the different, but physically relevant, interpretations that apply to each class.

I. Surface integrals of real-valued functions

In this class the surface integrals operate on scalar functions that are defined *on* a surface S and give the total amount of some quantity that is distributed over $S \subset \mathbb{R}^3$.

Corollary 4.1.1 (2D version) for $f(x, y) \geq 0$ provides a geometric interpretation of the double integral of f over a planar region D as

$$\iint_D f(x, y)\, \mathrm{d}A \;=\; \text{volume of body under } f \text{ over } D \subset \mathbb{R}^2.$$

If, however, $f(x, y)$ were interpreted as a surface density of some quantity, say charge/unit area, defined on $\mathbb{R}^2$ then the double integral would give the total amount of that quantity, Q, on the planar region D in the xy-plane (Figure 5.31):

$$\iint_D f(x, y)\, \mathrm{d}A \;=\; Q.$$

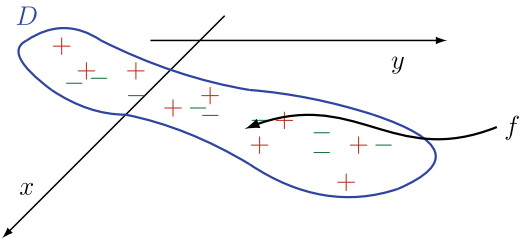


Figure 5.31 Physical interpretation of a double integral over a planar region D.

Now suppose that instead of a region in the plane we have a bounded surface $S \subset \mathbb{R}^3$ defined as the set of points

$$S = \{\boldsymbol{r}(u, v) \in \mathbb{R}^3 : (u, v) \in D \subset \mathbb{R}^2\}.$$

For now we may assume there is a one-to-one correspondence between points in the two-dimensional domain, D, and points on S (this can be altered to consider piecewise mappings of parts of S to subdomains if a one-to-one mapping of the whole of S is not possible).

Moreover, suppose we are given a continuous scalar function $f : \mathbb{R}^3 \longrightarrow \mathbb{R}$ defined on a 3D sub-domain in $\mathbb{R}^3$ containing S. Restricting f to the surface S within that sub-domain, whose points are uniquely determined by the pair of parameters, u and v, the function then becomes a composite vector function of those two variables:

$$f(x(u, v), y(u, v), z(u, v)) = f(\boldsymbol{r}(u, v)). \qquad \Big(= \boldsymbol{F}(u, v) \Big)$$

The function $f(\boldsymbol{r}(u, v)$, restricted to the bounded surface S, can be thought of as a summable surface area density of some quantity (say, a charge/unit area or a mass/unit area). Even though points $(u, v) \in D$ define points on S, f itself is a quantity defined on S rather than on D. Multiplying f with the area of a small segment of surface, ΔS, gives the total amount of that quantity carried by that segment of area.

Similarly to how we reasoned with line integrals, we can partition the surface S into n such small segments, ΔS_i, $i = 1, 2, ..., n$. This partitioning can be performed most conveniently by considering a network of intersecting curves of constant u and constant v, as shown in Figure 5.32. Within each segment a suitable point, (ξ_i, η_i, ζ_i), is identified.

With this information, an approximation to the total amount of a quantity, represented by f, carried by S can be established:

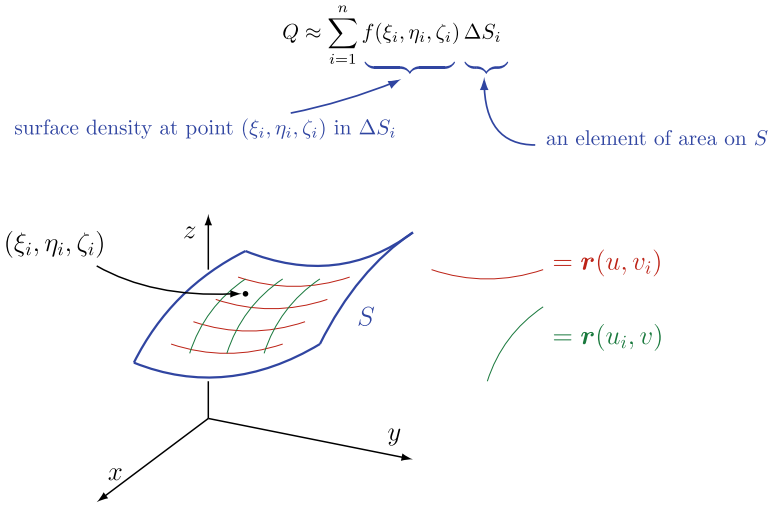


Figure 5.32 A partition of surface S using lines of constant u and v.

As we have done many times before (see Section 4.A), we refine the partition into smaller and smaller segments and, assuming that f is constant over ΔS_i, take the limit as $\Delta S_i \to 0$ and $n \to \infty$. Then, provided the limit exists the result is what is designated to be the surface integral of f over S:

$$\iint_S f(x, y, z)\, \mathrm{d}S.$$

—the limit exists if f is continuous and S is bounded (Theorem 3.2).

Remarks

* It is easily established (Corollary 4.1.6) that if $S = S_1 \cup \cdots \cup S_N$ then

$$\iint_S f\, \mathrm{d}S = \sum_{i=1}^{N} \iint_{S_i} f\, \mathrm{d}S.$$

  This is a useful result if S needs partitioning into parts to ensure the existence of one-to-one mappings of those parts onto suitable regions of $\mathbb{R}^2$, and the integral over S considered piecewise.

* If $f = 1$ then, as with Corollary 4.1.3, $\iint_S f \mathrm{d}S = \iint_S 1 \mathrm{d}S =$ area of S.

Evaluating a surface integral

• General surface parametrization

To evaluate the surface integral, assuming it is tractable, requires rewriting the area element $\mathrm{d}S$ in terms of known quantities that define the surface. For example, recall from Section 5.A, Page 302, that for a smooth surface parameterized by u and v, we can define tangent vectors $\dfrac{\partial \boldsymbol{r}}{\partial u}$ and $\dfrac{\partial \boldsymbol{r}}{\partial v}$ to constant v and constant u curves, respectively. If $\dfrac{\partial \boldsymbol{r}}{\partial u} \neq 0$, $\dfrac{\partial \boldsymbol{r}}{\partial v} \neq 0$, meaning that $\boldsymbol{r}(u, v_0)$ and $\boldsymbol{r}(u_0, v)$ are smooth curves, then S is a *smooth* surface.

The tangent vectors $\left\{ \begin{array}{l} \dfrac{\partial \boldsymbol{r}}{\partial u} \\ \dfrac{\partial \boldsymbol{r}}{\partial v} \end{array} \right.$ lead to differential line elements: $\left\{ \begin{array}{l} \dfrac{\partial \boldsymbol{r}}{\partial u}\,\mathrm{d}u \\ \dfrac{\partial \boldsymbol{r}}{\partial v}\,\mathrm{d}v \end{array} \right.$,

and their cross product leads to the differential area element:

$$\mathrm{d}S = \left| \frac{\partial \boldsymbol{r}}{\partial u} \times \frac{\partial \boldsymbol{r}}{\partial v} \right| \mathrm{d}u\,\mathrm{d}v.$$

Consequently, we arrive at a practical representation of the surface integral as a double integral over the planar domain, D, that defined the original S ($\mathrm{d}A = \mathrm{d}u\,\mathrm{d}v$).

$$Q = \underbrace{\iint_S f(\boldsymbol{r})\mathrm{d}S}_{\substack{\text{surface integral} \\ \text{of } f \text{ over } S \\ \text{—DEFINITION}}} = \underbrace{\iint_D f\big(\boldsymbol{r}(u,v)\big) \left| \frac{\partial \boldsymbol{r}}{\partial u} \times \frac{\partial \boldsymbol{r}}{\partial v} \right| \mathrm{d}A}_{\substack{\text{double integral of } f. \left| \cdots \times \cdots \right| \text{ over } D \\ \text{leading to an iterated integral} \\ \text{—PRACTICE}}}$$

The example below demonstrates how the rewrite of the surface integral as a double integral is exploited in practice. Admittedly, the task is made easier in this example by the fact that the surface parametrization is given. In other cases, that information would have to first be devised.

■ Example 5.15:

Evaluate the surface integral $\iint_S f(x,y,z)\mathrm{d}S$ where S is the parametric surface defined as the point set,

$$\begin{aligned} S &= \Big\{(x,y,z)\in\mathbb{R}^3 : x = t+\cos\theta, y = t+\sin\theta, z = t, \\ &\qquad t\in[-1,1],\ \theta\in[0,\pi/4]\Big\}. \end{aligned}$$

and $f(x,y,z) = x^2 - y^2 - 2z(x-y)$.

Solution:

Given the parameter representation, points on S are defined by the position vector,

$$\boldsymbol{r}(t,\theta) = (t+\cos\theta)\mathbf{i} + (t+\sin\theta)\mathbf{j} + t\mathbf{k}.$$

Orthogonal tangent vectors to S are therefore

$$\begin{cases} \dfrac{\partial \boldsymbol{r}}{\partial t} = \mathbf{i}+\mathbf{j}+\mathbf{k} \\ \dfrac{\partial \boldsymbol{r}}{\partial \theta} = -\sin\theta\mathbf{i} + \cos\theta\mathbf{j} + 0\mathbf{k}. \end{cases}$$

With these tangent vectors we obtain the local element of surface area,

$$\mathrm{d}S = \left|\left(\frac{\partial \boldsymbol{r}}{\partial t}\mathrm{d}t\right)\times\left(\frac{\partial \boldsymbol{r}}{\partial \theta}\mathrm{d}\theta\right)\right| = \left\|\begin{array}{ccc} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 1 & 1 & 1 \\ -\sin\theta & \cos\theta & 0 \end{array}\right\| \mathrm{d}t\mathrm{d}\theta$$

determinant

absolute value

$$= \Big|(-\cos\theta)\mathbf{i} + (-\sin\theta)\mathbf{j} + (\cos\theta-\sin\theta)\mathbf{k}\Big|\,\mathrm{d}t\mathrm{d}\theta$$

Expanding and simplifying the vector magnitude gives

$$\mathrm{d}S = \sqrt{2\,(1+\sin\theta\cos\theta)}\,\mathrm{d}t\mathrm{d}\theta.$$

The multivariable function, rewritten, and parameterized, becomes

$$\begin{aligned} f(x,y,z) &= x^2 - y^2 - 2z(x-y), \\ &= \left(x^2 - 2zx\right) - \left(y^2 - 2zy\right), \\ &= \left(x^2 - 2zx + z^2\right) - \left(y^2 - 2zy + z^2\right), \\ &= (x-z)^2 - (y-z)^2 = (x-t)^2 - (y-t)^2, \qquad (\text{since } z = t) \\ &= \cos^2\theta - \sin^2\theta = \cos 2\theta. \end{aligned}$$

Importing these results into the parameter-dependent version of the surface integral gives

$$\begin{aligned}
\iint_S f(x,y,z)\mathrm{d}S &= \iint_D \left(\cos^2\theta - \sin^2\theta\right)\sqrt{2(1+\sin\theta\cos\theta)}\,\mathrm{d}t\mathrm{d}\theta, \\
&= \sqrt{2}\int_{-1}^{1} 1\,\mathrm{d}t \int_0^{\pi/4} \left(\cos^2\theta - \sin^2\theta\right)\sqrt{1+\sin\theta\cos\theta}\,\mathrm{d}\theta, \\
&= \sqrt{2}\int_{-1}^{1} 1\,\mathrm{d}t \int_0^{\pi/4} \cos 2\theta\sqrt{1+\frac{1}{2}\sin 2\theta}\,\mathrm{d}\theta, \\
&= \sqrt{2}\Big[t\Big]_{-1}^{1} \int_1^{\frac{3}{2}} \sqrt{u}\,\mathrm{d}u, \qquad \text{(substituting } u = 1+\frac{1}{2}\sin 2\theta\text{)} \\
&= 2\sqrt{2}\left[\frac{2}{3}u^{\frac{3}{2}}\right]_1^{\frac{3}{2}} = \frac{4\sqrt{2}}{3}\left(\left(\frac{3}{2}\right)^{\frac{3}{2}} - 1\right).
\end{aligned}$$

As an incidental comment, the parametrization describes S as an oblique cylinder of radius 1 whose central axis lies along the line $(x, y, z) = (t, t, t)$.

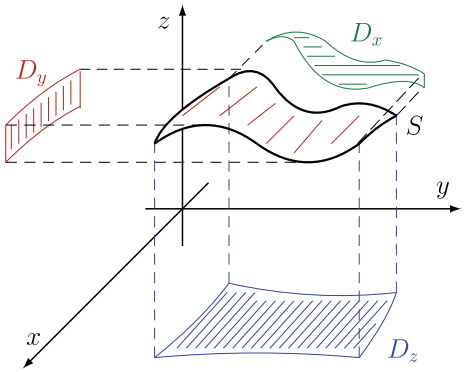
■

One doesn't need to know the specific parametrization of a surface in order to obtain a formula for the surface area element. Assuming a one-to-one relation between a point $\boldsymbol{r}$ on a surface and a point (u, v) in the plane and assuming that the surface is smooth, the complete and most general expression can be derived with respect to arbitrary orthogonal planar coordinates. The first step is to determine the vector $\boldsymbol{r}'_u \times \boldsymbol{r}'_v$. This task and subsequent steps towards the goal of $\mathrm{d}S$ is left to the reader in the next Mastery Check.

✍ Mastery Check 5.10:

For a general C^1 parametrization of a surface $S : \boldsymbol{r} = \boldsymbol{r}(u, v)$, derive the expression for $\dfrac{\partial \boldsymbol{r}}{\partial u} \times \dfrac{\partial \boldsymbol{r}}{\partial v}$. From your result derive the expression for $\mathrm{d}S$?

✍



(a) $\boldsymbol{r} = \big(x, y, q(x,y)\big)$ for the integral over D_z

(b) $\boldsymbol{r} = \big(x, g(x,z), z\big)$ for the integral over D_y

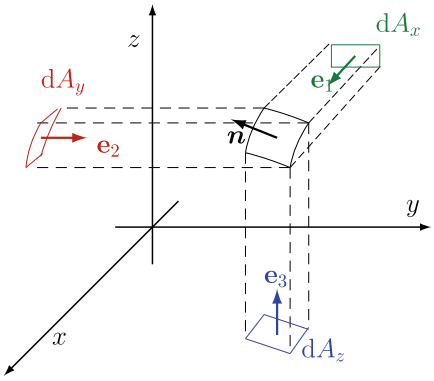
(c) $\boldsymbol{r} = \big(h(y,z), y, z\big)$ for the integral over D_x

Figure 5.33 Projections of S onto the three coordinate planes.

• **Cartesian coordinate representation**

The one and same surface *can* be parameterized, at least piecewise, in any of three different ways with respect to different pairwise combinations of the Cartesian coordinates, as shown in Figure 5.33.

From these different representations we have infinitesimal surface elements shown in Figure 5.34 below. It is important to note that in Figure 5.34 the vector $\boldsymbol{n}$ which appears is the local normal vector to S but is *not necessarily* a unit normal vector. That this, the formulae shown are general in that sense.



(a) $\mathrm{d}S = \dfrac{|\boldsymbol{n}|}{|\boldsymbol{n}\cdot\mathbf{e}_3|}\,\mathrm{d}x\,\mathrm{d}y$

(b) $\mathrm{d}S = \dfrac{|\boldsymbol{n}|}{|\boldsymbol{n}\cdot\mathbf{e}_2|}\,\mathrm{d}x\,\mathrm{d}z$

(c) $\mathrm{d}S = \dfrac{|\boldsymbol{n}|}{|\boldsymbol{n}\cdot\mathbf{e}_1|}\,\mathrm{d}y\,\mathrm{d}z$

Figure 5.34 Projections of a surface area element $\mathrm{d}S$ onto the three coordinate planes.

✍ Mastery Check 5.11:

Evaluate the surface area element $\mathrm{d}S$ in the three cases involving, respectively, the functions q, g, and h, described in Figure 5.33 as suggested by Figure 5.34. ✍

II. Surface integrals of vector fields

The above discussion on surface integrals of scalar functions can be extended directly to surface integrals of vector fields to give new vector quantities. Suppose $\boldsymbol{f} : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ is a vector field restricted to points $\boldsymbol{r} = (x, y, z)$ on a smooth surface S. Then the surface integral of the vector field $\boldsymbol{f}(\boldsymbol{r})$ over S is simply

$$\iint_S \boldsymbol{f}(\boldsymbol{r})\mathrm{d}S = \mathbf{i}\iint_S f_1(\boldsymbol{r})\mathrm{d}S + \mathbf{j}\iint_S f_2(\boldsymbol{r})\mathrm{d}S + \mathbf{k}\iint_S f_3(\boldsymbol{r})\mathrm{d}S.$$

That is, by appealing to the linear nature of Cartesian vectors and the linearity property of the integral operator one can determine the surface integral of a vector field as a vector sum of surface integrals of the components of that field. Despite the simple extension from a scalar to a vector integral quantity, the latter's significance is likely to be case specific. On the other hand, the following more important variant of a surface integral applicable to vector fields, is more prevalent in applications and has meaning that is not limited to any particular application.

One of the most useful qualities of vector fields is that of describing collective movement, in both direction and magnitude of motion. When things are moving, it is often of interest to know how much of some quantity passes through a given region or across a given boundary. For example,

- vehicular traffic through an area of a city or an entire city,
- water through a semi-permeable membrane, such as a plant cell wall,
- magnetic flux through a steel cooking pot, or
- X-ray photons through a body.

This "how much" is called the *flux*. To evaluate the flux we need two pieces of information:

(1) a vector description of the collective movement—this is $\boldsymbol{f}$.

(2) a vector description of the boundary across which the collective movement is to pass—the surface S and the normal vector $\boldsymbol{N}$.

To define the flux it suffices to use a simple situation. Let $\boldsymbol{f}$ be a uniform vector field whose magnitude $|\boldsymbol{f}|$ is a measure of the number of X-ray photons per unit area travelling in a given constant direction. Suppose we wanted to

know the number of photons entering a body whose boundary surface comprises a connected series of flat plates. A schematic of this situation is shown in Figure 5.35.

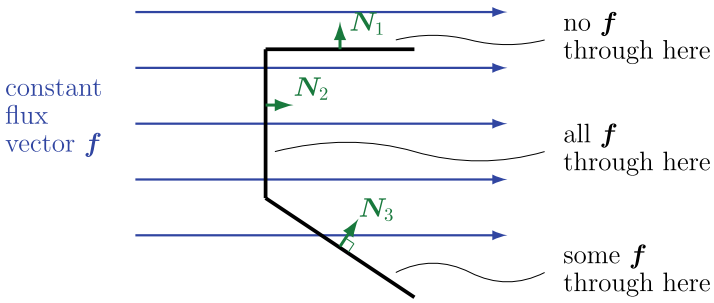


Figure 5.35 Flux of uniform field $\boldsymbol{f}$ relative to the boundary of a body.

Intuitively, the number of photons entering the body will depend on the area of its surface, A, exposed to the uniform field *as well as* the surface's orientation, $\boldsymbol{N}$, relative to the direction of the field. As suggested by Figure 5.35, the greatest number of photons will pass through the surface that is completely exposed. This is the surface whose *unit normal*, $\boldsymbol{N}_2$, is in the same direction as the field. In contrast, the surface admitting the least number of photons (*i.e.*, nil) will be the one that is oriented 90 degrees to the field. This is the surface with normal $\boldsymbol{N}_1$ perpendicular to $\boldsymbol{f}$. Intermediate between these extremes is the surface whose unit normal $\boldsymbol{N}_3$ makes some finite angle with the direction of $\boldsymbol{f}$.

A formula summarizing each of these cases (depicted in Figure 5.35) is then,

$$\begin{aligned} \text{flux} \quad &= \quad |\boldsymbol{f}|\, A\cos\theta = |\boldsymbol{f}||\boldsymbol{N}|\; A\cos\theta = |\boldsymbol{f}||\boldsymbol{N}|\cos\theta\, A, \\ &= (\boldsymbol{f}\cdot\boldsymbol{N})\, A = \boldsymbol{f}\cdot\big(\boldsymbol{N}A\big) = \boldsymbol{f}\cdot\boldsymbol{A}, \end{aligned}$$

where θ is the angle between the vector $\boldsymbol{f}$ and the surface normal $\boldsymbol{N}$.

Notice that at the first step in the above train of equalities $\boldsymbol{N}$ does not appear. The only contributing factors are the magnitude of $\boldsymbol{f}$, the area A, and the cosine of θ, the angle between $\boldsymbol{f}$ and the surface's orientation. The normal vector enters at the second step through its magnitude *which must be unity* so as not to alter the physically relevant total number of photons being determined. The scalar product of two vectors involves the magnitudes of *both* vectors, but the flux only requires the magnitude of $\boldsymbol{f}$. This is only possible if $|\boldsymbol{N}| = 1$. Hence, unless otherwise stated, $\boldsymbol{N}$ will denote the unit normal vector to a surface. Finally, by combining A with $\boldsymbol{N}$ we introduce a *vector surface area*, $\boldsymbol{A} = A\boldsymbol{N}$.

The preceding discussion assumes that $\boldsymbol{f}$ is a constant field and S is a (piecewise) planar surface. As such, $\boldsymbol{f}$ does not depend on position, and the surface normals $\boldsymbol{N}$ are constant vectors. For non-uniform fields and smoothly varying surfaces, as depicted in Figure 5.36, all of the above points of reasoning are still applicable when considered *locally*.

Suppose $\boldsymbol{f} : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ is again defined on a surface $S \subset \mathbb{R}^3$, and the smooth surface is parameterized with respect to parameters (u, v) defined on some region D:

$$S = \{\boldsymbol{r}(u, v) : (u, v) \in D \subset \mathbb{R}^2\}.$$

We now consider a differential element of area, $\mathrm{d}S$, with unit normal $\boldsymbol{N}$ defined at the point $\boldsymbol{r} \in S$. If $\mathrm{d}S$ is sufficiently small then over its (infinitesimal) extent $\boldsymbol{f}$ may be considered uniform and $\boldsymbol{N}$ may be assumed constant. Consequently, when considered locally at $\boldsymbol{r} \in S$ the flux of $\boldsymbol{f}$ through $\mathrm{d}S$ will have the same form as derived earlier, but be a function of position on the surface, $\boldsymbol{r}$. That is, the flux through $\mathrm{d}S$ will be

$$\boldsymbol{f}(\boldsymbol{r}) \cdot \boldsymbol{N}(\boldsymbol{r})\, \mathrm{d}S = \boldsymbol{f}(\boldsymbol{r}) \cdot \mathrm{d}\boldsymbol{S}.$$

Accumulating such contributions over the entire surface we get the total flux,

$$\iint_S (\boldsymbol{f} \cdot \boldsymbol{N})\, \mathrm{d}S = \iint_S \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S},$$

defined, as always, as the limit of a Riemann sum.

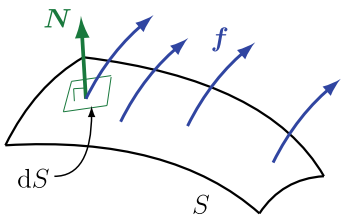


Figure 5.36 Depiction of flux of non-uniform $\boldsymbol{f}$ through curved S.

The integral $\iint_S (\boldsymbol{f} \cdot \boldsymbol{N})\, \mathrm{d}S$ is in the form of a surface integral of a scalar field, $\boldsymbol{f} \cdot \boldsymbol{N}$. This means that we can use the different approaches to surface integrals discussed on Pages 348 – 351 to evaluate this integral. Two of these possible approaches are included in the Remarks below.

Remarks

* Clearly, in considering a surface integral of a vector field $\boldsymbol{f}$, we take for granted that $\boldsymbol{f}$ is well defined over all of S. That is, that $\boldsymbol{f}$ is non-singular everywhere on S so that the integration can be established.

* If the surface S is defined by a level set equation (Section 1.F), *i.e.*, if S is defined as a set of points that produce a constant value of some function ϕ, as in $S = \{(x, y, z) : \phi(x, y, z) = C\}$, then the unit normal can be given as

$$\boldsymbol{N} = \frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|}.$$

The differential element of area may similarly be expressed in Cartesian coordinates. Choosing, say, the projection of S onto a region D in the xy-plane as the most convenient projection, then following Figure 5.34, we have that

$$\mathrm{d}S = \frac{|\boldsymbol{\nabla}\phi|}{|\boldsymbol{\nabla}\phi \cdot \mathbf{k}|}\,\mathrm{d}x\mathrm{d}y,$$

and therefore,

$$\begin{aligned} \iint_S \boldsymbol{f} \cdot \boldsymbol{N}\mathrm{d}S &= \iint_D \boldsymbol{f} \cdot \Big(\frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|}\Big) \frac{|\boldsymbol{\nabla}\phi|}{|\boldsymbol{\nabla}\phi \cdot \mathbf{k}|}\,\mathrm{d}x\,\mathrm{d}y, \\ &= \iint_D \big(\boldsymbol{f} \cdot \boldsymbol{\nabla}\phi\big) \frac{\mathrm{d}x\,\mathrm{d}y}{|\boldsymbol{\nabla}\phi \cdot \mathbf{k}|}. \end{aligned}$$

Analogous expressions follow from projections of S onto the other two coordinate planes.

* If the surface S is defined parametrically as $S = \{\boldsymbol{r}(u, v) : (u, v) \in D\}$, then

$$\boldsymbol{N} = \frac{\dfrac{\partial \boldsymbol{r}}{\partial u} \times \dfrac{\partial \boldsymbol{r}}{\partial v}}{\left|\dfrac{\partial \boldsymbol{r}}{\partial u} \times \dfrac{\partial \boldsymbol{r}}{\partial v}\right|}.$$

—*u* and *v can* be Cartesian coordinates!

In this case, recalling the formula for $\mathrm{d}S$ on Page 348 and inserting both expressions in the flux definition:

$$\iint_S \boldsymbol{f} \cdot \boldsymbol{N}\mathrm{d}S = \iint_D \boldsymbol{f} \cdot \underbrace{\frac{\Big(\dfrac{\partial \boldsymbol{r}}{\partial u} \times \dfrac{\partial \boldsymbol{r}}{\partial v}\Big)}{\left|\dfrac{\partial \boldsymbol{r}}{\partial u} \times \dfrac{\partial \boldsymbol{r}}{\partial v}\right|}}_{\boldsymbol{N}} \underbrace{\left|\frac{\partial \boldsymbol{r}}{\partial u} \times \frac{\partial \boldsymbol{r}}{\partial v}\right| \mathrm{d}u\,\mathrm{d}v}_{\mathrm{d}S},$$

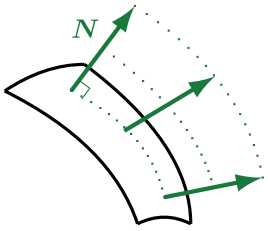
we arrive at the convenient and simpler double integral form,

$$\iint_S \boldsymbol{f} \cdot \boldsymbol{N}\mathrm{d}S = \iint_D \boldsymbol{f} \cdot \Big(\frac{\partial \boldsymbol{r}}{\partial u} \times \frac{\partial \boldsymbol{r}}{\partial v}\Big)\,\mathrm{d}u\,\mathrm{d}v.$$

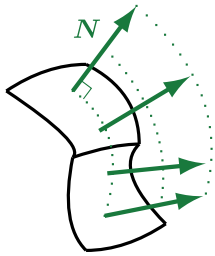
More about the surface normal

We argued earlier that a 3D, piecewise-smooth and otherwise continuous surface S implies the existence of a tangent plane at every point of S (except, of course, at points along any edges). This in turn ensures that a unit normal vector exists at every point on the smooth pieces of S and determined in the manner described above. The surface normal, thus guaranteed and thus generated, now assumes an additional role: that of defining a surface's *orientation*.

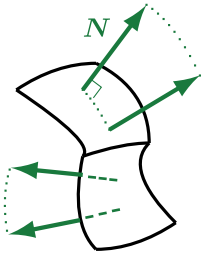
A surface can have two sides, as in two sides of a sheet of paper. A normal vector, *once determined*, points in only one direction. The surface normal vector, though, can be conveniently used to select one of those sides and therefore it can imbue the surface with an orientation. A surface is said to be *orientable* if it possesses a continuously varying normal or, perhaps more accurately stated, if it possesses a *consistently turning normal vector*, even across its pieces. A surface together with its continuously/consistently turning normal is said to be *oriented*. Figure 5.37 shows two examples of oriented surfaces and one example of a non-oriented surface.



(a) Continuously turning $\boldsymbol{N}$ on smooth S.



(b) Consistently turning $\boldsymbol{N}$ on piecewise smooth S.



(c) Inconsistently turning $\boldsymbol{N}$ on piecewise smooth S.

Figure 5.37 Oriented (a) and (b) and non-oriented (c) surfaces.

In Figure 5.37(c) the surface as a whole does not have a continuously or consistently turning normal, even though the two pieces, considered separately, do. This surface is not oriented.

If a smooth surface is defined parametrically as $\boldsymbol{r}(u, v)$, the surface's orientation is determined by the normal vector $\boldsymbol{r}'_u \times \boldsymbol{r}'_v$. Of course, a different parametric description could result in the opposite orientation. As a trivial example, $\boldsymbol{r}'_v \times \boldsymbol{r}'_u$ assigns the opposite orientation. Deciding which of a surface's two normal vectors to choose can be tied up with the naming convention of surfaces and, in the case of open surfaces, their boundaries.

For an open surface (such as a plane or the surface of a paraboloid), with a particular choice of $\boldsymbol{N}$ made, the side of S out of which $\boldsymbol{N}$ points is called the *positive side*. Analogously, if S is a closed surface (*e.g.*, a smooth sphere or a piecewise smooth cube) convention has the outside of S being the *positive side* with $\boldsymbol{N}$ as being the outward-pointing vector normal. In both open and closed cases, if the above conditions are satisfied then S is said to be *positively oriented*.

Remarks (on flux, continued)

* If S is closed we write
$$\oiint_S \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S} = \oiint_S (\boldsymbol{f} \cdot \boldsymbol{N}) \mathrm{d}S$$
and, as mentioned already, we adopt the convention that $\boldsymbol{N}$ is the *outward*-pointing unit normal.

* Why is orientation so important? Consider the uniform field $\boldsymbol{f}$ and the two open surfaces shown in Figure 5.38. Of course, for practical purposes we need to choose and determine an $\boldsymbol{N}$ for each surface, but once a choice is made we stick with it. In the case of both figures, the surfaces have a positive side out of which the respective $\boldsymbol{N}$ vectors point. Having chosen $\boldsymbol{N}$ in each case and hence defined the positively oriented S, we can now interpret the passage of $\boldsymbol{f}$ through S:
$$\begin{array}{llll} \text{if} & \boldsymbol{f} \cdot \boldsymbol{N} > 0 & \text{we say} & \boldsymbol{f} \text{ travels } \textit{out of } S, \\ \text{if} & \boldsymbol{f} \cdot \boldsymbol{N} < 0 & \text{we say} & \boldsymbol{f} \text{ travels } \textit{into } S. \end{array}$$

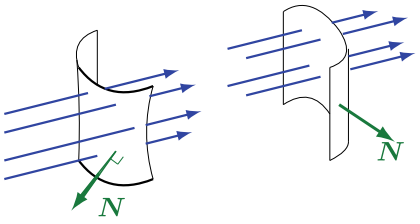


Figure 5.38 The relation between surface normal $\boldsymbol{N}$ and a vector field.

We end this section with two examples that illustrate the calculation of flux. The first example involves a closed surface and is formulated in terms of Cartesian coordinates. It highlights the need to divide up the surface so as to ensure a one-to-one relation between a point on the surface and a point in the projected domain. Consequently, two calculations are required, one for each hemisphere. Take note of how in the solution the normal vectors (and z's) are distinguished in the calculations. This same exercise is solved anew in the next section. The reader should contrast the difference in the efforts required in the two solutions.

The second example, which is followed by a characteristically similar Mastery Check, features a surface parametrization $\boldsymbol{r}(u, v)$ and so uses the parametric version of surface integral.

■ Example 5.16:

Determine the flux of the vector field $\boldsymbol{f} = (x, y, 2z)$ out through the surface S, defined by $x^2 + y^2 + z^2 = a^2$.

Solution:

Note that this surface shown in Figure 5.39 is a closed surface. Hence, we assume the usual convention of taking the *outward*-pointing normal.

We divide the surface into the upper hemisphere,

$$S_+ = \{(x, y, z) : z = g(x, y), 0 \leq x^2 + y^2 \leq a^2\}$$

with an upward pointing normal, and the lower hemisphere,

$$S_- = \{(x, y, z) : z = -g(x, y), 0 \leq x^2 + y^2 \leq a^2\}$$

with a downward pointing normal.

Here, $g(x, y) = \sqrt{a^2 - x^2 - y^2}$.

The flux integral over the closed sphere can then be written as the sum of two flux integrals:

$$\oiint_S \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S} = \iint_{S_+} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S} + \iint_{S_-} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S}.$$

With the Cartesian variables x and y as parameters, both S_+ and S_- are defined through a one-to-one relationship with points in the planar domain $D = \{(x, y) : 0 \leq x^2 + y^2 \leq a^2\}$.
Hence, the flux integral through S can be rewritten (see Equation (5.3)) as

$$\begin{aligned} \oiint_S \boldsymbol{f} \cdot d\boldsymbol{S} \quad = \quad & \iint_D \boldsymbol{f}(x, y, g(x, y)) \cdot \left(\frac{\partial \boldsymbol{r}_+}{\partial x} \times \frac{\partial \boldsymbol{r}_+}{\partial y} \right) \mathrm{d}x\, \mathrm{d}y \\ & + \iint_D \boldsymbol{f}(x, y, -g(x, y)) \cdot \left(-\frac{\partial \boldsymbol{r}_-}{\partial x} \times \frac{\partial \boldsymbol{r}_-}{\partial y} \right) \mathrm{d}x\, \mathrm{d}y \end{aligned}$$

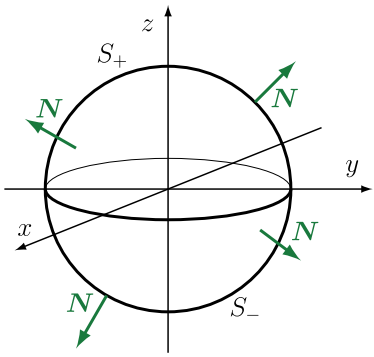


Figure 5.39 The sphere of radius a in Example 5.16.

where $\boldsymbol{r}_\pm = (x, y, \pm g(x, y))$, and a minus sign is introduced in the second flux integral to provide the correct surface normal direction.

Now, $\dfrac{\partial \boldsymbol{r}_\pm}{\partial x} = \left(1, 0, \pm\dfrac{\partial g}{\partial x}\right)$ and $\dfrac{\partial \boldsymbol{r}_\pm}{\partial y} = \left(0, 1, \pm\dfrac{\partial g}{\partial y}\right)$.

Thus,

$$\left(\frac{\partial \boldsymbol{r}_\pm}{\partial x} \times \frac{\partial \boldsymbol{r}_\pm}{\partial y}\right) = \left(\mp\frac{\partial g}{\partial x}, \mp\frac{\partial g}{\partial y}, 1\right),$$

where $\dfrac{\partial g}{\partial x} = \dfrac{1}{2}(a^2 - x^2 - y^2)^{-1/2}.(-2x) = \dfrac{-x}{\sqrt{a^2 - x^2 - y^2}} = \dfrac{-x}{g(x, y)}$, etc.

This gives the two normal vectors

$$\pm\left(\frac{\partial \boldsymbol{r}_\pm}{\partial x} \times \frac{\partial \boldsymbol{r}_\pm}{\partial y}\right) = \left(\frac{x}{g}, \frac{y}{g}, \pm 1\right),$$

and so

$$\begin{aligned}
\oiint_S \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S} \;&=\; \iint_D (x, y, 2g) \cdot \left(\frac{x}{g}, \frac{y}{g}, 1\right) \mathrm{d}x\,\mathrm{d}y \\
&\qquad + \iint_D (x, y, -2g) \cdot \left(\frac{x}{g}, \frac{y}{g}, -1\right) \mathrm{d}x\,\mathrm{d}y \\
&= \; 2\iint_D \left(\frac{x^2}{g} + \frac{y^2}{g} + 2g\right) \mathrm{d}x\,\mathrm{d}y \;=\; 2\iint_D \left(\frac{x^2 + y^2 + 2g^2}{g}\right) \mathrm{d}x\,\mathrm{d}y \\
&= \; 2\iint_D \left(\frac{2a^2 - x^2 - y^2}{\sqrt{a^2 - x^2 - y^2}}\right) \mathrm{d}x\,\mathrm{d}y.
\end{aligned}$$

Since D is a disc we can use polar coordinates:

$$x = r\cos\theta,\ y = r\sin\theta,\ \mathrm{d}x\,\mathrm{d}y = r\,\mathrm{d}r\,\mathrm{d}\theta,\ x^2+y^2 = r^2.$$

$$\begin{aligned}\oiint_S \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S} &= 2\int_0^{2\pi}\mathrm{d}\theta\int_0^a\left(\frac{2a^2-r^2}{\sqrt{a^2-r^2}}\right)r\mathrm{d}r\\ &= 4\pi\left\{a^2\int_0^a\frac{r\,\mathrm{d}r}{\sqrt{a^2-r^2}}+\int_0^a\sqrt{a^2-r^2}\,r\,\mathrm{d}r\right\}.\end{aligned}$$

The final integrals can be evaluated easily using the substitution $u = a^2 - r^2 \Longrightarrow \mathrm{d}u = -2r\,\mathrm{d}r$:

$$\begin{aligned}\oiint_S \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S} &= 4\pi\left\{a^2\left[-\frac{1}{2}u^{1/2}.2\right]_{a^2}^0+\left[-\frac{1}{2}u^{3/2}.\frac{2}{3}\right]_{a^2}^0\right\}\\ &= 4\pi\left\{a^2.a+a^3\frac{1}{3}\right\} = \frac{16}{3}\pi a^3.\end{aligned}$$

■

■ Example 5.17:

Calculate the flux of $\boldsymbol{f} = (x^2, y^2, z^2)$ through the surface

$$S = \{\boldsymbol{r} : z^2 = x^2+y^2, \qquad 1\le z\le 2\}$$

in the direction $\boldsymbol{N}\cdot\mathbf{e}_3 > 0$ (Figure 5.40(a)).

Solution:

We note that $\boldsymbol{f}(x,y,z)$ is defined over S, and that S is orientable (its positive side is up).

We start by parameterizing the surface S as (essentially cylindrical coordinates),

$$\boldsymbol{r}(u,v) = (u\cos v, u\sin v, u),\ 1\le u\le 2,\ 0\le v\le 2\pi.$$

(Check that $z^2 = x^2+y^2$.) Then $\boldsymbol{f} = (u^2\cos^2 v, u^2\sin^2 v, u^2)$ on S, and

$$\frac{\partial\boldsymbol{r}}{\partial u}\times\frac{\partial\boldsymbol{r}}{\partial v} = \begin{vmatrix}\mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3\\ \cos v & \sin v & 1\\ -u\sin v & u\cos v & 0\end{vmatrix} = (-u\cos v, -u\sin v, u).$$

We note that $\boldsymbol{N} = \dfrac{(-\cos v, -\sin v, 1)}{\sqrt{2}}$, and $\boldsymbol{N}\cdot\mathbf{e}_3 = \dfrac{1}{\sqrt{2}} > 0$ for $1\le u\le 2$, so we have chosen the parametrization correctly.

Now

$$\begin{aligned}
\iint_S \boldsymbol{f}\cdot\boldsymbol{N}\,\mathrm{d}S &= \iint_D \boldsymbol{f}\cdot\Big(\frac{\partial \boldsymbol{r}}{\partial u}\times\frac{\partial \boldsymbol{r}}{\partial v}\Big)\,\mathrm{d}u\,\mathrm{d}v \\
&= \int_1^2 \mathrm{d}u \int_0^{2\pi} (u^2\cos^2 v, u^2\sin^2 v, u^2)\cdot(-u\cos v, -u\sin v, u)\,\mathrm{d}v \\
&= \int_1^2 \mathrm{d}u \int_0^{2\pi} \big(-u^3\cos^3 v - u^3\sin^3 v + u^3\big)\,\mathrm{d}v \\
&= \int_1^2 u^3\mathrm{d}u \int_0^{2\pi} \big(-\cos^3 v - \sin^3 v + 1\big)\,\mathrm{d}v \\
&= \Big[\frac{1}{4}u^4\Big]_1^2 \int_0^{2\pi} \Big(-\frac{1}{4}(\cos 3v + 3\cos v - \sin 3v + 3\sin v) + 1\Big)\,\mathrm{d}v \\
&= \Big[2\pi\frac{u^4}{4}\Big]_1^2 = \frac{15\pi}{2}.
\end{aligned}$$

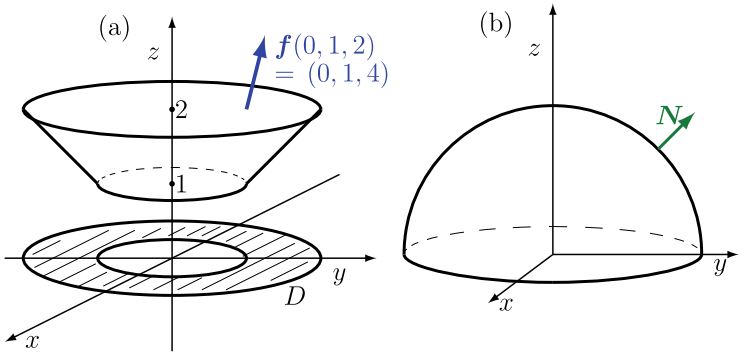


Figure 5.40 (a) The cone S and projection D in Example 5.D; (b) The hemisphere in MC 5.12.

✍ Mastery Check 5.12:

Determine the flux of $\boldsymbol{f} = (-y, x, x^2 + z)$ up through the surface (Figure 5.40(b))

$$S = \big\{(x, y, z) : x^2 + y^2 + z^2 = 1, \qquad z \geq 0\big\}.$$

✍

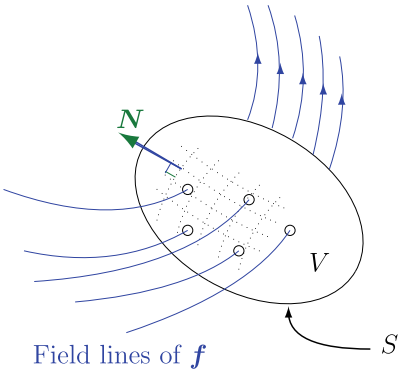


Figure 5.41 The field $\boldsymbol{f}$ passing into and out of a closed region S.

5.E Gauss's Theorem

Fluxes into, out of, or through, closed surfaces feature in a wide range of applications in diverse fields such as fluid dynamics, general relativity, electrodynamics nuclear physics and even traffic management. Despite their diversity, the treatment of flux in these applications can be represented in a common way. A schematic illustration of flux through a closed surface is shown in Figure 5.41. The key result of this section, Gauss's theorem, which is to be complemented by Stokes's and Green's theorems in the next section, is truly an impressive theoretical result finding uses in higher mathematical analysis. Supplementary Problems 5.28, 5.29, 5.38, 5.40, are examples of how Gauss's theorem enables novel theoretical results to be obtained. At the same time Gauss's theorem is also an incredibly powerful practical tool for solving problems, as we will see as we work through the exercises in this section. We offer a physical motivation for why the relationship in Gauss's theorem could be anticipated before proceeding with the statement and proof of the theorem itself.

Consider a C^1 field $\boldsymbol{f} : D_f \subset \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ and a *closed* surface S which is the boundary of a *bounded* volume $V \subset D_f$.

With S being closed there will be some flux of $\boldsymbol{f}$ into S and some flux out of S. Consequently, if we take $\boldsymbol{N}$ to be the outward normal to S, then $\oiint \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S}$will be a measure of the *net flux of* $\boldsymbol{f}$ *out of* S:

$$q = \oiint_S \boldsymbol{f} \cdot \boldsymbol{N} \, \mathrm{d}S.$$

Let's now place this q in a physical setting. Suppose $\boldsymbol{f}$ describes flow of water. Then

- if $q > 0$: this says that more water flows out of S than in, meaning that there is a *production* of water *inside* V;
- if $q < 0$: this says that less water flows out of S than in, meaning that there is a *destruction* of water *inside* V;
- if $q = 0$: this says that what flows in flows out of S, meaning that the amount of water in V is conserved.

From this interpretation one would naturally suspect that q contains information about what occurs *inside* V. That is, there is reason to suspect a relationship of the form

$$\iiint_V (\text{production of } \boldsymbol{f})\,\mathrm{d}V = \oiint_s \boldsymbol{f} \cdot \mathrm{d}S.$$

This is in fact exactly what Gauss's[1] theorem states:

Theorem 5.3
Suppose $\boldsymbol{f} : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ *is a* C^1 *vector field defined on and within a domain* V *which is bounded by a piecewise smooth closed surface* S *which in turn has a continuously varying outward unit normal* N*. Then*

$$\oiint_S \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S} = \iiint_V \left(\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} + \frac{\partial f_3}{\partial z}\right) \mathrm{d}V = \iiint_V (\boldsymbol{\nabla} \cdot \boldsymbol{f})\,\mathrm{d}V.$$

Remarks

- The theorem implies that the divergence $\boldsymbol{\nabla} \cdot \boldsymbol{f}$ is a measure of the *local production* or *local destruction* of $\boldsymbol{f}$ inside V: $\boldsymbol{\nabla} \cdot \boldsymbol{f}(\boldsymbol{x})$ is the *source or sink strength* per unit volume of $\boldsymbol{f}$ at $\boldsymbol{x} \in V$.
- The theorem holds true *only* if $\boldsymbol{N}$ is the unit normal pointing *away* from region V, as per the examples in Figure 5.42.

[1] This book uses this form of the possessive for proper names ending in "s", such as Gauss and Stokes [24, 25]. Some texts use the form "Gauss' theorem". The theorems are the same however they are described.

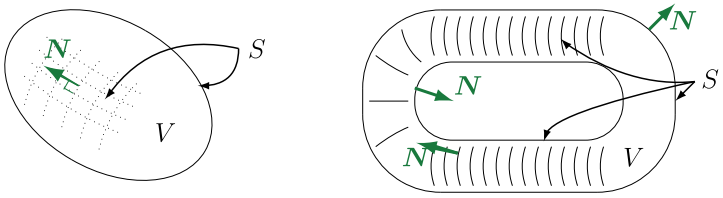


Figure 5.42 Two closed surfaces and their outward normals.

* The reference to "piecewise smooth" means that S can have edges, such as a rectangular prism, just as long as S is closed.

* Gauss's theorem is useful in rewriting relations involving surface and volume integrals so that all terms can be combined under one integral sign ([5] Chapter 18).

* If we apply the mean value theorem for multiple integrals to the volume integral in Gauss's theorem we get

$$\iiint_V (\boldsymbol{\nabla} \cdot \boldsymbol{f})\, \mathrm{d}V = \boldsymbol{\nabla} \cdot \boldsymbol{f}(P_0).V,$$

where $\boldsymbol{f} \in C^1$ and is bounded, and where P_0 is some point in V. If we now take the limit of this result as $V \to 0$ and $S \to 0$ so as to converge to the single point $\boldsymbol{x}$, which will coincide with P_0, then

$$\boldsymbol{\nabla} \cdot \boldsymbol{f}(\boldsymbol{x}) = \lim_{V \to 0} \frac{1}{V} \oiint_S \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S},$$

where $\boldsymbol{x}$ is common to V and S in this limit.
This result says that the divergence of a vector field $\boldsymbol{f}$ is the *flux per unit volume* of $\boldsymbol{f}$ out of a region of vanishing volume.

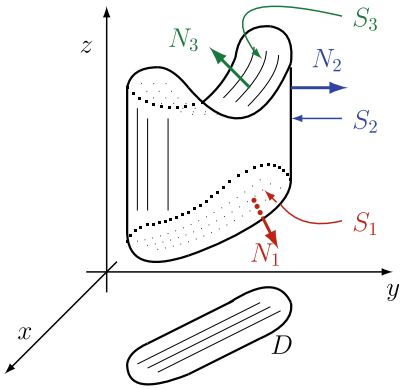


Figure 5.43 V as a z-simple region.

Sketch proof of Gauss's theorem

This simple proof assumes a convex body so that a vertical line does not intersect the surface in more than two places. Here, these intersection points are at $z = h(x, y)$ and $z = g(x, y)$. More elaborate circumstances, *i.e.*, non-convex closed surfaces, can be treated similarly, since it is always possible to treat S as the union of piecewise smooth surfaces and V as the union of simple domains (x-simple, y-simple, and z-simple) ([16], Chapter 5).

We start by splitting the surface and volume integrals into their component terms:

$$\begin{aligned} \oiint_S \boldsymbol{f}\cdot\boldsymbol{N}\,\mathrm{d}S &= \oiint_S (f_1\mathbf{e}_1)\cdot\mathrm{d}\boldsymbol{S} + \oiint_S (f_2\mathbf{e}_2)\cdot\mathrm{d}\boldsymbol{S} + \oiint_S (f_3\mathbf{e}_3)\cdot\mathrm{d}\boldsymbol{S} \\ \iiint_V \boldsymbol{\nabla}\cdot\boldsymbol{f}\,\mathrm{d}V &= \iiint_V \frac{\partial f_1}{\partial x}\mathrm{d}V + \iiint_V \frac{\partial f_2}{\partial y}\mathrm{d}V + \iiint_V \frac{\partial f_3}{\partial z}\mathrm{d}V. \end{aligned}$$

involves f_1 involves f_2 involves f_3

Suppose now that V is one of these cases, specifically a z-simple domain, as in Figure 5.43: $V = \{\boldsymbol{x} : h(x, y) \le z \le g(x, y),\ (x, y) \in D\}$.

On S_1: $S_1 = \{\boldsymbol{x} : (x, y) \in D,\ z = h(x, y)\}$, $\boldsymbol{N}_1 = \dfrac{\left(\frac{\partial h}{\partial x}, \frac{\partial h}{\partial y}, -1\right)}{\sqrt{\cdots\cdots\cdots}}$.

On S_2: $\boldsymbol{N}_2$ is orthogonal to $\mathbf{e}_3$.

On S_3: $S_3 = \{\boldsymbol{x} : (x, y) \in D,\ z = g(x, y)\}$, $\boldsymbol{N}_3 = \dfrac{\left(\frac{\partial g}{\partial x}, \frac{\partial g}{\partial y}, 1\right)}{\sqrt{\cdots\cdots\cdots}}$.

Now let's work with the f_3 component of the flux integral.

$$\begin{aligned} \oiint_S (f_3\mathbf{k})\cdot\mathrm{d}\boldsymbol{S} &= \iint_{S_1\cup S_2\cup S_3} (f_3\mathbf{k}\cdot\boldsymbol{N})\,\mathrm{d}S \\ &= \iint_{S_1} (f_3\mathbf{k}\cdot\boldsymbol{N}_1)\,\mathrm{d}S + \iint_{S_2} \underbrace{(f_3\mathbf{k}\cdot\boldsymbol{N}_2)}_{0}\,\mathrm{d}S + \iint_{S_3} (f_3\mathbf{k}\cdot\boldsymbol{N}_3)\,\mathrm{d}S \\ &= -\iint_D f_3(x, y, h)\,\mathrm{d}A + \iint_D f_3(x, y, g)\,\mathrm{d}A \\ &= \iint_D \Big(\int_{h(x,y)}^{g(x,y)} \frac{\mathrm{d}f_3}{\mathrm{d}z}\,\mathrm{d}z\Big)\,\mathrm{d}A \;=\; \iiint_V \frac{\partial f_3}{\partial z}\,\mathrm{d}V. \end{aligned}$$

We can manipulate the other cases in analogous ways. Adding these contributions we get the desired result.

■

To show the calculation power of Gauss's theorem we have the following example which calculates the flux in two ways. However, more striking is a revisit to the flux calculation of Example 5.16 which there required considerable labour. But with the help of Gauss's theorem the calculation can be accomplished in a single line:

$$\oiint_S \boldsymbol{f}\cdot \mathrm{d}\boldsymbol{S} = \iiint_V \boldsymbol{\nabla}\cdot\boldsymbol{f}\,\mathrm{d}V = \iiint_V (1+1+2)\,\mathrm{d}V = 4\iiint_V 1\mathrm{d}V = \frac{16\pi a^3}{3}!$$

Example 5.18:

Verify Gauss's theorem by calculating the flux of $\boldsymbol{f} = (x^3, y^3, z^3)$ out of the sphere in Figure 5.38: $S = \{(x,y,z) : x^2+y^2+z^2 = a^2\}$.

Solution:

Note first that the vector field $\boldsymbol{f}$ is clearly C^1 and S is a closed surface with a continuously varying (outward pointing) normal, $\boldsymbol{N}$. So the conditions of Gauss's theorem are satisfied.

Consequently, we shall first determine the flux according to Gauss's theorem, which means we evaluate the volume integral of the divergence, then confirm the result by a direct flux calculation. Gauss's theorem says

$$\begin{aligned}\oiint_S \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S} &= \iiint_V \boldsymbol{\nabla}\cdot\boldsymbol{f}\,\mathrm{d}V \\ &= \iiint_V \left(3x^2+3y^2+3z^2\right)\mathrm{d}V \;=\; 3\iiint_V \left(x^2+y^2+z^2\right)\mathrm{d}V.\end{aligned}$$

We naturally change to spherical coordinates. (See Example 5.3)

$$x = \rho\sin\phi\,\cos\theta,\;\; y = \rho\sin\phi\,\sin\theta,\;\; z = \rho\cos\phi,\;\; x^2+y^2+z^2 = \rho^2.$$

The values $0<\rho<a,\;\; 0\le\theta\le 2\pi,\;\; 0\le\phi\le\pi$ cover all points in V, the interior of S. The differential $\mathrm{d}V = \rho^2\sin\phi\,\mathrm{d}\rho\,\mathrm{d}\theta\,\mathrm{d}\phi$. Thus

$$\begin{aligned}\oiint_S \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S} &= 3\iiint_V \left(x^2+y^2+z^2\right)\mathrm{d}V \\ &= 3\int_0^{2\pi}\mathrm{d}\theta\int_0^{\pi}\mathrm{d}\phi\int_0^{a}\rho^2.\rho^2\sin\phi\,\mathrm{d}\rho \;=\; 3\int_0^{2\pi}\mathrm{d}\theta\int_0^{\pi}\frac{1}{5}a^5\sin\phi\,\mathrm{d}\phi \\ &= \frac{3}{5}a^5\int_0^{2\pi}\mathrm{d}\theta\Big[-\cos\phi\Big]_0^{\pi} \;=\; \frac{12\pi a^5}{5}.\end{aligned}$$

Now compare this with the direct flux calculation.

Using spherical coordinates, a point $\boldsymbol{r}$ on the surface of the sphere of radius a has coordinates,

$$x = a\sin\phi\,\cos\theta,\ y = a\sin\phi\,\sin\theta,\ z = a\cos\phi,\quad \theta\in[0,2\pi],\ \phi\in[0,\pi].$$

The vector element of area, $\mathrm{d}\boldsymbol{S} = \boldsymbol{N}\mathrm{d}S$, in spherical coordinates is

$$\begin{aligned}\mathrm{d}\boldsymbol{S} &= \left(\frac{\partial\boldsymbol{r}}{\partial\phi}\times\frac{\partial\boldsymbol{r}}{\partial\theta}\right)\mathrm{d}\phi\,\mathrm{d}\theta,\\ &= \begin{vmatrix}\mathbf{i} & \mathbf{j} & \mathbf{k}\\ a\cos\phi\cos\theta & a\cos\phi\sin\theta & -a\sin\phi\\ -a\sin\phi\sin\theta & a\sin\phi\cos\theta & 0\end{vmatrix}\mathrm{d}\phi\,\mathrm{d}\theta,\\ &= a^2\Big(\sin^2\phi\,\cos\theta\,\mathbf{i}+\sin^2\phi\,\sin\theta\,\mathbf{j}+\sin\phi\,\cos\theta\,\mathbf{k}\Big)\mathrm{d}\phi\,\mathrm{d}\theta.\end{aligned}$$

The vector field, expressed in spherical coordinates, becomes

$$\boldsymbol{f} = a^3\sin^3\phi\cos^3\theta\mathbf{i} + a^3\sin^3\phi\sin^3\theta\mathbf{j} + a^3\cos^3\phi\mathbf{k}.$$

Consequently, the flux is given by

$$\begin{aligned}\oiint_S \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S} &= a^5\left[\int_0^{\pi}\sin^5\phi\,\mathrm{d}\phi\int_0^{2\pi}\cos^4\theta\,\mathrm{d}\theta\right.\\ &\qquad+\int_0^{\pi}\sin^5\phi\,\mathrm{d}\phi\int_0^{2\pi}\sin^4\theta\,\mathrm{d}\theta\\ &\qquad\left.+\int_0^{\pi}\cos^4\phi\sin\phi\,\mathrm{d}\phi\int_0^{2\pi}1\,\mathrm{d}\theta\right].\end{aligned}$$

Using the integration methodology explained in Section 4.J, these trigonometric integrals are readily evaluated to result in the flux being

$$\begin{aligned}\oiint_S \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S} &= a^5\left[\frac{4}{5}.\frac{2}{3}.2.\frac{3}{4}.\frac{1}{2}.2\pi+\frac{4}{5}.\frac{2}{3}.2.\frac{3}{4}.\frac{1}{2}.2\pi+2\pi.\frac{2}{5}\right]\\ &= a^5\left[\frac{4\pi}{5}+\frac{4\pi}{5}+\frac{4\pi}{5}\right] = \frac{12\pi a^5}{5}.\end{aligned}$$

The flux calculation is thus confirmed and Gauss's theorem verified.

■

What is good about Gauss's theorem:

Assuming that the conditions of the theorem are satisfied, if we were asked to evaluate $\iiint_V g(x,y,z)\,\mathrm{d}V$, we could instead evaluate $\oiint_S \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S}$, where $\boldsymbol{\nabla}\cdot\boldsymbol{f}=g(x,y,z)$. On the other hand, if we were asked to evaluate $\oiint_S \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S}$, we could instead evaluate $\iiint_V g(x,y,z)\,\mathrm{d}V$.

In these cases we choose whichever integral is easiest to evaluate.

Example 5.19:

According to Corollary 4.1.3, volumes of regions are found when $g=1$. However, instead of a volume integral we can invoke Gauss's theorem and evaluate a flux integral. To get $g=1$ in the volume integral we could use $\boldsymbol{f}=\frac{1}{3}\boldsymbol{r}=\frac{1}{3}(x,y,z)$, or $=(x,0,0)$, or $=(0,y,0)$ in the flux integral.

■

What is NOT so good about Gauss's theorem:

The conditions on the theorem are strict. As given, the theorem states that

$$\oiint_S \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S}=\iiint_V \boldsymbol{\nabla}\cdot\boldsymbol{f}\,\mathrm{d}V$$

is true *only if* two necessary conditions are met.

a) Firstly, there is the condition that S be a closed surface. But not every problem that is posed involves a closed surface.

However, if the given S in a problem is not closed we can create a convenient closed surface by complementing S:

$$S \longrightarrow S_c = S\cup S_{\text{xtra}}$$

S_c: a closed surface; S_{xtra}: a complementing surface

and then apply Gauss's theorem on S_c since, by Corollary 5.2.1, we can argue that

$$\iint_S \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S}=\oiint_{S_c} \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S}-\iint_{S_{\text{xtra}}} \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S}=\iiint_V \boldsymbol{\nabla}\cdot\boldsymbol{f}\,\mathrm{d}V-\iint_{S_{\text{xtra}}} \boldsymbol{f}\cdot\mathrm{d}\boldsymbol{S}.$$

—by Gauss's theorem on S_c at the middle step

The above idea is demonstrated in the next example followed by a Mastery Check of the same type.

Example 5.20:

How to use Gauss's theorem when $\boldsymbol{f}$ is C^1 but S is not closed.

Use Gauss's theorem to find the flux of the vector field $\boldsymbol{f} = (-y, x, x^2 + z)$ up through the hemispherical surface $S = \{(x, y, z) : x^2 + y^2 + z^2 = 1,\ z \geq 0\}$ (Figure 5.44(b)).

Solution:

The surface S is not closed, although other conditions relevant to Gauss's theorem are satisfied. So, in order to apply Gauss's theorem we complement S with an additional surface. Set $S_b = \{(x, y, z) : x^2 + y^2 \leq 1,\ z = 0\}$.

The combined surface $S + S_b$ is closed and encloses volume

$$V = \{(x, y, z) : x^2 + y^2 + z^2 \leq 1,\ z \geq 0\}.$$

Gauss's theorem is now valid so we begin with the volume integral of the divergence of $\boldsymbol{f}$.

$$\begin{aligned}
\iiint_V \boldsymbol{\nabla} \cdot \boldsymbol{f}\, \mathrm{d}V &= \iiint_V (0 + 0 + 1)\, \mathrm{d}V \\
&\qquad \text{—Introduce spherical coordinates:} \\
&\qquad (x, y, z) \longrightarrow (\rho, \theta, \phi),\ |J| = \rho^2 \sin\phi \\
&= \int_0^1 \mathrm{d}\rho \int_0^{2\pi} \mathrm{d}\theta \int_0^{\pi/2} 1.\rho^2 \sin\phi\, \mathrm{d}\phi \\
&= \int_0^1 \mathrm{d}\rho \int_0^{2\pi} \rho^2\, \mathrm{d}\theta \;=\; \int_0^1 2\pi\rho^2\, \mathrm{d}\rho \;=\; \frac{2\pi}{3}.
\end{aligned}$$

We now need to evaluate the flux through the extra surface that we introduced. Fortunately, this is a relatively simple undertaking.

$$\begin{aligned}
\iint_{S_b} \boldsymbol{f} \cdot \boldsymbol{N}\mathrm{d}S &= \iint_{S_b} (-y, x, x^2 + z) \cdot (0, 0, -1)\, \mathrm{d}S \\
&\qquad \text{—Introduce 2D polar coordinates:} \\
&\qquad (x, y) \longrightarrow (r, \theta) \ \text{ on } \ z = 0,\ |J| = r \\
&\qquad \text{—Notice that the normal vector is chosen to} \\
&\qquad \text{point } \textit{out} \text{ from V, } \textit{i.e.}\text{, down.} \\
&= \int_0^1 \mathrm{d}r \int_0^{2\pi} (-r^2 \cos^2\theta) r\, \mathrm{d}\theta \\
&= -\int_0^1 \mathrm{d}r \int_0^{2\pi} r^3 \Big(\frac{1}{2} + \frac{1}{2}\cos 2\theta\Big)\, \mathrm{d}\theta \;=\; -\frac{\pi}{4}.
\end{aligned}$$

Finally, to get the actual flux that was required, *up* through the hemisphere, we subtract the latter result from the former:

$$\begin{aligned} \iint_S \boldsymbol{f}\cdot\boldsymbol{N}\,\mathrm{d}S &= \iiint_V \boldsymbol{\nabla}\cdot\boldsymbol{f}\,\mathrm{d}V - \iint_{S_b}\boldsymbol{f}\cdot\boldsymbol{N}\mathrm{d}S \\ &= \frac{2\pi}{3} - \left(-\frac{\pi}{4}\right) = \frac{11\pi}{12}. \end{aligned}$$

■

✍ Mastery Check 5.13:

Determine the flux of $\boldsymbol{f} = (xz^2, x, x^2)$ through the cylinder

$$S = \{\boldsymbol{x} : x^2 + y^2 = 1,\ |z| \le 1\}$$

with outward-pointing normal (Figure 5.44(a)).

✍

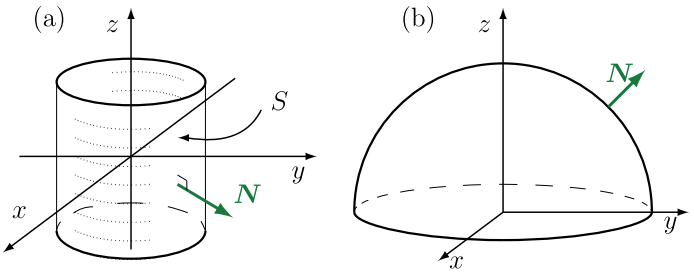


Figure 5.44 (a) The cylinder $x^2 + y^2 = 1$ in MC 5.13; (b) The unit hemisphere in Example 5.20.

b) The second strict condition is that $\boldsymbol{f}$ is C^1 in V (and C on S). In some problems $\boldsymbol{f}$ may be defined on S, so that one could in principle evaluate a flux integral, but $\boldsymbol{f}$ may not either be defined or if defined then not differentiable at some point P_0 within S, in V. Thus, Gauss's theorem cannot be applied.

However, the strategy that may be advanced here is that one can always *exclude* the singular point P_0 by enclosing it with another surface. Gauss's theorem would then be valid when applied to the bounded region *between* the surfaces.

For example, suppose S is closed and is the boundary of V containing the singular point P_0. Enclose P_0 in a new closed surface S^*, as shown in Figure 5.45.

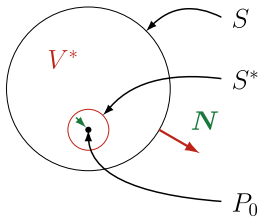


Figure 5.45 Exclusion of the singular point P_0.

The combined surface, $S \cup S^*$, is now the boundary of a volume $V^* \subset V$ such that $P_0 \notin V^*$. With the singular point now removed Gauss's theorem is applicable and, appealing to Corollary 5.2.1, the desired flux obtained:

$$\oiint_S \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S} = \oiint_{S \cup S^*} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S} - \oiint_{S^*} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S} = \iiint_{V^*} \boldsymbol{\nabla} \cdot \boldsymbol{f} \, \mathrm{d}V - \oiint_{S^*} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S}.$$

—by Gauss's theorem on $S \cup S^*$ at the middle step

Naturally, an additional flux integral is now required, but if S^* is chosen strategically that integral may not introduce too serious a complication. The process is similar to the preceding example and Mastery Check, so we leave to the reader the following exercise to complete for this scenario.

✍ Mastery Check 5.14:

How to use Gauss's theorem if S is closed but $\boldsymbol{f}$ is not C^1 at some point.

Determine the flux of $\boldsymbol{f} = -k\dfrac{\boldsymbol{r}}{|\boldsymbol{r}|^3}$ with $\boldsymbol{r} = (x, y, z)$, through *any* closed surface, Figure 5.46, enclosing a volume V which contains the point $(0, 0, 0)$. ✍

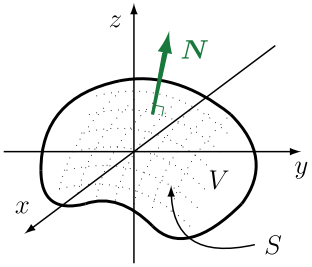


Figure 5.46 An arbitrary closed S enclosing $(0, 0, 0)$.

5.F Green's and Stokes's Theorems

Returning to the subject of line integrals of vector fields, but focusing interest on closed curves, we come to discuss Green's theorem and Stokes's theorem, which do for circulation of vector fields (Page 336) what Gauss's theorem does for net fluxes (Page 362). However, before introducing the theorems we shall first cover a few additional curve concepts.

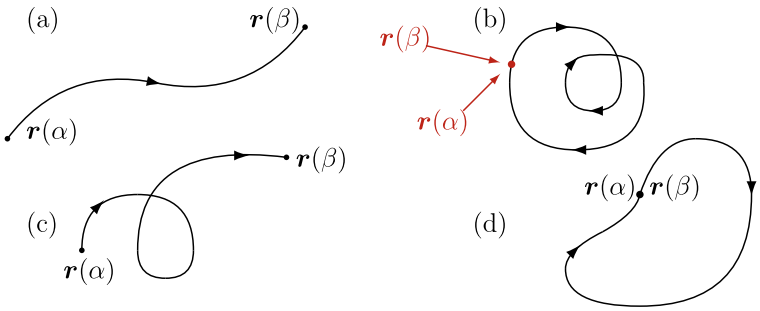


Figure 5.47 Curve types.

I. Additional notes on curves

(i) For any smooth curve (Figure 5.47(a)) we can find or construct a *parametrization* $\boldsymbol{r} = \boldsymbol{r}(t),\ \alpha \le t \le \beta$.

(ii) If $\boldsymbol{r}(\alpha) = \boldsymbol{r}(\beta)$ (Figure 5.47(b)), then the curve is *closed*.

(iii) If $\boldsymbol{r}(t_1) = \boldsymbol{r}(t_2)$ for some $\alpha < t_1 < t_2 < \beta$ (Figure 5.47(c)), the curve is *self-intersecting*.

(iv) If $\boldsymbol{r}(t_1) = \boldsymbol{r}(t_2)$ for some $\alpha \le t_1 < t_2 \le \beta \implies t_1 = \alpha, t_2 = \beta$ (Figure 5.47(d)), the curve is closed and non-intersecting. Such a curve is called *a simple closed curve*.

(v) Of strategic importance is the (obvious?) fact that a simple closed curve in 3D can be the boundary of many open 3D surfaces, as demonstrated in Figure 5.48 by the three example surfaces having the same boundary curve.

So, while a given *open* 3D surface has a unique, well-defined boundary, which must comprise at least one *simple closed curve* (an open cylinder has two simple closed curves for its boundary, one at each end), the converse is not true. In 3D, a given *simple closed curve* can be the boundary to an infinite number of surfaces. This becomes an important

and useful fact when considered in the context of Stokes's theorem to come (Page 381).

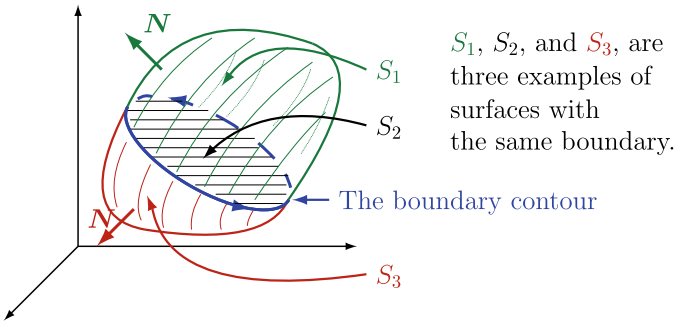


Figure 5.48 One simple closed contour, multiple surfaces.

(vi) In Section 5.C (Page 334), also in the context of line integration, the possible orientations of curves was discussed. In particular, it was highlighted that a given curve parametrization determines its orientation. For example, in Figure 5.49, for the parametrization with respect to t, $\boldsymbol{r}$ takes the path from $\boldsymbol{r}_0$ to $\boldsymbol{r}_1$, whereas the parametrization with respect to t^* $\boldsymbol{r}$ takes the opposite course:

$$\begin{aligned} t &: a \longrightarrow b \quad \Longrightarrow \quad \boldsymbol{r}_0 = \boldsymbol{r}(a) \longrightarrow \boldsymbol{r}(b) = \boldsymbol{r}_1 \\ t^* &: \alpha \longrightarrow \beta \quad \Longrightarrow \quad \boldsymbol{r}_1 = \boldsymbol{r}(\alpha) \longrightarrow \boldsymbol{r}(\beta) = \boldsymbol{r}_0. \end{aligned}$$

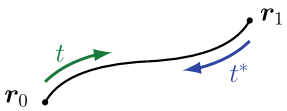


Figure 5.49 One non-closed curve, two alternative orientations.

For a non-closed curve choosing between the two alternative orientations is obvious once the start and end points are specified, as in Figure 5.49. For a closed curve there are also two alternative orientations, but in the absence of an additional criterion there remains an ambiguity of which to choose.

Fortunately, for an open surface S with (closed) boundary Γ there is an interdependent relation between the surface S, its surface normal $\boldsymbol{N}$, and its closed boundary Γ that assists in the choice.

Earlier we established that the side of a smooth surface S out of which points its normal vector is called *positive* and S itself is then said to be *positively oriented*. We can now extend that naming convention to include the closed curve boundary Γ, with one important caveat.

Suppose a little man, , walks around Γ, the boundary of S, so that a vector drawn from his feet to his head, 

, points in the same direction as $\boldsymbol{N}$, and also so that S is on the man's left, then Γ is said to be *positively oriented* (see Figure 5.50).

An equivalent, but more formal, phrasing of the above set of conditions is given in the following definition.

Definition 5.11
A closed curve, Γ*, the boundary of a* positively oriented surface*,* S*, is said to have* positive orientation *or be* positively oriented *if* Γ *is traversed so that the positive side of* S *lies to the left of the curve.*

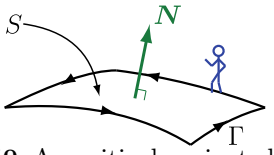


Figure 5.50 A positively oriented boundary.

Note that as a consequence of the above conditions, the direction of Γ's *positive orientation* will always be *counterclockwise* about an axis defined by the given normal vector $\boldsymbol{N}$, but *not* necessarily when viewed from the perspective of an external observer, *i.e.*, the reader.

The definition of a positively oriented curve is not simply for the sake of convention. A positively oriented curve is an essential requirement for the validity of both Green's and Stokes's theorems.

Example 5.21:

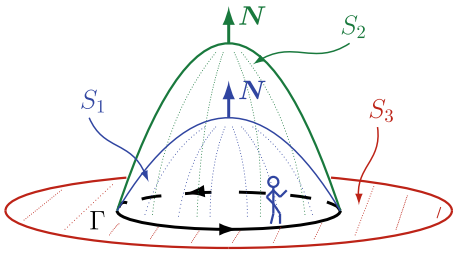


Figure 5.51 Surface and boundary orientation.

Γ in Figure 5.51 is a positively oriented boundary to S_1 and S_2, but not S_3!

II. Green's theorem

In the case of $\mathbb{R}^2$, the ambiguity between a simple closed contour and the surface it encloses vanishes; a simple closed, positively oriented curve defines and encloses a unique region (Figure 5.52). We take advantage of that fact in the next theorem which is valid for plane vector fields and plane regions (in 2D life is so much simpler).

We state and give a sketch proof of this important result, which was discovered by a gentleman having no formal education at the time [21].

Theorem 5.4
Green's theorem:
Let $\boldsymbol{f}(x,y) = f_1(x,y)\mathbf{e}_1 + f_2(x,y)\mathbf{e}_2$ *be a smooth 2D field defined on and within the* positively oriented simple closed boundary Γ *of a closed and bounded planar region* $D \subset \mathbb{R}^2$. *Then*

$$\underbrace{\oint_\Gamma \boldsymbol{f}\cdot \mathrm{d}\boldsymbol{r}}_{\text{line integral}} = \oint_\Gamma f_1(x,y)\,\mathrm{d}x + f_2(x,y)\,\mathrm{d}y = \underbrace{\iint_D \left(\frac{\partial f_2}{\partial x} - \frac{\partial f_1}{\partial y}\right)\mathrm{d}A}_{\text{double integral}}.$$

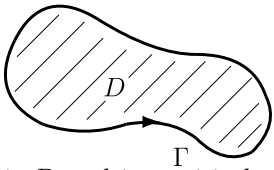


Figure 5.52 *Domain* D *and its positively oriented boundary* Γ.

Sketch proof of Green's theorem (for a simply-connected domain)

Suppose D is x-simple and y-simple. As depicted in Figure 5.53, functions ϕ_1, ϕ_2, ψ_1, and ψ_2 can be found such that

$$D = \{(x, y) : a \leq x \leq b,\ \phi_1(x) \leq y \leq \phi_2(x)\}$$

and

$$D = \{(x, y) : c \leq y \leq d,\ \psi_1(y) \leq x \leq \psi_2(y)\}.$$

Suppose also that all integrals exist.

We shall show that $\displaystyle\iint_D \frac{\partial f_2}{\partial x}\,\mathrm{d}A = \oint_\Gamma f_2\,\mathrm{d}y$:

Treating D as a y-simple domain we get

$$\begin{aligned}\iint_D \frac{\partial f_2}{\partial x}\,\mathrm{d}A &= \int_c^d \mathrm{d}y \int_{\psi_1(y)}^{\psi_2(y)} \frac{\partial f_2}{\partial x}\,\mathrm{d}x \\ &= \int_c^d f_2\big(\psi_2(y), y\big)\,\mathrm{d}y - \int_c^d f_2\big(\psi_1(y), y\big)\,\mathrm{d}y \\ &= \int_{\psi_2} f_2\,\mathrm{d}y + \int_{-\psi_1} f_2\,\mathrm{d}y \;=\; \oint_\Gamma f_2\,\mathrm{d}y.\end{aligned}$$

An analogous argument treating D as an x-simple domain will show that $\displaystyle\iint_D \frac{\partial f_1}{\partial y}\,\mathrm{d}A = -\oint_\Gamma f_1\,\mathrm{d}x$, and the theorem is proved.

■

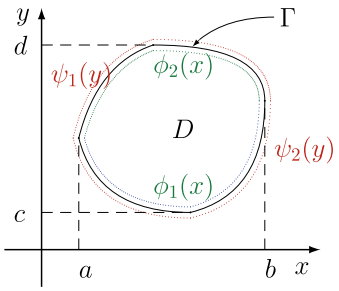


Figure 5.53 D as an x-simple and y-simple domain.

■ Example 5.22:

Verify Green's theorem for the vector field $\boldsymbol{f} = 3x^2\mathbf{i} - 4xy\mathbf{j}$ and the curve Γ, which is the boundary of the rectangle $D = \{(x, y) : x \in [0, 4], y \in [0, 1]\}$ in Figure 5.54.

Solution:

We first evaluate the line integral and then evaluate the double integral to verify.

The boundary is comprised of four sides: $\Gamma = C_1 \cup C_2 \cup C_3 \cup C_4$, where

$C_1 = \{(x, y) : x \in [0, 4],\ y = 0\}$, $C_2 = \{(x, y) : x = 4,\ y \in [0, 1]\}$,
$C_3 = \{(x, y) : x \in [0, 4],\ y = 1\}$, $C_4 = \{(x, y) : x = 0,\ y \in [0, 1]\}$.

On C_1, $\mathrm{d}\boldsymbol{r} = \mathrm{d}x\,\mathbf{i} + 0\mathbf{j}$;
on C_2, $\mathrm{d}\boldsymbol{r} = 0\mathbf{i} + \mathrm{d}y\,\mathbf{j}$;
on C_3, $\mathrm{d}\boldsymbol{r} = -\mathrm{d}x\,\mathbf{i} + 0\mathbf{j}$;
on C_4, $\mathrm{d}\boldsymbol{r} = 0\mathbf{i} - \mathrm{d}y\,\mathbf{j}$.

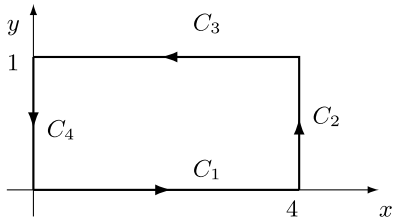


Figure 5.54 Rectangle Γ.

Note that the sides are parameterized such that Γ is traversed in a counterclockwise direction (inspect the 4 $\mathrm{d}\boldsymbol{r}$ designations). Then

$$\begin{aligned}\oint_\Gamma \boldsymbol{f}(\boldsymbol{r}) \cdot \mathrm{d}\boldsymbol{r} &= \int_{C_1} \boldsymbol{f}(\boldsymbol{r}) \cdot \mathrm{d}\boldsymbol{r} + \int_{C_2} \boldsymbol{f}(\boldsymbol{r}) \cdot \mathrm{d}\boldsymbol{r} + \int_{C_3} \boldsymbol{f}(\boldsymbol{r}) \cdot \mathrm{d}\boldsymbol{r} + \int_{C_4} \boldsymbol{f}(\boldsymbol{r}) \cdot \mathrm{d}\boldsymbol{r} \\ &= \int_0^4 3x^2\,\mathrm{d}x + \int_0^1 -16y\,\mathrm{d}y + \int_4^0 3x^2\,\mathrm{d}x + \int_1^0 0\,\mathrm{d}y \\ &= 64 - 8 - 64 + 0 \ = \ -8.\end{aligned}$$

Now consider the double integral expression in Green's theorem:

$$\begin{aligned}\iint_D \Big(\frac{\partial f_2}{\partial x} - \frac{\partial f_1}{\partial y}\Big)\,\mathrm{d}A &= \int_0^4 \mathrm{d}x \int_0^1 \big(-4y - 0\big)\,\mathrm{d}y \\ &= \int_0^4 \big(-2\big)\,\mathrm{d}x \ = \ -8,\end{aligned}$$

in agreement with the explicit line integral calculation, thus verifying Green's theorem:

$$\oint_\Gamma \Big(f_1 \mathrm{d}x + f_2 \mathrm{d}y\Big) = \iint_D \Big(\frac{\partial f_2}{\partial x} - \frac{\partial f_1}{\partial y}\Big).$$

■

Identical steps to those taken in the above example can be taken by the reader in the next Mastery Check to again verify Green's theorem, this time for a region with a curved boundary. Ensure that the curve is traversed in the correct direction.

✍ Mastery Check 5.15:

Verify Green's theorem for the curve integral

$$\oint_\Gamma (3x^2 - 8y^2)\,\mathrm{d}x + (4y - 6xy)\,\mathrm{d}y$$

where Γ is the boundary of the region D bounded by curves $y = \sqrt{x}$ and $y = x^2$ shown in Figure 5.55. ✍

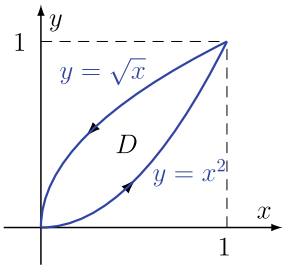


Figure 5.55 D and its boundary: $y = \sqrt{x}$ and $y = x^2$.

As always there are a number of consequences and thoughts to share with readers.

Remarks

* First, as with Gauss's theorem, Green's theorem asserts a relation between (differential) properties of $\boldsymbol{f}$ within a region and properties of $\boldsymbol{f}$ on the boundary. Explaining the nature of this relation will be postponed until we present Stokes's theorem. Meanwhile, we have the following related fact.

* If the plane field $\boldsymbol{f}$ is conservative then

$$\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = 0 \quad \Longrightarrow \quad \iint_D \left(\frac{\partial f_2}{\partial x} - \frac{\partial f_1}{\partial y}\right) \mathrm{d}A = 0,$$

which motivates the following important theorem about conservative fields.

Theorem 5.5
If the plane field $\boldsymbol{f} = (f_1, f_2)$ *satisfies* $\dfrac{\partial f_2}{\partial x} = \dfrac{\partial f_1}{\partial y}$ *in a simply-connected domain* D *then* $\boldsymbol{f}$ *is conservative in* D.

* Green's theorem is valid for more complicated regions. For example, it works in the case of annular domains such as shown in Figure 5.56.

Take good note of the indicated orientations of the inner and outer boundaries of the annular domain. In each case the curve complies with Definition 5.11 so that Green's theorem remains valid.

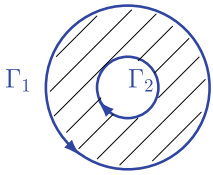


Figure 5.56 The composite boundary $\Gamma = \Gamma_1 \cup \Gamma_2$ and enclosed region.

∗ In precisely the same way as was noted in Example 5.E for Gauss's theorem, particular choices of 2D fields invoked in Green's theorem allow for the calculation of areas of planar regions using curve integrals.

■ Example 5.23:

Suppose Γ is the positively oriented boundary of a bounded connected 2D region D and suppose vector field $\boldsymbol{f} = \frac{1}{2}(-y\mathbf{i}+x\mathbf{j})$. Green's theorem then gives,

$$\begin{aligned}\oint_\Gamma \boldsymbol{f}\cdot \mathrm{d}\boldsymbol{r} &= \oint_\Gamma \Big(f_1\mathrm{d}x + f_2\mathrm{d}y\Big) = \frac{1}{2}\oint_\Gamma \Big(-y\mathrm{d}x + x\mathrm{d}y\Big),\\ &= \iint_D \Big(\frac{\partial f_2}{\partial x} - \frac{\partial f_1}{\partial y}\Big)\mathrm{d}x\mathrm{d}y = \frac{1}{2}\iint_D \Big(\frac{\partial x}{\partial x} - \frac{\partial(-y)}{\partial y}\Big)\mathrm{d}x\mathrm{d}y,\\ &= \iint_D 1\mathrm{d}x\mathrm{d}y = area\, of\, D.\end{aligned}$$

The result suggests an alternative way of evaluating the area of a 2D region D via a line integral of the vector field $\boldsymbol{f} = \frac{1}{2}(-y\mathbf{i} + x\mathbf{j})$. Alternative, vector fields are $\boldsymbol{f} = -y\mathbf{i}$ and $\boldsymbol{f} = x\mathbf{j}$.

This alternative may be particularly attractive for regions whose boundaries cannot be conveniently represented. This particular application of Green's theorem is the theoretical basis [3] for a mechanical and now digital instrument called a Planimeter used by land and aerial surveyors and cartographers for measuring areas of irregularly shaped regions.

If a boundary is parameterized: $\Gamma = \{(x(t), y(t)),\, t \in [0, T]\}$ then the curve integral in Green's formula may be expressed as the parameter integral,

$$\oint_\Gamma \boldsymbol{f}\cdot \mathrm{d}\boldsymbol{r} = \frac{1}{2}\int_0^T \Big(-y(t)\frac{\mathrm{d}x}{\mathrm{d}t} + x(t)\frac{\mathrm{d}y}{\mathrm{d}t}\Big)\mathrm{d}t.$$

And, if the irregularly shaped Γ is sampled N times in equal intervals $\Delta t = T/N$, then taking $\Delta x(i) \approx \dfrac{\mathrm{d}x}{\mathrm{d}t}(t_i)\Delta t$ and $\Delta y(i) \approx \dfrac{\mathrm{d}y}{\mathrm{d}t}(t_i)\Delta t$ the area of the irregularly shaped region may be estimated by the sum

$$\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} \approx \frac{1}{2}\sum_{i=1}^{N}\Big(- y(t_i)\Delta x(i) + x(t_i)\Delta y(i)\Big).$$

Note that although t is sampled uniformly, $\Delta t > 0$, this does not mean that the discrete increments $\Delta x(i)$ and $\Delta y(i)$ need be uniform nor even positive.

As an elementary and conveniently constructed example, the rectangle in Figure 5.54 has an area of 4 square units. If each side is sampled n times in equal increments of $\Delta t(j)$, $j = 1, \ldots, 4$, then starting from, but not including, the origin and ending at the origin the sampled points $(x(i), y(i))$ are

$$\begin{array}{lll}
\text{on } C_1: & (\dfrac{4i}{n}, 0) & \text{for } \ i = 1, \ldots, n \qquad \Delta x(i) = \frac{4}{n},\ \Delta y(i) = 0; \\
\text{on } C_2: & (4, \dfrac{(i-n)}{n}) & \text{for } \ i = n+1, \ldots, 2n \qquad \Delta x(i) = 0,\ \Delta y(i) = \frac{1}{n}; \\
\text{on } C_3: & (4 - 4\dfrac{(i-2n)}{n}, 1) & \text{for } \ i = 2n+1, \ldots, 3n \qquad \Delta x(i) = -\frac{4}{n},\ \Delta y(i) = 0; \\
\text{on } C_4: & (0, 1 - \dfrac{(i-3n)}{n}) & \text{for } \ i = 3n+1, \ldots, 4n \qquad \Delta x(i) = 0,\ \Delta y(i) = -\frac{1}{n}.
\end{array}$$

The area of the rectangle is then estimated by the four discrete line sums

$$\begin{aligned}
A \ \approx\ & \frac{1}{2}\sum_{i=1}^{n-1}\Big(0.\frac{4}{n} + \frac{4i}{n}.0\Big) + \frac{1}{2}\sum_{i=n+1}^{2n-1}\Big(- \frac{(i-n)}{n}.0 + 4\frac{1}{n}\Big) \\
& + \frac{1}{2}\sum_{i=2n+1}^{3n-1}\Big((-1)(-\frac{4}{n}) + 4 - 4\frac{(i-2n)}{n}.0\Big) \\
& + \frac{1}{2}\sum_{i=3n+1}^{4n-1}\Big(- \Big(1 - \frac{(i-3n)}{n}\Big).0 + 0.\Big(-\frac{1}{n}\Big)\Big) \\
=\ & \frac{2}{n}\left(\sum_{i=n+1}^{2n-1} 1 + \sum_{i=2n+1}^{3n-1} 1\right) = \frac{2}{n}(2n-2) = 4\left(1 - \frac{1}{n}\right).
\end{aligned}$$

The approximation improves as n increases. The error originates from the missed half-length segments at the corners of the rectangle.

■

III. Stokes's theorem

Generalizing Green's theorem to 3D we get what is commonly referred to as Stokes's theorem, which analogously relates properties of a vector field around a boundary of an (unclosed) surface to properties of the field, in this case the curl of the field, over that surface.

Theorem 5.6
Suppose S is an oriented surface, piecewise smooth in $\mathbb{R}^3$, with unit normal $\boldsymbol{N}$, and suppose that S is bounded by a piecewise smooth closed curve Γ with positive orientation. If $\boldsymbol{f} = \big(f_1(x,y,z), f_2(x,y,z), f_3(x,y,z)\big)$ is a 3D **smooth** *field defined* **on** *S, then*

$$\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = \iint_S (\boldsymbol{\nabla} \times \boldsymbol{f}) \cdot \boldsymbol{N}\, \mathrm{d}S.$$

Remarks

* In the same way we employed Gauss's theorem to derive a physical meaning for the divergence of a vector field (fifth remark following Theorem 5.3), we may use Stokes's theorem to provide an interpretation of the curl of a vector field.

  We apply the mean value theorem to the surface integral in Stokes's theorem:

  $$\iint_S (\boldsymbol{\nabla} \times \boldsymbol{f}) \cdot \mathrm{d}\boldsymbol{S} = (\boldsymbol{\nabla} \times \boldsymbol{f})\Big|_{\boldsymbol{r}_0} \cdot \boldsymbol{N}(\boldsymbol{r}_0) \iint_S \mathrm{d}S$$

  for $\boldsymbol{f} \in C^1$ and some point $\boldsymbol{r}_0 \in S$. In the limit as $S, |\Gamma| \longrightarrow 0$ (specifically shrinking to a point),

  $$(\boldsymbol{\nabla} \times \boldsymbol{f})\Big|_{\boldsymbol{r}} \cdot \boldsymbol{N}(\boldsymbol{x}) = \lim_{S \to 0} \frac{1}{S} \oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} \ (\boldsymbol{x} \text{ common to all } S \text{ in this limit})$$

  —the component of $\boldsymbol{\nabla} \times \boldsymbol{f}$ normal to S at $\boldsymbol{x} \in S$ is the work done per unit area in traversing an oriented contour Γ of vanishing length

* If $\boldsymbol{f} \in C^1(\mathbb{R}^3)$ is conservative, then by Theorem 5.2 $\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = 0$.
  By Stokes's theorem this now implies that $\iint_S (\boldsymbol{\nabla} \times \boldsymbol{f}) \cdot \mathrm{d}\boldsymbol{S} = 0$.

Conversely, if for $\boldsymbol{f} \in C^1(\mathbb{R}^3)$ we find that

$$\frac{\partial f_1}{\partial y} = \frac{\partial f_2}{\partial x}, \quad \frac{\partial f_3}{\partial x} = \frac{\partial f_1}{\partial z}, \quad \frac{\partial f_3}{\partial y} = \frac{\partial f_2}{\partial z}$$

in some simply-connected domain, then

$$\text{curl } \boldsymbol{f} = \boldsymbol{\nabla} \times \boldsymbol{f} = 0.$$

—the vector field $\boldsymbol{f}$ is said to be irrotational.

Stokes's theorem then implies that $\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = 0$ for all closed curves Γ in that domain. That is, $\boldsymbol{f}$ is *conservative*. This important result is an extension to 3D of Theorem 5.5 and warrants its own theorem status.

Theorem 5.7
If the C^1 vector field $\boldsymbol{f} = (f_1, f_2, f_3)$ satisfies $\boldsymbol{\nabla} \times \boldsymbol{f} = \boldsymbol{0}$ in a simply-connected domain $D \subset \mathbb{R}^3$, then $\boldsymbol{f}$ is conservative in D.

Example 5.24:

Verify Stokes's theorem for the C^1 vector field $\boldsymbol{f} = (xz, xy^2+2z, xy+z)$, where the contour Γ is that created by the intersection of the cone $x = 1-\sqrt{y^2+z^2}$ and the xy- and yz-planes, such that $0 \le x \le 1,\ -1 \le y \le 1,\ z \ge 0$.
Γ is oriented counterclockwise as seen from $(0, 0, 10)$.

Solution:

The geometrical situation is shown in Figure 5.57. The piecewise smooth curve Γ comprises three part curves: Γ_1, Γ_2, Γ_3, which are oriented as shown.

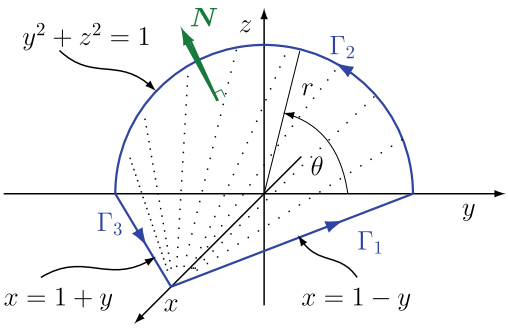


Figure 5.57 The cone $x = 1 - \sqrt{y^2+z^2}$.

Note that no surface with which to verify the theorem is specified. However, two possibilities come to mind: One is the curved surface of the cone lying above the xy-plane, while the other is the piecewise combination of the two planar pieces of the xy-plane and the yz-plane within the bottom triangle and semicircle, respectively.

First, the curve integral, $\oint_\Gamma \boldsymbol{f}\cdot \mathrm{d}\boldsymbol{r} \;=\; \Big(\int_{\Gamma_1}+\int_{\Gamma_2}+\int_{\Gamma_3}\Big)\boldsymbol{f}\cdot \mathrm{d}\boldsymbol{r}$, where

$$\begin{aligned}\int_{\Gamma_1}\boldsymbol{f}\cdot \mathrm{d}\boldsymbol{r} &= \int_{\Gamma_1} xz\,\mathrm{d}x+\big(xy^2+2z\big)\,\mathrm{d}y+\big(xy+z\big)\,\mathrm{d}z=\int_{\Gamma_1} xy^2\mathrm{d}y\\ &= \int_0^1 (1-y)y^2\,\mathrm{d}y \;=\; \frac{1}{3}-\frac{1}{4} \;=\; \frac{1}{12},\end{aligned}$$

since $z=dz=0$,

and, with $x=0,\; y=\cos\theta,\; z=\sin\theta$,

$$\begin{aligned}\int_{\Gamma_2}\boldsymbol{f}\cdot \mathrm{d}\boldsymbol{r} &= \int_0^\pi \boldsymbol{f}\big(\boldsymbol{r}(\theta)\big)\cdot\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}\theta}\mathrm{d}\theta=\int_0^\pi\Big(\big(2\sin\theta\big)\big(-\sin\theta\big)+\sin\theta\cos\theta\Big)\mathrm{d}\theta\\ &= -2\int_0^\pi \sin^2\theta\,\mathrm{d}\theta+\frac{1}{2}\int_0^\pi \sin 2\theta\,\mathrm{d}\theta \;=\; -2.\frac{1}{2}.\pi \;=\; -\pi,\end{aligned}$$

$$\int_{\Gamma_3}\boldsymbol{f}\cdot \mathrm{d}\boldsymbol{r} \;=\; \int_{\Gamma_3} xy^2\,\mathrm{d}y \;=\; \int_{-1}^0 (1+y)y^2\,\mathrm{d}y \;=\; \frac{1}{3}-\frac{1}{4} \;=\; \frac{1}{12}.$$

Therefore, adding these contributions we get

$$\int_\Gamma \boldsymbol{f}\cdot \mathrm{d}\boldsymbol{r} \;=\; \frac{1}{12}-\pi+\frac{1}{12} \;=\; \frac{1}{6}-\pi.$$

Now consider the surface integral, $\iint_S(\boldsymbol{\nabla}\times\boldsymbol{f})\cdot\boldsymbol{N}\,\mathrm{d}S$.

The correct orientation of the cone surface is with $\boldsymbol{N}$ pointing to +ve z.

$$\boldsymbol{\nabla}\times\boldsymbol{f} \;=\; \begin{vmatrix}\mathbf{i} & \mathbf{j} & \mathbf{k}\\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z}\\ xz & xy^2+2z & xy+z\end{vmatrix} \;=\; (x-2)\mathbf{i}+(x-y)\mathbf{j}+y^2\mathbf{k}.$$

Consider the cone parametrization

$x = 1 - r,\ y = r\cos\theta,\ z = r\sin\theta;\ D = \{0 \le \theta \le \pi,\ 0 \le r \le 1\}.$

$$\frac{\partial \boldsymbol{r}}{\partial r} \times \frac{\partial \boldsymbol{r}}{\partial \theta} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ -1 & \cos\theta & \sin\theta \\ 0 & -r\sin\theta & r\cos\theta \end{vmatrix} = r\mathbf{i} + r\cos\theta\mathbf{j} + r\sin\theta\mathbf{k}.$$

$$\begin{aligned} \iint_S (\boldsymbol{\nabla} \times \boldsymbol{f}) \cdot \boldsymbol{N}\, \mathrm{d}S &= \iint_D (\boldsymbol{\nabla} \times \boldsymbol{f}) \cdot \left(\frac{\partial \boldsymbol{r}}{\partial r} \times \frac{\partial \boldsymbol{r}}{\partial \theta}\right) \mathrm{d}r\, \mathrm{d}\theta \quad \text{(see Page 355)} \\ &= \int_0^{\pi} \int_0^1 \left(1 - r - 2, 1 - r - r\cos\theta, r^2\cos^2\theta\right) \cdot \left(r, r\cos\theta, r\sin\theta\right) \mathrm{d}r\, \mathrm{d}\theta \\ &= \int_0^{\pi} \int_0^1 \Big(- r(1+r) + r\cos\theta(1 - r - r\cos\theta) + r^3\cos^2\theta\sin\theta \Big) \mathrm{d}r\, \mathrm{d}\theta \\ &= \int_0^{\pi} \Big(- \frac{5}{6} + \frac{1}{6}\cos\theta - \frac{1}{3}\cos^2\theta + \frac{1}{4}\cos^2\theta\sin\theta \Big) \mathrm{d}\theta. \end{aligned}$$

So,

$$\iint_S (\boldsymbol{\nabla} \times \boldsymbol{f}) \cdot \boldsymbol{N}\, \mathrm{d}S = -\frac{5\pi}{6} + 0 - \frac{1}{3}.\frac{1}{2}.\pi + \frac{1}{4}.\frac{1}{3}.2 = \frac{1}{6} - \pi,$$

and the theorem is verified.

The reader should redo the surface integral calculation using the piecewise planar combination alternative.

Be mindful of choosing the correct surface orientation.

■

The next and final Mastery Check offers another opportunity for the reader to try their hand at a straightforward application of Stokes's theorem.

✍ Mastery Check 5.16:

Determine $\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}$, where $\boldsymbol{f} = (y, x, xy)$ and Γ is the curve of intersection of the plane $x + y + z = 1$ and the planes $x = y = z = 0$ in Figure 5.58.

Orientation of Γ: counterclockwise seen from $(10, 10, 10)$.

✍

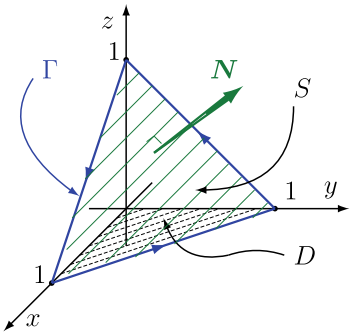


Figure 5.58 The intersection of $x + y + z = 1$ and the coordinate planes.

What is good about Stokes's theorem:

Assuming that the conditions of the theorem are satisfied, if we were asked to evaluate the work $\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}$ around a closed contour, we could instead evaluate $\iint_S (\boldsymbol{\nabla} \times \boldsymbol{f}) \cdot \mathrm{d}\boldsymbol{S}$ through *any* convenient surface that has Γ as its boundary.

Alternatively, if we were asked to evaluate $\iint_S (\boldsymbol{\nabla} \times \boldsymbol{f}) \cdot \mathrm{d}\boldsymbol{S}$ through a given S, we could instead evaluate the flux integral through any surface that has the same curve Γ as its boundary.

—there is an infinity of choices provided $\boldsymbol{f}$ is not singular

Or, we could evaluate $\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}$, if $\boldsymbol{f}$ could be deduced from the given expression $\boldsymbol{\nabla} \times \boldsymbol{f}$.

In these cases we choose whichever integral is easiest to evaluate. (See Mastery Check 5.16.)

What is NOT so good about Stokes's theorem:

The conditions on the theorem are strict. As given, the theorem states that

$$\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = \iint_S (\boldsymbol{\nabla} \times \boldsymbol{f}) \cdot \mathrm{d}\boldsymbol{S}$$

is true *only if* two necessary conditions are met.

(a) The first condition is that Γ be a closed contour. Unfortunately, not every problem posed involves a closed curve. However, if the given curve Γ is not closed, we may create a conveniently closed contour by complementing Γ:

$$\Gamma \longrightarrow \Gamma_c = \Gamma \cup \Gamma_{\text{xtra}}$$

a closed contour — a complementary contour

We can then apply Stokes's theorem on Γ_c since, by Corollary 5.2.1, it is reasonable to argue that

$$\int_{\Gamma} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = \oint_{\Gamma_c} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} - \int_{\Gamma_{\text{xtra}}} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = \iint_S (\boldsymbol{\nabla} \times \boldsymbol{f}) \cdot \mathrm{d}\boldsymbol{S} - \int_{\Gamma_{\text{xtra}}} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}.$$

—by Stokes's theorem on Γ_c at the middle step

(b) The second strict condition is that $\boldsymbol{f}$ be non-singular on S or Γ. If $\boldsymbol{f}$ is singular on Γ or $\boldsymbol{\nabla} \times \boldsymbol{f}$ is singular on S, then it is harder to deal with, and success will depend on the problem.

On the other hand, if we are asked to evaluate $\oint_{\Gamma} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}$, and $\boldsymbol{f}$ is singular on the given S, we can introduce an extra closed contour Γ_ϵ of small size ϵ around the singular point on S so as to exclude it: $\Gamma \longrightarrow \Gamma_c = \Gamma \cup \Gamma_\epsilon$. Introducing this new contour on S defines a new surface S_c bounded by the composite boundary Γ_c. Hence, with the singular point now removed we can argue, again by appealing to Corollary 5.2.1, that

$$\oint_{\Gamma} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = \oint_{\Gamma_c} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} - \oint_{\Gamma_\epsilon} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r} = \iint_{S_c} \boldsymbol{\nabla} \times \boldsymbol{f} \cdot \boldsymbol{N}\, \mathrm{d}S - \oint_{\Gamma_\epsilon} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}.$$

—by Stokes's theorem on Γ_c at the middle step

We then need to consider the contribution from the curve integral around Γ_ϵ in the limit $\epsilon \to 0$ to regain the original surface S.

5.G Epilogue: The Summation Convention

In many of the Supplementary Problems it proves convenient to replace the conventional notation of coordinates x, y, and z, with coordinate notation denoted by subscripts. Beginning with that change we can take advantage of

the very useful *summation convention*[2]. The foundation for the convention is the following set of identifications and definitions,

- $(x, y, z) \Longrightarrow (x_1, x_2, x_3)$, and $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\} \Longrightarrow \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$;
- $[\boldsymbol{A}]_i$ or A_i, as the ith component of the vector $\boldsymbol{A}$.
- $\delta_{ij} = 0$ for $i \neq j$ or 1 for $i = j$. This is called the *Kronecker delta*;
- $$\varepsilon_{ijk} = \begin{cases} -1, & \text{if } i,j,k \text{ is a noncyclic (or odd) permutation of 1, 2, 3,} \\ 0, & \text{if any index is repeated,} \\ 1, & \text{if } i,j,k \text{ is a cyclic (or even) permutation of 1, 2, 3.} \end{cases}$$

  This is called the *Levi-Civita density* or *Levi-Civita symbol*.

  By *cyclic or even* permutation we mean that i, j, k are all different and occur sequentially anywhere in the repeated sequence 12312312.... An example would be the index group $ijk = 312$. For this selection, which arises in the sequence (underlined), an *even* number of pairwise interchanges will result in the numbers appearing in the order 123 (*e.g.*, two exchanges: swap 3 and 1, then swap 3 and 2). By *noncyclic or odd* permutation we mean the numbers assigned to ijk being in any other order. For example, the index group $ijk = 213$ does not arise in the above repeated sequence. Moreover, it requires an *odd* number of pairwise interchanges to give the sequence 123 (*e.g.*, one swap of just the first two numbers);
- $\varepsilon_{ijk}\varepsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$.

This notation was introduced to deal with so-called curvilinear coordinates (*e.g.*, spherical coordinates) and tensors (*i.e.*, higher dimensional vectors) in differential geometry and general relativity, neither topic of which concerns us explicitly here. However, the power of this convention is evident even in our relatively mediocre setting of vectors and vector functions. What is important to always keep in mind is that essentially we have only just changed notation. We are still dealing with Cartesian coordinates and vectors in a Cartesian frame of reference.

Before attempting the Supplementary Problems we take the opportunity to familiarize ourselves with the summation convention itself. Basically, the convention is based on the idea that if an expression exhibits a repeated index, then a summation over that index is implied.

[2]Due to Ricci and Levi-Civita (1900), and introduced into physics by Einstein (1916). It is commonly called the Einstein summation convention.

For example, consider the standard expression of a vector in $\mathbb{R}^3$. In standard notation, the vector $\boldsymbol{u}$ would be written $\boldsymbol{u} = u_1\mathbf{i} + u_2\mathbf{j} + u_3\mathbf{k}$. However, with the index notation it becomes $u_1\mathbf{e}_1 + u_2\mathbf{e}_2 + u_3\mathbf{e}_3$. This is in the form of a sum, which can be written explicitly, as is done below. At that point the convention comes into play: the summation is simply implied rather than written out explicitly. In the notation of the convention, the vector $\boldsymbol{u}$ becomes

$$\boldsymbol{u} \quad = \quad \underbrace{u_1\mathbf{e}_1 + u_2\mathbf{e}_2 + u_3\mathbf{e}_3}_{\text{index form}} = \underbrace{\sum_{i=1}^{3} u_i\mathbf{e}_i}_{\text{explicit sum}} = \underbrace{u_i\mathbf{e}_i}_{\text{implied summation}}.$$

According to the convention, we drop the summation sign and consider the repeated index (here i) as an indicator that a summation is implied. The true power of the convention is not immediately evident from this simple rewrite. But even at this stage we can appreciate the convenience of a shorthand way of writing vectors component-wise.

In a similar fashion the usual scalar product of two vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ becomes

$$\boldsymbol{u} \cdot \boldsymbol{v} = u_1v_1 + u_2v_2 + u_3v_3 = \sum_{i=1}^{3} u_iv_i = u_iv_i.$$

Again the summation sign has been dropped and the repeated index now indicates an implied summation. There is, of course, nothing special about the index i. The scalar product may equivalently be written

$$\boldsymbol{u} \cdot \boldsymbol{v} = u_iv_i = u_jv_j = u_lv_l.$$

The repeated index (i, j, or l) is referred to as a dummy index in that it can be replaced by any other index. We shall often do just that for the following reason. Any index occurring twice in an expression implies a summation over the three values 1, 2, and 3. Consequently, no index should appear more than twice in an expression (except in extraordinary circumstances which will not arise in this book). If it does occur, the expression needs to be treated carefully if a summation is intended. For example, consider the vector expression $(\boldsymbol{x} \cdot \boldsymbol{u})\boldsymbol{v}$. Simplistically, allocating each vector the same subscript index i would lead to the confusing and incorrect expression $x_iu_iv_i$, for the ith component which is not permitted in the convention. In fact, since the intention was for a summation to occur between the first two factors (the scalar product), but not the third vector, a more rigorous formatting (and some forward thinking) would instead have led to the unequivocal expression $x_ku_kv_i$. The end result is interpreted as the ith component of a new vector, which is composed of the original ith component multiplied by the scalar product of the first two vectors.

We now move on to the new symbols. The *Kronecker delta* is the easier one to explain. From its definition it is clear that $\delta_{11} = \delta_{22} = \delta_{33} = 1$ and $\delta_{12} = \delta_{32} = \delta_{13} = 0$. However, according to the summation convention, although δ_{ij} is either 1 or 0, δ_{ii} has a repeated index, i, which means that a summation is implied. Indeed, we have the following summation property:

$$\delta_{ii} = \delta_{11} + \delta_{22} + \delta_{33} = 1 + 1 + 1 = 3.$$

A more important property and function of δ_{ij} is the so-called substitution property. Suppose in an expression the index j appears and is not repeated, if we multiply the expression by δ_{ij}, the result will now have a repeated index, j, implying a summation over j. In that sum, the only term that will *not* be zero will be the term when the j is equal to i. The end result will then be the ith component of the original expression (prior to the multiplication by δ_{ij}) multiplied by 1. The result is then essentially just a substitution of the index j with the index i. We demonstrate this explicitly. Suppose we start with A_{kj} which is then multiplied by δ_{ij}. The repeated index, j, indicates a summation. We then get

$$A_{kj}\delta_{ij} = \sum_{j=1}^{3} A_{kj}\delta_{ij} = (A_{k1}\delta_{i1} + A_{k2}\delta_{i2} + A_{k3}\delta_{i3}) = \begin{cases} A_{k1}, & \text{if } i = 1, \\ A_{k2}, & \text{if } i = 2, \\ A_{k3}, & \text{if } i = 3, \end{cases}$$

Depending on what i is, two of the three terms in that sum will vanish leaving only the term corresponding to the index i. The end result is then simply A_{ki}. All that has occurred, effectively, is that the index j has been replaced by the index i. And this has occurred independent of the index k.

For future reference note the relation emerging from the properties of the unit vectors.

$$\delta_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j.$$

We shall make use of this and similar results in our solutions to Supplementary Problems 5.9, 5.10 and 5.13.

The Levi-Civita symbol, ε_{ijk}, arises in the definition of the vector product of two vectors, but is more easily motivated by considering the scalar triple product. Let $\boldsymbol{u}$, $\boldsymbol{v}$, and $\boldsymbol{w}$ by three non-coplanar vectors. Then, according to the summation convention, their scalar triple product is

$$(\boldsymbol{u} \times \boldsymbol{v}) \cdot \boldsymbol{w} = ((u_i\mathbf{e}_i) \times (v_j\mathbf{e}_j)) \cdot (w_k\mathbf{e}_k) = u_i v_j w_k \, (\mathbf{e}_i \times \mathbf{e}_j) \cdot \mathbf{e}_k.$$

Note that all three indices are repeated which implies a sum of 27 terms.

However, consider closely the factors $(\mathbf{e}_i \times \mathbf{e}_j) \cdot \mathbf{e}_k$. Given the properties of the scalar triple product and the orthogonality properties of the unit vectors, $\boldsymbol{e}_j$, it may readily be deduced that $(\mathbf{e}_i \times \mathbf{e}_j) \cdot \mathbf{e}_k$ corresponding to $i = j$ and $i = k$ and $j = k$ is zero. On the other hand, for i, j, k all different *and* listed in the *order of the right-handed coordinate system*, $(\mathbf{e}_i \times \mathbf{e}_j) \cdot \mathbf{e}_k = 1$. For all

remaining combinations $(\mathbf{e}_i \times \mathbf{e}_j) \cdot \mathbf{e}_k = -1$. It may readily be verified that this agrees with the definition of the Levi-Civita symbol. Hence, we may state that

$$\varepsilon_{ijk} = (\mathbf{e}_i \times \mathbf{e}_j) \cdot \mathbf{e}_k.$$

Consequently, the triple scalar product can be written simply as

$$(\boldsymbol{u} \times \boldsymbol{v}) \cdot \boldsymbol{w} = \varepsilon_{ijk} u_i v_j w_k.$$

Note the locations of the vectors on the left-hand side, while on the right-hand side note (i) the order of the indices in the Levi-Civita density plus (ii) the vector components to which the respective indices have been assigned.

We remark that many algebraic results involving the Kronecker delta and the Levi-Civita symbol can be deduced, but we leave these to the student reader. Instead we discuss the last relevant topic here.

The summation convention is not only useful in vector algebra but also in vector calculus. In particular, we are interested in differentiation of vector fields (and sometimes their integration). The partial derivative with respect to x_j of a scalar function $\phi(x_1, x_2, x_3)$ is obviously $\dfrac{\partial \phi}{\partial x_j}$. Using the convention we can then readily write the gradient of ϕ as

$$\boldsymbol{\nabla}\phi \quad = \quad \underbrace{\frac{\partial \phi}{\partial x_1}\mathbf{e}_1 + \frac{\partial \phi}{\partial x_2}\mathbf{e}_2 + \frac{\partial \phi}{\partial x_3}\mathbf{e}_3}_{\text{index form}} = \underbrace{\sum_{i=1}^{3} \frac{\partial \phi}{\partial x_i}\mathbf{e}_i}_{\text{explicit sum}} = \underbrace{\frac{\partial \phi}{\partial x_i}\mathbf{e}_i}_{\text{implied sum}}.$$

Similarly, the divergence of a vector field $\boldsymbol{F}(x_1, x_2, x_3)$ becomes simply

$$\boldsymbol{\nabla} \cdot \boldsymbol{F} = \sum_{i=1}^{3} \frac{\partial F_i}{\partial x_i} = \frac{\partial F_i}{\partial x_i}.$$

And finally the curl of the vector field $\boldsymbol{F}(x_1, x_2, x_3)$ is then

$$\boldsymbol{\nabla} \times \boldsymbol{F} = \varepsilon_{ijk} \frac{\partial F_k}{\partial x_j} \mathbf{e}_i.$$

As with algebraic relations, relations involving derivatives of vector fields can be most easily proved using the notation just described. The power of the summation convention is demonstrated in the solutions of Supplementary Problems 5.9, 5.10, 5.13, and 5.28.

As an incidental remark, it can be immediately verified that

$$\delta_{ij} = \frac{\partial x_i}{\partial x_j} = \frac{\partial x_j}{\partial x_i} = \delta_{ji},$$

and

$$\frac{\partial x_i}{\partial x_i} = \frac{\partial x_1}{\partial x_1} + \frac{\partial x_2}{\partial x_2} + \frac{\partial x_3}{\partial x_3} = 3.$$

With regard to the last item in our bullet point list, this is a relation that may be confirmed through successive consideration of the indices on both sides of the equation. The relation itself is invaluable because of the substitution properties of the Kronecker delta, as the reader will see in the solutions to some of the Supplementary Problems. As a final comment, the reader should practice the use of the convention by proving some of the more simple identities on page 314 of the text.

■ Example 5.25:

For smooth scalar functions ψ and ϕ, verify that

$$\boldsymbol{\nabla} \times (\phi \boldsymbol{\nabla} \psi) = \boldsymbol{\nabla}\phi \times \boldsymbol{\nabla}\psi.$$

Solution:

The things to note here are, firstly, the outcome is a vector. In the summation convention it will have the form $A_i \boldsymbol{e}_i$ which, as is customary, we represent with the index i. Any and all other indices must then be dummy indices, appearing in pairs.

Secondly, a vector product is involved (on both sides of the equation), so a Levi-Civita density symbol will appear and must be carried through to the end of the calculation.

Thirdly, partial derivatives of a product of functions are involved, so we anticipate multiple terms arising (despite there being only one term on the right-hand side).

We start with the reinterpretation of the left-hand side of the given relation in summation convention notation:

$$\boldsymbol{\nabla} \times (\phi \boldsymbol{\nabla} \psi) = \varepsilon_{ijk} \frac{\partial}{\partial x_j} \left(\phi \frac{\partial \psi}{\partial x_k} \right) \boldsymbol{e}_i.$$

final vector index

1st vector index

2nd vector index

The final vector index is the very first index in the Levi-Civita density. The density's second index is also that of the first vector, the gradient's partial derivative $\dfrac{\partial}{\partial x_j}$. The density's third index is repeated as the index of the second vector, $\phi \dfrac{\partial \psi}{\partial x_k}$. The two repeated indices j and k indicate two implied summations.

Now expand on the derivative operation.

$$\begin{aligned}
\boldsymbol{\nabla}\times(\phi\boldsymbol{\nabla}\psi) &= \varepsilon_{ijk}\frac{\partial}{\partial x_j}\left(\phi\frac{\partial\psi}{\partial x_k}\right)\boldsymbol{e}_i,\\
&= \varepsilon_{ijk}\left(\frac{\partial\phi}{\partial x_j}\frac{\partial\psi}{\partial x_k}+\phi\frac{\partial^2\psi}{\partial x_j\partial x_k}\right)\boldsymbol{e}_i, \qquad (*)\\
&\qquad\qquad \text{—using the product rule of differentiation}\\
&= \varepsilon_{ijk}\frac{\partial\phi}{\partial x_j}\frac{\partial\psi}{\partial x_k}\boldsymbol{e}_i=\boldsymbol{\nabla}\phi\times\boldsymbol{\nabla}\psi \quad \text{—reverting back to vector notation.}
\end{aligned}$$

We have arrived at the required identity noting in line $(*)$ that for smooth functions, ϕ and ψ, the second-order mixed partial derivatives are equal. Hence,

$$\begin{aligned}
\frac{\partial^2\psi}{\partial x_j\partial x_k}=\frac{\partial^2\psi}{\partial x_k\partial x_j}\Longrightarrow\varepsilon_{ijk}\frac{\partial^2\psi}{\partial x_j\partial x_k} &= \frac{1}{2}\left(\varepsilon_{ijk}\frac{\partial^2\psi}{\partial x_j\partial x_k}+\varepsilon_{ijk}\frac{\partial^2\psi}{\partial x_j\partial x_k}\right),\\
&= \frac{1}{2}\left(\varepsilon_{ijk}\frac{\partial^2\psi}{\partial x_j\partial x_k}+\varepsilon_{ijk}\frac{\partial^2\psi}{\partial x_k\partial x_j}\right),\\
&\qquad \text{—swapping the order of partial derivatives}\\
&= \frac{1}{2}\left(\varepsilon_{ijk}\frac{\partial^2\psi}{\partial x_j\partial x_k}-\varepsilon_{ikj}\frac{\partial^2\psi}{\partial x_k\partial x_j}\right),\\
&\qquad \text{—one exchange of indices in } \varepsilon_{ijk}\\
&= 0,
\end{aligned}$$

since repeated (dummy) indices simply indicate summation and otherwise hold no special significance.

As a bonus, with the summation convention notation we readily see that,

$$\varepsilon_{ijk}\frac{\partial\phi}{\partial x_j}\frac{\partial\psi}{\partial x_k}=-\varepsilon_{ikj}\frac{\partial\phi}{\partial x_j}\frac{\partial\psi}{\partial x_k}=-\varepsilon_{ikj}\frac{\partial}{\partial x_k}\left(\psi\frac{\partial\phi}{\partial x_j}\right)=-\left[\boldsymbol{\nabla}\times(\psi\boldsymbol{\nabla}\phi)\right]_i.$$

■

In this next example, we demonstrate the benefit of the most useful relation between the Levi-Civita density and the Kronecker delta.

■ Example 5.26:

For the C^2 vector field $\boldsymbol{F}$, verify that

$$\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{F})=\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{F})-\boldsymbol{\nabla}^2\boldsymbol{F}.$$

Solution:

On the left-hand side of this, there are two vector products. So, in the language of the summation convention there will appear two Levi-Civita densities. Observe the number and use of repeated indices. No index appears more

than twice. We adhere to the principle, applied in the previous example, of assigning indices according to the order in which the vectors appear in each of the vector products.

$$\begin{aligned}
\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{F}) &= \varepsilon_{ijk}\frac{\partial}{\partial x_j}\left(\varepsilon_{klm}\frac{\partial}{\partial x_l}F_m\right)\boldsymbol{e}_i \\
&= \varepsilon_{ijk}\varepsilon_{klm}\frac{\partial^2 F_m}{\partial x_j\partial x_l}\boldsymbol{e}_i = \varepsilon_{kij}\varepsilon_{klm}\frac{\partial^2 F_m}{\partial x_j\partial x_l}\boldsymbol{e}_i, \\
&\qquad \text{—perform a cyclic permutation of the indices of the first density} \\
&= \left(\delta_{il}\delta_{jm}-\delta_{im}\delta_{jl}\right)\frac{\partial^2 F_m}{\partial x_j\partial x_l}\boldsymbol{e}_i, \\
&\qquad\qquad \text{—the product of Levi-Civita densities is replaced} \\
&= \delta_{il}\delta_{jm}\frac{\partial^2 F_m}{\partial x_j\partial x_l}\boldsymbol{e}_i-\delta_{im}\delta_{jl}\frac{\partial^2 F_m}{\partial x_j\partial x_l}\boldsymbol{e}_i, \\
&= \frac{\partial}{\partial x_i}\frac{\partial F_m}{\partial x_m}\boldsymbol{e}_i-\frac{\partial^2}{\partial x_l\partial x_l}F_i\boldsymbol{e}_i, \\
&\qquad\qquad \text{—we invoke the Kronecker delta substitution} \\
&\qquad\qquad\qquad \text{property for each delta, in each term} \\
&= \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{F})-\boldsymbol{\nabla}^2\boldsymbol{F}, \quad \text{—reverting back to vector notation}
\end{aligned}$$

which confirms the vector identity, as required.

■

To fully appreciate the power and convenience of the summation convention, the reader should solve the above examples using standard notation.

5.H Supplementary Problems

§5.A.1. Given a C^2 curve in $\mathbb{R}^3$ representing the trajectory of a particle and described by the parametrization

$$\boldsymbol{r}(t) = x(t)\mathbf{i}+y(t)\mathbf{j}+z(t)\mathbf{k},\ 0\le t\le T,$$

express the position, velocity, and acceleration of the particle in terms of the local unit vectors $\boldsymbol{T}$, $\boldsymbol{N}$, and $\boldsymbol{B}$, the curvature κ and torsion τ of the curve, and the speed v of the particle. Give an interpretation of your result for the particle's acceleration.
Conversely, express κ and τ in terms of $\boldsymbol{v}$ and $\boldsymbol{a}$.

2. Find the curvature and torsion of the following smooth curves:
(a) $\boldsymbol{r}(t) = (t^3, t^2, t)$, when $t = 1$,

(b) $\boldsymbol{r}(t) = (\mathrm{e}^t, 3t, \mathrm{e}^{-2t})$, when $t = 1$,

(c) $\boldsymbol{r}(t) = (t, t^2, \frac{2}{3}t^3)$, for general t.

3. Prove that $\boldsymbol{N}'(t) = -\kappa(t)\,|\boldsymbol{r}'(t)|\,\boldsymbol{T}(t) + \tau(t)\,|\boldsymbol{r}'(t)|\,\boldsymbol{B}(t)$.
Hint: Differentiate $\boldsymbol{N}(t) = \boldsymbol{B}(t) \times \boldsymbol{T}(t)$ with respect to t. See Rule (f) on Page 296.

4. Suppose a smooth curve is to be parameterized specifically in terms of arc length s rather than t. From the equations derived earlier, express $\boldsymbol{T}$, $\boldsymbol{N}$, and $\boldsymbol{B}$ in terms of s. Consequently, derive formulae for $\boldsymbol{T}'(s)$, $\boldsymbol{N}'(s)$, and $\boldsymbol{B}'(s)$ corresponding to those for $\boldsymbol{T}'(t)$, $\boldsymbol{N}'(t)$, and $\boldsymbol{B}'(t)$ appearing in Definitions 5.4 and 5.5, and the preceding exercise.
The formulae for $\boldsymbol{T}'(s)$, $\boldsymbol{N}'(s)$, and $\boldsymbol{B}'(s)$ are called *Frenet-Serret* formulae and are fundamental to the differential geometry of space curves.

5. Consider the 3D circle of radius a with centre at $\boldsymbol{r}_0$ described by

$$\mathbf{r}(\theta) = \mathbf{r_0} + a(\sin\phi\cos\theta, \sin\phi\sin\theta, \cos\phi) \text{ with } \phi = f(\theta) \text{ and } \theta \in [0, 2\pi],$$

where θ and ϕ are spherical polar angle variables. Show that it has constant curvature, $\kappa(\theta) = 1/a$ and that the curve's torsion $\tau(\theta) = 0$.

Hint: It may help to consider a few simple cases of circles.
(With this exercise we provide some detail to the claims made in Example 5.2.)

6. The *catenary* curve in Figure 5.59(a) is the shape taken by a chain, of uniform density per unit length, which is allowed to hang under its own weight.

Such a curve may be described by the vector function

$$\boldsymbol{r}(t) = at\mathbf{i} + a\cosh t\,\mathbf{j}, \ -1 \le t \le 1,$$

where $a > 0$ is a constant.

Calculate the length of this curve.

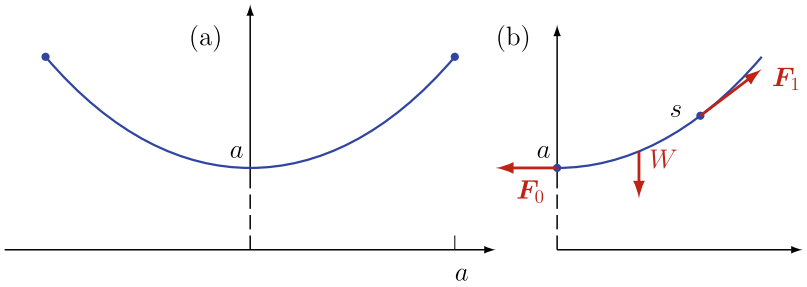


Figure 5.59 (a) The curve $\boldsymbol{r}(t)\mathbf{i} + a\cosh t\mathbf{j}$ in Problem 6; (b) The catenary curve in Problem 7.

7. Suppose a piece of chain is allowed to hang under its own weight, anchored at $(0, a)$, $a > 0$, by a force acting horizontally in the negative direction, and at some point (x, y), $x > 0$, $y > a$, by a force tangential to the curve adopted by the chain.

   Let the piece of chain have length s and let the curve be defined as $\boldsymbol{r}(t) = x(t)\,\mathbf{i} + y(t)\,\mathbf{j}$, $t \geq 0$. Assume the density of the chain is ρ per unit length, and that it is at rest while subject to tangential tension forces at each end.

   These two tension forces $\boldsymbol{F}_0$ and $\boldsymbol{F}_1$ are shown in Figure 5.59(b).

   Assume (from elementary mechanics) that the horizontal components of these forces are equal and opposite, while the sum of the vertical components is equal to the weight $W = -\rho g s\mathbf{j}$ of that portion of the chain (acting through its centre of gravity).

   Show that if the forces are in equilibrium then the curve adopted by the chain is the catenary curve as defined in the last problem, with a suitable choice of constants. Use the following steps:

   (i) Show that $\dfrac{\mathrm{d}y}{\mathrm{d}x} = \dfrac{s}{\lambda}$ for some constant λ.

   (ii) From $\dfrac{\mathrm{d}s}{\mathrm{d}t} = |\boldsymbol{r}'(t)|$ derive $\dfrac{\mathrm{d}s}{\mathrm{d}x} = \dfrac{\sqrt{\lambda^2 + s^2}}{\lambda}$, and similarly for $\dfrac{\mathrm{d}s}{\mathrm{d}y}$.

   (iii) Determine x and y in terms of s.

   (iv) Show that these equations are solved by setting $x = \lambda t$, $y = \lambda\cosh t$. That is, the curve is as described with the appropriate choice of constants.

*8. A projectile of mass m is fired with initial velocity $\mathbf{v}_0$ in a direction that makes an angle α to the horizontal, landing on the same horizontal plane some distance away. During its flight the projectile

experiences air resistance proportional to the projectile's instantaneous velocity, $\mathbf{v}(t)$, but with coefficient that diminishes exponentially with height. That is, the resistance force is

$$\mathbf{F}(\mathbf{v}, z) = -\left[b\mathrm{e}^{-z/h}\right]\mathbf{v},$$

where b is a (constant) resistance coefficient, h is a (constant) length scale. The path taken by the projectile is described by Newton's second law of motion:

$$m\ddot{\mathbf{r}}(t) = -mg\mathbf{j} + \mathbf{F}(\dot{\mathbf{r}}(t), z(t)).$$

Derive a closed-form expression for the trajectory (*i.e.*, $\mathbf{r} = \mathbf{r}(t)$) and compare this with the trajectory found assuming a uniform atmospheric resistance.

Determine the angle of projection α required to achieve the maximum range of the projectile and determine the latter.

Compare your results with the corresponding angle and range obtained for a projectile passing through a uniformly resisting atmosphere.

§5.B.9. For the C^1 fields $\boldsymbol{F}$ and $\boldsymbol{G}$, using the summation convention or directly, verify that

(a) $\boldsymbol{\nabla}(\boldsymbol{F}\cdot\boldsymbol{G}) = (\boldsymbol{F}\cdot\boldsymbol{\nabla})\boldsymbol{G} + (\boldsymbol{G}\cdot\boldsymbol{\nabla})\boldsymbol{F} + \boldsymbol{F}\times(\boldsymbol{\nabla}\times\boldsymbol{G}) + \boldsymbol{G}\times(\boldsymbol{\nabla}\times\boldsymbol{F})$,

(b) $\boldsymbol{\nabla}\times(\boldsymbol{F}\times\boldsymbol{r}) = \boldsymbol{F} - (\boldsymbol{\nabla}\cdot\boldsymbol{F})\boldsymbol{r} + \boldsymbol{\nabla}(\boldsymbol{F}\cdot\boldsymbol{r}) - \boldsymbol{r}\times(\boldsymbol{\nabla}\times\boldsymbol{F})$.

10. Show that in 3D a field proportional to $\dfrac{\boldsymbol{r}}{|\boldsymbol{r}|^3}$ is conservative. Show also that this field is solenoidal.

11. Show that the 2D electrostatic field $\boldsymbol{E} = \dfrac{\rho}{2\pi\epsilon_0|\boldsymbol{r}|^2}\,\boldsymbol{r}$ (a field due to a uniformly charged wire of infinite length) is conservative.

12. Derive and solve the equations for the field lines corresponding to the 3D vector field $\dfrac{\boldsymbol{r}}{|\boldsymbol{r}|^3}$, $\boldsymbol{r}\neq\mathbf{0}$. Hence, show that these correspond to radial lines emanating from the origin.

13. Determine the two-parameter family of field lines of the vector field

$$\boldsymbol{f}(\boldsymbol{r}) = -\frac{Ay}{(x^2+y^2)}\mathbf{i} + \frac{Ax}{(x^2+y^2)}\mathbf{j} + \mathbf{k}.$$

14. Suppose the C^1 vector field $\boldsymbol{F}$ satisfies $\boldsymbol{\nabla}\cdot\boldsymbol{F} = 0$ in a domain $D\subset\mathbb{R}^3$. If

$$\boldsymbol{G}(x,y,z) = \int_0^1 t\boldsymbol{F}\left(\boldsymbol{r}(t)\right)\times\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}\mathrm{d}t$$

with $\boldsymbol{r}(t) = (xt, yt, zt)$ for $t \in [0,1]$, show that $\boldsymbol{\nabla} \times \boldsymbol{G} = \boldsymbol{F}$. This shows that $\boldsymbol{G}$ is a vector potential for the solenoidal field $\boldsymbol{F}$ for points $(x, y, z) \in D$.

§5.C.15. Evaluate the following line integrals along the given curves

(a) $\displaystyle\int_{(0,2)}^{(4,0)} (x^2 + y^2)\,\mathrm{d}x$ along the path $y = \sqrt{4 - x}$.

(b) $\displaystyle\int_{(0,2)}^{(4,0)} (x^2 + y^2)\,\mathrm{d}\boldsymbol{r}$ along the path $y = \sqrt{4 - x}$.

(c) $\displaystyle\int_{(-1,0)}^{(1,0)} y(1 + x)\,\mathrm{d}y$ along the x-axis.

(d) $\displaystyle\int_{(-1,0)}^{(1,0)} y(1 + x)\,\mathrm{d}y$ along the parabola $y = 1 - x^2$.

16. Let

$$\begin{aligned} \boldsymbol{F}_1(x, y, z) &= yx\mathbf{i} + (xz + y)\mathbf{j} + (1 + xz)\mathbf{k}, \\ \boldsymbol{F}_2(x, y, z) &= \left(2xy + 3yz^2\right)\mathbf{i} + \left(x^2 + 2yz + 3xz^2\right)\mathbf{j} + \left(y^2 + 6xyz\right)\mathbf{k}, \end{aligned}$$

be two C^∞ vector fields, and suppose Γ is the straight-line segment from the origin to an arbitrary point (x, y, z).

(a) For each vector field compute the line integral $f(x, y, z) = \displaystyle\int_\Gamma \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{r}$.

(b) In each case evaluate $\boldsymbol{\nabla} f$.

(c) Discuss your findings.

17. Along what curve of the family $y = kx(1 - x)$ does the integral

$$\int_{(0,0)}^{(1,0)} y(x - y)\,\mathrm{d}x$$

have the largest value?

18. Suppose a particle experiences a force directed to the origin with magnitude inversely proportional to its distance from the origin. Evaluate the work done by the force if the particle traverses the helical path $\boldsymbol{r}(t) = (a\cos t, a\sin t, bt)$ for $t \in [0, 2\pi]$.

19. Compute $\displaystyle\int_\Gamma \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{r}$, where $\boldsymbol{A} = -y\mathbf{i} + 2x\mathbf{j} + x\mathbf{k}$, and Γ is a circle in the plane $x = y$ with centre $(1, 1, 0)$ and radius 1.

Orientation: Γ is traversed counterclockwise as seen from $(1,0,0)$ (Figure 5.60(a)).

20. Compute $\displaystyle\int_\Gamma \boldsymbol{A}\cdot \mathrm{d}\boldsymbol{r}$, where $\boldsymbol{A} = x^2\mathbf{i}+(x^2+y^2)\mathbf{j}+(x^2+y^2+z^2)\mathbf{k}$, and Γ is the boundary of $\{(x,y,z) : x+y+z=1, x\geq 0,\ y\geq 0,\ z\geq 0\}$. Orientation: Γ is traversed counterclockwise seen from point $(1,1,1)$ (Figure 5.58).

21. Evaluate the line integral $\displaystyle\int_\Gamma \boldsymbol{F}\cdot \mathrm{d}\boldsymbol{r}$, where

$$\boldsymbol{F} = (3x^2y^2 + 2xy - \mathrm{e}^z y)\mathbf{i} + (2x^3y + x^2 + 1 + \mathrm{e}^z x)\mathbf{j} + x^3y^2\mathbf{k},$$

and Γ is one quarter cycle of the circular helix of unit radius starting at $(1,0,0)$ and ending at $(0,1,\pi/2)$.

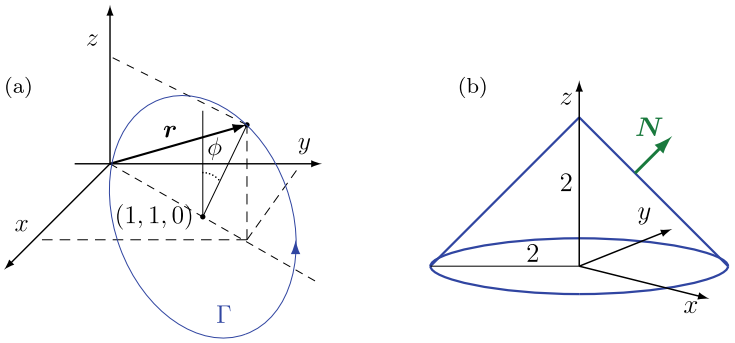


Figure 5.60 (a) The circle Γ of Problem 19. (b) The surface $x^2 + y^2 = (z-2)^2$ of Problem 28.

22. If C is the curve of intersection of the surfaces $z = \ln(1+x)$ and $y = x$, directed from $(0,0,0)$ to $(1,1,\ln 2)$, evaluate

$$\int_C \left(2x\sin(\pi y) - e^z\right)dx + \left(\pi x^2\cos(\pi y) - 3e^z\right)dy - xe^z dz.$$

23. If f and g are C^1 scalar fields defined on a connected domain $D \subset \mathbb{R}^3$, show that

$$\int_C f\boldsymbol{\nabla} g\cdot \mathrm{d}\boldsymbol{r} + \int_C g\boldsymbol{\nabla} f\cdot \mathrm{d}\boldsymbol{r} = f(Q)g(Q) - f(P)g(P)$$

for any piecewise smooth curve in D from point directed from P to point Q on C.

24. Let C be a piecewise smooth curve in the xy-plane not passing through the origin and let $\theta(x,y)$ be the polar angle coordinate of the point $P(x,y)$ on C, not restricted to any interval of length 2π,

but varying continuously as P moves along C. Derive $\boldsymbol{\nabla}\theta$. If C is a closed curve show that

$$w(C) = \frac{1}{2\pi}\oint_C \frac{x\,dy - y\,dx}{x^2+y^2}$$

has an integer value.
(Defined in this way, w is called the *winding number* of C about the origin: w(C) counts the number of times C winds around the origin, positive if counterclockwise and negative is clockwise.)

25. Evaluate the curve integral $I = \oint_C \boldsymbol{F}\cdot \mathrm{d}\boldsymbol{r}$ for the following fields and curves C.

(a) $\begin{cases} \boldsymbol{r}(t) = & (1+\cos t)\mathbf{i} + (1+\sin t)\mathbf{j} + (1-\cos t-\sin t)\mathbf{k}, \quad 0\le t\le 2\pi, \\ \boldsymbol{F}(\boldsymbol{r}) = & y\mathrm{e}^x\mathbf{i} + \left(x^2+y^2+\mathrm{e}^x\right)\mathbf{j} + z^2\mathrm{e}^z\mathbf{k}. \end{cases}$

(b) $\begin{cases} \boldsymbol{r}(t) = & \sin(\pi t/2)\,\mathbf{i} + \left(1-2(t-1)^2\right)\mathbf{j} + 2t^3\mathbf{k}, \quad 0\le t\le 1, \\ \boldsymbol{F}(\boldsymbol{r}) = & z\left(2xy^2z^2+1\right)\mathbf{i} + \left(2x^2yz^3+1\right)\mathbf{j} + x\left(3xy^2z^2+1\right)\mathbf{k}. \end{cases}$

§5.D.26. Evaluate the surface integral $\iint_S f(x,y,z)\,\mathrm{d}S$ for the following fields and surfaces.

(a) $\begin{cases} f(x,y,z) = & (2x+y-3z^2), \\ \boldsymbol{r}(u,v) = & u\mathbf{i}+v\mathbf{j}+u\mathbf{k}, \quad 0\le u,v\le 1. \end{cases}$

(b) $\begin{cases} f(x,y,z) = & (6x+y-x^2), \\ \boldsymbol{r}(u,v) = & u\mathbf{i}+u^2\mathbf{j}+v\mathbf{k}, \quad 0\le u,v\le 1. \end{cases}$

*27. Let S be the ellipsoid

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}+\frac{z^2}{c^2} = 1,$$

and $p(x,y,z)$ be the length of the perpendicular from the plane, that is tangent to S at $(x,y,z)\in S$, to the origin. Show that

$$\iint_S \frac{\mathrm{d}S}{p} = \frac{4}{3}\pi abc\left(\frac{1}{a^2}+\frac{1}{b^2}+\frac{1}{c^2}\right).$$

§5.E.28. Use Gauss's theorem to determine the flux of the vector field $\boldsymbol{f} = (x^2+y^2, y^2+z^2, z^2+x^2)$ through the surface of the cone $S = \{(x,y,z) : x^2+y^2-(z-2)^2 = 0,\ 0\le z\le 2,\ \boldsymbol{N}\cdot\mathbf{e}_3 > 0\}$ (Figure 5.60(b)).

29. Suppose the region $D \subset \mathbb{R}^3$ is bounded by a closed surface S. Using Gauss's theorem as a basis, prove the following variants of the theorem:

$$\text{(a)} \quad \iiint_D (\boldsymbol{\nabla} \times \boldsymbol{F})\, \mathrm{d}V = \oiint_S (\boldsymbol{N} \times \boldsymbol{F})\, \mathrm{d}S,$$

$$\text{(b)} \quad \iiint_D (\boldsymbol{\nabla} \phi)\, \mathrm{d}V = \oiint_S (\phi \boldsymbol{N})\, \mathrm{d}S.$$

30. Let A be the area of a region D of the surface of a sphere of radius R centred at the origin. Let V be the volume of the solid cone comprising all rays from the origin to points on D. Show that

$$V = \frac{1}{3} AR.$$

31. Show that the electric intensity due to a uniformly charged sphere at points outside the sphere is the same as if the charge were concentrated at the centre, while at points inside the sphere it is proportional to the distance from the centre.

32. Let S be a surface with boundary $\partial S = C_1 \cup C_2$, where

$$\begin{aligned} C_1 &= \{(x, y, z) : y = z = 0, -1 \leq x \leq 1\}, \\ C_2 &= \left\{(x, y, z) : z = 0, y \geq 0, x^2 + y^2 = 1\right\}. \end{aligned}$$

Determine constants a and b for which the upward flux of the vector field
$\boldsymbol{F} = (ax^2 - z)\mathbf{i} + (xy + y^3 + z)\mathbf{j} + by^2(z+1)\mathbf{k}$ through S is independent of S. Determine the flux in that case, confirming independence of S.

33. Through what closed, oriented surface in $\mathbb{R}^3$ does the vector field

$$\mathbf{F}(\mathbf{r}) = \left(4x + 2x^3 z\right)\mathbf{i} - y\left(x^2 + z^2\right)\mathbf{j} - \left(3x^2 z^2 + 4y^2 z\right)\mathbf{k}$$

have the greatest flux?

34. Consider the vector field $\boldsymbol{A} = \boldsymbol{\nabla}\phi$ where $\phi = |\boldsymbol{r}|^4$, and let S be the surface
$x^2 + y^2 = 1$ between $z = 0$ and $z = 1$. Evaluate $\displaystyle\iint_S \mathbf{A} \cdot \mathrm{d}\mathbf{S}$.

35. A solid V has boundary S defined as the intersection of two finite surfaces,
$S_1 = \{(x, y, z) \in D : z = 4 - x^2 - y^2\}$ and $S_2 = \{(x, y, z) \in D : z = 2x + 1\}$, where D is a finite domain in $\mathbb{R}^3$. Determine the flux of $\boldsymbol{F} = y^3\mathbf{i} + z^2\mathbf{j} + x\mathbf{k}$:

(a) out of S,

(b) upward through S_1 (*i.e.*, such that $\boldsymbol{N}_1 \cdot \mathbf{k} > 0$), and

(c) upward through S_2 (*i.e.*, such that $\boldsymbol{N}_2 \cdot \mathbf{k} > 0$).

36. For the following vector fields, $\boldsymbol{F}$, compute the flux out through the sphere of radius R centred at the origin. Also compute the fluxes through the positive and negative hemispheres, which are completed with the plane at $z = 0$.

(a) $\boldsymbol{F} = 2zx\mathbf{i} + 2xy\mathbf{j} + (a^2 + z^2 - x^2 - y^2)\mathbf{k}$, with $a > 0$,

(b) $\boldsymbol{F} = \dfrac{1}{|\boldsymbol{r} - a\mathbf{k}|^3}\big(x\mathbf{i} + y\mathbf{j} + (z-a)\mathbf{k}\big)$, with $a > 0$.

*37. By direct calculation, determine the flux of $\boldsymbol{F}(\boldsymbol{r}) = m\dfrac{\boldsymbol{r}}{|\boldsymbol{r}|^3}$ out of the surface of the cube $-a \le x, y, z \le a$ for $a > 0$. Verify your result using Gauss's theorem.

38. Determine the total flux of the vector field $\boldsymbol{F}(x, y, z) = \dfrac{\boldsymbol{r}}{|\boldsymbol{r}|^3} + z\mathbf{i} - x\mathbf{k}$ through the half ellipsoid $S = \big\{(x, y, z) : x^2 + y^2/2 + z^2 = 1, y \ge 0\big\}$ in the direction $\mathbf{N} \cdot \mathbf{j} > 0$.

39. Suppose ϕ, f, and g satisfy the following conditions

(a) ϕ, f, and g are continuous in $\overline{\Omega}$ and have continuous second derivatives in a compact region Ω bounded by the smooth closed surface S,

(b) $\boldsymbol{\nabla} \cdot \boldsymbol{\nabla}\phi = \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} f = \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} g = 0$ in Ω,

(c) $\phi = 0$ and $f = g$ on S.

Consequently, evaluate $\iiint_\Omega |\boldsymbol{\nabla}\phi|^2 dV$, and show that $f = g$ in Ω (as well as on S).

40. Let B, c, T, ω be positive constants with $\omega = 2\pi/T$, and consider the function of four variables ($r = |\boldsymbol{x}|$),

$$\phi(x, y, z, t) = B\frac{1}{r}\sin\left(\omega\left(t - \frac{r}{c}\right)\right).$$

(a) Determine the vector field $\boldsymbol{F}(\boldsymbol{r})$ defined by

$$\boldsymbol{F}(x, y, z) = -\frac{1}{T}\int_0^T \left(\frac{\partial\phi}{\partial t}\boldsymbol{\nabla}\phi\right) \mathrm{d}t.$$

(b) Evaluate the flux of $\boldsymbol{F}$ out through *any* closed surface *not* passing through the origin.

41. Show that for the conditions of Gauss's theorem and for two C^2 functions $\phi, \psi : \mathbb{R}^3 \longrightarrow \mathbb{R}$, the following integral identity holds:

$$\iiint_V \left(\psi \boldsymbol{\nabla}^2 \phi - \phi \boldsymbol{\nabla}^2 \psi\right) \mathrm{d}V = \oiint_S \left(\psi \boldsymbol{\nabla}\phi - \phi \boldsymbol{\nabla}\psi\right) \cdot \boldsymbol{N} \mathrm{d}S.$$

This is known as Green's second identity ([9]) or Green's formula ([16]).

§5.F.42. Verify Green's theorem for the following integrals and paths.

(a) $\oint_\Gamma (x^2 + y)\,\mathrm{d}x - xy^2\,\mathrm{d}y$, where Γ is the boundary of the square with vertices $(0,0),\ (1,0),\ (1,1),\ (0,1)$.

(b) $\oint_\Gamma (x - y)\,\mathrm{d}x + (x + y)\,\mathrm{d}y$, where Γ is the boundary of the first quadrant region between the curves $y = x^2$ and $y^2 = x$, taken anticlockwise (Figure 5.61).

(c) $\oint_\Gamma (x - 2y)\,\mathrm{d}x + x\,\mathrm{d}y$, where Γ is the boundary of the unit circle $x^2 + y^2 = 1$ taken anticlockwise.

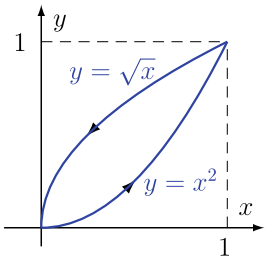


Figure 5.61 The closed contour Γ of Problem 41(b).

43. Use Green's theorem to evaluate

$$\oint_\Gamma (2xy + y^2)\,\mathrm{d}x + (x^2 + xy)\,\mathrm{d}y,$$

where Γ is the boundary taken anticlockwise of the region cutoff from the first quadrant by the curve $y^2 = 1 - x^3$.

44. The intersection of the ellipsoid $x^2/2 + y^2 + (z-1)^2/4 = 1$ and the plane $z + 2x = 2$ is a closed curve. Let Γ be that part of the curve

lying above the xy-plane directed from, and including, $(1, -\frac{1}{2}, 0)$ to, and including, $(1, \frac{1}{2}, 0)$. Evaluate $\oint_\Gamma \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{r}$ if

$$\boldsymbol{F}(x, y, z) = \left(z^2 + \frac{2}{3}xy^3\right)\mathbf{i} + \left(x^2y^2\right)\mathbf{j} + \left(\frac{1}{4}z^2y^4 + \frac{1}{2}y^2\right)\mathbf{k}.$$

45. Let Γ be the curve of intersection of the surfaces

$$S_1 = \{(x, y, z) : 4x^2 + 4y^2 + z^2 = 40\},$$
$$S_2 = \{(x, y, z) : x^2 + y^2 - z^2 = 0, z > 0\}.$$

Evaluate $\oint_\Gamma \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{r}$ if

$$\boldsymbol{F}(x, y, z) = \left(\frac{y}{x^2 + y^2} - z\right)\mathbf{i} + \left(x - \frac{x}{x^2 + y^2}\right)\mathbf{j} + \left(y + x^2\right)\mathbf{k}.$$

46. Suppose Γ is the curve of intersection of surfaces $x^2 + y^2 = x$ and $1 - x^2 - y^2 = z$, while vector field $\boldsymbol{f} = (y, 1, x)$. Evaluate $\oint_\Gamma \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{r}$.

*47. Let $\boldsymbol{A}$ be a C^2 vector field everywhere except at $(0, 0, 0)$ where it is singular. Show that $I = \iint_S (\boldsymbol{\nabla} \times \boldsymbol{A}) \cdot \boldsymbol{N} \mathrm{d}S = 0$, where S is the unit sphere centred at the origin, and $\boldsymbol{N}$ is the outward-pointing normal to S.

*48. Consider the vector field

$$\boldsymbol{F}(x, y, z) = \left(y^3 + y^2 - (2 - x^2)y\right)\boldsymbol{i} + \left(x^2 + x(1 + 2y^2)\right)\boldsymbol{j} + \left(\frac{1}{4}z^2y^4 + \frac{1}{2}y^2\right)\boldsymbol{k}.$$

The intersection of a sphere of radius 3 and the $xy-$plane is a closed curve, Γ, oriented anticlockwise as seen from the point $(0, 0, 11)$. Determine the sphere's centre so that the circulation $\oint_\Gamma \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{r}$ is as large as possible.

*49 The ellipsoid,

$$\frac{(x - x_0)^2}{a^2} + \frac{(y - y_0)^2}{b^2} + \frac{(z - z_0)^2}{c^2} = 1,$$

with semi-axis lengths $a = \dfrac{4}{\sqrt{3}}$, $b = \dfrac{2}{\sqrt{3}}$, and $c = 2$, intersects the xy-plane to give a closed curve, C, oriented counterclockwise as seen from $(0, 0, 11)$. Determine the 3D position(s) of the ellipsoid's centre which result in the greatest value of the circulation, $\oint_C \boldsymbol{F} \cdot$

$\mathrm{d}\boldsymbol{r}$, where $\boldsymbol{F}$ is the smooth vector field,

$$\boldsymbol{F}(\boldsymbol{r}) = \big(y(x^2+2x)+4y^2\big)\,\mathbf{i}+\big(4-x^2+4x(y^2-1)\big)\,\mathbf{j}+\big(z^2x+2y^2z\big)\,\mathbf{k}.$$

50. Let Γ be the curve of intersection of surfaces $x^2+y^2+z^2=1$ and $x^2+\left(z-\frac{1}{2}\right)^2=\dfrac{1}{4}$, with $y\geq 0$. Show that the vector field $\boldsymbol{F}(\boldsymbol{r})=\boldsymbol{f}\times\boldsymbol{g}$ has zero circulation $\oint_\Gamma \boldsymbol{F}\cdot\mathrm{d}\boldsymbol{r}=0$, when $\boldsymbol{f}$ and $\boldsymbol{g}$ take the forms

$$\boldsymbol{f}=f(y)\mathbf{j}+\alpha\mathbf{k} \quad ; \quad \boldsymbol{g}=g(z)\mathbf{i}+\beta\mathbf{j},$$

for any single-variable scalar functions f and g and real-valued constants α and β.

*51. Let Γ be the curve of intersection of surfaces $x^2+y^2+z^2=1$ and $y^2+\left(z-\frac{1}{2}\right)^2=\dfrac{1}{4}$, with $x\geq 0$. If the vector field $\boldsymbol{F}$ is defined as the cross product $\boldsymbol{F}(\boldsymbol{r})=\boldsymbol{f}\times\boldsymbol{g}$, where

$$\boldsymbol{f}=f(y)\mathbf{j}+\alpha\mathbf{k} \quad \text{and} \quad \boldsymbol{g}=g(z)\mathbf{i}+\beta\mathbf{j},$$

for real-valued constants α and β, determine single-variable scalar functions f and g so that $\boldsymbol{F}$ has zero circulation, *i.e.*, $\oint_\Gamma \boldsymbol{F}\cdot\mathrm{d}\boldsymbol{r}=0$.

Glossary of symbols

$a, b, c, a_1, ..., b_1, ...$	Scalar constants (usually).
x, y, z, u, v, w, s, t	Variables, assumed continuous.
$\boldsymbol{u}, \boldsymbol{v}, \underset{\sim}{\mathrm{u}}, \underset{\sim}{\mathrm{v}}, \vec{u}, \vec{v}$	Vector variables or vector constants.
f, g, h, F, G, H	Functions (usually).
$F^{(k)}(x)$	The kth-order derivative of $F(x)$.
m, n, ℓ	Discrete integer variables.
$\mathbb{R}$	Real one-dimensional space; the real line.
$\mathbb{R}^n,\ n = 2, 3, \ldots$	Real n-dimensional space. $\mathbb{R}^3$ is the 3-dimensional space we inhabit.
V, S	A volume region, and a surface embedded, in $\mathbb{R}^n$, $n \geq 3$.
D_f; D, R	Domain of a function f; a general region and a rectangular region, respectively, (of integration) in $\mathbb{R}^n$.
M	A subset of $\mathbb{R}^n$; n is usually specified in context.
$M^c, \partial M$	The complement, and the boundary, of a set M.
$\overline{M}$	The closure of a set M: $\overline{M} = M \cup \partial M$.
$\boldsymbol{N}, \boldsymbol{n}$	Unit normal vector and non-unit normal vector to a surface $S \subset \mathbb{R}^3$.

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$Q(\boldsymbol{h})$	Quadratic form of argument $\boldsymbol{h} = (h, k, l, \dots)$.
$\lvert x\rvert, \lvert \boldsymbol{u}\rvert$	Absolute value of scalar x, and the magnitude of vector $\boldsymbol{u}$.
$\lvert A\rvert$	Determinant of square matrix A.
$\mathbf{i}, \mathbf{j}, \mathbf{k}$	Unit vectors in the x-, y-, & z-directions, respectively.
$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$	Another way of writing $\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$, respectively.
θ, ϕ	Angles (usually). The symbol ϕ is also used to denote a scalar potential field in $\mathbb{R}^n$ $n \geq 2$.
α, β, γ	Components of a fixed vector (usually). Angles (sometimes).
$\Gamma(x)$	The gamma function of argument x.
$\beta(m, n)$	The beta function of two arguments, m and n.
δ_{ij}	Kronecker delta.
ε_{ijk}	The Levi-Civita density or Levi-Civita symbol.
$\equiv, \exists, \forall$	"equivalent to", "there exists", and "for all".
$\in$	"belongs to" or "is a member of".
$\subset$	"is a subset of" or "is contained within".
$\cap$	$A \cap B$ is the intersection of two sets A, B.
$\cup$	$A \cup B$ is the union of two sets A, B.
$(\cdot)$	An undefined, undeclared, or generic, argument of a function.
s.t.	"such that".
:	(Inside a set-builder like $\{x : x < 0\}$) "such that".
w.r.t.	"with respect to".
$\dfrac{\mathrm{d}f}{\mathrm{d}x} \equiv f'(x)$	Notation for the total derivative of a function f of x.

$(f \circ g)(x)$	Composite function; equivalent to $f\big(g(x)\big)$.
$\dfrac{\partial f}{\partial x} \equiv f_x$	The partial derivative w.r.t. x of a function f of two or more variables.
$C^n(\mathbb{R}^m)$	The set of continuous functions defined on the space $\mathbb{R}^m$ $(m \geq 1)$ having continuous derivatives of order up to & including n.
$\boldsymbol{\nabla}$	The vector differential operator, "del".
$\boldsymbol{\nabla} f$	The gradient of a scalar function f, "grad f".
$\boldsymbol{\nabla} \cdot \boldsymbol{f}$	The divergence of a vector function $\boldsymbol{f}$, "div $\boldsymbol{f}$".
$\boldsymbol{\nabla} \times \boldsymbol{f}$	The rotation vector of a vector field f, "curl $\boldsymbol{f}$".
J	The Jacobian determinant (usually).
L	A linear operator, a level set, a line, or a length, depending on context.
$\Longrightarrow,\ \Rightarrow$	Implication: "this implies" or "this results in".
$\Longleftrightarrow$	"if and only if" or "equivalent to".
$\perp$	"is orthogonal to", "is perpendicular to", or "is at right-angles to".
$\parallel$	"is parallel to".
$\ll$	"is much less than".
$\gtrless$	"is greater than and also less than".
$\longmapsto,\ \mapsto$	$f : x \longmapsto y$ (or $f : x \mapsto y$) "function f maps point x to point y" (point mapping).
$\longrightarrow,\ \rightarrow$	Context dependent: $f : A \longrightarrow B$ (or $f : A \rightarrow B$) "function f maps from set A into set B" (set mapping); $x \longrightarrow 0$ (or $x \rightarrow 0$) "x converges to 0"; "tends to".
Field	A scalar or vector function on $\mathbb{R}^n$, $n \geq 2$.
Theorem	A proposition that can be proved to be true.
Corollary	A result that follows immediately from a theorem.

1D, 2D, 3D	"one dimension" or "one-dimensional", etc.
ODE	"ordinary differential equation".
PDE	"partial differential equation".
b.c.	"boundary condition".
b.v.p.	"boundary-value problem".

Bibliography

Any serious scientist, engineer or mathematician should be in possession of a decent personal library of reference books. Likewise, a university or college library worthy of its name should have a ready and sufficient store of text books. Although hard-copy books are becoming unfashionable (perhaps, at least, to be replaced by electronic literature — "eBooks"), it is important for the student to follow up on the material presented here by reading some of the more specialist books. The list given below is far from exhaustive, but these books do cover the areas we have discussed as well as being some of my favourites.

I have attempted to categorize the books according to the present requirements. However, some books span multiple areas and are therefore of broader practical benefit. For example, Adams's book [5] covers both single and multivariable calculus as well as some elements of linear algebra. The book by Jeffreys and Jeffreys [16] similarly covers elements of single variable calculus, multivariable calculus, linear algebra, differential equations, and more.

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