Natural Sciences Tripos: IB Mathematical Methods I

Contents

0 Introduction

0.1 Schedule

The schedules, or syllabuses, are determined by a committee which has input from all the Physical Science subjects in the Natural Sciences and from Computer Science and is agreed by the Faculty of Mathematics. The schedules are minimal for lecturing and maximal for examining; that is to say, all the material in the schedules will be lectured and only this material will be examined.

Below is a copy from the booklet of schedules.[1] The numbers in square brackets at the end of paragraphs indicate roughly (I emphasise *roughly*) the number of lectures that will be devoted to the material in the paragraph.

Please note that the committee responsible for the schedules has recently asked me to lecture the section on *Partial differential equations* after the section on the *Fourier transform* (instead of before the section on *Green's functions*).

Part IB: Mathematics

This course comprises Mathematical Methods I, Mathematical Methods II and Mathematical Methods III and six Computer Practicals. The material in Course A from Part IA will be assumed in the lectures for this course.[2] *Topics marked with asterisks should be lectured, but questions will not be set on them in examinations.*

The material in the course will be as well illustrated as time allows with examples and applications of Mathematical Methods to the Physical Sciences.[3] *Separate occasional examples classes will be given as stated in the lecture list.*

Mathematical Methods I **24 lectures, Michaelmas term**

Vector calculus
Vector calculus Suffix notation. Einstein summation convention. Contractions using δ_{ij} and ε_{ijk}. Reminder of vector products, grad, div, curl, Δ^2, and their representations using suffix notation. Divergence theorem and Stokes' theorem. Vector differential operators in orthogonal curvilinear coordinates, e.g. cylindrical and spherical polar coordinates. Jacobians. [**6**]

Green's functions
Response to impulses, delta function (treated heuristically), Green's functions for initial and boundary value problems. [**3**]

Fourier transform
Fourier transforms; relation to Fourier series, simple properties and examples, convolution theorem, correlation functions, Parseval's theorem and power spectra. [**2**]

Partial differential equations
Partial differential equations Linear second-order partial differential equations; physical examples of occurrence, the method of separation of variables (Cartesian coordinates only). [**2**]

Matrices
N-–dimensional vector spaces, matrices, scalar product, transformation of basis vectors. Eigenvalues and eigenvectors of a matrix; degenerate case, stationary property of eigenvalues. Orthogonal and unitary transformations. Quadratic and Hermitian forms, quadric surfaces. [**5**]

[1] See
https://www.maths.cam.ac.uk/undergradnst/files/misc/NSTschedules.pdf
and also
https://www.maths.cam.ac.uk/undergradnst/currentstudents.

[2] However, if you took course A rather than B, then you might like to recall the following extract from the schedules: *The material from course A is assumed. Students are nevertheless advised that if they have taken course A in Part IA, they should consult their Director of Studies about suitable reading during the Long Vacation before embarking upon part IB Mathematics.*

[3] Time is always short.

Elementary Analysis
Idea of convergence and limits. O notation. Statement of Taylor's theorem with discussion of remainder. Convergence of series; comparison and ratio tests. Power series of a complex variable; circle of convergence. Analytic functions: Cauchy-Riemann equations, rational functions and $\exp(z)$. Zeros, poles and essential singularities. [**3**]

Series solutions of ordinary differential equations
Homogeneous equations; solution by series (without full discussion of logarithmic singularities), exemplified by Legendre's equation. Classification of singular points. Indicial equation and local behaviour of solutions near singular points. [**3**]

0.2 Books

An extract from the schedules.

> *There are very many books which cover the sort of mathematics required by Natural Scientists. The following should be helpful as general reference; further advice will be given by Lecturers. Books which can reasonably be used as principal texts for the course are marked with a dagger. The prices given are intended as a guide only, and are subject to change.*

† G Arfken & H Weber *Mathematical Methods for Physicists, 6th edition.* Elsevier, 2005 (£44.09).

† J W Dettman *Mathematical Methods in Physics and Engineering.* Dover, 1988 (£23.99 paperback).

H F Jones *Groups, Representation and Physics, 2nd edition.* Institute of Physics Publishing, 1998 (£45.99 paperback)

E Kreyszig *Advanced Engineering Mathematics, 8th edition.* Wiley, 1999 (10th edition available, £46.59 hardback)

† J Mathews & R L Walker *Mathematical Methods of Physics, 2nd edition.* Pearson/Benjamin Cummings, 1970 (From £42.00 used).

† K F Riley, M P Hobson & S J Bence *Mathematical Methods for Physics and Engineering.* 3nd ed., Cambridge University Press, 2002 (£39.99 paperback).

R N Snieder *A guided tour of mathematical methods for the physical sciences, 2nd edition.* Cambridge University Press, 2004 (£34.19 paperback)

There is likely to be a resemblance between my notes and Riley, Hobson & Bence. This is because we both used the same source, i.e. previous Cambridge lecture notes.[4]

Of the other books, I like Mathews & Walker, but it might be a little mathematical for some. Also, the first time I gave a 'service' mathematics course (over 35 years ago to aeronautics students at Imperial), my notes bore a resemblance to Kreyszig ... and that was not because we were using a common source!

0.3 Course Website

See the `NST Part IB: Mathematics` Moodle course at

https://www.vle.cam.ac.uk/course/view.php?id=78772

The direct link to this term's section is

https://www.vle.cam.ac.uk/course/view.php?id=78772&sectionid=4279112

but this might break if someone changes the number of sections!

[4] When I lectured this course two decades ago, a student hoped that Riley *et al.* were getting royalties from my lecture notes; my hope is that my lecturers from 45 years ago are getting royalties from Riley *et al.*!

0.4 Lectures

- Lectures will start at 11:05 promptly with a summary of the last lecture. If attending in-person (which I highly recommend on educational grounds), please be on time since it is distracting to have people walking in late.
- I will aim to finish by 11:55, but am not going to stop dead in the middle of a long proof/explanation.
- I welcome *constructive* heckling. Hence, if I am inaudible, illegible, unclear (e.g. you spot a typo or I use jargon you do not understand), or just plain wrong, then please speak up. I will endeavour to stay around for a few minutes at the front after lectures in order to answer questions. Questions and comments, particularly longer ones, can also be emailed to me at S.J.Cowley@maths.cam.ac.uk.
- I want you to learn. I will do my best to be clear but you *must* read through and understand your notes before the next lecture . . . otherwise you will get hopelessly lost. An understanding of your notes will not diffuse into you just because you have carried your notes around for a week, or put them under your pillow, or watched them (possibly more than once) online (especially if done at double speed).
- I aim to avoid the words *trivial*, *easy*, *obvious* and *yes*[5]. Let me know if I fail. I will occasionally use *straightforward* or *similarly to last time*; if it is not, email me at S.J.Cowley@maths.cam.ac.uk, or catch me at the end of the next lecture.
- Sometimes I may confuse both you and *myself*, and may not be able to extract myself in the middle of a lecture. Under such circumstances I will have to plough on as a result of time constraints; however I will clear up any problems at the beginning of the next lecture.
- This is a 'service' course, so you will not get pure mathematical levels of rigour. However, I will give some justification for a method, rather than just a recipe, because if you are to use a method efficiently and effectively, or extend it as might be necessary in research, you need to understand *why* a method works, as well as *how* to apply it.
- If anyone is colour blind please tell me which colours you cannot read.

0.5 Lecture Notes

- The lecture notes should be online [just] before the relevant lecture. If I manage to get organised, there may be a sign-up sheet for hard-copies, but please do not ask for hard-copies unless you really need them (since paper copies are not environmentally friendly).
- An advantage of typeset notes is that you can listen to me rather than having to scribble things down. However, a disadvantage is that you can lose concentration. Hence, with one or two exceptions figures/diagrams are deliberately omitted from the notes. I was taught to do this at my teaching course on *How To Lecture* . . . the aim being that it might help you to stay awake if you have to write something down from time to time. Indeed, as an aid to concentration, you may wish to copy my scribbles on the visualisers.
- There are a number of unlectured worked examples in the notes. In the past I have been tempted to not include these because I was worried that students would be unhappy with material in the notes that was not lectured. However, a vote in an earlier year was overwhelming in favour of including unlectured worked examples.
- Please email corrections to the notes to me at S.J.Cowley@maths.cam.ac.uk.
- If it is not in the typeset notes, or on the example sheets, it should not be in the exam.

[5] But I will fail miserably in the case of *yes*.

0.6 Example Sheets

- There will be five Example Sheets. They will be available on Moodle at about the same time as you can do them.
- You should be able to complete the revision example sheet, i.e. Example Sheet 0, immediately (although you might like to wait until the end of lecture 2 for a couple of the questions).
- You should be able to complete Example Sheets 1/2/3/4 after lectures 6/12/18/24 respectively (or thereabouts). Please bear this in mind when arranging supervisions.
- There are sketch answers to the sheets. I will make these available to you on Moodle at the end of weeks 1, 3, 5, 7 and 9 (where I count weeks from 0, with week 0 starting on the Sunday before the Tuesday on which Full Term starts). If I forget to do this, please remind me by email.
- The good news for supervisors is that the sheets are the same as last year other than for some rearrangement caused by moving the lecture material on *Partial differential equations* to later. Supervisors can have access to the answers almost immediately, as indicated on the Moodle site.

0.7 Examples Classes

There will be Examples Classes on Wednesday 2 November and Wednesday 23 November from 14:00 to 16:00 in the Cockcroft Lecture Theatre.

0.8 Computational Exercises

I have been asked to remind you that there is a Computational Projects element to the course that you need to register on the course Moodle by 23 October 2022.

0.9 Election of Student Representatives

The Faculty Board of Mathematics asked DAMTP to set up a Staff-Student Committee for Mathematics in the Natural Sciences to provide an opportunity for discussion of matters relating to the courses. The Committee has four staff and three student members, the latter being drawn from the A and B courses in Part IA and from the Part IB course.

Hence, this Consultative Committee for NST Mathematics will need an elected undergraduate member drawn from this course. I have been asked to conduct an election. It has been suggested that a week's notice be given and that nominations are asked for in writing, countersigned by the nominee as a guarantee of willingness to serve. It has been proposed that the election can take place by a show of hands at the start of a designated lecture.

Please could you hand me nominations in writing, countersigned by the nominee, by the end of the lecture on Monday 17 October?

If you would prefer that the election take place by other than a show of hands, please could you email an alternative suggestion to S.J.Cowley@maths.cam.ac.uk.

0.10 Feedback

Comments and administrative/organisational queries on the course, lectures and the examples sheets can be made via the email address NST@maths.cam.ac.uk.

Comments received will be edited and passed on anonymously to the relevant lecturer and others concerned. They will also be considered at the next meeting of the Staff Student Consultative Committee. Queries will either be answered directly or passed on to the relevant lecturer.

0.11 Acknowledgements

The Lecture Notes and Example Sheets were adapted from those of Paul Townsend, Stuart Dalziel, Mike Proctor, Paul Metcalfe and Henrik Latter.

0.12 Assumed Knowledge

Familiarity with the following topics at the level of Course A of Part IA Mathematics for Natural Sciences will be assumed.

- Algebra of complex numbers
- Algebra of vectors (including scalar and vector products)
- Algebra of matrices
- Eigenvalues and eigenvectors of matrices
- Taylor series and the geometric series
- Calculus of functions of several variables
- Line, surface and volume integrals
- The Gaussian integral
- First-order ordinary differential equations
- Second-order linear ODEs with constant coefficients
- Fourier series
- Permutations

More specifically, you should check that you recall the following.

The Greek alphabet.

A	α	alpha
B	β	beta
Γ	γ	gamma
Δ	δ	delta
E	ϵ	epsilon
Z	ζ	zeta
H	η	eta
Θ	θ	theta
I	ι	iota
K	κ	kappa
Λ	λ	lambda
M	μ	mu
N	ν	nu
Ξ	ξ	xi
O	o	omicron
Π	π	pi
P	ρ	rho
Σ	σ	sigma
T	τ	tau
Υ	υ	upsilon
Φ	ϕ	phi
X	χ	chi
Ψ	ψ	psi
Ω	ω	omega

There are also typographic variations on epsilon (i.e. ε), theta (i.e. ϑ), pi (i.e. ϖ), rho (i.e. ϱ), sigma (i.e. ς) and phi (i.e. φ).

The first fundamental theorem of calculus. The first fundamental theorem of calculus states that the derivative of the integral of f is f, i.e. if f is suitably 'nice' (e.g. f is continuous) then

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\int_{x_1}^{x} f(t)\,\mathrm{d}t\right) = f(x)\,. \tag{0.1}$$

Key Result

The second fundamental theorem of calculus. The second fundamental theorem of calculus states that the integral of the derivative of f is f, e.g. if f is differentiable then

$$\int_{x_1}^{x_2} \frac{\mathrm{d}f}{\mathrm{d}x}\,\mathrm{d}x = f(x_2) - f(x_1)\,. \tag{0.2}$$

Key Result

The Gaussian. The function

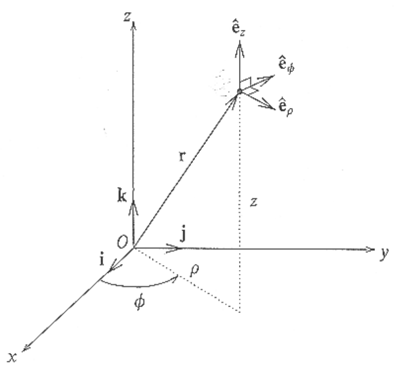
$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\Big(-\frac{x^2}{2\sigma^2}\Big) \tag{0.3}$$

is called a *Gaussian* of width σ; in context of probability theory σ is the standard deviation. The area under this curve is unity, i.e.

$$\frac{1}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty}\exp\Big(-\frac{x^2}{2\sigma^2}\Big)\,\mathrm{d}x = 1\,. \tag{0.4}$$

Key Result

Cylindrical polar co-ordinates (ρ, ϕ, z).



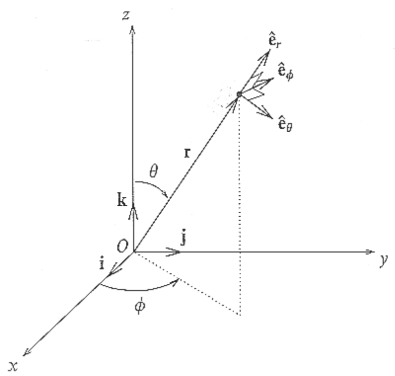
In cylindrical polar co-ordinates the position vector $\mathbf{r}$ is given in terms of a radial distance ρ from an axis $\mathbf{e}_z$, a polar angle ϕ, and the distance z along the axis:

$$\begin{aligned} \mathbf{r} &= \rho\cos\phi\,\mathbf{e}_x + \rho\sin\phi\,\mathbf{e}_y + z\,\mathbf{e}_z & \text{(0.5a)}\\ &= \rho\,\mathbf{e}_\rho + z\,\mathbf{e}_z\,, & \text{(0.5b)}\end{aligned}$$

where $0 \leqslant \rho < \infty$, $0 \leqslant \phi \leqslant 2\pi$ and $-\infty < z < \infty$.

Remark. Often r and/or θ are used in place of ρ and/or ϕ respectively (but then there is potential confusion with the different definitions of r and θ in spherical polar co-ordinates).

Spherical polar co-ordinates (r, θ, ϕ).



In spherical polar co-ordinates the position vector $\mathbf{r}$ is given in terms of a radial distance r from the origin, a 'latitude' angle θ, and a 'longitude' angle ϕ:

$$\begin{aligned} \mathbf{r} &= r\sin\theta\cos\phi\,\mathbf{e}_x + r\sin\theta\sin\phi\,\mathbf{e}_y + r\cos\theta\,\mathbf{e}_z & \text{(0.6a)}\\ &= r\mathbf{e}_r\,, & \text{(0.6b)}\end{aligned}$$

where $0 \leqslant r < \infty$, $0 \leqslant \theta \leqslant \pi$ and $0 \leqslant \phi \leqslant 2\pi$.

Taylor's theorem for functions of more than one variable. Let $f(x, y)$ be a function of two variables, then

$$\begin{aligned} f(x+\delta x, y+\delta y) &= f(x,y) + \delta x\frac{\partial f}{\partial x} + \delta y\frac{\partial f}{\partial y}\\ &\quad + \frac{1}{2!}\left((\delta x)^2\frac{\partial^2 f}{\partial x^2} + 2\delta x\delta y\frac{\partial^2 f}{\partial x\partial y} + (\delta y)^2\frac{\partial^2 f}{\partial y^2}\right)\dots\,. \end{aligned} \tag{0.7}$$

Exercise. Let $g(x, y, z)$ be a function of three variables. Expand $g(x+\delta x, y+\delta y, z+\delta z)$ correct to $O(\delta x, \delta y, \delta z)$.

Partial differentiation. For variables q_1, q_2, q_3,

$$\left(\frac{\partial q_1}{\partial q_1}\right)_{q_2,q_3} = 1\,, \quad \left(\frac{\partial q_1}{\partial q_2}\right)_{q_1,q_3} = 0\,, \quad \text{etc.}\,, \tag{0.8a}$$

and hence

$$\frac{\partial q_i}{\partial q_j} = \delta_{ij}\,, \tag{0.8b}$$

Key Result

where δ_{ij} is the Kronecker delta:

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}\,. \tag{0.9}$$

The chain rule. Let $h(x, y)$ be a function of two variables, and suppose that x and y are themselves functions of a variable s, then

$$\frac{\mathrm{d}h}{\mathrm{d}s} = \frac{\partial h}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}s} + \frac{\partial h}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}s}\,. \tag{0.10a}$$

Suppose instead that h depends on n variables x_i ($i = 1, \ldots, n$), so that $h = h(x_1, x_2, \ldots, x_n)$. If the x_i depend on m variables s_j ($j = 1, \ldots, m$), then for $j = 1, \ldots, m$

$$\frac{\partial h}{\partial s_j} = \sum_{i=1}^{n} \frac{\partial h}{\partial x_i}\frac{\partial x_i}{\partial s_j}\,. \tag{0.10b}$$

Key Result

Vector identities. Suppose that vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ have components (a_1, a_2, a_3), (b_1, b_2, b_3) and (c_1, c_2, c_3) respectively.

Scalar or dot product. The *scalar product* for $\mathbf{a}$ and $\mathbf{b}$ is given by

$$\mathbf{a}\cdot\mathbf{b} = \sum_{i=1}^{n} a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3\,. \tag{0.11a}$$

Vector or cross product. The *vector product* for $\mathbf{a}$ and $\mathbf{b}$ is given by

$$\mathbf{a}\times\mathbf{b} = (a_2\, b_3 - a_3\, b_2,\ a_3\, b_1 - a_1\, b_3,\ a_1\, b_2 - a_2\, b_1)\,. \tag{0.11b}$$

Scalar triple product. The *scalar triple product* for $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ is given by

$$(\mathbf{a}\times\mathbf{b})\cdot\mathbf{c} = a_1\, b_2\, c_3 + a_2\, b_3\, c_1 + a_3\, b_1\, c_2 - a_1\, b_3\, c_2 - a_2\, b_1\, c_3 - a_3\, b_2\, c_1 \tag{0.11c}$$

$$= \begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix}\,. \tag{0.11d}$$

Vector triple product. The *vector triple product* for $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ is given by

$$\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = (\mathbf{a}\cdot\mathbf{c})\mathbf{b} - (\mathbf{a}\cdot\mathbf{b})\mathbf{c}\,. \tag{0.11e}$$

Line integrals. Let $\mathcal{C}$ be a smooth curve, then

$$\int_{\mathcal{C}} \mathrm{d}\mathbf{r} = -\int_{-\mathcal{C}} \mathrm{d}\mathbf{r}\,. \tag{0.6}$$

Key Result

The transpose of a matrix. Let A be a 3×3 matrix:

$$\mathsf{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}\,. \tag{0.7a}$$

Then the transpose, A^{T}, of this matrix is given by

$$\mathsf{A}^{\mathrm{T}} = \begin{pmatrix} A_{11} & A_{21} & A_{31} \\ A_{12} & A_{22} & A_{32} \\ A_{13} & A_{23} & A_{33} \end{pmatrix}\,. \tag{0.7b}$$

Fourier series. Let $f(x)$ be a function with period $\mathcal{L}$, i.e. a function such that $f(x+\mathcal{L}) = f(x)$. Then the Fourier series expansion of $f(x)$ is given by

$$f(x) = \tfrac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi n x}{\mathcal{L}}\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{2\pi n x}{\mathcal{L}}\right), \tag{0.8a}$$

Key Result

where

$$a_n = \frac{2}{\mathcal{L}} \int_{x_0}^{x_0+\mathcal{L}} f(x) \cos\left(\frac{2\pi n x}{\mathcal{L}}\right) \mathrm{d}x\,, \tag{0.8b}$$

$$b_n = \frac{2}{\mathcal{L}} \int_{x_0}^{x_0+\mathcal{L}} f(x) \sin\left(\frac{2\pi n x}{\mathcal{L}}\right) \mathrm{d}x\,, \tag{0.8c}$$

and x_0 is an arbitrary constant. Also recall the orthogonality conditions

$$\int_0^{\mathcal{L}} \sin\frac{2\pi n x}{\mathcal{L}} \sin\frac{2\pi m x}{\mathcal{L}}\,\mathrm{d}x = \frac{\mathcal{L}}{2}\,\delta_{nm}\,, \tag{0.9a}$$

$$\int_0^{\mathcal{L}} \cos\frac{2\pi n x}{\mathcal{L}} \cos\frac{2\pi m x}{\mathcal{L}}\,\mathrm{d}x = \frac{\mathcal{L}}{2}\,\delta_{nm}\,, \tag{0.9b}$$

$$\int_0^{\mathcal{L}} \sin\frac{2\pi n x}{\mathcal{L}} \cos\frac{2\pi m x}{\mathcal{L}}\,\mathrm{d}x = 0\,. \tag{0.9c}$$

Let $g_{\mathrm{e}}(x)$ be an even function, i.e. a function such that $g_{\mathrm{e}}(-x) = g_{\mathrm{e}}(x)$, with period $\mathcal{L} = 2L$. Then the Fourier series expansion of $g_{\mathrm{e}}(x)$ can be expressed as

$$g_{\mathrm{e}}(x) = \tfrac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi x}{L}\right), \tag{0.10a}$$

where

$$a_n = \frac{2}{L}\int_0^L g_{\mathrm{e}}(x)\cos\left(\frac{n\pi x}{L}\right)\mathrm{d}x\,. \tag{0.10b}$$

Let $g_{\mathrm{o}}(x)$ be an odd function, i.e. a function such that $g_{\mathrm{o}}(-x) = -g_{\mathrm{o}}(x)$, with period $\mathcal{L} = 2L$. Then the Fourier series expansion of $g_{\mathrm{o}}(x)$ can be expressed as

$$g_{\mathrm{o}}(x) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right), \tag{0.11a}$$

where

$$b_n = \frac{2}{L}\int_0^L g_{\mathrm{o}}(x)\sin\left(\frac{n\pi x}{L}\right)\mathrm{d}x\,. \tag{0.11b}$$

Recall that if integrated over a half period, the 'orthogonality' conditions require care since

$$\int_0^L \sin\frac{n\pi x}{L}\sin\frac{m\pi x}{L}\,\mathrm{d}x = \frac{L}{2}\,\delta_{nm}\,, \tag{0.12a}$$

$$\int_0^L \cos\frac{n\pi x}{L}\cos\frac{m\pi x}{L}\,\mathrm{d}x = \frac{L}{2}\,\delta_{nm}\,, \tag{0.12b}$$

but

$$\int_0^L \sin\frac{n\pi x}{L}\cos\frac{m\pi x}{L}\,\mathrm{d}x = \begin{cases} 0 & \text{if } n+m \text{ is even,} \\ \dfrac{2nL}{\pi(n^2-m^2)} & \text{if } n+m \text{ is odd.} \end{cases} \tag{0.12c}$$

Permutations A permutation of degree n is a function that rearranges n distinct objects, such as the first n strictly positive integers $\{1, 2, \ldots, n\}$, amongst themselves.

An *even (odd) permutation* is one consisting of an even (odd) number of transpositions (interchanges of two neighbouring objects).

If $n = 3$ there are 6 permutations (including the identity permutation) that re-arrange $\{1, 2, 3\}$ to

$$\{1, 2, 3\},\ \{2, 3, 1\},\ \{3, 1, 2\}, \tag{0.13a}$$

$$\{1, 3, 2\},\ \{2, 1, 3\},\ \{3, 2, 1\}. \tag{0.13b}$$

(0.13a) and (0.13b) are, respectively, even and odd permutations of $\{1, 2, 3\}$.

Suggestions.

Examples.

1. Include Ampere's law, Faraday's law, etc., somewhere (see 1997 Vector Calculus notes).

Additions/Subtractions?

1. Remove all the `\enlargethispage` commands.
2. 2D divergence theorem, Green's theorem (e.g. as a special case of Stokes' theorem).
3. Add Fourier transforms of $\cos x$, $\sin x$ and periodic functions.
4. Check that the addendum at the end of § 3 has been incorporated into the main section.
5. Swap § 4.7.1 and § 3.5.
6. Swap § 5.2 and § 5.4.
7. Explain that observables in quantum mechanics are Hermitian operators.
8. Come up with a better explanation of why for a transformation matrix, say A, $\det \mathsf{A} \neq 0$.

1 Vector Calculus

1.0 Why Study This?

Scientific quantities can be of different kinds.

- Many scientific quantities just have a magnitude (and sign), e.g. time, temperature, mass, density, concentration, energy. Such quantities can be completely specified by a single number. We refer to such numbers as *scalars*. You have learnt how to manipulate such scalars (e.g. by addition, subtraction, multiplication, differentiation) since your first day in school (or possibly before that).

- However other quantities have both a magnitude and a direction, e.g. the position of a particle, the velocity of a particle, the direction of propagation of a wave, a force, an electric field, a magnetic field. You need to know how to manipulate these quantities (e.g. by addition, subtraction, multiplication, differentiation) if you are to be able to describe them mathematically.

A *field* is a quantity that depends continuously on position (and possibly on time). Examples include:

- air pressure in this room (scalar field)

- electric field in this room (vector field)

Vector calculus is concerned with scalar and vector fields. The spatial variation of fields is described by *vector differential operators*, which appear in the *partial differential equations* governing the fields.

Vector calculus is most easily done in Cartesian coordinates, but other systems (*curvilinear coordinates*) are better suited for some problems because of symmetries or boundary conditions.

1.1 Vectors and Bases

1.1.1 Three-dimensional Euclidean space, points and vectors

This is a close approximation to our physical space:

- *points* are the elements of the space

- *vectors* are translatable, directed line segments

- *Euclidean* means that lengths and angles obey the classical results of geometry

Definition. A quantity that is specified by a [positive] magnitude and a direction in space is called a *vector*.

Example. A point P in 3D (or 2D) space can be specified by giving its *position vector*, $\mathbf{r}$, from some chosen origin 0.

1.1.2 Bases

Points and vectors have a geometrical existence without reference to any coordinate system. However, it is often very useful to describe them in term of a *basis* for the space. Three non-zero vectors $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ can form a basis in 3D space if they do not all lie in a plane, i.e. they are *linearly independent*. Any vector can be expressed uniquely in terms of scalar multiples of the basis vectors:

$$\mathbf{v} \quad = \quad v_1\mathbf{e}_1 + v_2\mathbf{e}_2 + v_3\mathbf{e}_3. \tag{1.1}$$

The v_i $(i = 1, 2, 3)$ are said to the *components* of the vector $\mathbf{v}$ with respect to this basis.

Remark. The choice of basis is not unique. The components of a vector are different with respect to two different bases.

Definition. The $\mathbf{e}_i$ $(i = 1, 2, 3)$ need not have unit magnitude and/or be orthogonal. However calculations, etc. are much simpler if the $\mathbf{e}_i$ $(i = 1, 2, 3)$ define a *orthonormal basis*, for which the basis vectors have unit magnitude and are mutually orthogonal, i.e.

$$\mathbf{e}_1\cdot\mathbf{e}_1 = \mathbf{e}_2\cdot\mathbf{e}_2 = \mathbf{e}_3\cdot\mathbf{e}_3 = 1\,, \tag{1.2a}$$

$$\mathbf{e}_1\cdot\mathbf{e}_2 = \mathbf{e}_2\cdot\mathbf{e}_3 = \mathbf{e}_3\cdot\mathbf{e}_1 = 0\,, \tag{1.2b}$$

or equivalently

$$|\mathbf{e}_i| = 1\,, \quad \mathbf{e}_i \cdot \mathbf{e}_j = 0 \quad \text{if } i \neq j, \quad i, j = 1, 2, 3. \tag{1.2c}$$

The orthonormal basis is *right-handed* if

$$\mathbf{e}_1 \times \mathbf{e}_2 = \mathbf{e}_3, \tag{1.3}$$

so that the *ordered* triple scalar product of the basis vectors is positive:

$$[\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3] = \mathbf{e}_1 \times \mathbf{e}_2 \cdot \mathbf{e}_3 = 1\,. \tag{1.4}$$

Exercise. Show using (1.2c) and (1.3) that

$$\mathbf{e}_2 \times \mathbf{e}_3 = \mathbf{e}_1 \quad \text{and that} \quad \mathbf{e}_3 \times \mathbf{e}_1 = \mathbf{e}_2\,. \tag{1.5}$$

1.1.3 Cartesian Coordinate Systems

We can set up a *Cartesian coordinate system* by identifying $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ with unit vectors pointing in the x, y and z directions respectively. The position vector $\mathbf{r}$ is then given by

$$\mathbf{r} = x\,\mathbf{e}_1 + y\,\mathbf{e}_2 + z\,\mathbf{e}_3 \tag{1.6a}$$

$$= (x, y, z)\,, \tag{1.6b}$$

where (x, y, z) are the *Cartesian components* of the position vector.

Remarks.

1. We shall sometimes write x_1 for x, x_2 for y and x_3 for z.
2. Alternative notations for a Cartesian basis in $\mathbb{R}^3$ (i.e. 3D) include

$$\mathbf{e}_1 = \mathbf{e}_x = \mathbf{i} = \hat{\mathbf{i}} = \hat{\mathbf{x}} = \widehat{\mathbf{x}}_1\,, \quad \mathbf{e}_2 = \mathbf{e}_y = \mathbf{j} = \hat{\mathbf{j}} = \hat{\mathbf{y}} = \widehat{\mathbf{x}}_2 \quad \text{and} \quad \mathbf{e}_3 = \mathbf{e}_z = \mathbf{k} = \hat{\mathbf{k}} = \hat{\mathbf{z}} = \widehat{\mathbf{x}}_3\,, \tag{1.7}$$

for the unit vectors in the x, y and z directions respectively. Hence from (1.2c) and (1.5)

$$\mathbf{i}.\mathbf{i} = \mathbf{j}.\mathbf{j} = \mathbf{k}.\mathbf{k} = 1\,, \quad \mathbf{i}.\mathbf{j} = \mathbf{j}.\mathbf{k} = \mathbf{k}.\mathbf{i} = 0\,, \tag{1.8a}$$

$$\mathbf{i} \times \mathbf{j} = \mathbf{k}\,, \quad \mathbf{j} \times \mathbf{k} = \mathbf{i}\,, \quad \mathbf{k} \times \mathbf{i} = \mathbf{j}\,. \tag{1.8b}$$

3. Two different bases, if both orthonormal and right-handed, are simply related by a rotation.
4. The Cartesian components of a vector are different with respect to two different Cartesian bases.

1.2 Suffix Notation

So far we have used *dyadic notation* for vectors. *Suffix notation* is an alternative means of expressing vectors (and tensors). Once familiar with suffix notation, it is generally easier to manipulate vectors using suffix notation.[6]

An alternative to the notation used for the vector (1.1), is to write

$$\mathbf{v} = v_1\mathbf{e}_1 + v_2\mathbf{e}_2 + v_3\mathbf{e}_3 = (v_1, v_2, v_3) \tag{1.9a}$$

$$= \{v_i\} \quad \text{for} \quad i = 1, 2, 3\,. \tag{1.9b}$$

Suffix notation. We will refer to $\mathbf{v}$ as $\{v_i\}$, with the $i = 1, 2, 3$ understood; i is then termed a *free suffix.*

Remark. Sometimes we will denote the i^{th} component of the vector $\mathbf{v}$ by $(\mathbf{v})_i$, i.e. $(\mathbf{v})_i = v_i$.

Example: the position vector. The position vector $\mathbf{r}$ can be written as

$$\mathbf{r} = (x, y, z) = (x_1, x_2, x_3) = \{x_i\}\,. \tag{1.10}$$

Remark. The use of $\mathbf{x}$, rather than $\mathbf{r}$, for the position vector in dyadic notation possibly seems more understandable given the above expression for the position vector in suffix notation. Henceforth we will use $\mathbf{x}$ and $\mathbf{r}$ interchangeably.

1.2.1 Dyadic and suffix equivalents

If two vectors $\mathbf{a}$ and $\mathbf{b}$ are equal, we write

$$\mathbf{a} = \mathbf{b}\,, \tag{1.11a}$$

or equivalently in component form

$$a_1 = b_1\,, \tag{1.11b}$$

$$a_2 = b_2\,, \tag{1.11c}$$

$$a_3 = b_3\,. \tag{1.11d}$$

In suffix notation we express this equality as

$$a_i = b_i \quad \text{for} \quad i = 1, 2, 3\,. \tag{1.11e}$$

This is a vector equation; when we omit the 'for $i = 1, 2, 3$', it is understood that the one free suffix i ranges through $1, 2, 3$ (or $1, 2$ in 2D) so as to give three component equations. Similarly

$$\begin{aligned} \mathbf{c} = \lambda\mathbf{a} + \mu\mathbf{b} \quad &\Leftrightarrow \quad c_i = \lambda a_i + \mu b_i \\ &\Leftrightarrow \quad c_j = \lambda a_j + \mu b_j \\ &\Leftrightarrow \quad c_\alpha = \lambda a_\alpha + \mu b_\alpha \\ &\Leftrightarrow \quad c_{¥} = \lambda a_{¥} + \mu b_{¥}\,, \end{aligned}$$

where is is assumed that i, j, α and ¥, respectively, range through $(1, 2, 3)$.[7]

Remark. It does not matter what letter, or symbol, is chosen for the free suffix, but it must be the same in each term.

Dummy suffices. In suffix notation the scalar product becomes

$$\begin{aligned} \mathbf{a}\cdot\mathbf{b} &= a_1b_1 + a_2b_2 + a_3b_3 \\ &= \sum_{i=1}^{3} a_ib_i \\ &= \sum_{k=1}^{3} a_kb_k\,, \quad \text{etc.,} \end{aligned}$$

[6] Although there are dissenters to that view.

[7] In higher dimensions the suffices would be assumed to range through the number of dimensions.

where the i, k, etc. are referred to as *dummy suffices* since they are 'summed out' of the equation. Similarly

$$\mathbf{a}\cdot\mathbf{b}=\lambda \quad \Leftrightarrow \quad \sum_{\alpha=1}^{3} a_\alpha b_\alpha = \lambda\,,$$

where we note that the equivalent equation on the right hand side has no free suffices since the dummy suffix (in this case α) has again been summed out.

Further examples.

(i) As another example consider the equation $(\mathbf{a}\cdot\mathbf{b})\mathbf{c}=\mathbf{d}$. In suffix notation this becomes

$$\sum_{k=1}^{3}(a_k b_k)\,c_i = \sum_{k=1}^{3} a_k b_k c_i = d_i\,, \tag{1.12}$$

where k is the dummy suffix, and i is the free suffix that is assumed to range through $(1,2,3)$. It is essential that we used different symbols for both the dummy and free suffices!

(ii) In suffix notation the expression $(\mathbf{a}\cdot\mathbf{b})(\mathbf{c}\cdot\mathbf{d})$ becomes

$$\begin{aligned}(\mathbf{a}\cdot\mathbf{b})(\mathbf{c}\cdot\mathbf{d}) &= \left(\sum_{i=1}^{3} a_i b_i\right)\left(\sum_{j=1}^{3} c_j d_j\right)\\ &= \sum_{i=1}^{3}\sum_{j=1}^{3} a_i b_i c_j d_j\,,\end{aligned}$$

where, especially after the rearrangement, it is essential that the dummy suffices are different.

1.2.2 Summation convention

In the case of free suffices we are assuming that they range through $(1,2,3)$ without the need to explicitly say so. Under Einstein's summation convention the explicit sum, $\sum$, can be omitted for dummy suffices.[8] In particular

- if a suffix appears once it is taken to be a free suffix and ranged through,
- if a suffix appears twice it is taken to be a dummy suffix and summed over,
- if a suffix appears more than twice *in one term* of an equation, ***something has gone wrong*** (unless there is an explicit sum).

Remark. This notation is powerful because it is highly abbreviated (and so aids calculation, especially in examinations), but the above rules *must* be followed, and remember to check your answers (e.g. the free suffices should be identical on each side of an equation).

Examples. Under suffix notation and the summation convention

$$\begin{aligned}\mathbf{a}+\mathbf{b}=\mathbf{c} &\quad \text{can be written as} \quad a_i+b_i=c_i\,,\\ (\mathbf{a}\cdot\mathbf{b})\mathbf{c}=\mathbf{d} &\quad \text{can be written as} \quad a_i\,b_i\,c_j=d_j\,,\\ ((\mathbf{a}\cdot\mathbf{b})\mathbf{c}-(\mathbf{a}\cdot\mathbf{c})\mathbf{b})_j &\quad \text{can be written as} \quad a_i\,b_i\,c_j-a_k\,c_k\,b_j\,,\\ &\quad \text{or can be written as} \quad a_i\,b_i\,c_j-a_i\,c_i\,b_j\,,\\ &\quad \text{or can be written as} \quad a_i(b_i\,c_j-c_i\,b_j)\,.\end{aligned}$$

[8] Learning to omit the explicit sum is a bit like learning to change gear when starting to drive. At first you have to remind yourself that the sum is there, in the same way that you have to think consciously where to move gear knob. **With practice** you will learn to note the existence of the sum unconsciously, in the same way that an experienced driver changes gear unconsciously; however you will crash a few gears on the way!

Under suffix notation the following equations make no sense

$$a_k = b_j \qquad \text{because the free suffices are different,}$$

$$((\mathbf{a}\cdot\mathbf{b})\mathbf{c})_i = a_i\, b_i\, c_i \qquad \text{because } i \text{ is repeated more than twice in one term on the left-hand side.}$$

Under suffix notation the following equation is problematical (and probably best avoided unless you will always remember to double count the i on the right-hand side)

$$n_i\, n_i = n_i^2 \quad \text{because } i \text{ occurs twice on the left-hand side and only once on the right-hand side.}$$

01/22 *Remark.* If the summation convention is *not* being used, this should be noted explicitly.

1.2.3 Matrix expressions

Transpose of a matrix (A):

$$(\mathsf{A}^{\mathrm{T}})_{ij} = A_{ji}\,.$$

Trace of a matrix (A):

$$\operatorname{tr}\mathsf{A} = A_{ii}\,.$$

Matrix (A) times vector (x):

$$\mathsf{y} = \mathsf{A}\mathsf{x} \quad \Leftrightarrow \quad y_i = A_{ij}x_j\,.$$

Matrix (B) times matrix (C):

$$\mathsf{A} = \mathsf{B}\mathsf{C} \quad \Leftrightarrow \quad A_{ij} = B_{ik}C_{kj}\,.$$

Determinant of a (3×3) matrix (A), where (if you have not met it before) ε_{ijk} is defined in (1.18) below:

$$\det\mathsf{A} = \varepsilon_{ijk}A_{1i}A_{2j}A_{3k}\,.$$

1.2.4 Kronecker delta

The Kronecker delta, δ_{ij}, $i,j = 1,2,3$, is a set of nine numbers defined by

$$\delta_{11} = 1\,,\quad \delta_{22} = 1\,,\quad \delta_{33} = 1\,, \tag{1.13a}$$

$$\delta_{ij} = 0 \quad \text{if} \quad i \neq j\,. \tag{1.13b}$$

This can be written as a *matrix* equation:

$$\begin{pmatrix} \delta_{11} & \delta_{12} & \delta_{13} \\ \delta_{21} & \delta_{22} & \delta_{23} \\ \delta_{31} & \delta_{32} & \delta_{33} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathsf{1}\,. \tag{1.13c}$$

Properties.

(i) δ_{ij} is symmetric, i.e.

$$\delta_{ij} = \delta_{ji}\,.$$

(ii) Using the definition of the delta function:

$$\begin{aligned} a_i\delta_{i1} &= \sum_{i=1}^{3} a_i\delta_{i1} = a_1\delta_{11} + a_2\delta_{21} + a_3\delta_{31} \\ &= a_1\,. \end{aligned} \tag{1.14a}$$

i.e. $\mathsf{a}\mathsf{1} = \mathsf{a}$. Similarly

$$a_i\delta_{ij} = a_j\,, \tag{1.14b}$$

$$a_j\delta_{ij} = a_i\,. \tag{1.14c}$$

(iii)

$$\delta_{ij}\delta_{jk} = \sum_{j=1}^{3} \delta_{ij}\delta_{jk} = \delta_{ik}\,. \tag{1.14d}$$

(iv)

$$\delta_{ii} = \sum_{i=1}^{3} \delta_{ii} = \delta_{11} + \delta_{22} + \delta_{33} = 3\,. \tag{1.14e}$$

(v)

$$a_p\,\delta_{pq}\,b_q = a_p\,b_p = a_q\,b_q = \mathbf{a}\cdot\mathbf{b}\,. \tag{1.14f}$$

(vi) From (1.2c)

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}\,. \tag{1.14g}$$

Contraction. Contraction is an operation by which we set one free index equal to another, so that it is summed over. For example, the contraction of a_{ij} is a_{ii}. Contraction is equivalent to multiplication by a Kronecker delta:

$$a_{ij}\delta_{ij} = a_{11} + a_{22} + a_{33} = a_{ii}\,. \tag{1.15}$$

1.2.5 More on basis vectors (Unlectured)

An alternative notation to $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ is $\mathbf{e}^{(1)}$, $\mathbf{e}^{(2)}$ and $\mathbf{e}^{(3)}$, where the use of superscripts may help emphasise that the 1, 2 and 3 are labels rather than components.

Then in terms of the superscript notation

$$\mathbf{e}^{(i)} \cdot \mathbf{e}^{(j)} = \delta_{ij}\,, \tag{1.16a}$$

$$\mathbf{a} \cdot \mathbf{e}^{(i)} = a_i\,. \tag{1.16b}$$

Thus the ith component of $\mathbf{e}^{(j)}$ is given by

$$\begin{aligned} \left(\mathbf{e}^{(j)}\right)_i &= \mathbf{e}^{(j)} \cdot \mathbf{e}^{(i)} \\ &= \delta_{ij}\,. \end{aligned} \tag{1.16c}$$

Similarly

$$\left(\mathbf{e}^{(i)}\right)_j = \delta_{ij}\,, \tag{1.16d}$$

and equivalently

$$\left(\mathbf{e}_j\right)_i = \left(\mathbf{e}_i\right)_j = \delta_{ij}\,. \tag{1.16e}$$

1.2.6 The Levi-Civita symbol or alternating tensor

Revision. A permutation of degree n is a function that rearranges n distinct objects (taken in our case to be the first n strictly positive integers $\{1, 2, \ldots, n\}$) amongst themselves.

If $n = 3$ there are 6 permutations (including the identity permutation) that re-arrange $\{1, 2, 3\}$ to

$$\{1,2,3\},\ \{2,3,1\},\ \{3,1,2\}, \tag{1.17a}$$

$$\{1,3,2\},\ \{2,1,3\},\ \{3,2,1\}. \tag{1.17b}$$

An *even (odd) permutation* is one consisting of an even (odd) number of transpositions (interchanges of two neighbouring objects). Hence, (1.17a) and (1.17b) are, respectively, even and odd permutations of $\{1, 2, 3\}$.

Definition 1.1. *We define the Levi-Civita permutation symbol, ε_{ijk} $(i, j, k = 1, 2, 3)$, to be the set of 27 quantities such that*

$$\varepsilon_{ijk} = \begin{cases} 1 & \textit{if } i\,j\,k \textit{ is an even permutation of } 1,\,2,\,3; \\ -1 & \textit{if } i\,j\,k \textit{ is an odd permutation of } 1,\,2,\,3; \\ 0 & \textit{otherwise} \end{cases} \tag{1.18}$$

The non-zero components of ε_{ijk} are therefore

$$\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1 \tag{1.19a}$$

$$\varepsilon_{132} = \varepsilon_{213} = \varepsilon_{321} = -1 \tag{1.19b}$$

Further

$$\varepsilon_{ijk} = \varepsilon_{jki} = \varepsilon_{kij} = -\varepsilon_{ikj} = -\varepsilon_{kji} = -\varepsilon_{jik}\,. \tag{1.19c}$$

Worked exercise.

For a symmetric tensor s_{ij}, $i, j = 1, 2, 3$, such that $s_{ij} = s_{ji}$ evaluate $\varepsilon_{ijk} s_{ij}$.

Solution. By relabelling the dummy suffices we have from (1.19c) and the symmetry of s_{ij} that

$$\sum_{i=1}^{3}\sum_{j=1}^{3} \varepsilon_{ijk} s_{ij} = \sum_{a=1}^{3}\sum_{b=1}^{3} \varepsilon_{abk} s_{ab} = \sum_{j=1}^{3}\sum_{i=1}^{3} \varepsilon_{jik} s_{ji} = \sum_{i=1}^{3}\sum_{j=1}^{3} - \varepsilon_{ijk} s_{ij}\,, \tag{1.20a}$$

or equivalently by using the summation convention

$$\varepsilon_{ijk} s_{ij} = \varepsilon_{abk} s_{ab} = \varepsilon_{jik} s_{ji} = -\varepsilon_{ijk} s_{ij}\,, \tag{1.20b}$$

where we have successively relabelled $i \to a \to j$ and $j \to b \to i$. Hence we conclude that

$$\varepsilon_{ijk} s_{ij} = 0\,. \tag{1.20c}$$

1.2.7 The vector product in suffix notation

We claim that

$$(\mathbf{a} \times \mathbf{b})_i = \sum_{j=1}^{3}\sum_{k=1}^{3} \varepsilon_{ijk}\, a_j\, b_k = \varepsilon_{ijk}\, a_j\, b_k\,, \tag{1.21}$$

where we note that there is one free suffix and two dummy suffices.

Check.

$$(\mathbf{a} \times \mathbf{b})_1 = \sum_{j=1}^{3}\sum_{k=1}^{3} \varepsilon_{1jk}\, a_j\, b_k = \varepsilon_{123}\, a_2\, b_3 + \varepsilon_{132}\, a_3\, b_2 = a_2\, b_3 - a_3\, b_2\,,$$

in agreement with (0.11b). Do we need to do more?

Remark. Equivalently

$$\begin{aligned} \mathbf{a} \times \mathbf{b} &= \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} \\ &= \varepsilon_{ijk} \mathbf{e}_i a_j b_k\,. \end{aligned} \tag{1.22}$$

Example. From (1.14b), (1.16e) and (1.21)

$$\begin{aligned} \left(\mathbf{e}_j \times \mathbf{e}_k\right)_i &= \varepsilon_{ilm} \left(\mathbf{e}_j\right)_l \left(\mathbf{e}_k\right)_m \\ &= \varepsilon_{ilm}\, \delta_{jl}\, \delta_{km} \\ &= \varepsilon_{ijk}\,. \end{aligned} \tag{1.23}$$

1.2.8 The product of two Levi-Civita symbols

We claim that

$$\varepsilon_{ijk}\varepsilon_{lmn} = \begin{vmatrix} \delta_{il} & \delta_{im} & \delta_{in} \\ \delta_{jl} & \delta_{jm} & \delta_{jn} \\ \delta_{kl} & \delta_{km} & \delta_{kn} \end{vmatrix}\,. \tag{1.24}$$

As proof we observe that the value of both the LHS and the RHS:

(i) is 0 when any of (i, j, k) are equal (two rows equal in a determinant), or when any of (l, m, n) are equal (two columns equal in a determinant);

(ii) is 1 when $(i, j, k) = (l, m, n) = (1, 2, 3)$;

(iii) changes sign when any of (i, j, k) are interchanged (row interchange in a determinant), or when any of (l, m, n) are interchanged (column interchange in a determinant). □

Remark. The first property is implied by the third.

A contracted identity. We contract the identity (1.24) once by setting $l = i$, then using (1.14d) and (1.14e):

$$\begin{aligned}\varepsilon_{ijk}\varepsilon_{imn} &= \begin{vmatrix}\delta_{ii} & \delta_{im} & \delta_{in}\\ \delta_{ji} & \delta_{jm} & \delta_{jn}\\ \delta_{ki} & \delta_{km} & \delta_{kn}\end{vmatrix}\\ &= \delta_{ii}(\delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}) + \delta_{im}(\delta_{jn}\delta_{ki} - \delta_{ji}\delta_{kn}) + \delta_{in}(\delta_{ji}\delta_{km} - \delta_{jm}\delta_{ki})\\ &= 3(\delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}) + (\delta_{jn}\delta_{km} - \delta_{jm}\delta_{kn}) + (\delta_{jn}\delta_{km} - \delta_{jm}\delta_{kn})\\ &= \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}\end{aligned} \tag{1.25a}$$

This is the most useful form to remember:

$$\boxed{\varepsilon_{ijk}\varepsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}} \tag{1.25b}$$

Remarks.

(i) There are four free suffices/indices on each side, with i as a dummy suffix on the left-hand side. Hence (1.25b) represents 3^4 equations.

(ii) Given any product of two epsilons with one common index, the indices can be permuted cyclically into this form, for instance:

$$\varepsilon_{\alpha\beta\gamma}\varepsilon_{\mu\nu\beta} = \varepsilon_{\beta\gamma\alpha}\varepsilon_{\beta\mu\nu} = \delta_{\gamma\mu}\delta_{\alpha\nu} - \delta_{\gamma\nu}\delta_{\alpha\mu} \tag{1.25c}$$

Contracted^2 and contracted^3 identities. A further contraction of the identity (1.24) yields from (1.25b)

$$\begin{aligned}\varepsilon_{ijk}\varepsilon_{ijn} &= \delta_{jj}\delta_{kn} - \delta_{jn}\delta_{kj}\\ &= 3\delta_{kn} - \delta_{kn}\\ &= 2\delta_{kn}\,,\end{aligned} \tag{1.26a}$$

while a further contraction yields

$$\varepsilon_{ijk}\varepsilon_{ijk} = 6\,. \tag{1.26b}$$

Example. Show that

$$(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{c}\times\mathbf{d}) = (\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{d}) - (\mathbf{a}\cdot\mathbf{d})(\mathbf{b}\cdot\mathbf{c})\,.$$

Solution.

$$\begin{aligned}(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{c}\times\mathbf{d}) &= (\mathbf{a}\times\mathbf{b})_i(\mathbf{c}\times\mathbf{d})_i\\ &= (\varepsilon_{ijk}a_jb_k)(\varepsilon_{ilm}c_ld_m) && \text{from (1.21)}\\ &= \varepsilon_{ijk}\varepsilon_{ilm}a_jb_kc_ld_m\\ &= (\delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl})a_jb_kc_ld_m && \text{from (1.25b)}\\ &= a_jb_kc_jd_k - a_jb_kc_kd_j && \text{from (1.14b) and (1.14c)}\\ &= (a_jc_j)(b_kd_k) - (a_jd_j)(b_kc_k)\\ &= (\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{d}) - (\mathbf{a}\cdot\mathbf{d})(\mathbf{b}\cdot\mathbf{c})\,.\end{aligned}$$

Scalar triple product. In suffix notation the scalar triple product is given by

$$\begin{aligned}\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) &= a_i(\mathbf{b}\times\mathbf{c})_i\\ &= \varepsilon_{ijk}\,a_i\,b_j\,c_k\,.\end{aligned} \tag{1.27a}$$

Vector triple product. Using suffix notation for the vector triple product, we recover in agreement with (0.11e):

$$\begin{aligned}\big(\mathbf{a}\times(\mathbf{b}\times\mathbf{c})\big)_i &= \varepsilon_{ijk}\,a_j\,(\mathbf{b}\times\mathbf{c})_k\\ &= \varepsilon_{ijk}\,a_j\,\varepsilon_{klm}\,b_l\,c_m && \text{only two identical sufficies}\\ &= \varepsilon_{kij}\,\varepsilon_{klm}\,a_j\,b_l\,c_m && \text{from (1.19c) permutate the sufficies}\\ &= (\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl})\,a_j\,b_l\,c_m && \text{from (1.25b)}\\ &= a_j\,b_i\,c_j - a_j\,b_j\,c_i && \text{from (1.14b) and (1.14c)}\\ &= \big((\mathbf{a}\cdot\mathbf{c})\mathbf{b} - (\mathbf{a}\cdot\mathbf{b})\mathbf{c}\big)_i\,.\end{aligned} \tag{1.27b}$$

1.2.9 A proof of Schwarz's inequality (Unlectured)

There is an elegant proof of Schwarz's inequality (which works in n-dimensions) using the summation convention:

$$\begin{aligned}\|\mathbf{x}\|^2\|\mathbf{y}\|^2 - |\mathbf{x}\cdot\mathbf{y}|^2 &= x_i x_i y_j y_j - x_i y_i x_j y_j \\ &= \tfrac{1}{2}x_i x_i y_j y_j + \tfrac{1}{2}x_j x_j y_i y_i - x_i y_i x_j y_j \qquad \text{relabel indicies in half the first term} \\ &= \tfrac{1}{2}(x_i y_j - x_j y_i)(x_i y_j - x_j y_i) \qquad \text{factorize} \\ &\geqslant 0\,.\end{aligned}$$

1.3 Vector Calculus in Cartesian Coordinates.

1.3.1 The Gradient of a Scalar Field

Let $\psi(\mathbf{r})$ be a *scalar field*, i.e. a scalar function of position $\mathbf{r} = (x, y, z)$.

Examples of scalar fields include temperature and density.

Consider a small change to the position $\mathbf{r}$, say to $\mathbf{r} + \delta\mathbf{r}$. This small change in position will generally produce a small change in ψ. We estimate this change in ψ using the Taylor series for a function of many variables, as follows:

$$\begin{aligned}\delta\psi \equiv \psi(\mathbf{r}+\delta\mathbf{r}) - \psi(\mathbf{r}) &= \psi(x+\delta x, y+\delta y, z+\delta z) - \psi(x,y,z) \\ &= \frac{\partial\psi}{\partial x}\delta x + \frac{\partial\psi}{\partial y}\delta y + \frac{\partial\psi}{\partial z}\delta z + \dots \\ &= \left(\frac{\partial\psi}{\partial x}\mathbf{e}_x + \frac{\partial\psi}{\partial y}\mathbf{e}_y + \frac{\partial\psi}{\partial z}\mathbf{e}_z\right)\cdot(\delta x\,\mathbf{e}_x + \delta y\,\mathbf{e}_y + \delta z\,\mathbf{e}_z) + \dots \\ &= \boldsymbol{\nabla}\psi\cdot\delta\mathbf{r} + \dots\,, \end{aligned} \tag{1.28a}$$

where, using the shorthand $\sum_j$ for $\sum_{j=1}^3$, the *gradient* of ψ is defined by

$$\begin{aligned}\operatorname{grad}\psi \equiv \boldsymbol{\nabla}\psi &= \frac{\partial\psi}{\partial x}\mathbf{e}_x + \frac{\partial\psi}{\partial y}\mathbf{e}_y + \frac{\partial\psi}{\partial z}\mathbf{e}_z \\ &= \sum_j \frac{\partial\psi}{\partial x_j}\mathbf{e}_j\,. \end{aligned} \tag{1.28b}$$

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In the limit when $\delta\bullet$ becomes infinitesimal we write $\mathrm{d}\bullet$ for $\delta\bullet$.[9] Thus we have that

$$\mathrm{d}\psi = \boldsymbol{\nabla}\psi\cdot\mathrm{d}\mathbf{r}\,. \tag{1.29}$$

We can define the vector differential operator $\boldsymbol{\nabla}$ (pronounced 'grad') independently of ψ by writing

$$\boldsymbol{\nabla} \equiv \mathbf{e}_x\frac{\partial}{\partial x} + \mathbf{e}_y\frac{\partial}{\partial y} + \mathbf{e}_z\frac{\partial}{\partial z} = \sum_j \mathbf{e}_j\frac{\partial}{\partial x_j} \tag{1.30a}$$

Key Results

$$= \mathbf{e}_j\frac{\partial}{\partial x_j}\,, \qquad \text{using the summation convention.} \tag{1.30b}$$

[9] This is a bit of a 'fudge' because, strictly, a differential $\mathrm{d}\bullet$ need not be small ... but there is no quick way out.

1.3.2 Example

Find $\boldsymbol{\nabla} f$, where $f(r)$ is a function of $r = |\mathbf{r}|$. *We will use this result later.*

Answer. First recall that $r^2 = x^2 + y^2 + z^2$. Hence

$$2r\frac{\partial r}{\partial x} = 2x\,, \quad \text{i.e.} \quad \frac{\partial r}{\partial x} = \frac{x}{r}\,. \tag{1.31a}$$

Similarly, by use of the permutations $x \to y$, $y \to z$ and $z \to x$,

$$\frac{\partial r}{\partial y} = \frac{y}{r}\,, \quad \frac{\partial r}{\partial z} = \frac{z}{r}\,. \tag{1.31b}$$

Hence, from the definition of gradient (1.28b),

$$\boldsymbol{\nabla} r = \left(\frac{\partial r}{\partial x}, \frac{\partial r}{\partial y}, \frac{\partial r}{\partial z}\right) = \left(\frac{x}{r}, \frac{y}{r}, \frac{z}{r}\right) = \frac{\mathbf{r}}{r}\,. \tag{1.32}$$

Key Result

Similarly, from the definition of gradient (1.28b) (and from standard results for the derivative of a function of a function),

$$\begin{aligned}
\boldsymbol{\nabla} f(r) &= \left(\frac{\partial f(r)}{\partial x}, \frac{\partial f(r)}{\partial y}, \frac{\partial f(r)}{\partial z}\right) \\
&= \left(\frac{\mathrm{d}f}{\mathrm{d}r}\frac{\partial r}{\partial x}, \frac{\mathrm{d}f}{\mathrm{d}r}\frac{\partial r}{\partial y}, \frac{\mathrm{d}f}{\mathrm{d}r}\frac{\partial r}{\partial z}\right) \\
&= f'(r)\boldsymbol{\nabla} r & (1.33a)\\
&= f'(r)\frac{\mathbf{r}}{r}\,. & (1.33b)
\end{aligned}$$

1.3.3 The Geometrical Significance of Gradient

The directional derivative. Consider the rate of change of ψ in the direction given by the unit vector $\mathbf{l}$. If we regard $\psi(\mathbf{r}+s\mathbf{l})$ as a function of the single variable s, then a Taylor series expansion yields

$$\delta\psi = \psi(\mathbf{r} + \delta s\,\mathbf{l}) - \psi(\mathbf{r}) = \delta s\,\frac{\mathrm{d}}{\mathrm{d}s}\psi(\mathbf{r}+s\mathbf{l})\bigg|_{s=0} + \dots\,,$$

or in the limit of δs becoming infinitesimal,

$$\mathrm{d}\psi = \mathrm{d}s\,\frac{\mathrm{d}}{\mathrm{d}s}\psi(\mathbf{r}+s\mathbf{l})\bigg|_{s=0}\,. \tag{1.34a}$$

But from (1.29) with $\mathrm{d}\mathbf{r} = \mathrm{d}s\,\mathbf{l}$,

$$\mathrm{d}\psi = \mathrm{d}s\,(\mathbf{l}\cdot\boldsymbol{\nabla}\psi)\,. \tag{1.34b}$$

Since (1.34a) and (1.34b) hold for all $\mathrm{d}s$, it follows that

$$\mathbf{l}\cdot\boldsymbol{\nabla}\psi = \frac{\mathrm{d}}{\mathrm{d}s}\psi(\mathbf{r}+s\mathbf{l})\bigg|_{s=0}\,. \tag{1.35}$$

Hence $\mathbf{l}\cdot\boldsymbol{\nabla}\psi$ is the rate of change of ψ in the direction $\mathbf{l}$. It is referred to as a *directional derivative*.

Remarks.

(i) More generally, the rate of change of ψ with arclength s along a curve is $\mathrm{d}\psi/\mathrm{d}s = \mathbf{l}\cdot\operatorname{grad}\psi$, where $\mathbf{l} = \mathrm{d}\mathbf{r}/\mathrm{d}s$ is the unit tangent vector to the curve.

(ii) When the directional derivative is zero, i.e. $\mathbf{l}\cdot\boldsymbol{\nabla}\psi = 0$, it follows that if $\boldsymbol{\nabla}\psi \neq 0$, then ψ does not change in the direction of $\mathbf{l}$; hence $\mathbf{l}$ is a tangent to the surface $\psi = \text{constant}$.

(iii) Moreover, we deduce that when $\boldsymbol{\nabla}\psi \neq 0$ at a point, $\boldsymbol{\nabla}\psi$ is orthogonal/normal to *all* tangents of the surface $\psi = \mathsf{constant}$ at that point. Hence, if $\widehat{\mathbf{n}}$ is the unit normal to a surface of constant ψ, then (up to a sign)

$$\widehat{\mathbf{n}} = \frac{\boldsymbol{\nabla}\psi}{|\boldsymbol{\nabla}\psi|}\,. \tag{1.36}$$

(iv) The directional derivative is maximal when $\mathbf{l}$ is parallel to $\boldsymbol{\nabla}\psi$; hence *$\boldsymbol{\nabla}\psi$ is a vector field pointing in the*
01/02 *direction in which ψ is changing most rapidly.*
01/03

1.3.4 Applications

1. Find the unit normal at the point $\mathbf{r}(x, y, z)$ to the surface

$$\psi(\mathbf{r}) \equiv xy + yz + zx = -c\,, \tag{1.37}$$

where c is a positive constant. Hence find the points where the tangents to the surface are parallel to the (x, y) plane.

Answer. First calculate

$$\boldsymbol{\nabla}\psi = (y + z, x + z, y + x)\,. \tag{1.38a}$$

Then from (1.36) the unit normal is given by

$$\widehat{\mathbf{n}} = \frac{\boldsymbol{\nabla}\psi}{|\boldsymbol{\nabla}\psi|} = \frac{(y + z, x + z, y + x)}{\sqrt{2(x^2 + y^2 + z^2 + xy + xz + yz}}\,. \tag{1.38b}$$

The tangents to the surface $\psi(\mathbf{r}) = -c$ are parallel to the (x, y) plane when the normal is parallel to the z-axis, i.e. when $\widehat{\mathbf{n}} = (0, 0, 1)$ or $\widehat{\mathbf{n}} = (0, 0, -1)$, i.e. when

$$y = -z \quad \text{and} \quad x = -z\,. \tag{1.38c}$$

Hence from the equation for the surface, i.e. (1.37), the points where the tangents to the surface are parallel to the (x, y) plane satisfy

$$z^2 = c\,, \tag{1.38d}$$

so from (1.38c)

$$\mathbf{r} = \pm(-c, -c, c)\,. \tag{1.38e}$$

01/04

2. *Unlectured.* A mountain's height $z = h(x, y)$ depends on Cartesian coordinates x, y according to $h(x, y) = 1 - x^4 - y^4 \geqslant 0$. Find the point at which the slope in the plane $y = 0$ is greatest.

Answer. The slope of a path is the rate of change in the vertical direction divided by the rate of change in the horizontal direction. So consider a path on the mountain parameterised by s:

$$\mathbf{r}(s) = (x(s), y(s), h(x(s), y(s)))\,. \tag{1.39}$$

As s varies, the rate of change with s in the vertical direction is $\frac{\mathrm{d}h}{\mathrm{d}s}$, while the rate of change with s in the horizontal direction is $\sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}s}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}s}\right)^2}$.

Hence the slope of the path is given by

$$\begin{aligned}
\text{slope} &= \frac{\frac{\mathrm{d}h}{\mathrm{d}s}}{\sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}s}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}s}\right)^2}} \\
&= \frac{\frac{\partial h}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}s} + \frac{\partial h}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}s}}{\sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}s}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}s}\right)^2}} && \text{from (0.10a)} \\
&= \mathbf{l} \cdot \boldsymbol{\nabla} h\,, && (1.40\text{a})
\end{aligned}$$

where

$$\mathbf{l} = \frac{1}{\sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}s}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}s}\right)^2}} \left(\frac{\mathrm{d}x}{\mathrm{d}s}, \frac{\mathrm{d}y}{\mathrm{d}s}, 0\right). \tag{1.40b}$$

Thus the *slope is a directional derivative*. On $y = 0$

$$\text{slope} = \frac{-4x^3 \frac{\mathrm{d}x}{\mathrm{d}s}}{\left|\frac{\mathrm{d}x}{\mathrm{d}s}\right|} = -4x^3 \operatorname{sign}\left(\frac{\mathrm{d}x}{\mathrm{d}s}\right). \tag{1.40c}$$

Therefore the magnitude of the slope is largest where $|x|$ is largest, i.e. at the edge of the mountain $|x| = 1$. It follows that $\max|\text{slope}| = 4$.

1.4 The Divergence and Curl

1.4.1 Vector fields

$\boldsymbol{\nabla}\psi$ is an example of a *vector field*, i.e. a vector specified at each point $\mathbf{r}$ in space. More generally, we have for a vector field $\mathbf{F}(\mathbf{r})$,

$$\mathbf{F}(\mathbf{r}) = F_x(\mathbf{r})\mathbf{e}_x + F_y(\mathbf{r})\mathbf{e}_y + F_z(\mathbf{r})\mathbf{e}_z = \sum_j F_j(\mathbf{r})\mathbf{e}_j\,, \tag{1.41}$$

where F_x, F_y, F_z, or alternatively F_j $(j = 1, 2, 3)$, are the *components* of $\mathbf{F}$ in this Cartesian coordinate system. Examples of vector fields include current, electric and magnetic fields, and fluid velocities.

We can apply the $\boldsymbol{\nabla}$ vector operator to vector fields by means of dot and cross products.

1.4.2 The Divergence and Curl of a Vector Field

Divergence. The *divergence* of $\mathbf{F}$ is the *scalar field*

$$\begin{aligned}
\operatorname{div}\mathbf{F} \;\equiv\; \boldsymbol{\nabla}\cdot\mathbf{F} &= \left(\mathbf{e}_x\frac{\partial}{\partial x} + \mathbf{e}_y\frac{\partial}{\partial y} + \mathbf{e}_z\frac{\partial}{\partial z}\right)\cdot\left(F_x\mathbf{e}_x + F_y\mathbf{e}_y + F_z\mathbf{e}_z\right) \\
&= \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} && (1.42\text{a}) \\
&= \frac{\partial F_j}{\partial x_j}\,, && \text{(s.c.)}\ \ (1.42\text{b})
\end{aligned}$$

Key Result

from using (1.14g) and (1.30a), and remembering that in a Cartesian coordinate system the basis vectors do not depend on position and hence do not need to be differentiated.

Curl. The *curl* of $\mathbf{F}$ is the *vector field*

$$\begin{aligned}
\operatorname{curl}\mathbf{F} \;\equiv\; \boldsymbol{\nabla}\times\mathbf{F} &= \left(\mathbf{e}_x\frac{\partial}{\partial x} + \mathbf{e}_y\frac{\partial}{\partial y} + \mathbf{e}_z\frac{\partial}{\partial z}\right)\times\left(F_x\mathbf{e}_x + F_y\mathbf{e}_y + F_z\mathbf{e}_z\right) \\
&= \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z}\right)\mathbf{e}_x + \left(\frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x}\right)\mathbf{e}_y + \left(\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y}\right)\mathbf{e}_z && (1.43\text{a}) \\
&= \begin{vmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ \partial_x & \partial_y & \partial_z \\ F_x & F_y & F_z \end{vmatrix} = \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ \partial_{x_1} & \partial_{x_2} & \partial_{x_3} \\ F_1 & F_2 & F_3 \end{vmatrix} && (1.43\text{b}) \\
&= \varepsilon_{ijk}\mathbf{e}_i\frac{\partial F_k}{\partial x_j}\,, && \text{(s.c.)}\ \ (1.43\text{c})
\end{aligned}$$

Key Result

from using (1.3) and (1.5), and remembering that in a Cartesian coordinate system the basis vectors do not depend on position. Here

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$$\frac{\partial}{\partial x} \equiv \partial_x\,, \ \frac{\partial}{\partial y} \equiv \partial_y\,, \ \frac{\partial}{\partial z} \equiv \partial_z \qquad \text{and} \qquad \frac{\partial}{\partial x_j} \equiv \partial_{x_j} \equiv \partial_j\,. \tag{1.43d}$$

1.4.3 Examples

1. *Unlectured.* Find the divergence and curl of the vector field $\mathbf{F} = (x^2y, y^2z, z^2x)$.

   Answer.

$$\boldsymbol{\nabla}\cdot\mathbf{F} = \frac{\partial(x^2y)}{\partial x} + \frac{\partial(y^2z)}{\partial y} + \frac{\partial(z^2x)}{\partial z} = 2xy + 2yz + 2zx\,. \tag{1.44}$$

$$\begin{aligned}\boldsymbol{\nabla}\times\mathbf{F} &= \begin{vmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ \partial_x & \partial_y & \partial_z \\ x^2y & y^2z & z^2x \end{vmatrix} \\ &= -y^2\mathbf{e}_x - z^2\mathbf{e}_y - x^2\mathbf{e}_z \\ &= -(y^2, z^2, x^2)\,. \end{aligned} \tag{1.45}$$

2. Find $\boldsymbol{\nabla}\cdot\mathbf{r}$ and $\boldsymbol{\nabla}\times\mathbf{r}$.

   Answer. From the definition of divergence (1.42a), and recalling that $\mathbf{r} = (x, y, z) = (x_1, x_2, x_3)$, it follows that

$$\boldsymbol{\nabla}\cdot\mathbf{r} = \frac{\partial x}{\partial x} + \frac{\partial y}{\partial y} + \frac{\partial z}{\partial z} = 3\,. \tag{1.46a}$$

   or equivalently from (1.42b)

$$\boldsymbol{\nabla}\cdot\mathbf{r} = \frac{\partial x_i}{\partial x_i} = \delta_{ii} = 3\,, \qquad \text{since, from Example Sheet 0,} \qquad \frac{\partial x_i}{\partial x_j} = \delta_{ij}\,. \tag{1.46b}$$

   Next, from the definition of curl (1.43a) it follows that

$$\boldsymbol{\nabla}\times\mathbf{r} = \left(\frac{\partial z}{\partial y} - \frac{\partial y}{\partial z}, \frac{\partial x}{\partial z} - \frac{\partial z}{\partial x}, \frac{\partial y}{\partial x} - \frac{\partial x}{\partial y}\right) = 0. \tag{1.46c}$$

   or equivalently from (1.43c)

$$\boldsymbol{\nabla}\times\mathbf{r} = \varepsilon_{ijk}\mathbf{e}_i\frac{\partial x_k}{\partial x_j} = \varepsilon_{ijk}\mathbf{e}_i\delta_{jk} = \varepsilon_{ijj}\mathbf{e}_i = 0\,. \tag{1.46d}$$

1.4.4 $\mathbf{F}\cdot\boldsymbol{\nabla}$.

In (1.42a) we defined the divergence of a vector field $\mathbf{F}$, i.e. the scalar $\boldsymbol{\nabla}\cdot\mathbf{F}$. The order of the operator $\boldsymbol{\nabla}$ and the vector field $\mathbf{F}$ is important here. If we invert the order then we obtain the scalar operator

$$(\mathbf{F}\cdot\boldsymbol{\nabla}) \equiv F_x\frac{\partial}{\partial x} + F_y\frac{\partial}{\partial y} + F_z\frac{\partial}{\partial z} = F_j\frac{\partial}{\partial x_j}\,. \qquad \text{(s.c.)} \tag{1.47a}$$

Remark. As far as notation is concerned, for scalar ψ

$$\mathbf{F}\cdot(\boldsymbol{\nabla}\psi) = F_j\left(\frac{\partial\psi}{\partial x_j}\right) = \left(F_j\frac{\partial}{\partial x_j}\right)\psi = (\mathbf{F}\cdot\boldsymbol{\nabla})\psi\,. \qquad \text{(s.c.)} \tag{1.47b}$$

However, the right hand form is preferable. This is because for a vector $\mathbf{G}$, the ith component of $(\mathbf{F}\cdot\boldsymbol{\nabla})\mathbf{G}$ is unambiguous, namely

$$((\mathbf{F}\cdot\boldsymbol{\nabla})\mathbf{G})_i = \sum_j F_j\frac{\partial G_i}{\partial x_j}\,, \tag{1.47c}$$ Key Result

while the ith component of $\mathbf{F}\cdot(\boldsymbol{\nabla}\mathbf{G})$ is not, i.e. it is not clear whether the ith component of $\mathbf{F}\cdot(\boldsymbol{\nabla}\mathbf{G})$ is

$$\sum_j F_j\frac{\partial G_i}{\partial x_j} \quad \text{or} \quad \sum_j F_j\frac{\partial G_j}{\partial x_i}\,.$$

1.5 Vector Differential Identities

Calculations involving $\boldsymbol{\nabla}$ can be much sped up when certain vector identities are known. There are a large number of these! A short list is given below of the most common. Here ψ is a scalar field and $\mathbf{F}$, $\mathbf{G}$ are vector fields.

$$\begin{aligned}
\boldsymbol{\nabla}\cdot(\psi\,\mathbf{F}) &= \psi\,\boldsymbol{\nabla}\cdot\mathbf{F}+(\mathbf{F}\cdot\boldsymbol{\nabla})\psi\,, && \text{(1.48a)}\\
\boldsymbol{\nabla}\times(\psi\mathbf{F}) &= \psi\,(\boldsymbol{\nabla}\times\mathbf{F})+(\boldsymbol{\nabla}\psi)\times\mathbf{F}\,, && \text{(1.48b)}\\
\boldsymbol{\nabla}\cdot(\mathbf{F}\times\mathbf{G}) &= \mathbf{G}\cdot(\boldsymbol{\nabla}\times\mathbf{F})-\mathbf{F}\cdot(\boldsymbol{\nabla}\times\mathbf{G})\,, && \text{(1.48c)}\\
\boldsymbol{\nabla}\times(\mathbf{F}\times\mathbf{G}) &= \mathbf{F}\,(\boldsymbol{\nabla}\cdot\mathbf{G})-\mathbf{G}\,(\boldsymbol{\nabla}\cdot\mathbf{F})+(\mathbf{G}\cdot\boldsymbol{\nabla})\mathbf{F}-(\mathbf{F}\cdot\boldsymbol{\nabla})\mathbf{G}\,, && \text{(1.48d)}\\
\boldsymbol{\nabla}(\mathbf{F}\cdot\mathbf{G}) &= (\mathbf{F}\cdot\boldsymbol{\nabla})\mathbf{G}+(\mathbf{G}\cdot\boldsymbol{\nabla})\mathbf{F}+\mathbf{F}\times(\boldsymbol{\nabla}\times\mathbf{G})+\mathbf{G}\times(\boldsymbol{\nabla}\times\mathbf{F})\,. && \text{(1.48e)}
\end{aligned}$$

Example Verifications.

(1.48a):

$$\begin{aligned}
\boldsymbol{\nabla}\cdot(\psi\,\mathbf{F}) &= \frac{\partial(\psi\,F_i)}{\partial x_i} && \text{from (1.42b)}\\
&= \psi\,\frac{\partial F_i}{\partial x_i}+F_i\,\frac{\partial\psi}{\partial x_i}\\
&= \psi\,\boldsymbol{\nabla}\cdot\mathbf{F}+(\mathbf{F}\cdot\boldsymbol{\nabla})\psi && \text{from (1.42b) and (1.47a).}
\end{aligned}$$

Unlectured. (1.48c):

$$\begin{aligned}
\boldsymbol{\nabla}\cdot(\mathbf{F}\times\mathbf{G}) &= \frac{\partial}{\partial x_i}\,(\varepsilon_{ijk}F_jG_k) && \text{from (1.42b) and (1.21)}\\
&= G_k\,\varepsilon_{ijk}\frac{\partial F_j}{\partial x_i}+F_j\,\varepsilon_{ijk}\frac{\partial G_k}{\partial x_i}\\
&= G_k\,\varepsilon_{kij}\frac{\partial F_j}{\partial x_i}-F_j\,\varepsilon_{jik}\frac{\partial G_k}{\partial x_i} && \text{from (1.19c)}\\
&= \mathbf{G}\cdot(\boldsymbol{\nabla}\times\mathbf{F})-\mathbf{F}\cdot(\boldsymbol{\nabla}\times\mathbf{G})\,. && \text{from (1.43c).}
\end{aligned}$$

(1.48d):

$$\begin{aligned}
(\boldsymbol{\nabla}\times(\mathbf{F}\times\mathbf{G}))_i &= \varepsilon_{ijk}\frac{\partial}{\partial x_j}\,(\varepsilon_{klm}F_lG_m) && \text{from (1.21) and (1.43c)}\\
&= (\delta_{il}\delta_{jm}-\delta_{im}\delta_{jl})\left(F_l\frac{\partial G_m}{\partial x_j}+G_m\frac{\partial F_l}{\partial x_j}\right) && \text{from (1.25b)}\\
&= F_i\frac{\partial G_j}{\partial x_j}+G_j\frac{\partial F_i}{\partial x_j}-F_j\frac{\partial G_i}{\partial x_j}-G_i\frac{\partial F_j}{\partial x_j} && \text{from (1.14b) and (1.14c)}\\
&= \left(\mathbf{F}\,(\boldsymbol{\nabla}\cdot\mathbf{G})-\mathbf{G}\,(\boldsymbol{\nabla}\cdot\mathbf{F})+(\mathbf{G}\cdot\boldsymbol{\nabla})\mathbf{F}-(\mathbf{F}\cdot\boldsymbol{\nabla})\mathbf{G}\right)_i && \text{from (1.42b) and (1.47a).}
\end{aligned}$$

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Warnings.

1. Always remember what terms the differential operator is acting on, e.g. is it all terms to the right or just some?

2. Be very very careful when using standard vector identities where you have just replaced a vector with $\boldsymbol{\nabla}$. Sometimes it works, sometimes it does not! For instance for constant vectors $\mathbf{D}$, $\mathbf{F}$ and $\mathbf{G}$

$$\mathbf{F}\cdot(\mathbf{D}\times\mathbf{G}) \;=\; \mathbf{D}\cdot(\mathbf{G}\times\mathbf{F})=-\mathbf{D}\cdot(\mathbf{F}\times\mathbf{G})\,.$$

However for $\boldsymbol{\nabla}$ and vector functions $\mathbf{F}$ and $\mathbf{G}$

$$\mathbf{F}\cdot(\boldsymbol{\nabla}\times\mathbf{G})\neq\boldsymbol{\nabla}\cdot(\mathbf{G}\times\mathbf{F})=-\boldsymbol{\nabla}\cdot(\mathbf{F}\times\mathbf{G})\,,$$

since

$$\mathbf{F} \cdot (\boldsymbol{\nabla} \times \mathbf{G}) = F_i\, \varepsilon_{ijk} \frac{\partial G_k}{\partial x_j}\,,$$

while

$$\begin{aligned} \boldsymbol{\nabla} \cdot (\mathbf{G} \times \mathbf{F}) &= \frac{\partial}{\partial x_j} (\varepsilon_{jki} G_k F_i) \\ &= F_i\, \varepsilon_{ijk} \frac{\partial G_k}{\partial x_j} + G_k\, \varepsilon_{ijk} \frac{\partial F_i}{\partial x_j}\,. \end{aligned}$$

1.6 Second-Order Vector Differential Operators

1.6.1 curl grad **and** div curl

Using the definitions grad, div and curl, i.e. (1.28b), (1.42a) and (1.43a), and assuming the equality of mixed derivatives, we have that (cf. (1.20c) where we showed that $\varepsilon_{ijk} s_{ij} = 0$ is s_{ij} is symmetric)

$$\begin{aligned} \operatorname{curl}(\operatorname{grad}\psi) \;=\; \boldsymbol{\nabla} \times (\boldsymbol{\nabla}\psi) &= \varepsilon_{ijk} \partial_{x_j} (\partial_{x_k} \psi) && \\ &= \varepsilon_{ikj} \partial_{x_k} \partial_{x_j} \psi && \text{relabel dummy suffices } j \text{ and } k \\ &= -\varepsilon_{ijk} \partial_{x_j} \partial_{x_k} \psi && \text{permutate } ikj \text{ in } \varepsilon_{ikj} \text{ \& swap partials} \\ &= 0 && \text{quantity equals its negative.} \qquad (1.49a) \end{aligned}$$

Similarly,

$$\begin{aligned} \operatorname{div}(\operatorname{curl}\mathbf{F}) \;=\; \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \times \mathbf{F}) &= \partial_{x_i} \varepsilon_{ijk} \partial_{x_j} F_k && \\ &= \partial_{x_j} \varepsilon_{jik} \partial_{x_i} F_k && \text{relabel dummy suffices } i \text{ and } j \\ &= -\partial_{x_i} \varepsilon_{ijk} \partial_{x_j} F_k && \text{permutate } jik \text{ in } \varepsilon_{jik} \text{ \& swap partials} \\ &= 0\,. && \text{quantity equals its negative} \qquad (1.49b) \end{aligned}$$

Remarks.

1. Since by the standard rules for scalar triple products $\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \times \mathbf{F}) \equiv (\boldsymbol{\nabla} \times \boldsymbol{\nabla}) \cdot \mathbf{F}$, we can summarise both of these identities by
$$\boldsymbol{\nabla} \times \boldsymbol{\nabla} \equiv 0\,. \qquad (1.50)$$
Key Result

2. There are important converses to (1.49a) and (1.49b). The following two assertions can be proved (but not here).

   (a) Suppose that $\boldsymbol{\nabla} \times \mathbf{F} = 0$; the vector field $\mathbf{F}(\mathbf{r})$ is said to be *irrotational*. Then there exists a *scalar potential*, $\varphi(\mathbf{r})$, such that
   $$\mathbf{F} = \boldsymbol{\nabla}\varphi\,. \qquad (1.51)$$
   Application. A force field $\mathbf{F}$ such that $\boldsymbol{\nabla} \times \mathbf{F} = 0$ is said to the *conservative*. Gravity is a conservative force field. The above result shows that we can define a gravitational potential φ such that $\mathbf{F} = \boldsymbol{\nabla}\varphi$.

   (b) Suppose that $\boldsymbol{\nabla} \cdot \mathbf{B} = 0$; the vector field $\mathbf{B}(\mathbf{r})$ is said to be *solenoidal*. Then there exists a non-unique *vector potential*, $\mathbf{A}(\mathbf{r})$, such that
   $$\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}\,. \qquad (1.52)$$
   Application. One of Maxwell's equations for a magnetic field, $\mathbf{B}$, states that $\boldsymbol{\nabla} \cdot \mathbf{B} = 0$. The above result shows that we can define a magnetic vector potential, $\mathbf{A}$, such that $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$.

Example. Evaluate $\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}p \times \boldsymbol{\nabla}q)$, where p and q are scalar fields. *We will use this result later.*

Answer. Identify $\boldsymbol{\nabla}p$ and $\boldsymbol{\nabla}q$ with $\mathbf{F}$ and $\mathbf{G}$ respectively in the vector identity (1.48c). Then it follows from using (1.50) that

$$\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}p \times \boldsymbol{\nabla}q) = \boldsymbol{\nabla}q \cdot (\boldsymbol{\nabla} \times \boldsymbol{\nabla}p) - \boldsymbol{\nabla}p \cdot (\boldsymbol{\nabla} \times \boldsymbol{\nabla}q) = 0\,. \qquad (1.53)$$

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1.6.2 The Laplacian Operator ∇^2

From the definitions of div and grad

$$\operatorname{div}(\operatorname{grad}\psi) = \boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\psi) = \frac{\partial}{\partial x_i}\left(\frac{\partial}{\partial x_i}\psi\right)$$

$$= \frac{\partial^2\psi}{\partial x_i^2} \tag{1.54a}$$

$$= \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\right)\psi\,. \tag{1.54b}$$

Define the *Laplacian operator* to be $\nabla^2 = \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}$; then in *Cartesian coordinates* it is given by

$$\nabla^2 = \boldsymbol{\nabla}\cdot\boldsymbol{\nabla} = \frac{\partial^2}{\partial x_i^2} = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\,. \tag{1.54c}$$

Remarks.

1. The Laplacian operator ∇^2 is very important in the natural sciences. For instance it occurs in

   (a) Poisson's equation for a potential $\varphi(\mathbf{r})$:

   $$\nabla^2\varphi = \rho\,, \tag{1.55a}$$

   where (with a suitable normalisation)

   i. $\rho(\mathbf{r})$ is charge density in electromagnetism (when (1.55a) relates charge and electric potential);

   ii. $\rho(\mathbf{r})$ is mass density in gravitation (when (1.55a) relates mass and gravitational potential).

   (b) Schrödinger's equation for a non-relativistic quantum mechanical particle of mass m in a potential $V(\mathbf{r})$:

   $$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{r})\psi = \mathrm{i}\hbar\frac{\partial\psi}{\partial t}\,, \tag{1.55b}$$

   where ψ is the quantum mechanical wave function and $\hbar$ is Planck's constant divided by 2π.

   (c) Helmholtz's equation

   $$\nabla^2 f + \omega^2 f = 0\,, \tag{1.55c}$$

   which governs the propagation of fixed frequency waves (e.g. fixed frequency sound waves). Helmholtz's equation is a 3D generalisation of the simple harmonic resonator

   $$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + \omega^2 f = 0\,.$$

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2. Although the Laplacian has been introduced by reference to its effect on a scalar field (in our case ψ), it also has meaning when applied to vectors. *However some care is needed.* On the first example sheet you will prove the vector identity

   $$\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{F}) = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{F}) - \nabla^2\mathbf{F}\,. \tag{1.56a}$$

   The Laplacian acting on a vector is conventionally defined by rearranging this identity to obtain

   $$\nabla^2\mathbf{F} = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{F}) - \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{F})\,. \tag{1.56b}$$

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1.6.3 Examples

1. Find $\nabla^2 r^n = \operatorname{div}(\boldsymbol{\nabla} r^n)$. *We will use this result later.*

   Answer. Put $f(r) = r^n$ in (1.33b) to obtain

$$\boldsymbol{\nabla} r^n \quad = \quad n r^{n-1}\,\frac{\mathbf{r}}{r} \;=\; n r^{n-2}\,(x_1, x_2, x_3)\,. \tag{1.57}$$

   So from the definition of divergence (1.42a):

$$\begin{aligned}
\nabla^2 r^n = \boldsymbol{\nabla}\cdot(\boldsymbol{\nabla} r^n) &= \frac{\partial(n r^{n-2} x_i)}{\partial x_i} \\
&= n r^{n-2}\,\frac{\partial x_i}{\partial x_i} + n x_i \frac{\partial r^{n-2}}{\partial x_i} \\
&= 3 n r^{n-2} + n x_i (n-2) r^{n-3}\,\frac{x_i}{r} && \text{using (1.31a)} \\
&= n(n+1) r^{n-2}\,. && (1.58)
\end{aligned}$$

   Check. Note that from setting $n = 2$ in (1.57) we have that $\boldsymbol{\nabla} r^2 = 2\mathbf{r}$. It follows that, with $n = 2$, (1.58) reproduces (1.46a).

2. *Unlectured.* Find the Laplacian of $\frac{\sin r}{r}$.

   Answer. Since the Laplacian consists of first taking a gradient, we first note from using result (1.33a), i.e. $\boldsymbol{\nabla} f(r) = f'(r)\boldsymbol{\nabla} r$, that

$$\boldsymbol{\nabla}\left(\frac{\sin r}{r}\right) = \left(\frac{\cos r}{r} - \frac{\sin r}{r^2}\right)\boldsymbol{\nabla} r\,. \tag{1.59a}$$

   Further, we recall from (1.32) that

$$\boldsymbol{\nabla} r = \frac{\mathbf{r}}{r}\,, \tag{1.59b}$$

   and also from (1.58) with $n = 1$ that

$$\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla} r) = \frac{2}{r}\,. \tag{1.59c}$$

   Hence

$$\begin{aligned}
\nabla^2\left(\frac{\sin r}{r}\right) &= \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\left(\frac{\sin r}{r}\right) \\
&= \boldsymbol{\nabla}\cdot\left(\left(\frac{\cos r}{r} - \frac{\sin r}{r^2}\right)\boldsymbol{\nabla} r\right) && \text{from (1.59a)} \\
&= \left(\frac{\cos r}{r} - \frac{\sin r}{r^2}\right)\boldsymbol{\nabla}\cdot\boldsymbol{\nabla} r + \boldsymbol{\nabla} r\cdot\boldsymbol{\nabla}\left(\frac{\cos r}{r} - \frac{\sin r}{r^2}\right) && \text{from identity (1.48a)} \\
&= 2\left(\frac{\cos r}{r^2} - \frac{\sin r}{r^3}\right) + \frac{\mathbf{r}}{r}\cdot\boldsymbol{\nabla}\left(\frac{\cos r}{r} - \frac{\sin r}{r^2}\right) && \text{from (1.59b) \& (1.59c)} \\
&= 2\left(\frac{\cos r}{r^2} - \frac{\sin r}{r^3}\right) + \frac{\mathbf{r}}{r}\cdot\left(-\frac{\sin r}{r} - \frac{2\cos r}{r^2} + \frac{2\sin r}{r^3}\right)\boldsymbol{\nabla} r && \text{using (1.33a) again} \\
&= -\frac{\sin r}{r}\,. && (1.60)
\end{aligned}$$

   Remarks.

   (i) It follows that $f = \frac{\sin r}{r}$ satisfies Helmholtz's equation (1.55c) for $\omega = 1$.

   (ii) It is arguably easier to derive this result using suffix notation.

1.7 The Big Integral Theorems

These are two very important integral theorems for vector fields that have many scientific applications.

1.7.1 The Divergence Theorem (Gauss' Theorem)

Divergence Theorem. Let $\mathcal{S}$ be a 'nice' surface[10] enclosing a volume $\mathcal{V}$ in $\mathbb{R}^3$, with a normal $\widehat{\mathbf{n}}$ that points outwards from $\mathcal{V}$. Let $\mathbf{u}$ be a 'nice' vector field.[11] Then

$$\iiint\limits_{\mathcal{V}} \boldsymbol{\nabla}\cdot\mathbf{u}\,\mathrm{d}V = \iint\limits_{\mathcal{S}(\mathcal{V})} \mathbf{u}\cdot\mathrm{d}\mathbf{S}\,, \tag{1.61}$$ Key Result

where $\mathrm{d}V$ is the volume element, $\mathrm{d}\mathbf{S} = \widehat{\mathbf{n}}\mathrm{d}S$ is the vector surface element, $\widehat{\mathbf{n}}$ is the unit normal to the surface $\mathcal{S}$ and $\mathrm{d}S$ is a small element of surface area. In *Cartesian coordinates*

$$\mathrm{d}V = \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,, \tag{1.62a}$$

and

$$\mathrm{d}\mathbf{S} = \sigma_x \mathrm{d}y\,\mathrm{d}z\,\mathbf{e}_x + \sigma_y \mathrm{d}z\,\mathrm{d}x\,\mathbf{e}_y + \sigma_z \mathrm{d}x\,\mathrm{d}y\,\mathbf{e}_z\,, \tag{1.62b}$$

where $\sigma_x = \mathrm{sign}(\widehat{\mathbf{n}}\cdot\mathbf{e}_x)$, $\sigma_y = \mathrm{sign}(\widehat{\mathbf{n}}\cdot\mathbf{e}_y)$ and $\sigma_z = \mathrm{sign}(\widehat{\mathbf{n}}\cdot\mathbf{e}_z)$.

At a point on the surface, $\mathbf{u}\cdot\widehat{\mathbf{n}}$ is the *flux* of $\mathbf{u}$ across the surface at that point. Hence the divergence theorem states that $\boldsymbol{\nabla}\cdot\mathbf{u}$ integrated over a volume $\mathcal{V}$ is equal to the total flux of $\mathbf{u}$ across the closed surface $\mathcal{S}$ surrounding the volume.

Remark. The divergence theorem relates a triple integral to a double integral. This is analogous to the second fundamental theorem of calculus, i.e.

$$\int_{h_1}^{h_2} \frac{\mathrm{d}f}{\mathrm{d}z}\,\mathrm{d}z = f(h_2) - f(h_1)\,, \tag{1.63}$$

02/01 which relates a single integral to a function.

Outline Proof. Suppose that $\mathcal{S}$ is a surface enclosing a volume $\mathcal{V}$ such that Cartesian axes can be chosen so that any line parallel to any one of the axes meets $\mathcal{S}$ in just one or two points (e.g. a convex surface). We observe that

$$\iiint\limits_{\mathcal{V}} \boldsymbol{\nabla}\cdot\mathbf{u}\,\mathrm{d}V = \iiint\limits_{\mathcal{V}} \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}\right)\mathrm{d}V\,,$$

comprises of three terms; we initially concentrate on the $\iiint_{\mathcal{V}} \frac{\partial u_z}{\partial z}\mathrm{d}V$ term.

Let region $\mathcal{A}$ be the projection of $\mathcal{S}$ onto the xy-plane. Let the lower/upper surfaces, $\mathcal{S}_1/\mathcal{S}_2$ respectively, be parameterised by

$$\begin{aligned} \mathcal{S}_1: \quad \mathbf{r} &= (x, y, h_1(x,y)) \\ \mathcal{S}_2: \quad \mathbf{r} &= (x, y, h_2(x,y))\,. \end{aligned}$$

[10] For instance, a bounded, piecewise smooth, orientated, non-intersecting surface.
[11] For instance a vector field with continuous first-order partial derivatives throughout $\mathcal{V}$.

Then using the second fundamental theorem of calculus (1.63)

$$\iiint\limits_{\mathcal{V}} \frac{\partial u_z}{\partial z}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \iint\limits_{\mathcal{A}} \left[\int_{z=h_1}^{h_2} \frac{\partial u_z}{\partial z}\mathrm{d}z\right]\mathrm{d}x\,\mathrm{d}y$$

$$= \iint\limits_{\mathcal{A}} \left(u_z(x,y,h_2(x,y)) - u_z(x,y,h_1(x,y)\right)\mathrm{d}x\,\mathrm{d}y\,. \tag{1.64}$$

Now consider the projection of a surface element $\mathrm{d}\mathbf{S}$ on the upper surface onto the xy plane. It follows geometrically that $\mathrm{d}x\,\mathrm{d}y = |\cos\alpha|\,\mathrm{d}S$, where α is the angle between $\mathbf{e}_z$ and the unit normal $\widehat{\mathbf{n}}$; hence on $\mathcal{S}_2$

$$\mathrm{d}x\,\mathrm{d}y = \mathbf{e_z}\cdot\widehat{\mathbf{n}}\,\mathrm{d}S = \mathbf{e_z}\cdot\mathrm{d}\mathbf{S}\,. \tag{1.65a}$$

On the lower surface $\mathcal{S}_1$ we need to dot $\widehat{\mathbf{n}}$ with $-\mathbf{e}_z$ in order to get a positive area; hence

$$\mathrm{d}x\,\mathrm{d}y = -\mathbf{e_z}\cdot\mathrm{d}\mathbf{S}\,. \tag{1.65b}$$

We note that (1.65a) and (1.65b) are consistent with (1.62b) once the tricky issue of signs is sorted out. Using (1.62a), (1.65a) and (1.65b), equation (1.64) can be rewritten as

$$\iiint\limits_{\mathcal{V}} \frac{\partial u_z}{\partial z}\,\mathrm{d}V = \iint\limits_{\mathcal{S}_2} u_z\,\mathbf{e}_z\cdot\mathrm{d}\mathbf{S} + \iint\limits_{\mathcal{S}_1} u_z\,\mathbf{e}_z\cdot\mathrm{d}\mathbf{S} = \iint\limits_{\mathcal{S}} u_z\,\mathbf{e}_z\cdot\mathrm{d}\mathbf{S}\,, \tag{1.66a}$$

since $\mathcal{S}_1+\mathcal{S}_2=\mathcal{S}$. Similarly by permutation (i.e. $x\to y$, $y\to z$ and $z\to x$),

$$\iiint\limits_{\mathcal{V}} \frac{\partial u_y}{\partial y}\,\mathrm{d}V = \iint\limits_{\mathcal{S}} u_y\,\mathbf{e}_y\cdot\mathrm{d}\mathbf{S}\,, \qquad \iiint\limits_{\mathcal{V}} \frac{\partial u_x}{\partial x}\,\mathrm{d}V = \iint\limits_{\mathcal{S}} u_x\,\mathbf{e}_x\cdot\mathrm{d}\mathbf{S}\,. \tag{1.66b}$$

Adding the above results we obtain the divergence theorem (1.61):

$$\iiint\limits_{\mathcal{V}} \boldsymbol{\nabla}\cdot\mathbf{u}\,\mathrm{d}V = \iint\limits_{\mathcal{S}} \mathbf{u}\cdot\mathrm{d}\mathbf{S}\,. \tag{1.67}$$

The generalisation for a scalar field. For a scalar field $\psi(\mathbf{x})$ with continuous first-order partial derivatives in $\mathcal{V}$,

$$\iiint\limits_{\mathcal{V}} \boldsymbol{\nabla}\psi\,\mathrm{d}V = \iint\limits_{\mathcal{S}} \psi\,\mathrm{d}\mathbf{S}\,. \tag{1.68a}$$

Proof. Set $\mathbf{u}=\psi\,\mathbf{a}$ in (1.67), where $\mathbf{a}$ is an arbitrary constant vector. Then from (1.48a)

$$\mathbf{a}.\iiint\limits_{\mathcal{V}} \boldsymbol{\nabla}\psi\,\mathrm{d}V = \mathbf{a}.\iint\limits_{\mathcal{S}} \psi\,\mathrm{d}\mathbf{S}\,. \tag{1.68b}$$

Since $\mathbf{a}$ is arbitrary, (1.68a) follows.[12] Alternatively, choose $\mathbf{a}=\mathbf{e}_i$ to obtain the component form

$$\iiint\limits_{\mathcal{V}} \frac{\partial\psi}{\partial x_i}\,\mathrm{d}V = \iint\limits_{\mathcal{S}} \psi n_i\,\mathrm{d}S\,. \tag{1.68c}$$

Key Result

The generalisation for a vector potential. For a vector potential $\mathbf{A}$ with continuous first-order partial derivatives in $\mathcal{V}$,

$$\iiint\limits_{\mathcal{V}} \boldsymbol{\nabla}\times\mathbf{A}\,\mathrm{d}V = \iint\limits_{\mathcal{S}} \widehat{\mathbf{n}}\times\mathbf{A}\,\mathrm{d}S\,. \tag{1.69}$$

Proof (unlectured). Either set $\mathbf{u}=\mathbf{a}\times\mathbf{A}$ in (1.67), where where $\mathbf{a}$ is an arbitrary constant vector, and then proceed as above, or let $\psi=\varepsilon_{ijk}A_j$ in (1.68c), to recover (1.69) in component form.

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[12] If $\mathbf{a}\cdot\mathbf{b}=0$ for every $\mathbf{a}$, choose $\mathbf{a}=\mathbf{b}$. Then $\mathbf{b}\cdot\mathbf{b}=\|\mathbf{b}\|^2=0$ implies $\mathbf{b}=0$.

1.7.2 Stokes' Theorem

Let $\mathcal{S}$ be *any* 'nice' open surface bounding the 'nice' closed curve $\mathcal{C}$.[13] Let $\mathbf{u}(\mathbf{r})$ be a 'nice' vector field.[14] Then

$$\iint\limits_{\mathcal{S}} \boldsymbol{\nabla} \times \mathbf{u} \cdot \mathrm{d}\mathbf{S} = \oint\limits_{\mathcal{C}} \mathbf{u} \cdot \mathrm{d}\mathbf{r}\,, \tag{1.70a}$$

Key Result

where the line integral is taken in the direction of $\mathcal{C}$ as specified by the 'right-hand rule'.

Remark. Stokes' theorem thus states that the flux of $\boldsymbol{\nabla} \times \mathbf{u}$ across an open surface $\mathcal{S}$ is equal to the *circulation* of $\mathbf{u}$ round the bounding curve $\mathcal{C}$.

Planar surface. For a surface in the (x, y) plane, so that $\mathrm{d}\mathbf{S} = \mathrm{d}x\mathrm{d}y\,\mathbf{e}_z$, Stokes' theorem reduces to *Green's theorem in the plane*:

$$\iint_{\mathcal{A}} \left(\frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y}\right) \mathrm{d}x\mathrm{d}y = \int_{\mathcal{C}} (u_x\,\mathrm{d}x + u_y\,\mathrm{d}y)\,, \tag{1.70b}$$

where $\mathcal{A}$ is the region of the plane bounded by the curve $\mathcal{C}$, and the line integral follows a positive sense.

Outline Proof. First prove Green's theorem for a rectangle using the second fundamental theorem of calculus. Second, subdivide $\mathcal{S}$ into small planar rectangles to any desired accuracy (cf. subdividing the range in a standard line integral). Finally, apply Green's theorem to all these subdivisions, noting that when the integrals are added together, the circulations along internal curve segments cancel out, leaving only the circulation around C.

1.7.3 Examples and Applications

Archimedes' Principle. A body is acted on by a hydrostatic pressure force $p = -\rho g z$, where ρ is the density of the surrounding fluid, g is gravity and z is the vertical coordinate. Find a simplified expression for the pressure force on the body starting from

$$\mathbf{F} = -\iint\limits_{\mathcal{S}} p\;\mathrm{d}\mathbf{S}\,. \tag{1.71}$$

Answer. Consider the individual components of $\mathbf{u}$ and use the divergence theorem. Then

$$\mathbf{e}_z \cdot \mathbf{F} = -\iint\limits_{\mathcal{S}} p\,\mathbf{e}_z \cdot \mathrm{d}\mathbf{S} = -\iiint\limits_{\mathcal{V}} \boldsymbol{\nabla} \cdot (p\,\mathbf{e}_z)\,\mathrm{d}V = -\iiint\limits_{\mathcal{V}} \frac{\partial(-\rho g z)}{\partial z}\,\mathrm{d}V = g\iiint\limits_{\mathcal{V}} \rho\,\mathrm{d}V = Mg\,, \tag{1.72a}$$

where M is the mass of the fluid displaced by the body. Similarly

$$\mathbf{e}_x \cdot \mathbf{F} = -\iiint\limits_{\mathcal{V}} \boldsymbol{\nabla} \cdot (p\,\mathbf{e}_x)\,\mathrm{d}V = -\iiint\limits_{\mathcal{V}} \frac{\partial(-\rho g z)}{\partial x}\,\mathrm{d}V = 0\,, \tag{1.72b}$$

and $\mathbf{e}_y \cdot \mathbf{F} = 0$. Hence we have *Archimedes' Principle* that an immersed body experiences a loss of weight equal to the weight of the fluid displaced:

$$\mathbf{F} = Mg\,\mathbf{e}_z\,. \tag{1.72c}$$

[13] Or to be slightly more precise: let $\mathcal{S}$ be a piecewise smooth, open, orientated, non-intersecting surface bounded by a simple, piecewise smooth, closed curve $\mathcal{C}$.

[14] For instance a vector field with continuous first-order partial derivatives on $\mathcal{S}$.

Gradient theorem. Show that provided there are no singularities, the integral

$$\int_{\mathcal{C}} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r}\,, \tag{1.73}$$

where φ is a scalar field and $\mathcal{C}$ is an open path joining two fixed points A and B, is independent of the path chosen between the points.

Answer. Consider two such paths: $\mathcal{C}_1$ and $\mathcal{C}_2$. Form a closed curve $\widehat{\mathcal{C}}$ from these two curves. Then using Stokes' Theorem and the result (1.49a) that a curl of a gradient is zero, we have that

$$\begin{aligned}\int\limits_{\mathcal{C}_1} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r} - \int\limits_{\mathcal{C}_2} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r} &= \oint\limits_{\widehat{\mathcal{C}}} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r} \\ &= \iint\limits_{\widehat{\mathcal{S}}} \boldsymbol{\nabla} \times (\boldsymbol{\nabla}\varphi) \cdot \mathrm{d}\mathbf{S} \\ &= 0\,,\end{aligned}$$

where $\widehat{\mathcal{S}}$ is a nice open surface bounding $\widehat{\mathcal{C}}$. Hence

$$\int\limits_{\mathcal{C}_1} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r} = \int\limits_{\mathcal{C}_2} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r}\,. \tag{1.74}$$

Application. Suppose that φ is the gravitational potential, then $\mathbf{g} = -\boldsymbol{\nabla}\varphi$ is the gravitational force, and $\int_{\mathcal{C}}(-\boldsymbol{\nabla}\varphi) \cdot \mathrm{d}\mathbf{r}$ is the work done against gravity in moving from A to B. The above result demonstrates that the work done is independent of path. Indeed, from (1.29), i.e. $\boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r} = \mathrm{d}\varphi$,

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$$\int_{\mathcal{C}} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r} = \int_{\mathcal{C}} \mathrm{d}\varphi = \varphi(B) - \varphi(A)\,. \tag{1.75}$$

1.7.4 Interpretation of divergence

Let a volume $\mathcal{V}$ be enclosed by a surface $\mathcal{S}$, and consider a limit process in which the greatest diameter of $\mathcal{V}$ tends to zero while keeping the point $\mathbf{r}_0$ inside $\mathcal{V}$. Then from Taylor's theorem with $\mathbf{r} = \mathbf{r}_0 + \boldsymbol{\delta}\mathbf{r}$,

$$\iiint_{\mathcal{V}} \boldsymbol{\nabla} \cdot \mathbf{u}(\mathbf{r})\, \mathrm{d}V = \iiint_{\mathcal{V}} (\boldsymbol{\nabla} \cdot \mathbf{u}(\mathbf{r}_0) + \dots)\, \mathrm{d}V = \boldsymbol{\nabla} \cdot \mathbf{u}(\mathbf{r}_0)\, |\mathcal{V}| + \dots\,,$$

where $|\mathcal{V}|$ is the volume of $\mathcal{V}$. Thus using the divergence theorem (1.61)

$$\boldsymbol{\nabla} \cdot \mathbf{u} = \lim_{|\mathcal{V}| \to 0} \frac{1}{|\mathcal{V}|} \iint\limits_{\mathcal{S}} \mathbf{u} \cdot \mathrm{d}\mathbf{S}\,, \tag{1.76}$$

where $\mathcal{S}$ is any 'nice' small closed surface enclosing a volume $\mathcal{V}$. It follows that $\boldsymbol{\nabla} \cdot \mathbf{u}$ can be interpreted as the net rate of flux outflow at $\mathbf{r}_0$ per unit volume.

Application. Suppose that $\mathbf{v}$ is a velocity field. Then

$$\begin{array}{llll}\boldsymbol{\nabla} \cdot \mathbf{v} > 0 \quad \Rightarrow & \iint\limits_{\mathcal{S}} \mathbf{v} \cdot \mathrm{d}\mathbf{S} > 0 & \Rightarrow \text{net positive flux} & \Rightarrow \text{there exists a source at } \mathbf{r}_0; \\ \boldsymbol{\nabla} \cdot \mathbf{v} < 0 \quad \Rightarrow & \iint\limits_{\mathcal{S}} \mathbf{v} \cdot \mathrm{d}\mathbf{S} < 0 & \Rightarrow \text{net negative flux} & \Rightarrow \text{there exists a sink at } \mathbf{r}_0.\end{array}$$

1.7.5 Interpretation of curl

Let an open smooth surface $\mathcal{S}$ be bounded by a curve $\mathcal{C}$. Consider a limit process in which the point $\mathbf{r}_0$ remains on $\mathcal{S}$, the greatest diameter of $\mathcal{S}$ tends to zero, and the normals at all points on the surface tend to a specific direction (i.e. the value of $\widehat{\mathbf{n}}$ at $\mathbf{r}_0$). Then from Taylor's theorem with $\mathbf{r} = \mathbf{r}_0 + \boldsymbol{\delta}\mathbf{r}$,

$$\iint\limits_{\mathcal{S}} (\boldsymbol{\nabla} \times \mathbf{u}(\mathbf{r})) \cdot \mathrm{d}\mathbf{S} = \iint\limits_{\mathcal{S}} (\boldsymbol{\nabla} \times \mathbf{u}(\mathbf{r}_0) + \dots) \cdot \mathrm{d}\mathbf{S} = \boldsymbol{\nabla} \times \mathbf{u}(\mathbf{r}_0) \cdot \widehat{\mathbf{n}}\, |\mathcal{S}| + \dots\,,$$

where $|\mathcal{S}|$ is the area of $\mathcal{S}$. Thus using Stokes' theorem (1.70a)

$$\widehat{\mathbf{n}} \cdot (\boldsymbol{\nabla} \times \mathbf{u}) = \lim_{\mathcal{S} \to 0} \frac{1}{|\mathcal{S}|} \oint_C \mathbf{u} \cdot \mathrm{d}\mathbf{r}\,, \tag{1.77}$$

where $\mathcal{S}$ is any 'nice' small open surface with a bounding curve $\mathcal{C}$. It follows that $\widehat{\mathbf{n}} \cdot (\boldsymbol{\nabla} \times \mathbf{u})$ can be interpreted
03/03 as the circulation about $\widehat{\mathbf{n}}$ at $\mathbf{r}_0$ per unit area.

Application.

Consider a rigid body rotating with angular velocity $\boldsymbol{\omega}$ about an axis through 0. Then the velocity at a point $\mathbf{r}$ in the body is given by

$$\mathbf{v} = \boldsymbol{\omega} \times \mathbf{r}\,. \tag{1.78a}$$

Suppose that $\mathcal{C}$ is a circle of radius a in a plane normal to $\boldsymbol{\omega}$. Then the circulation of $\mathbf{v}$ around $\mathcal{C}$ is

$$\oint_C \mathbf{v} \cdot \mathrm{d}\mathbf{r} = \int_0^{2\pi} (\omega a)\, a\, \mathrm{d}\phi = 2\pi a^2 \omega\,. \tag{1.78b}$$

Hence from (1.77)

$$\widehat{\boldsymbol{\omega}} \cdot (\boldsymbol{\nabla} \times \mathbf{v}) = \lim_{a \to 0} \frac{1}{\pi a^2} \oint_C \mathbf{v} \cdot \mathrm{d}\mathbf{r} = 2\omega\,. \tag{1.78c}$$

We conclude that the curl is a measure of the local rotation of a vector field.

03/04 *Exercise.* Show by direct evaluation that if $\mathbf{v} = \boldsymbol{\omega} \times \mathbf{r}$ then $\boldsymbol{\nabla} \times \mathbf{v} = 2\boldsymbol{\omega}$.

1.8 Orthogonal Curvilinear Coordinates

1.8.1 What Are Orthogonal Curvilinear Coordinates?

There are many ways to describe the position of points in space. One way is to define three independent sets of surfaces, each parameterised by a single variable (for Cartesian coordinates these are orthogonal planes parameterised, say, by the point on the axis that they intercept). Then any point has 'coordinates' given by the labels for the three surfaces that intersect at that point.

The unit vectors analogous to $\mathbf{e}_1$, etc. are the unit normals to these surfaces. Such coordinates are called *curvilinear*. They are generally of most use when the orthonormality condition (1.14g), i.e. $\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$, holds; in which case they are called *orthogonal curvilinear coordinates*. Common examples are spherical and cylindrical polar coordinates. For instance in the case of spherical polar coordinates the independent sets of surfaces are spherical shells and planes of constant latitude and longitude.

It is very important to realise that there is a key difference between Cartesian coordinates and other orthogonal curvilinear coordinates. In Cartesian coordinates the *directions* of the basis vectors $\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ are *independent of position*. This is not the case in other coordinate systems; for instance, $\mathbf{e}_r$ the normal to a spherical shell changes direction with position on the shell. It is sometimes helpful to display this dependence on position explicitly: Key Point

$$\mathbf{e}_i \equiv \mathbf{e}_i(\mathbf{r})\,. \tag{1.79}$$

1.8.2 Relationships Between Coordinate Systems

Suppose that we have *non-Cartesian* coordinates, q_i $(i = 1, 2, 3)$. Since we can express one coordinate system in term of another, there will be a functional dependence of the q_i on, say, Cartesian coordinates x, y, z, i.e.

$$q_i \equiv q_i(x, y, z) \quad (i = 1, 2, 3)\,. \tag{1.80}$$

For cylindrical polar coordinates and spherical polar coordinates we know that:

	Cylindrical Polar Coordinates	Spherical Polar Coordinates
q_1	$\rho = (x^2 + y^2)^{1/2}$	$r = (x^2 + y^2 + z^2)^{1/2}$
q_2	$\phi = \tan^{-1}\left(\frac{y}{x}\right)$	$\theta = \tan^{-1}\left(\frac{(x^2+y^2)^{1/2}}{z}\right)$
q_3	z	$\phi = \tan^{-1}(y/x)$

Remarks

1. Note that $q_i = c_i$ $(i = 1, 2, 3)$, where the c_i are constants, define three independent sets of surfaces, each 'labelled' by a parameter (i.e. the c_i). As discussed above, any point has 'coordinates' given by the labels for the three surfaces that intersect at that point.
2. The equation (1.80) can be viewed as three simultaneous equations for three unknowns x, y, z. In general these equations can be solved to yield the position vector $\mathbf{r}$ as a function of $\mathbf{q} = (q_1, q_2, q_3)$, i.e. $\mathbf{r} \equiv \mathbf{r}(\mathbf{q})$ or
$$x = x(q_1, q_2, q_3)\,, \quad y = y(q_1, q_2, q_3)\,, \quad z = z(q_1, q_2, q_3)\,. \tag{1.81}$$
For instance:

	Cylindrical Polar Coordinates	Spherical Polar Coordinates
x	$\rho\cos\phi$	$r\cos\phi\sin\theta$
y	$\rho\sin\phi$	$r\sin\phi\sin\theta$
z	z	$r\cos\theta$

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1.8.3 Incremental Change in Position or Length.

Consider an infinitesimal change in position. Then, by the chain rule, the change $\mathrm{d}x_i$ in $x_i(q_1, q_2, q_3)$ due to changes $\mathrm{d}q_j$ in q_j $(i = 1, 2, 3)$ is

$$\mathrm{d}x_i = \frac{\partial x_i}{\partial q_1}\mathrm{d}q_1 + \frac{\partial x_i}{\partial q_2}\mathrm{d}q_2 + \frac{\partial x_i}{\partial q_3}\mathrm{d}q_3 = \frac{\partial x_i}{\partial q_j}\,\mathrm{d}q_j \quad (i = 1, 2, 3). \qquad \text{(s.c.)} \tag{1.82}$$

Anticipating a crisis in notation, we let $\mathbf{e}_x = \widehat{\mathbf{x}}_1$, $\mathbf{e}_y = \widehat{\mathbf{x}}_2$ and $\mathbf{e}_z = \widehat{\mathbf{x}}_3$. Then the vector displacement $\mathrm{d}\mathbf{r}$ can be written as

$$\begin{aligned}\mathrm{d}\mathbf{r} \equiv \mathrm{d}x_i\,\widehat{\mathbf{x}}_\mathbf{i} &= \frac{\partial x_i}{\partial q_j}\,\mathrm{d}q_j\,\widehat{\mathbf{x}}_\mathbf{i} \\ &= \left(\frac{\partial x_i}{\partial q_j}\,\widehat{\mathbf{x}}_\mathbf{i}\right)\mathrm{d}q_j \\ &= \mathbf{h}_j\,\mathrm{d}q_j\,,\end{aligned} \tag{1.83a}$$

where

$$\mathbf{h}_j = \frac{\partial x_i}{\partial q_j}\,\widehat{\mathbf{x}}_\mathbf{i} = \frac{\partial \mathbf{r}(\mathbf{q})}{\partial q_j} \quad (j = 1, 2, 3)\,. \tag{1.83b}$$

Thus the infinitesimal change in position $\mathrm{d}\mathbf{r}$ is a vector sum of displacements $\mathbf{h}_j(\mathbf{r})\,\mathrm{d}q_j$ 'along' each of the three q-axes through $\mathbf{r}$. The vectors $\mathbf{h}_j$ are not necessarily unit vectors, so it is convenient to write (suspending the s.c.)

$$\mathbf{h}_j = h_j\,\mathbf{e}_j \quad (j=1,2,3)\,, \qquad \textbf{(no s.c.)} \quad (1.84a)$$

where the $h_j = |\mathbf{h_j}|$ are the lengths of the $\mathbf{h}_j$, and the $\mathbf{e}_j$ are *unit vectors*, i.e.

$$h_j = \left|\frac{\partial \mathbf{r}}{\partial q_j}\right| \quad \text{and} \quad \mathbf{e}_j = \frac{1}{h_j}\frac{\partial \mathbf{r}}{\partial q_j} \quad (j=1,2,3)\,. \qquad \textbf{(no s.c.)} \quad (1.84b)$$

Remarks.

(i) The $\mathbf{h}_j$ will, in general, *depend on position* $\mathbf{r}$. Consequently, the $\mathbf{e}_j(\mathbf{r})$ will vary in space (cf. the $\widehat{\mathbf{x}}_i$), and the q-axes will be *curves* rather than straight lines. The coordinate system is said to be *curvilinear.*

(ii) The *scale factors* or *metric coefficients*, h_j, convert co-ordinate increments into lengths. Any point at
05/22 which $h_j = 0$ is a *coordinate singularity* at which the coordinate system breaks down.

1.8.4 The Jacobian

The *Jacobian matrix*, J, of the transformation from coordinates (x_1, x_2, x_3) to (q_1, q_2, q_3) is defined as

$$\mathsf{J} = \begin{pmatrix} \frac{\partial x}{\partial q_1} & \frac{\partial x}{\partial q_2} & \frac{\partial x}{\partial q_3} \\ \frac{\partial y}{\partial q_1} & \frac{\partial y}{\partial q_2} & \frac{\partial y}{\partial q_3} \\ \frac{\partial z}{\partial q_1} & \frac{\partial z}{\partial q_2} & \frac{\partial z}{\partial q_3} \end{pmatrix}. \qquad (1.85a)$$

The *Jacobian* of (x,y,z) with respect to (q_1,q_2,q_3) is defined as the determinant of this matrix:

$$J \equiv \frac{\partial(x,y,z)}{\partial(q_1,q_2,q_3)} = |\mathsf{J}| = \begin{vmatrix} \frac{\partial x}{\partial q_1} & \frac{\partial x}{\partial q_2} & \frac{\partial x}{\partial q_3} \\ \frac{\partial y}{\partial q_1} & \frac{\partial y}{\partial q_2} & \frac{\partial y}{\partial q_3} \\ \frac{\partial z}{\partial q_1} & \frac{\partial z}{\partial q_2} & \frac{\partial z}{\partial q_3} \end{vmatrix}. \qquad (1.85b)$$

The columns of the above matrix are the vectors $\mathbf{h}_i$ defined in (1.83b). Therefore the Jacobian is equal to the scalar triple product

$$J = [\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3] = \mathbf{h}_1\cdot\mathbf{h}_2 \times \mathbf{h}_3\,. \qquad (1.85c)$$

Given a point with curvilinear coordinates (q_1,q_2,q_3), consider three small displacements $\mathrm{d}\mathbf{r}_1 = \mathbf{h}_1\,\mathrm{d}q_1$, $\mathrm{d}\mathbf{r}_2 = \mathbf{h}_2\,\mathrm{d}q_2$ and $\mathrm{d}\mathbf{r}_3 = \mathbf{h}_3\,\mathrm{d}q_3$ along the three curvilinear coordinate directions. They span a parallelepiped of volume

$$\mathrm{d}V = |[\mathrm{d}\mathbf{r}_1, \mathrm{d}\mathbf{r}_2, \mathrm{d}\mathbf{r}_3]| = |J|\,\mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3\,. \qquad (1.86a)$$

Hence the *volume element* in a general curvilinear coordinate system is

$$\mathrm{d}V = \left|\frac{\partial(x,y,z)}{\partial(q_1,q_2,q_3)}\right|\mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3\,. \qquad (1.86b)$$ Key Result

The Jacobian therefore appears when changing variables in a multiple integral:

$$\iiint \Phi\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \int \Phi\,\mathrm{d}V = \iiint \Phi\left|\frac{\partial(x,y,z)}{\partial(q_1,q_2,q_3)}\right|\mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3 \iiint \Phi\,J\,\mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}q_3\,. \qquad (1.86c)$$

Remarks.

(i) If $|J| = 0$ in the range of variables, the coordinate transformation is singular and care is needed.

(ii) Jacobians are defined similarly for transformations in any number of dimensions. If curvilinear coordinates (q_1,q_2) are introduced in the (x,y)-plane, the area element is

$$\mathrm{d}A = |J|\,\mathrm{d}q_1\,\mathrm{d}q_2\,, \qquad (1.87a)$$

where

$$J = \frac{\partial(x,y)}{\partial(q_1,q_2)} = \begin{vmatrix} \frac{\partial x}{\partial q_1} & \frac{\partial x}{\partial q_2} \\ \frac{\partial y}{\partial q_1} & \frac{\partial y}{\partial q_2} \end{vmatrix}. \qquad (1.87b)$$

(iii) The equivalent rule for a one-dimensional integral is

$$\int f(x)\,\mathrm{d}x = \int f(x(q)) \left|\frac{\mathrm{d}x}{\mathrm{d}q}\right| \mathrm{d}q\,, \tag{1.88}$$

where the direction of integration of the limits needs to be consistent with the use of the modulus. Indeed, care is needed in transforming the limits in any of the above integrals.

1.8.5 Properties of Jacobians

Consider now three sets of variables α_i, β_i and γ_i, with $1 \leqslant i \leqslant n$, none of which need be Cartesian coordinates. According to the chain rule of partial differentiation,

$$\frac{\partial \alpha_i}{\partial \gamma_j} = \frac{\partial \alpha_i}{\partial \beta_k}\frac{\partial \beta_k}{\partial \gamma_j}\,. \qquad \text{(s.c.)} \tag{1.89}$$

The left-hand side is the ij-component of the Jacobian matrix of the transformation from α_i to γ_i. The equation states that this matrix is the product of the Jacobian matrices of the transformations from α_i to β_i and from β_i to γ_i, i.e. the Jacobian matrix of a composite transformation is the product of the Jacobian matrices of the transformations of which it is composed.

The chain rule for Jacobians. Taking the determinant of (1.89), we recover the chain rule for Jacobians:

$$\frac{\partial(\alpha_1,\cdots,\alpha_n)}{\partial(\gamma_1,\cdots,\gamma_n)} = \frac{\partial(\alpha_1,\cdots,\alpha_n)}{\partial(\beta_1,\cdots,\beta_n)}\frac{\partial(\beta_1,\cdots,\beta_n)}{\partial(\gamma_1,\cdots,\gamma_n)}\,. \tag{1.90}$$

The inverse transformation for Jacobians. In the special case in which $\gamma_i = \alpha_i$ for all i, the left-hand side is 1 (the determinant of the unit matrix), and so we obtain

$$\frac{\partial(\alpha_1,\cdots,\alpha_n)}{\partial(\beta_1,\cdots,\beta_n)} = \left[\frac{\partial(\beta_1,\cdots,\beta_n)}{\partial(\alpha_1,\cdots,\alpha_n)}\right]^{-1}\,. \tag{1.91}$$

Hence, the Jacobian of an inverse transformation is the reciprocal of that of the forward transformation. This is a multidimensional generalization of the result $\mathrm{d}x/\mathrm{d}y = (\mathrm{d}y/\mathrm{d}x)^{-1}$.

1.8.6 Orthogonality

For a general q_j coordinate system the $\mathbf{e}_j$ are not necessarily mutually orthogonal, i.e. in general

$$\mathbf{e}_i \cdot \mathbf{e}_j \neq 0 \quad \text{for } i \neq j\,.$$

However, for *orthogonal curvilinear coordinates* the $\mathbf{e}_i$ are *required* to be mutually orthogonal at all points in space, i.e.

$$\mathbf{e}_i \cdot \mathbf{e}_j = 0 \quad \text{if} \quad i \neq j\,.$$

Since by definition the $\mathbf{e}_j$ are unit vectors, we thus have that

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}\,. \tag{1.92}$$

Handedness. It is conventional to order the q_i so that the coordinate system is *right-handed.*

Incremental Distance. In an orthogonal curvilinear coordinate system the expression for the incremental distance, $|\mathrm{d}\mathbf{r}|^2$ simplifies. We find that (noting that the s.c. does not work)

$$\begin{aligned} |\mathrm{d}\mathbf{r}|^2 = \mathrm{d}\mathbf{r}\cdot\mathrm{d}\mathbf{r} &= \left(\sum_i h_i \mathrm{d}q_i\,\mathbf{e}_i\right)\cdot\left(\sum_j h_j \mathrm{d}q_j\,\mathbf{e}_j\right) && \text{from (1.83a) and (1.84a)} \\ &= \sum_{i,j} (h_i \mathrm{d}q_i)(h_j \mathrm{d}q_j)\,\delta_{ij} && \text{from (1.92)} \\ &= \sum_i h_i^2 (\mathrm{d}q_i)^2\,. && \text{from (1.14c)} \end{aligned} \tag{1.93}$$

Key Result

1.8.7 Spherical Polar Coordinates

In this case $q_1 = r$, $q_2 = \theta$, $q_3 = \phi$, and in term of Cartesian co-ordinates

$$\mathbf{r} = (r\sin\theta\cos\phi,\ r\sin\theta\sin\phi,\ r\cos\theta)\,. \tag{1.94a}$$

Hence

$$\begin{aligned}
\frac{\partial\mathbf{r}}{\partial q_1} &= \frac{\partial\mathbf{r}}{\partial r} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)\,,\\
\frac{\partial\mathbf{r}}{\partial q_2} &= \frac{\partial\mathbf{r}}{\partial \theta} = (r\cos\theta\cos\phi, r\cos\theta\sin\phi, -r\sin\theta)\,,\\
\frac{\partial\mathbf{r}}{\partial q_3} &= \frac{\partial\mathbf{r}}{\partial \phi} = (-r\sin\theta\sin\phi, r\sin\theta\cos\phi, 0)\,.
\end{aligned}$$

It follows from (1.84b) that

$$h_1 = h_r = \left|\frac{\partial\mathbf{r}}{\partial q_1}\right| = 1\,, \qquad \mathbf{e}_1 = \mathbf{e}_r = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)\,, \tag{1.94b}$$

$$h_2 = h_\theta = \left|\frac{\partial\mathbf{r}}{\partial q_2}\right| = r\,, \qquad \mathbf{e}_2 = \mathbf{e}_\theta = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta)\,, \tag{1.94c}$$

$$h_3 = h_\phi = \left|\frac{\partial\mathbf{r}}{\partial q_3}\right| = r\sin\theta\,, \qquad \mathbf{e}_3 = \mathbf{e}_\phi = (-\sin\phi, \cos\phi, 0)\,. \tag{1.94d}$$

Remarks.

(i) $\mathbf{e}_i\cdot\mathbf{e}_j = \delta_{ij}$ and $\mathbf{e}_1\times\mathbf{e}_2 = \mathbf{e}_3$, i.e. spherical polar coordinates are a right-handed orthogonal curvilinear coordinate system. If we had chosen, say, $q_1 = r$, $q_2 = \phi$, $q_3 = \theta$, then we would have ended up with a left-handed system.

(ii) $\mathbf{e}_r$, $\mathbf{e}_\theta$ and $\mathbf{e}_\phi$ are functions of position.

(iii) Spherical polars are singular at $r = 0$, $\theta = 0$ and $\theta = \pi$, i.e. on the 'north-south' axis.

(iv) Recalling from (1.83a) and (1.84a) that the h_j give the components of the displacement vector $\mathrm{d}\mathbf{r}$ along the r, θ, and ϕ axes, we have that

$$\mathrm{d}\mathbf{r} = \sum_j h_j\,\mathrm{d}q_j\,\mathbf{e}_j = \mathrm{d}r\,\mathbf{e}_r + r\,\mathrm{d}\theta\,\mathbf{e}_\theta + r\sin\theta\,\mathrm{d}\phi\,\mathbf{e}_\phi\,. \tag{1.95}$$

1.8.8 Cylindrical Polar Coordinates

In this case $q_1 = \rho$, $q_2 = \phi$, $q_3 = z$, and in term of Cartesian co-ordinates

$$\mathbf{r} = (\rho\cos\phi,\ \rho\sin\phi, z)\,. \tag{1.96a}$$

Exercise. Show that

$$\begin{aligned}
\frac{\partial\mathbf{r}}{\partial q_1} &= \frac{\partial\mathbf{r}}{\partial \rho} = (\cos\phi, \sin\phi,\ 0)\,,\\
\frac{\partial\mathbf{r}}{\partial q_2} &= \frac{\partial\mathbf{r}}{\partial \phi} = (-\rho\sin\phi,\ \rho\cos\phi,\ 0)\,,\\
\frac{\partial\mathbf{r}}{\partial q_3} &= \frac{\partial\mathbf{r}}{\partial z} = (0, 0, 1)\,.
\end{aligned}$$

and hence that

$$h_1 = h_\rho = \left|\frac{\partial \mathbf{r}}{\partial q_1}\right| = 1\,, \qquad \mathbf{e}_1 = \mathbf{e}_\rho = (\cos\phi, \sin\phi, 0)\,, \tag{1.96b}$$

$$h_2 = h_\phi = \left|\frac{\partial \mathbf{r}}{\partial q_2}\right| = \rho\,, \qquad \mathbf{e}_2 = \mathbf{e}_\phi = (-\sin\phi, \cos\phi, 0)\,, \tag{1.96c}$$

$$h_3 = h_z = \left|\frac{\partial \mathbf{r}}{\partial q_3}\right| = 1\,, \qquad \mathbf{e}_3 = \mathbf{e}_z = (0, 0, 1)\,. \tag{1.96d}$$

Remarks.

(i) $\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$ and $\mathbf{e}_1 \times \mathbf{e}_2 = \mathbf{e}_3$, i.e. cylindrical polar coordinates are a right-handed orthogonal curvilinear coordinate system.

(ii) $\mathbf{e}_\rho$ and $\mathbf{e}_\phi$ are functions of position.

(iii) Cylindrical polars are singular on the axis $\rho = 0$.

(iv) As noted in the section on *Assumed Knowledge*, §0.12, in the case of cylindrical polar coordinates, sometimes r and/or θ are used in place of ρ and/or ϕ respectively (but then there is potential confusion with the different definitions of r and θ in spherical polar co-ordinates). Further, in order to maximise confusion, instead of ρ (which, admittedly, can be useful for other things, such as density), some authors use R, s or ϖ.

1.8.9 Volume and Surface Elements in Orthogonal Curvilinear Coordinates

Volume element. For *orthogonal* curvilinear coordinate systems it follows from (1.86a) that

$$\begin{aligned} \mathrm{d}V &= \mathrm{d}\mathbf{r}_1 \times \mathrm{d}\mathbf{r}_2 \cdot \mathrm{d}\mathbf{r}_3 \\ &= h_1 h_2 h_3\, \mathrm{d}q_1 \mathrm{d}q_2 \mathrm{d}q_3\, \mathbf{e}_1 \times \mathbf{e}_2 \cdot \mathbf{e}_3 \\ &= h_1 h_2 h_3\, \mathrm{d}q_1 \mathrm{d}q_2 \mathrm{d}q_3\,. \end{aligned} \tag{1.97a}$$

Example: Spherical Polar Coordinates. In the case of spherical polar coordinates we have from (1.94b), (1.94c), (1.94d) and (1.97a) that

$$\mathrm{d}V = r^2 \sin\theta\, \mathrm{d}r \mathrm{d}\theta \mathrm{d}\phi\,. \tag{1.97b}$$

The volume of the sphere of radius a is therefore

$$\iiint\limits_{\mathcal{V}} \mathrm{d}V = \int_0^a \mathrm{d}r \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\ r^2 \sin\theta = \frac{4}{3}\pi a^3. \tag{1.97c}$$

Surface element. The surface element can also be deduced for arbitrary orthogonal curvilinear coordinates. First consider the special case when $\mathrm{d}\mathbf{S} \,||\, \mathbf{e}_3$, then

$$\begin{aligned} \mathrm{d}\mathbf{S} &= (h_1 \mathrm{d}q_1 \mathbf{e}_1) \times (h_2 \mathrm{d}q_2 \mathbf{e}_2) \\ &= h_1 h_2\, \mathrm{d}q_1 \mathrm{d}q_2\, \mathbf{e}_3\,. \end{aligned} \tag{1.98a}$$

In general

$$\mathrm{d}\mathbf{S} = \mathrm{sign}(\widehat{\mathbf{n}} \cdot \mathbf{e}_1) h_2 h_3\, \mathrm{d}q_2 \mathrm{d}q_3\, \mathbf{e}_1 + \mathrm{sign}(\widehat{\mathbf{n}} \cdot \mathbf{e}_2) h_3 h_1\, \mathrm{d}q_3 \mathrm{d}q_1\, \mathbf{e}_2 + \mathrm{sign}(\widehat{\mathbf{n}} \cdot \mathbf{e}_3) h_1 h_2\, \mathrm{d}q_1 \mathrm{d}q_2\, \mathbf{e}_3\,, \tag{1.98b}$$

so that

04/02 $$dS = \widehat{\mathbf{n}} \cdot \mathrm{d}\mathbf{S} = h_2 h_3\, \mathrm{d}q_2 \mathrm{d}q_3\, |\widehat{\mathbf{n}} \cdot \mathbf{e}_1| + h_3 h_1\, \mathrm{d}q_3 \mathrm{d}q_1\, |\widehat{\mathbf{n}} \cdot \mathbf{e}_2| + h_1 h_2\, \mathrm{d}q_1 \mathrm{d}q_2\, |\widehat{\mathbf{n}} \cdot \mathbf{e}_2| > 0 \quad \text{if } \mathrm{d}q_j > 0\,. \tag{1.98c}$$
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1.8.10 Gradient in Orthogonal Curvilinear Coordinates

First we recall from (1.29) that for Cartesian coordinates and infinitesimal displacements $\mathrm{d}\psi = \boldsymbol{\nabla}\psi \cdot \mathrm{d}\mathbf{r}$.

Definition. For curvilinear orthogonal coordinates (for which the basis vectors are in general functions of position), we define $\boldsymbol{\nabla}\psi$ to be the vector such that for all $\mathrm{d}\mathbf{r}$

$$\mathrm{d}\psi = \boldsymbol{\nabla}\psi \cdot \mathrm{d}\mathbf{r}\,. \tag{1.99}$$

In order to determine the components of $\boldsymbol{\nabla}\psi$ when ψ is viewed as a function of $\mathbf{q}$ rather than $\mathbf{r}$, write

$$\boldsymbol{\nabla}\psi = \sum_i \mathbf{e}_i \alpha_i \,, \tag{1.100a}$$

then from (1.83a), (1.84a), (1.92), (1.14c) and (1.99)

$$\mathrm{d}\psi = \nabla\psi \cdot \mathrm{d}\mathbf{r} = \sum_i \mathbf{e}_i\alpha_i \cdot \sum_j h_j \mathbf{e}_j \mathrm{d}q_j = \sum_{i,j} \alpha_i \left(h_j \mathrm{d}q_j\right) \mathbf{e}_i \cdot \mathbf{e}_j = \sum_i \alpha_i \left(h_i \mathrm{d}q_i\right). \tag{1.100b}$$

But according to the chain rule, an infinitesimal change $\mathrm{d}\mathbf{q}$ to $\mathbf{q}$ will lead to the following infinitesimal change in $\psi \equiv \psi(q_1, q_2, q_3)$

$$\mathrm{d}\psi = \sum_i \frac{\partial\psi}{\partial q_i}\mathrm{d}q_i = \sum_i \left(\frac{1}{h_i}\frac{\partial\psi}{\partial q_i}\right)\left(h_i \mathrm{d}q_i\right). \tag{1.100c}$$

Hence, since (1.100b) and (1.100c) must hold for all $\mathrm{d}q_i$,

$$\alpha_i = \frac{1}{h_i}\,\frac{\partial\psi}{\partial q_i}\,, \tag{1.100d}$$

and from (1.100a)

$$\boldsymbol{\nabla}\psi = \sum_i \frac{\mathbf{e}_i}{h_i}\,\frac{\partial\psi}{\partial q_i} = \left(\frac{1}{h_1}\frac{\partial\psi}{\partial q_1}, \frac{1}{h_2}\frac{\partial\psi}{\partial q_2}, \frac{1}{h_3}\frac{\partial\psi}{\partial q_3}\right). \tag{1.100e}$$

Remark. Each term has dimensions 'ψ/length'.

As before, we can consider $\boldsymbol{\nabla}\psi$ to be the result of acting on ψ with the vector differential operator

$$\boldsymbol{\nabla} = \sum_i \mathbf{e}_i \frac{1}{h_i}\frac{\partial}{\partial q_i}\,. \tag{1.101}$$

Key Result

1.8.11 Examples of Gradients

Cylindrical Polar Coordinates. In cylindrical polar coordinates, the gradient is given from (1.96b), (1.96c) and (1.96d) to be

$$\boldsymbol{\nabla} = \mathbf{e}_\rho \frac{\partial}{\partial\rho} \;+\; \mathbf{e}_\phi \frac{1}{\rho}\frac{\partial}{\partial\phi} \;+\; \mathbf{e}_z \frac{\partial}{\partial z}\,. \tag{1.102a}$$

Spherical Polar Coordinates. In spherical polar coordinates the gradient is given from (1.94b), (1.94c) and (1.94d) to be

$$\boldsymbol{\nabla} = \mathbf{e}_r \frac{\partial}{\partial r} \;+\; \mathbf{e}_\theta \frac{1}{r}\frac{\partial}{\partial\theta} \;+\; \mathbf{e}_\phi \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\,. \tag{1.102b}$$

1.8.12 Divergence and Curl

We can now use (1.101) to compute $\boldsymbol{\nabla}\cdot\mathbf{F}$ and $\boldsymbol{\nabla}\times\mathbf{F}$ in orthogonal curvilinear coordinates. However, first we need a preliminary result which is complementary to (1.84b). Since

$$\frac{\partial q_i}{\partial q_j} = \delta_{ij}\,, \tag{1.103a}$$

it follows from (1.101) that

$$\boldsymbol{\nabla} q_i = \sum_j \mathbf{e}_j \frac{1}{h_j}\,\frac{\partial q_i}{\partial q_j} = \sum_j \frac{\mathbf{e}_j}{h_j}\,\delta_{ij} = \frac{\mathbf{e}_i}{h_i}\,, \quad \text{i.e. that} \quad \mathbf{e}_i = h_i \boldsymbol{\nabla} q_i\,. \tag{1.103b}$$

We also recall that the $\mathbf{e}_i$ form an orthonormal right-handed basis; thus $\mathbf{e}_1 = \mathbf{e}_2 \times \mathbf{e}_3$ (and cyclic permutations). Hence from (1.103b)

$$\mathbf{e}_1 = h_2 \boldsymbol{\nabla} q_2 \times h_3 \boldsymbol{\nabla} q_3\,, \quad \text{and cyclic permutations.} \tag{1.103c}$$

Divergence. We have with a little bit of inspired rearrangement, and remembering to differentiate the $\mathbf{e}_i$ because they are position dependent:

$$\begin{aligned}
\boldsymbol{\nabla}\cdot\mathbf{F} &= \boldsymbol{\nabla}\cdot\left(\sum_i F_i\mathbf{e}_i\right)\\
&= \boldsymbol{\nabla}\cdot\left((h_2h_3F_1)\left(\frac{\mathbf{e}_1}{h_2h_3}\right)\right) + \text{cyclic permutations}\\
&= \frac{\mathbf{e}_1}{h_2h_3}\cdot\boldsymbol{\nabla}(h_2h_3F_1) + h_2h_3F_1\boldsymbol{\nabla}\cdot\left(\frac{\mathbf{e}_1}{h_2h_3}\right) + \text{cyclic permutations} && \text{using (1.48a)}\\
&= \frac{\mathbf{e}_1}{h_2h_3}\cdot\sum_j \mathbf{e}_j\left(\frac{1}{h_j}\frac{\partial}{\partial q_j}(h_2h_3F_1)\right) + h_2h_3F_1\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}q_2\times\boldsymbol{\nabla}q_3)\\
&\qquad + \text{cyclic permutations}\,. && \text{using (1.101) \& (1.103c)}
\end{aligned}$$

Recall from (1.92) that $\mathbf{e}_1\cdot\mathbf{e}_j = \delta_{1j}$, and from example (1.53), with $p = q_2$ and $q = q_3$, that

$$\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}q_2\times\boldsymbol{\nabla}q_3) = 0\,.$$

It follows that

$$\boldsymbol{\nabla}\cdot\mathbf{F} = \frac{1}{h_1h_2h_3}\left(\frac{\partial}{\partial q_1}(h_2h_3F_1) + \frac{\partial}{\partial q_2}(h_3h_1F_2) + \frac{\partial}{\partial q_3}(h_1h_2F_3)\right). \tag{1.104}$$

Key Result

Cylindrical Polar Coordinates. From (1.96b), (1.96c), (1.96d) and (1.104)

$$\operatorname{div}\mathbf{F} = \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho F_\rho) + \frac{1}{\rho}\frac{\partial F_\phi}{\partial\phi} + \frac{\partial F_z}{\partial z}\,. \tag{1.105a}$$

Spherical Polar Coordinates. From (1.94b), (1.94c), (1.94d) and (1.104)

$$\operatorname{div}\mathbf{F} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2F_r\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\; F_\theta) + \frac{1}{r\sin\theta}\frac{\partial F_\phi}{\partial\phi}\,. \tag{1.105b}$$

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Curl. Again with a little bit of inspired rearrangement we have that

$$\begin{aligned}
\boldsymbol{\nabla}\times\mathbf{F} &= \boldsymbol{\nabla}\times\left(\sum_i F_i\mathbf{e}_i\right)\\
&= \sum_i \boldsymbol{\nabla}\times\left((h_iF_i)\left(\frac{\mathbf{e}_i}{h_i}\right)\right)\\
&= \sum_i \boldsymbol{\nabla}(h_iF_i)\times\frac{\mathbf{e}_i}{h_i} + \sum_i h_iF_i\,(\boldsymbol{\nabla}\times\boldsymbol{\nabla}q_i) && \text{using (1.48b) \& (1.103b)}\\
&= \sum_i\sum_j\left(\frac{1}{h_ih_j}\frac{\partial(h_iF_i)}{\partial q_j}\right)\mathbf{e}_j\times\mathbf{e}_i\,. && \text{using (1.49a) \& (1.101)}
\end{aligned}$$

But $\mathbf{e}_1\times\mathbf{e}_2 = \mathbf{e}_3$ and cyclic permutations, and $\mathbf{e}_k\times\mathbf{e}_k = 0$, hence

$$\begin{aligned}
\boldsymbol{\nabla}\times\mathbf{F} \quad = \quad & \frac{\mathbf{e}_1}{h_2h_3}\left(\frac{\partial(h_3F_3)}{\partial q_2} - \frac{\partial(h_2F_2)}{\partial q_3}\right) + \frac{\mathbf{e}_2}{h_3h_1}\left(\frac{\partial(h_1F_1)}{\partial q_3} - \frac{\partial(h_3F_3)}{\partial q_1}\right)\\
& + \frac{\mathbf{e}_3}{h_1h_2}\left(\frac{\partial(h_2F_2)}{\partial q_1} - \frac{\partial(h_1F_1)}{\partial q_2}\right).
\end{aligned} \tag{1.106a}$$

All three components of the curl can be written in the concise form

$$\boldsymbol{\nabla}\times\mathbf{F} = \frac{1}{h_1h_2h_3}\begin{vmatrix} h_1\mathbf{e}_1 & h_2\mathbf{e}_2 & h_3\mathbf{e}_3\\ \frac{\partial}{\partial q_1} & \frac{\partial}{\partial q_2} & \frac{\partial}{\partial q_3}\\ h_1F_1 & h_2F_2 & h_3F_3\end{vmatrix}\,. \tag{1.106b}$$

Key Result

06/22

Cylindrical Polar Coordinates. From (1.96b), (1.96c), (1.96d) and (1.106b)

$$\nabla \times \mathbf{F} = \frac{1}{\rho} \begin{vmatrix} \mathbf{e}_\rho & \rho\,\mathbf{e}_\phi & \mathbf{e}_z \\ \partial_\rho & \partial_\phi & \partial_z \\ F_\rho & \rho\,F_\phi & F_z \end{vmatrix} \tag{1.107a}$$

$$= \left(\frac{1}{\rho}\frac{\partial F_z}{\partial \phi} - \frac{\partial F_\phi}{\partial z}, \frac{\partial F_\rho}{\partial z} - \frac{\partial F_z}{\partial \rho}, \frac{1}{\rho}\frac{\partial(\rho F_\phi)}{\partial \rho} - \frac{1}{\rho}\frac{\partial F_\rho}{\partial \phi} \right). \tag{1.107b}$$

Spherical Polar Coordinates. From (1.94b), (1.94c), (1.94d) and (1.106b)

$$\nabla \times \mathbf{F} = \frac{1}{r^2 \sin\theta} \begin{vmatrix} \mathbf{e}_r & r\mathbf{e}_\theta & r\sin\theta\mathbf{e}_\phi \\ \partial_r & \partial_\theta & \partial_\phi \\ F_r & rF_\theta & r\sin\theta F_\phi \end{vmatrix} \tag{1.108a}$$

$$= \left(\frac{1}{r\sin\theta}\left(\frac{\partial(\sin\theta\, F_\phi)}{\partial\theta} - \frac{\partial F_\theta}{\partial\phi} \right), \frac{1}{r\sin\theta}\frac{\partial F_r}{\partial\phi} - \frac{1}{r}\frac{\partial(rF_\phi)}{\partial r}, \frac{1}{r}\frac{\partial(rF_\theta)}{\partial r} - \frac{1}{r}\frac{\partial F_r}{\partial\theta} \right). \tag{1.108b}$$

Remarks.

1. Each term in a divergence and curl has dimensions 'F/length'.
2. The above formulae can also be derived in a more physical manner using the divergence theorem and Stokes' theorem respectively.

1.8.13 Laplacian in Orthogonal Curvilinear Coordinates

Suppose we substitute $\mathbf{F} = \nabla\psi$ into formula (1.104) for the divergence. Then since from (1.100e)

$$F_i = \frac{1}{h_i}\frac{\partial\psi}{\partial q_i},$$

we have that

$$\nabla^2\psi \equiv \nabla\cdot\nabla\psi = \frac{1}{h_1h_2h_3}\left(\frac{\partial}{\partial q_1}\left(\frac{h_2h_3}{h_1}\frac{\partial\psi}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(\frac{h_3h_1}{h_2}\frac{\partial\psi}{\partial q_2}\right) + \frac{\partial}{\partial q_3}\left(\frac{h_1h_2}{h_3}\frac{\partial\psi}{\partial q_3}\right) \right). \tag{1.109}$$

We thereby deduce that in a general orthogonal curvilinear coordinate system

$$\nabla^2 = \frac{1}{h_1h_2h_3}\left(\frac{\partial}{\partial q_1}\left(\frac{h_2h_3}{h_1}\frac{\partial}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(\frac{h_3h_1}{h_2}\frac{\partial}{\partial q_2}\right) + \frac{\partial}{\partial q_3}\left(\frac{h_1h_2}{h_3}\frac{\partial}{\partial q_3}\right) \right). \tag{1.110}$$

Cylindrical Polar Coordinates. From (1.96b), (1.96c), (1.96d) and (1.110)

$$\nabla^2\psi = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2}. \tag{1.111a}$$

Spherical Polar Coordinates. From (1.94b), (1.94c), (1.94d) and (1.110)

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}, \tag{1.111b}$$

$$= \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}. \tag{1.111c}$$

Remark. We have found here only the form of ∇^2 as a differential operator on *scalar* fields. As noted earlier, the action of the Laplacian on a *vector* field $\mathbf{F}$ is most easily defined using the vector identity

$$\nabla^2\mathbf{F} = \nabla(\nabla\cdot\mathbf{F}) - \nabla\times(\nabla\times\mathbf{F}). \tag{1.112}$$

Alternatively $\nabla^2\mathbf{F}$ can be evaluated by recalling that

$$\nabla^2\mathbf{F} = \nabla^2(F_1\mathbf{e}_1 + F_2\mathbf{e}_2 + F_3\mathbf{e}_3)\,,$$

and remembering (a) that the derivatives implied by the Laplacian act on the unit vectors too, and (b) that because the unit vectors are generally functions of position $(\nabla^2\mathbf{F})_i \neq \nabla^2 F_i$ (the exception being Cartesian coordinates).

1.8.14 Further Examples

Evaluate $\boldsymbol{\nabla}\cdot\mathbf{r}$, $\boldsymbol{\nabla}\times\mathbf{r}$, and $\nabla^2\left(\frac{1}{r}\right)$ in spherical polar coordinates, where $\mathbf{r} = r\,\mathbf{e}_r$. From (1.105b)

$$\boldsymbol{\nabla}\cdot\mathbf{r} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\cdot r\right) = 3\,,\quad \text{as in (1.46a).} \tag{1.113a}$$

From (1.108b)

$$\boldsymbol{\nabla}\times\mathbf{r} = \left(0\,,\frac{1}{r\sin\theta}\frac{\partial r}{\partial\phi}\,,-\frac{1}{r}\frac{\partial r}{\partial\theta}\right) = (0,0,0)\,,\quad \text{as in (1.46c).} \tag{1.113b}$$

From (1.111c) for $r\neq 0$

$$\nabla^2\left(\frac{1}{r}\right) \;=\; \frac{1}{r}\frac{\partial^2}{\partial r^2}\left(r\left(\frac{1}{r}\right)\right) = 0\,,\quad \text{as in (1.58) with } n=-1. \tag{1.113c}$$

P.T.O.

1.8.15 Aide Memoire

Orthogonal Curvilinear Coordinates.

$$\boldsymbol{\nabla} = \sum_i \mathbf{e}_i \frac{1}{h_i}\frac{\partial}{\partial q_i}\,.$$

$$\operatorname{div}\mathbf{F} = \frac{1}{h_1h_2h_3}\left(\frac{\partial}{\partial q_1}(h_2h_3F_1) + \frac{\partial}{\partial q_2}(h_3h_1F_2) + \frac{\partial}{\partial q_3}(h_1h_2F_3)\right)\,.$$

$$\operatorname{curl}\mathbf{F} = \frac{1}{h_1h_2h_3}\begin{vmatrix} h_1\mathbf{e}_1 & h_2\mathbf{e}_2 & h_3\mathbf{e}_3 \\ \frac{\partial}{\partial q_1} & \frac{\partial}{\partial q_2} & \frac{\partial}{\partial q_3} \\ h_1F_1 & h_2F_2 & h_3F_3 \end{vmatrix}\,.$$

$$\nabla^2\psi = \frac{1}{h_1h_2h_3}\left(\frac{\partial}{\partial q_1}\left(\frac{h_2h_3}{h_1}\frac{\partial\psi}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(\frac{h_3h_1}{h_2}\frac{\partial\psi}{\partial q_2}\right) + \frac{\partial}{\partial q_3}\left(\frac{h_1h_2}{h_3}\frac{\partial\psi}{\partial q_3}\right)\right)\,.$$

Cylindrical Polar Coordinates: $q_1 = \rho$, $h_1 = 1$, $q_2 = \phi$, $h_2 = \rho$, $q_3 = z$, $h_3 = 1$.

$$\boldsymbol{\nabla} = \mathbf{e}_\rho\frac{\partial}{\partial\rho} \;+\; \mathbf{e}_\phi\frac{1}{\rho}\frac{\partial}{\partial\phi} \;+\; \mathbf{e}_z\frac{\partial}{\partial z}\,.$$

$$\operatorname{div}\mathbf{F} = \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho F_\rho) + \frac{1}{\rho}\frac{\partial F_\phi}{\partial\phi} + \frac{\partial F_z}{\partial z}\,.$$

$$\begin{aligned}\operatorname{curl}\mathbf{F} &= \frac{1}{\rho}\begin{vmatrix} \mathbf{e}_\rho & \rho\,\mathbf{e}_\phi & \mathbf{e}_z \\ \partial_\rho & \partial_\phi & \partial_z \\ F_\rho & \rho\,F_\phi & F_z \end{vmatrix} \\ &= \left(\frac{1}{\rho}\frac{\partial F_z}{\partial\phi} - \frac{\partial F_\phi}{\partial z}, \frac{\partial F_\rho}{\partial z} - \frac{\partial F_z}{\partial\rho}, \frac{1}{\rho}\frac{\partial(\rho F_\phi)}{\partial\rho} - \frac{1}{\rho}\frac{\partial F_\rho}{\partial\phi}\right).\end{aligned}$$

$$\nabla^2\psi = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2}\,.$$

Spherical Polar Coordinates: $q_1 = r$, $h_1 = 1$, $q_2 = \theta$, $h_2 = r$, $q_3 = \phi$, $h_3 = r\sin\theta$.

$$\boldsymbol{\nabla} = \mathbf{e}_r\frac{\partial}{\partial r} \;+\; \mathbf{e}_\theta\frac{1}{r}\frac{\partial}{\partial\theta} \;+\; \mathbf{e}_\phi\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\,.$$

$$\operatorname{div}\mathbf{F} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2F_r\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\,F_\theta) + \frac{1}{r\sin\theta}\frac{\partial F_\phi}{\partial\phi}\,.$$

$$\begin{aligned}\operatorname{curl}\mathbf{F} &= \frac{1}{r^2\sin\theta}\begin{vmatrix} \mathbf{e}_r & r\mathbf{e}_\theta & r\sin\theta\mathbf{e}_\phi \\ \partial_r & \partial_\theta & \partial_\phi \\ F_r & rF_\theta & r\sin\theta F_\phi \end{vmatrix} \\ &= \left(\frac{1}{r\sin\theta}\left(\frac{\partial(\sin\theta\,F_\phi)}{\partial\theta} - \frac{\partial F_\theta}{\partial\phi}\right), \frac{1}{r\sin\theta}\frac{\partial F_r}{\partial\phi} - \frac{1}{r}\frac{\partial(rF_\phi)}{\partial r}, \frac{1}{r}\frac{\partial(rF_\theta)}{\partial r} - \frac{1}{r}\frac{\partial F_r}{\partial\theta}\right).\end{aligned}$$

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\,.$$

2 Green's Functions

2.0 Why Study This?

Numerous scientific phenomena are described by differential equations. This section is about extending your armoury for solving ordinary differential equations, such as those that arise in quantum mechanics and electrodynamics. In particular, we will be interested in how to model an idealized point charge or point mass, or a localized source of heat, waves, etc.

2.0.1 Physical motivation

Newton's second law for a particle of mass m moving in one dimension subject to a force $F(t)$ is

$$\frac{\mathrm{d}p}{\mathrm{d}t} = F\,, \tag{2.1a}$$

where

$$p = m\frac{\mathrm{d}x}{\mathrm{d}t}\,, \tag{2.1b}$$

is the momentum. Suppose that the force is applied only in the time interval $0 < t < \delta t$. The total change in momentum, termed the *impulse*, is

$$\delta p = \int_0^{\delta t} F(t)\,\mathrm{d}t = I\,. \tag{2.1c}$$

We may wish to represent mathematically a situation in which the momentum is changed instantaneously, e.g. if the particle experiences a collision. To achieve this, F must tend to infinity while δt tends to zero, in such a way that its integral I is finite and non-zero. The delta function is introduced to meet these and similar requirements.

2.1 The Dirac Delta Function (a.k.a. Alchemy)

2.1.1 The Delta Function as the Limit of a Sequence

Consider the discontinuous 'top-hat' function $\delta_\varepsilon(x)$ defined for $\varepsilon > 0$ by

$$\delta_\varepsilon(x) = \begin{cases} 0 & x < -\varepsilon \\ \frac{1}{2\varepsilon} & -\varepsilon \leqslant x \leqslant \varepsilon \\ 0 & \varepsilon < x \end{cases}\,. \tag{2.2a}$$

Then for *all* values of ε, including the limit $\varepsilon \to 0+$,

$$\int_{-\infty}^{\infty} \delta_\varepsilon(x)\,\mathrm{d}x = 1\,. \tag{2.2b}$$

Further we note that for any differentiable function $g(x)$ and constant ξ

$$\begin{aligned} \int_{-\infty}^{\infty} \delta_\varepsilon(x-\xi)g'(x)\,\mathrm{d}x &= \int_{\xi-\varepsilon}^{\xi+\varepsilon} \frac{1}{2\varepsilon}\,g'(x)\,\mathrm{d}x \\ &= \frac{1}{2\varepsilon}\Big[g(x)\Big]_{\xi-\varepsilon}^{\xi+\varepsilon} \\ &= \frac{1}{2\varepsilon}\left(g(\xi+\varepsilon) - g(\xi-\varepsilon)\right)\,. \end{aligned}$$

In the limit $\varepsilon \to 0+$ we recover, from using Taylor's theorem and writing $g'(x) = f(x)$,

$$\begin{aligned} \lim_{\varepsilon\to 0+}\int_{-\infty}^{\infty} \delta_\varepsilon(x-\xi)f(x)\,\mathrm{d}x &= \lim_{\varepsilon\to 0+}\frac{1}{2\varepsilon}\Big(\; g(\xi) + \varepsilon g'(\xi) + \tfrac{1}{2}\varepsilon^2 g''(\xi) + \dots \\ &\qquad\qquad -g(\xi) + \varepsilon g'(\xi) - \tfrac{1}{2}\varepsilon^2 g''(\xi) + \dots\Big) \\ &= f(\xi)\,. \end{aligned} \tag{2.2c}$$

We will view the *delta function*, $\delta(x)$, as the limit as $\varepsilon \to 0+$ of $\delta_\varepsilon(x)$, i.e.

$$\delta(x) = \lim_{\varepsilon \to 0+} \delta_\varepsilon(x) \,. \tag{2.3}$$

Applications. Delta functions (as mathematical objects of infinite density and zero spatial extension but having a non-zero integral effect) are a mathematical way of modelling point objects/properties, e.g. point charges, point masses, point forces, point sinks/sources.

2.1.2 Some Properties of the Delta Function

Taking (2.3) as our 'definition' of a delta function, we infer the following.

(i) From (2.2a) we see that the delta function has an *infinitely sharp peak of zero width*, i.e.

$$\delta(x) = \begin{cases} \infty & x = 0 \\ 0 & x \neq 0 \end{cases} \,. \tag{2.4a}$$

(ii) From (2.2b) it follows that the delta function has *unit area*, i.e.

$$\int_{-\alpha}^{\beta} \delta(x)\,\mathrm{d}x = 1 \quad \text{for any } \alpha > 0\,,\ \beta > 0\,. \tag{2.4b}$$

(iii) From (2.2c), and a sneaky interchange of the limit and the integration, we conclude that the delta function can perform 'surgical strikes' on integrands picking out the value of the integrand at one particular point, i.e.

$$\int_{-\infty}^{\infty} \delta(x-\xi) f(x)\,\mathrm{d}x = f(\xi)\,. \tag{2.4c}$$

Remark. This result is equivalent to the *substitution property* of the Kronecker delta:

$$\sum_{j=1}^{3} \delta_{ij} a_j = a_i\,.$$

The Dirac delta function can be understood as the equivalent of the Kronecker delta symbol for functions of a continuous variable.

2.1.3 An Alternative (And Better) View

- The delta function $\delta(x)$ is *not* a function, but a *distribution* or *generalised function*.
- (2.4c) is not really a property of the delta function, but its *definition*. In other words $\delta(x)$ is the generalised function such that for all 'nice' functions $f(x)$[15]

$$\int_{-\infty}^{\infty} \delta(x-\xi) f(x)\,\mathrm{d}x = f(\xi)\,. \tag{2.5}$$

- Given that $\delta(x)$ is defined within an integrand as a linear operator, it should always be employed in
8/02 an integrand as a linear operator.[16]
8/04

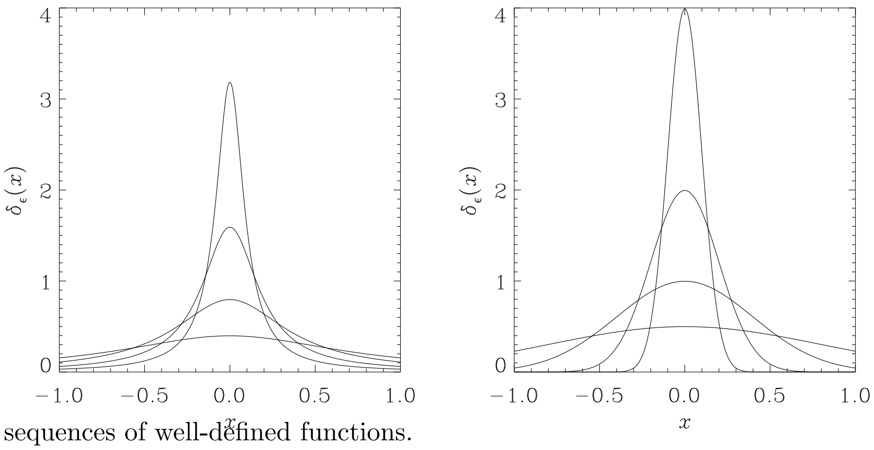
[15] By 'nice' we mean, for instance, that $f(x)$ is everywhere differentiable any number of times, and that

$$\int_{-\infty}^{\infty} \left|\frac{\mathrm{d}^n f}{\mathrm{d}x^n}\right|^2 \mathrm{d}x < \infty \quad \text{for all integers } n \geqslant 0.$$

[16] However we will not always be holier than thou: see (2.6d).

2.1.4 The Delta Function as the Limit of Other Sequences

The top-hat sequence, (2.2a), is not unique in tending to the delta function in an appropriate limit; there are many such sequences of well-defined functions.



The Witch of Agnesi.

For instance we could have alternatively defined $\delta_\varepsilon(x)$ by

$$\delta_\varepsilon(x) = \frac{\varepsilon}{\pi(x^2+\varepsilon^2)}\,. \tag{2.6a}$$

By substituting $x = \varepsilon y$, we recover (2.2b), i.e.

$$\int_{-\infty}^{\infty} \delta_\varepsilon(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} \frac{1}{\pi(y^2+1)}\,\mathrm{d}y = \frac{1}{\pi}\Big[\arctan y\Big]_{-\infty}^{\infty} = 1\,.$$

8/03 Also, by means of the substitution $x = (\xi + \varepsilon z)$ followed by an application of Taylor's theorem, the analogous result to (2.2c) follows, namely

$$\begin{aligned}
\lim_{\varepsilon\to0+}\int_{-\infty}^{\infty} \delta_\varepsilon(x-\xi) f(x)\,\mathrm{d}x &= \lim_{\varepsilon\to0+}\int_{-\infty}^{\infty} \delta_\varepsilon(\varepsilon z) f(\xi+\varepsilon z)\,\varepsilon\mathrm{d}z \\
&= \lim_{\varepsilon\to0+}\int_{-\infty}^{\infty} \frac{1}{\pi(z^2+1)}\left(f(\xi)+\varepsilon z f'(\xi)+\ldots\right)\mathrm{d}z \\
&= f(\xi)\,.
\end{aligned}$$

An equivalent sequence. We note that

$$\begin{aligned}
\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\imath kx-\varepsilon|k|}\,\mathrm{d}k &= \frac{1}{2\pi}\left(\int_{-\infty}^{0} \mathrm{e}^{\imath kx+\varepsilon k}\,\mathrm{d}k + \int_{0}^{\infty} \mathrm{e}^{\imath kx-\varepsilon k}\,\mathrm{d}k\right) \\
&= \frac{1}{2\pi}\left(\frac{1}{\imath x+\varepsilon} - \frac{1}{\imath x-\varepsilon}\right) \\
&= \frac{\varepsilon}{\pi(x^2+\varepsilon^2)}\,.
\end{aligned} \tag{2.6b}$$

Hence from (2.6a)

$$\delta_\varepsilon(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\imath kx-\varepsilon|k|}\,\mathrm{d}k \tag{2.6c}$$

It follows that if we are willing to break the injunction that $\delta(x)$ should always be employed in an integrand as a linear operator, we infer from (2.6c) that

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\imath kx}\,\mathrm{d}k\,. \tag{2.6d}$$

The Gaussian (unlectured).

Another popular choice for $\delta_\varepsilon(x)$ is the Gaussian of width ε:

$$\delta_\varepsilon(x) = \frac{1}{\sqrt{2\pi\varepsilon^2}} \exp\left(-\frac{x^2}{2\varepsilon^2}\right). \tag{2.7a}$$

The analogous result to (2.2b) follows by means of the substitution $x = \sqrt{2}\,\varepsilon y$:

$$\int_{-\infty}^{\infty} \delta_\varepsilon(x)\,\mathrm{d}x = \frac{1}{\sqrt{2\pi\varepsilon^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{2\varepsilon^2}\right) \mathrm{d}x = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp\left(-y^2\right) \mathrm{d}y = 1\,. \tag{2.7b}$$

The equivalent result to (2.2c) can also be recovered by the substitution $x = (\xi + \sqrt{2}\,\varepsilon z)$ followed by an application of Taylor's theorem.

2.1.5 Further Properties of the Delta Function

The following properties hold for all the definitions of $\delta_\varepsilon(x)$ above (i.e. (2.2a), (2.6a), (2.6c) and (2.7a)), and thence for δ by the limiting process. Alternatively they can be deduced from (2.6d).

(i) $\delta(x)$ is symmetric. From (2.6d) it follows using the substitution $k = -\ell$ that

$$\delta(-x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx}\,\mathrm{d}k = -\frac{1}{2\pi} \int_{\infty}^{-\infty} \mathrm{e}^{\imath \ell x}\,\mathrm{d}\ell = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{\imath \ell x}\,\mathrm{d}\ell = \delta(x)\,. \tag{2.8a}$$

(ii) $\delta(x)$ is real. From (2.6d) and (2.8a), with * denoting a complex conjugate, it follows that

$$\delta^*(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx}\,\mathrm{d}k = \delta(-x) = \delta(x)\,. \tag{2.8b}$$

2.1.6 The Heaviside Step Function

The Heaviside step function, $H(x)$, is defined for $x \neq 0$ by

$$H(x) = \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases}. \tag{2.9}$$

This function, which is sometimes written $\theta(x)$, is *discontinuous* at $x = 0$:

$$\lim_{x\to 0-} H(x) = 0 \neq 1 = \lim_{x \to 0+} H(x)\,.$$

There are various conventions for the value of the Heaviside step function at $x = 0$, but it is not uncommon to take $H(0) = \frac{1}{2}$.

The Heaviside function is closely related to the Dirac delta function, since from (2.4a) and (2.4b)

$$H(x) = \int_{-\infty}^{x} \delta(\xi)\,\mathrm{d}\xi. \tag{2.10a}$$

By analogy with the first fundamental theorem of calculus (0.1), this suggests that

$$H'(x) = \delta(x)\,. \tag{2.10b}$$

Unlectured Remark. As a check on (2.10b) we see from integrating by parts that

$$\begin{aligned}
\int_{-\infty}^{\infty} H'(x-\xi) f(x)\,\mathrm{d}x &= \Big[H(x-\xi)f(x)\Big]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} H(x-\xi) f'(x)\,\mathrm{d}x \\
&= f(\infty) - \int_{\xi}^{\infty} f'(x)\,\mathrm{d}x \\
&= f(\infty) - \Big[f(x)\Big]_{\xi}^{\infty} \\
&= f(\xi)\,.
\end{aligned}$$

Hence from the definition the delta function (2.5) we may identify $H'(x)$ with $\delta(x)$.

Application. The idealized impulsive force in § 2.0.1) can be represented as

$$F(t) = I\,\delta(t)\,,$$

i.e. a spike of strength I localized at $t = 0$. If the particle is at rest before the impulse, the solution for its momentum is

8/01 $$p = I\,H(t).$$

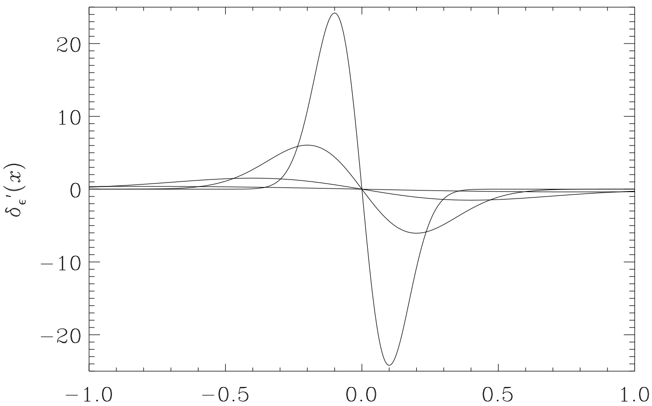
2.1.7 The Derivative of the Delta Function

We can define the derivative of $\delta(x)$ by using (2.4a), (2.4c) and a formal integration by parts:

$$\int_{-\infty}^{\infty} \delta'(x-\xi) f(x)\,\mathrm{d}x = \Big[\delta(x-\xi) f(x)\Big]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \delta(x-\xi) f'(x)\,\mathrm{d}x = -f'(\xi)\,, \tag{2.11}$$

where $f(x)$ is any differentiable function.

Alternatively, the derivative[s] of the delta function can be defined as the limits of sequences of functions. The generating functions for $\delta'(x)$ are the derivatives of (smooth) functions (e.g. Gaussians) that generate



$\delta(x)$, and have both positive and negative 'spikes' localized at $x = 0$.

Remark (unlectured). Not all operations are permitted on generalized functions. In particular, two generalized functions of the same variable cannot be multiplied together, e.g. $H(x)\delta(x)$ is meaningless. However $\delta(x)\delta(y)$ is permissible and represents a point source in a two-dimensional space.

2.2 Second-Order Linear Ordinary Differential Equations

The general *second-order linear* ordinary differential equation (ODE) for $y(x)$ can, wlog, be written as

$$y'' + p(x)y' + q(x)y = f(x) \qquad \text{or} \qquad L\,y(x) = f(x)\,, \tag{2.12a}$$

where L is the differential operator

$$L = \frac{\mathrm{d}^2}{\mathrm{d}x^2} + p(x)\frac{\mathrm{d}}{\mathrm{d}x} + q(x)\,, \tag{2.12b}$$

If $f(x) = 0$ the equation is said to be *homogeneous* (unforced), otherwise it is said to be *inhomogeneous* (forced).

2.2.1 Homogeneous Second-Order Linear ODEs

If $f = 0$ then any two solutions of

$$y'' + py' + qy = 0\,, \tag{2.13a}$$

can be *superposed* to give a third, i.e. if y_1 and y_2 are two solutions then for $\alpha, \beta \in \mathbb{R}$ another solution is

$$y = \alpha y_1 + \beta y_2\,. \tag{2.13b}$$

Further, suppose that y_1 and y_2 are two *linearly independent* solutions, where by linearly independent we mean that

$$\alpha y_1(x) + \beta y_2(x) \equiv 0 \quad \Rightarrow \quad \alpha = \beta = 0\,. \tag{2.13c}$$

Then since (2.13a) is second order, the *general solution* of (2.13a) will be of the form (2.13b). $y_1(x)$ and $y_2(x)$ are often referred to as *complementary functions*, while the parameters α and β can be viewed as the two integration constants. This means that in order to find the general solution of a second order linear homogeneous ODE we need to find two linearly-independent solutions.

Remark. If y_1 and y_2 are linearly dependent then $y_2 = \gamma y_1$ for some $\gamma \in \mathbb{R}$, in which case (2.13b) becomes

$$y = (\alpha + \beta\gamma) y_1\,, \tag{2.14}$$

and we have, in effect, a solution with only one integration constant $\sigma = (\alpha + \beta\gamma)$.

2.2.2 Inhomogeneous Second-Order Linear ODEs

If $y_0(x)$ is *any* solution of the real inhomogeneous equation (2.12a), i.e. if

$$Ly_0 \equiv y_0'' + p(x)y_0' + q(x)y_0 = f(x)\,, \tag{2.15a}$$

then the general solution of (2.12a) has the form

$$y(x) = y_0(x) + \alpha y_1(x) + \beta y_2(x)\,, \tag{2.15b}$$

since

$$\begin{aligned} Ly &= Ly_0 + \alpha L y_1 + \beta L y_2 &\quad (2.15c)\\ &= f + 0 + 0\,. &\quad (2.15d)\end{aligned}$$

Here $y_1(x)$ and $y_2(x)$ are complementary functions, while $y_0(x)$ is referred to as a *particular solution*, or a
07/22 *particular integral.*

2.2.3 The Wronskian

If y_1 and y_2 are linearly dependent (i.e. $y_2 = \gamma y_1$ for some γ), then so are y_1' and y_2' (since, from differentiating, $y_2' = \gamma y_1'$). Hence y_1 and y_2 are linearly dependent only if the equation

$$\begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0\,, \tag{2.16a}$$

has a non-zero solution for α and β. Conversely, if this equation has a solution then y_1 and y_2 are linearly dependent. It follows that non-zero functions y_1 and y_2 are linearly independent if and only if

$$\begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \quad \Rightarrow \quad \alpha = \beta = 0\,. \tag{2.16b}$$

Define the *Wronskian*, $W(x)$, of the two solutions to be the function

$$W[y_1, y_2] = y_1 y_2' - y_2 y_1'\,. \tag{2.17a}$$

Since $\mathsf{A}\mathsf{x} = 0$ only has a zero solution if and only if $\det \mathsf{A} \neq 0$, we conclude that y_1 and y_2 are linearly independent if and only if

$$\left\| \begin{matrix} y_1 & y_2 \\ y_1' & y_2' \end{matrix} \right\| = y_1 y_2' - y_2 y_1' = W \neq 0\,, \tag{2.17b}$$

i.e. the Wronskian is non-zero.

2.2.4 Initial-value and boundary-value problems

Two *boundary conditions* (BCs) must be specified to determine fully the solution of a second-order ODE. A boundary condition is usually an equation relating the values of y and y' at one point.

Remark. Without loss of generality we can assume that the BCs do not involve y'' and higher derivatives, since the ODE allows y'' and higher derivatives to be expressed in terms of y and y'.

The general form of a *linear* BC at a point $x = a$ is

$$Ay(a) + By'(a) = E\,, \tag{2.18}$$

where A, B and E are constants, and A and B are not both zero. If $E = 0$ the BC is said to be *homogeneous*.

Initial-value problem. If both BCs are specified at the same point we have an *initial-value problem*, e.g. solve

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = F(t) \quad \text{for } t \geqslant 0, \text{ subject to } x = \frac{\mathrm{d}x}{\mathrm{d}t} = 0 \text{ at } t = 0. \tag{2.19a}$$

Boundary-value problem. If the BCs are specified at different points we have a *two-point boundary-value problem*, e.g. solve

$$y''(x) + y(x) = f(x) \quad \text{for } a \leqslant x \leqslant b, \text{ subject to } y(a) = y(b) = 0\,. \tag{2.19b}$$

2.3 Differential equations containing delta functions

If a differential equation involves a step function or delta function, this generally implies a lack of smoothness in the solution. The equation can be solved separately on either side of the discontinuity and the two parts of the solution connected by applying the appropriate matching conditions. Consider, as an example, the linear second-order ODE

$$\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + y = \delta(x)\,. \tag{2.20}$$

If x represents time, this equation could represent the behaviour of a simple harmonic oscillator in response to an impulsive force. In each of the regions $x < 0$ and $x > 0$ separately, the right-hand side vanishes and the general solution is a linear combination of $\cos x$ and $\sin x$. We may write

$$y = \begin{cases} \alpha_- \cos x + \beta_- \sin x, & x < 0 \\ \alpha_+ \cos x + \beta_+ \sin x, & x > 0 \end{cases}.$$

Since the general solution of a second-order ODE should contain only two arbitrary constants, it should be possible to relate α_+ and β_+ to α_- and β_-.

What is the nature of the non-smoothness in y? Integrate (2.20) from $x = -\varepsilon$ to $x = \varepsilon$ to obtain

$$\int_{-\varepsilon}^{\varepsilon} \frac{\mathrm{d}^2y}{\mathrm{d}x^2}\,\mathrm{d}x \;+\; \int_{-\varepsilon}^{\varepsilon} y(x)\,\mathrm{d}x \;=\; \int_{-\varepsilon}^{\varepsilon} \delta(x)\,\mathrm{d}x\,, \tag{2.21a}$$

i.e.

$$y'(\varepsilon) - y'(-\varepsilon) \;+\; \int_{-\varepsilon}^{\varepsilon} y(x)\,\mathrm{d}x \;=\; 1\,. \tag{2.21b}$$

Now let $\varepsilon \to 0$. If we assume that y is bounded, then the integral term makes no contribution and we get

$$\left[\frac{\mathrm{d}y}{\mathrm{d}x}\right] \equiv \lim_{\varepsilon\to 0}\left[\frac{\mathrm{d}y}{\mathrm{d}x}\right]_{x=-\varepsilon}^{x=\varepsilon} = 1\,. \tag{2.21c}$$

Since there is only a finite jump in the derivative of y, we may further conclude that y is continuous, in which case the jump conditions are

$$[y] = 0, \qquad \left[\frac{\mathrm{d}y}{\mathrm{d}x}\right] = 1 \qquad \text{at } x = 0\,. \tag{2.21d}$$

Applying these conditions, we obtain

$$\alpha_+ - \alpha_- = 0 \quad \text{and} \quad \beta_+ - \beta_- = 1\,. \tag{2.22}$$

Hence the general solution is

$$y = \begin{cases} \alpha_- \cos x + \beta_- \sin x & x < 0 \\ \alpha_- \cos x + (\beta_- + 1)\sin x & x > 0 \end{cases}. \tag{2.23}$$

In particular, if the oscillator is at rest before the impulse occurs, then $\alpha_- = \beta_- = 0$ and the solution is $y = H(x)\sin x$.

2.4 Green's Functions

2.4.1 The Green's Function for two-point homogeneous boundary-value problems

Suppose that we wish to solve (2.12a), i.e.

$$L\, y(x) = f(x)\,, \tag{2.24a}$$

where L is the general second-order linear differential operator in x, i.e.

$$L = \frac{\mathrm{d}^2}{\mathrm{d}x^2} + p(x)\frac{\mathrm{d}}{\mathrm{d}x} + q(x)\,, \tag{2.24b}$$

with p and q being continuous functions. To fix ideas we will assume that the solution should satisfy *homogeneous* boundary conditions at $x = a$ and $x = b$, i.e.

$$Ay(a) + By'(a) = 0\,, \tag{2.25a}$$

$$Cy(b) + Dy'(b) = 0\,. \tag{2.25b}$$

where A, B, C and D are constants such that A and B are not both zero, and C and D are not both zero.

Next, suppose that we can find a solution $G(x;\zeta)$ that is the response of the system to *forcing at a point* ζ, i.e. $G(x;\zeta)$ is the solution to

$$\mathcal{L}\, G(x;\zeta) = \delta(x-\zeta)\,, \tag{2.26a}$$

subject to the boundary conditions (cf. (2.25a) and (2.25b))

$$A\, G(a;\zeta) + B\, G_x(a;\zeta) = 0 \quad \text{and} \quad C\, G(b;\zeta) + D\, G_x(b;\zeta) = 0\,, \tag{2.26b}$$

where

$$\mathcal{L} = \frac{\partial^2}{\partial x^2} + p(x)\frac{\partial}{\partial x} + q(x)\,, \tag{2.26c}$$

$$G_x(x;\zeta) = \frac{\partial G}{\partial x}(x;\zeta)\,, \tag{2.26d}$$

and we have used $\frac{\partial}{\partial x}$ rather than $\frac{\mathrm{d}}{\mathrm{d}x}$ since G is a function of both x and ζ. Then we claim that the solution of the original problem (2.24a) is

$$y(x) = \int_a^b G(x;\zeta) f(\zeta)\,\mathrm{d}\zeta\,. \tag{2.27}$$

To see this we first note that (2.27) satisfies the boundary conditions (2.25a) and (2.25b), since from (2.26b)

$$Ay(a) + By'(a) = \int_a^b \left(A\, G(a;\zeta) + B\, G_x(a;\zeta)\right) f(\zeta)\,\mathrm{d}\zeta = 0\,, \tag{2.28a}$$

$$Cy(b) + Dy'(b) = \int_a^b \left(C\, G(b;\zeta) + D\, G_x(b;\zeta)\right) f(\zeta)\,\mathrm{d}\zeta = 0\,. \tag{2.28b}$$

Further, (2.27) also satisfies the inhomogeneous equation (2.24a) because

$$\begin{aligned} \mathcal{L}\, y(x) &= \int_a^b \mathcal{L}\, G(x;\zeta)\; f(\zeta)\,\mathrm{d}\zeta && \text{differential wrt } x\text{, integral wrt } \zeta \\ &= \int_a^b \delta(x-\zeta)\; f(\zeta)\,\mathrm{d}\zeta && \text{from (2.26a)} \\ &= f(x) && \text{from (2.5)}\,. \end{aligned} \tag{2.28c}$$

21/02 The function $G(x;\zeta)$ is called the *Green's function* of $\mathcal{L}$ for the given homogeneous boundary conditions.

2.4.2 Two Properties Green's Functions

In the next subsection we will construct a Green's function. However, first we need to derive two properties of $G(x;\zeta)$. Suppose that we integrate equation (2.26a) from $\zeta-\varepsilon$ to $\zeta+\varepsilon$ for $\varepsilon>0$ and consider the limit $\varepsilon\to 0$ (cf. (2.21a)). From (2.5) the right hand side is equal to 1, and hence

$$\begin{aligned}
1 &= \lim_{\varepsilon\to0}\int_{\zeta-\varepsilon}^{\zeta+\varepsilon}\mathcal{L}G\,\mathrm{d}x \\
&= \lim_{\varepsilon\to0}\int_{\zeta-\varepsilon}^{\zeta+\varepsilon}\left(\frac{\partial^2 G}{\partial x^2}+p\frac{\partial G}{\partial x}+q\,G\right)\mathrm{d}x && \text{from (2.24b)}\\
&= \lim_{\varepsilon\to0}\int_{\zeta-\varepsilon}^{\zeta+\varepsilon}\frac{\partial}{\partial x}\left(\frac{\partial G}{\partial x}+p\,G\right)\mathrm{d}x+\lim_{\varepsilon\to0}\int_{\zeta-\varepsilon}^{\zeta+\varepsilon}\left(-\frac{\mathrm{d}p}{\mathrm{d}x}G+q\,G\right)\mathrm{d}x && \text{rearrange}\\
&= \lim_{\varepsilon\to0}\left[\frac{\partial G}{\partial x}+p\,G\right]_{x=\zeta-\varepsilon}^{x=\zeta+\varepsilon}-\lim_{\varepsilon\to0}\int_{\zeta-\varepsilon}^{\zeta+\varepsilon}\left(\frac{\mathrm{d}p}{\mathrm{d}x}-q\right)G\,\mathrm{d}x\,. && (2.29)
\end{aligned}$$

How can this equation be satisfied? Taking the lead from (2.21d), suppose that $G(x;\zeta)$ is bounded near $x=\zeta$, then since p and q are continuous, (2.29) reduces to

$$\lim_{\varepsilon\to0}\left[\frac{\partial G}{\partial x}+p\,G\right]_{x=\zeta-\varepsilon}^{x=\zeta+\varepsilon}=1\,.$$

This implies that the jump in the derivative of G is bounded (cf. the unit jump in the Heaviside step function (2.9) at $x=0$). In turn, this means that G must be continuous. We conclude that

$$\lim_{\varepsilon\to0}\Big[G(x;\zeta)\Big]_{\zeta-\varepsilon}^{\zeta+\varepsilon}=0\qquad\text{and}\qquad\lim_{\varepsilon\to0}\left[\frac{\partial G}{\partial x}\right]_{x=\zeta-\varepsilon}^{x=\zeta+\varepsilon}=1\,.\tag{2.30}$$

i.e. G is continuous and there is a unit jump in the derivative of G at $x=\zeta$.

21/01 *Remark.* A function can be continuous and its derivative discontinuous, but not vice versa.

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2.4.3 Construction of the Green's Function

$G(x;\zeta)$ can be constructed by the following procedure. First we note that when $x\neq\zeta$, G satisfies the homogeneous equation, and hence G should be the sum of two linearly independent solutions, say y_1 and y_2, of the homogeneous equation. So let

$$G(x;\zeta)=\begin{cases}\alpha_-(\zeta)y_1(x)+\beta_-(\zeta)y_2(x) & \text{for } a\leqslant x<\zeta,\\ \alpha_+(\zeta)y_1(x)+\beta_+(\zeta)y_2(x) & \text{for } \zeta\leqslant x\leqslant b.\end{cases}\tag{2.31}$$

By construction this satisfies (2.26a) for $x\neq\zeta$. Next we obtain equations relating $\alpha_\pm(\zeta)$ and $\beta_\pm(\zeta)$ by requiring at $x=\zeta$ that G is continuous and $\frac{\partial G}{\partial x}$ has a unit discontinuity. It follows from (2.30) that

$$\begin{aligned}
\big[\alpha_+(\zeta)y_1(\zeta)+\beta_+(\zeta)y_2(\zeta)\big]-\big[\alpha_-(\zeta)y_1(\zeta)+\beta_-(\zeta)y_2(\zeta)\big]&=0\,,\\
\big[\alpha_+(\zeta)y_1'(\zeta)+\beta_+(\zeta)y_2'(\zeta)\big]-\big[\alpha_-(\zeta)y_1'(\zeta)+\beta_-(\zeta)y_2'(\zeta)\big]&=1\,,
\end{aligned}$$

i.e., grouping the y_1 and y_2 terms,

$$\begin{aligned}
y_1(\zeta)\big[\alpha_+(\zeta)-\alpha_-(\zeta)\big]+y_2(\zeta)\big[\beta_+(\zeta)-\beta_-(\zeta)\big]&=0\,,\\
y_1'(\zeta)\big[\alpha_+(\zeta)-\alpha_-(\zeta)\big]+y_2'(\zeta)\big[\beta_+(\zeta)-\beta_-(\zeta)\big]&=1\,,
\end{aligned}$$

i.e.

$$\begin{pmatrix} y_1 & y_2\\ y_1' & y_2'\end{pmatrix}\begin{pmatrix}\alpha_+-\alpha_-\\ \beta_+-\beta_-\end{pmatrix}=\begin{pmatrix}0\\1\end{pmatrix}.\tag{2.32}$$

A solution exists to this equation if, see (2.17b),

$$W\equiv\left\|\begin{matrix} y_1 & y_2\\ y_1' & y_2'\end{matrix}\right\|\neq0\,,$$

i.e. if y_1 and y_2 are linearly independent; if so then

$$\alpha_+-\alpha_-=-\frac{y_2(\zeta)}{W(\zeta)}\quad\text{and}\quad\beta_+-\beta_-=\frac{y_1(\zeta)}{W(\zeta)}\,.\tag{2.33}$$ 08/22

Finally we impose the boundary conditions. For instance, suppose that the solution y is required to satisfy (cf. (2.19b))

$$y(a) = y(b) = 0\,. \tag{2.34a}$$

Then the appropriate boundary conditions for G would be

$$G(a;\zeta) = G(b;\zeta) = 0\,, \tag{2.34b}$$

i.e. $A = C = 1$ and $B = D = 0$ in (2.26b). It follows from (2.31) that we would require

$$\alpha_-(\zeta)y_1(a) + \beta_-(\zeta)y_2(a) = 0\,, \tag{2.35a}$$

$$\alpha_+(\zeta)y_1(b) + \beta_+(\zeta)y_2(b) = 0\,. \tag{2.35b}$$

$\alpha_\pm$, $\beta_\pm$ could then be determined from the four equations in (2.33), (2.35a) and (2.35b).

More generally, for the homogeneous boundary conditions (2.25a) and (2.25b), i.e.

$$Ay(a) + By'(a) = 0 \quad \text{and} \quad Cy(b) + Dy'(b) = 0\,, \tag{2.36a}$$

the appropriate boundary conditions for G are

$$AG(a;\zeta) + B\frac{\partial G}{\partial x}(a;\zeta) = 0 \tag{2.36b}$$

$$CG(b;\zeta) + D\frac{\partial G}{\partial x}(b;\zeta) = 0\,. \tag{2.36c}$$

For simplicity construct complementary functions y_1 and y_2 so that they satisfy the boundary condition at a and b respectively, i.e. choose y_1 and y_2 so that

$$Ay_1(a) + By_1'(a) = 0 \quad \text{and} \quad Cy_2(b) + Dy_2'(b) = 0\,. \tag{2.37a}$$

Then

$$\alpha_+ = \beta_- = 0\,, \tag{2.37b}$$

and the solution (2.31) simplifies to

$$G(x;\zeta) = \begin{cases} \alpha_-(\zeta)y_1(x), & a \leqslant x < \zeta\,, \\ \beta_+(\zeta)y_2(x), & \zeta \leqslant x \leqslant b\,, \end{cases} \tag{2.37c}$$

and thence from (2.33)

$$\alpha_- = \frac{y_2(\zeta)}{W(\zeta)} \quad \text{and} \quad \beta_+ = \frac{y_1(\zeta)}{W(\zeta)}\,. \tag{2.37d}$$

It follows from (2.31) that

$$G(x;\zeta) = \begin{cases} \dfrac{y_1(x)y_2(\zeta)}{W(\zeta)} & \text{for } a \leqslant x < \zeta, \\[2ex] \dfrac{y_1(\zeta)y_2(x)}{W(\zeta)} & \text{for } \zeta \leqslant x \leqslant b. \end{cases} \tag{2.37e}$$

Remark. This method fails if the Wronskian $W[y_1, y_2]$ vanishes. This happens if y_1 is proportional to y_2, i.e. if there is a complementary function that happens to satisfy the homogeneous boundary conditions both at $x = a$ and $x = b$. In this case the equation $Ly = f$ may not have a solution satisfying the boundary conditions; if it does, the solution will not be unique (cf. resonance).

2.4.4 Examples of Green's Functions

(i) Find the Green's function in $0 < a < b$ for

$$\mathcal{L} = \frac{\partial^2}{\partial x^2} + \frac{1}{x}\frac{\partial}{\partial x} - \frac{n^2}{x^2}\,, \tag{2.38a}$$

with homogeneous boundary conditions

$$G(a;\zeta) = 0 \quad \text{and} \quad \frac{\partial G}{\partial x}(b;\zeta) = 0\,, \tag{2.38b}$$

i.e. with $A = D = 1$ and $B = C = 0$ in (2.26b).

Answer. Seek solutions to the homogeneous equation $\mathcal{L}\, y = 0$ of the form $y = x^r$. Then we require that

$$r(r-1) + r - n^2 = 0\,, \quad \text{i.e.} \quad r = \pm n\,. \tag{2.39a}$$

Let

$$y_1 = \left(\frac{x}{a}\right)^n - \left(\frac{a}{x}\right)^n \quad \text{and} \quad y_2 = \left(\frac{x}{b}\right)^n + \left(\frac{b}{x}\right)^n, \tag{2.39b}$$

where we have constructed y_1 and y_2 so that $y_1(a) = 0$ and $y_2'(b) = 0$ as is appropriate for boundary conditions (2.38b). Since we require that $G(a;\zeta) = 0$ from (2.38b), and by construction $y_1(a) = 0$, it follows that $\beta_- = 0$ in (2.31). Similarly, since we require that $\frac{\partial G}{\partial x}(b;\zeta) = 0$ from (2.38b), and by construction $y_2'(b) = 0$, it follows that $\alpha_+ = 0$. Hence, as in (2.37c),

$$G(x;\zeta) = \begin{cases} \alpha_-(\zeta) y_1(x) & \text{for } a \leqslant x < \zeta, \\ \beta_+(\zeta) y_2(x) & \text{for } \zeta \leqslant x \leqslant b. \end{cases}$$

We also require that G is continuous and $\frac{\partial G}{\partial x}$ has a unit discontinuity at $x = \zeta$, hence

$$\beta_+(\zeta) y_2(\zeta) = \alpha_-(\zeta) y_1(\zeta) \quad \text{and} \quad \beta_+(\zeta) y_2'(\zeta) - \alpha_-(\zeta) y_1'(\zeta) = 1\,. \tag{2.40}$$

Thus, as in (2.37d) and (2.37e),

$$\alpha_- = \frac{y_2(\zeta)}{W(\zeta)}\,, \quad \beta_+ = \frac{y_1(\zeta)}{W(\zeta)} \quad \text{and} \quad G(x;\zeta) = \begin{cases} \dfrac{y_1(x) y_2(\zeta)}{W(\zeta)} & \text{for } a \leqslant x < \zeta, \\[2ex] \dfrac{y_1(\zeta) y_2(x)}{W(\zeta)} & \text{for } \zeta \leqslant x \leqslant b. \end{cases} \tag{2.41}$$

(ii) Find the Green's function for the two-point boundary-value problem

$$y''(x) + y(x) = f(x), \qquad y(0) = y(1) = 0\,. \tag{2.42}$$

Answer. The complementary functions satisfying left and right boundary conditions are

$$y_1 = \sin x \quad \text{and} \quad y_2 = \sin(x-1) \tag{2.43}$$

respectively. The Wronskian is thus

$$W = y_1 y_2' - y_2 y_1' = \sin x \cos(x-1) - \sin(x-1)\cos x = \sin 1\,. \tag{2.44}$$

Thus

$$G(x;\zeta) = \begin{cases} \dfrac{\sin x \sin(\zeta - 1)}{\sin 1} & 0 \leqslant x \leqslant \zeta\,, \\[2ex] \dfrac{\sin\zeta \sin(x-1)}{\sin 1} & \zeta \leqslant x \leqslant 1\,. \end{cases} \tag{2.45}$$

So, being careful to choose the correct expression for G depending on whether $x \leqslant \zeta$ or $x \geqslant \zeta$,

$$\begin{aligned} y(x) &= \int_0^1 G(x;\zeta) f(\zeta)\, \mathrm{d}\zeta \\ &= \frac{\sin(x-1)}{\sin 1} \int_0^x \sin\zeta\, f(\zeta)\, \mathrm{d}\zeta + \frac{\sin x}{\sin 1} \int_x^1 \sin(\zeta - 1) f(\zeta)\, \mathrm{d}\zeta\,. \end{aligned} \tag{2.46}$$

2.4.5 The Green's Function for homogeneous initial-value problems

Suppose that instead of the two-point boundary conditions (2.25a) and (2.25b), we require that

$$y(a) = y'(a) = 0\,. \tag{2.47a}$$

We then require, by analogy with (2.26b), that

$$G(a;\zeta) = \frac{\partial G}{\partial x}(a;\zeta) = 0\,. \tag{2.47b}$$

Choose the complementary functions so that $y_1(a) = 0$ and $y_2'(a) = 0$ (which can be shown to be linearly independent and always possible), then (2.31) simplifies to

$$G(x;\zeta) = \begin{cases} 0 & \text{for } a \leqslant x < \zeta, \\ \alpha_+(\zeta)y_1(x) + \beta_+(\zeta)y_2(x) & \text{for } \zeta \leqslant x \leqslant b, \end{cases} \tag{2.48}$$

i.e. $\alpha_- = \beta_- = 0$. The conditions that G be continuous and $\frac{\partial G}{\partial x}$ has a unit discontinuity then give that

$$\alpha_+(\zeta)y_1(\zeta) + \beta_+(\zeta)y_2(\zeta) = 0\,, \tag{2.49a}$$
$$\alpha_+(\zeta)y_1'(\zeta) + \beta_+(\zeta)y_2'(\zeta) = 1\,. \tag{2.49b}$$

Or in matrix form

$$\begin{bmatrix} y_1(\zeta) & y_2(\zeta) \\ y_1'(\zeta) & y_2'(\zeta) \end{bmatrix} \begin{bmatrix} \alpha_+(\zeta) \\ \beta_+(\zeta) \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{2.50a}$$

with solution

$$\begin{bmatrix} \alpha_+(\zeta) \\ \beta_+(\zeta) \end{bmatrix} = \frac{1}{W(\zeta)} \begin{bmatrix} y_2'(\zeta) & -y_2(\zeta) \\ -y_1'(\zeta) & y_1(\zeta) \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -y_2(\zeta)/W(\zeta) \\ y_1(\zeta)/W(\zeta) \end{bmatrix} \tag{2.50b}$$

The Green's function is therefore

$$G(x;\zeta) = \begin{cases} 0 & \text{for } a \leqslant x < \zeta, \\ \dfrac{y_1(\zeta)y_2(x) - y_1(x)y_2(\zeta)}{W(\zeta)} & \text{for } \zeta \leqslant x \leqslant b. \end{cases} \tag{2.51}$$

Example. Find the Green's function for the initial-value problem

$$y''(x) + y(x) = f(x), \qquad y(0) = y'(0) = 0\,. \tag{2.52}$$

Answer. The complementary functions that satisfy the boundary conditions are $y_1 = \sin x$ and $y_2 = \cos x$, with Wronskian

$$W = y_1y_2' - y_2y_1' = -\sin^2 x - \cos^2 x = -1\,. \tag{2.53a}$$

Further

$$y_1(\zeta)y_2(x) - y_1(x)y_2(\zeta) = \sin\zeta\cos x - \sin x\cos\zeta = \sin(\zeta - x)\,. \tag{2.53b}$$

Thus

$$G(x;\zeta) = \begin{cases} 0 & 0 \leqslant x \leqslant \zeta\,, \\ \sin(x-\zeta) & x > \zeta\,, \end{cases} \tag{2.53c}$$

and thus

$$y(x) = \int_0^x \sin(x-\zeta)f(\zeta)\,\mathrm{d}\zeta \tag{2.53d}$$

2.4.6 Inhomogeneous boundary conditions

So far we only considered problems with homogeneous boundary conditions. One can also use Green's functions to solve problems with inhomogeneous boundary conditions. The trick is to solve the homogeneous equation $Ly_{ibc} = 0$ for a function y_{ibc} which satisfies the *inhomogeneous* boundary conditions. Then solve the inhomogeneous equation $Ly_{hbc} = f$, perhaps using the Green's function method discussed in this chapter, imposing *homogeneous* boundary conditions on y_{hbc}. Then linearity means that $y_{ibc} + y_{hbc}$ satisfies the inhomogeneous equation with inhomogeneous boundary conditions.

3 Fourier Transforms

3.0 Why Study This?

Fourier series tell you about the *spectral* (or harmonic) properties of functions/signals that are periodic; if the period is L, then the harmonics have frequencies n/L where n is an integer. The Fourier transform generalizes this idea to functions that are not periodic. The 'harmonics' can then have any frequency.

The Fourier transform has innumerable applications in diverse fields such as astronomy, optics, signal processing, data analysis, statistics and number theory. Furthermore, the Fourier transform provides a complementary way of looking at a function. Certain operations on a function are more easily computed 'in the Fourier domain'. This idea is particularly useful in solving certain kinds of differential equation.

3.1 The Fourier Transform

3.1.1 Definition

Given a function $f(x)$ such that

$$\int_{-\infty}^{\infty} |f(x)|\,\mathrm{d}x \;<\; \infty\,,$$

we define its *Fourier transform*, $\widetilde{f}(k)$, by

$$\widetilde{f}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} f(x)\,\mathrm{d}x\,. \tag{3.1}$$

Notation. Sometimes it is clearer to denote the Fourier transform of a function f by $\mathcal{F}[f]$ rather than $\widetilde{f}$, i.e.

$$\mathcal{F}[\bullet] \equiv \widetilde{\bullet}\,. \tag{3.2}$$

Remark. There are differing normalisations of the Fourier transform. Hence you will encounter definitions where the $(2\pi)^{-\frac{1}{2}}$ is either not present or replaced by $(2\pi)^{-1}$, and other definitions where the $-\imath kx$ is replaced by $+\imath kx$.

Property. If the function $f(x)$ is real the Fourier transform $\widetilde{f}(k)$ is not necessarily real. However if f is both *real and even*, i.e. $f^*(x) = f(x)$ and $f(x) = f(-x)$ respectively, then by using these properties and the substitution $x = -y$ it follows that $\widetilde{f}$ is *real*:

$$\begin{aligned}
\widetilde{f}^*(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{\imath kx} f^*(x)\,\mathrm{d}x && \text{from c.c. of (3.1)}\\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{\imath kx} f(-x)\,\mathrm{d}x && \text{since } f^*(x) = f(-x)\\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{-\imath ky} f(y)\,\mathrm{d}y && \text{let } x = -y\\
&= \widetilde{f}(k)\,. && \text{from (3.1)}
\end{aligned} \tag{3.3}$$

Similarly we can show that if f is both *real and odd*, then $\widetilde{f}$ is *purely imaginary*, i.e. $\widetilde{f}^*(k) = -\widetilde{f}(k)$. Conversely it is possible to show using the Fourier inversion theorem (see below) that

- if both f and $\widetilde{f}$ are real, then f is even;
- if f is real and $\widetilde{f}$ is purely imaginary, then f is odd.

3.1.2 Examples of Fourier Transforms

The Fourier Transform (FT) of $\mathrm{e}^{-b|x|}$ $(b > 0)$. First, from (2.6b) we already have that

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\imath kx - \varepsilon|k|}\,\mathrm{d}k = \frac{\varepsilon}{\pi(x^2+\varepsilon^2)}\,.$$

For what follows it is helpful to rewrite this result by making the transformations $x \to -\ell$, $k \to x$ and $\varepsilon \to b$ to obtain

$$\int_{-\infty}^{\infty} \mathrm{e}^{-\imath \ell x - b|x|}\,\mathrm{d}x = \frac{2b}{\ell^2+b^2}\,. \tag{3.4}$$

We deduce from the definition of a Fourier transform, (3.1), and (3.4) with $\ell = k$, that

$$\mathcal{F}[\mathrm{e}^{-b|x|}] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx - b|x|}\,\mathrm{d}x = \frac{1}{\sqrt{2\pi}}\,\frac{2b}{k^2+b^2}\,. \tag{3.5}$$

The FTs of $\cos(ax)\,\mathrm{e}^{-b|x|}$ **and** $\sin(ax)\,\mathrm{e}^{-b|x|}$ $(b>0)$**.** *Unlectured.* From (3.1), the definition of cosine, and (3.4) first with $\ell = a-k$ and then with $\ell = a+k$, it follows that

$$\begin{aligned}\mathcal{F}[\cos(ax)\,\mathrm{e}^{-b|x|}] &= \frac{1}{2\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\mathrm{e}^{\imath ax} + \mathrm{e}^{-\imath ax}\right) \mathrm{e}^{-\imath kx - b|x|}\,\mathrm{d}x \\ &= \frac{b}{\sqrt{2\pi}} \left(\frac{1}{(a-k)^2+b^2} + \frac{1}{(a+k)^2+b^2} \right).\end{aligned} \tag{3.6a}$$

This is real, as it has to be since $\cos(ax)\,\mathrm{e}^{-b|x|}$ is even.

Similarly, from (3.1), the definition of sine, and (3.4) first with $\ell = a-k$ and then with $\ell = a+k$, it follows that

$$\begin{aligned}\mathcal{F}[\sin(ax)\,\mathrm{e}^{-b|x|}] &= \frac{1}{2\imath\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\mathrm{e}^{\imath ax} - \mathrm{e}^{-\imath ax}\right) \mathrm{e}^{-\imath kx - b|x|}\,\mathrm{d}x \\ &= \frac{-\imath b}{\sqrt{2\pi}} \left(\frac{1}{(a-k)^2+b^2} - \frac{1}{(a+k)^2+b^2} \right).\end{aligned} \tag{3.6b}$$

09/22 This is purely imaginary, as it has to be since $\sin(ax)\,\mathrm{e}^{-b|x|}$ is odd.

The FT of a Gaussian. From the definition (3.1), the completion of a square, and the substitution $x = (\varepsilon y - \imath\varepsilon^2 k)$,[17] it follows that

$$\begin{aligned}\mathcal{F}\left[\frac{1}{\sqrt{2\pi\varepsilon^2}} \exp\left(-\frac{x^2}{2\varepsilon^2}\right)\right] &= \frac{1}{2\pi\varepsilon} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{2\varepsilon^2} - \imath kx\right) \mathrm{d}x \\ &= \frac{1}{2\pi\varepsilon} \int_{-\infty}^{\infty} \exp\left(-\tfrac{1}{2}\left(\frac{x}{\varepsilon} + \imath\varepsilon k\right)^2 - \tfrac{1}{2}\varepsilon^2 k^2\right) \mathrm{d}x \\ &= \frac{1}{2\pi} \exp\left(-\tfrac{1}{2}\varepsilon^2 k^2\right) \int_{-\infty}^{\infty} \exp\left(-\tfrac{1}{2}y^2\right) \mathrm{d}y \\ &= \frac{1}{\sqrt{2\pi}} \exp\left(-\tfrac{1}{2}\varepsilon^2 k^2\right).\end{aligned} \tag{3.7}$$

Hence the FT of a Gaussian of width (standard deviation) ε is a Gaussian of width ε^{-1}. This illustrates a property of the Fourier transform: the narrower the function of x, the wider the function of k.

The FT of the delta function. From definitions (2.5) and (3.1) it follows that

$$\begin{aligned}\mathcal{F}[\delta(x-a)] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x-a)\mathrm{e}^{-\imath kx}\,\mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{-\imath ka}\,.\end{aligned} \tag{3.8a}$$

Hence the Fourier transform of $\delta(x)$ is $1/\sqrt{2\pi}$. Recalling the description of a delta function as a limit of a Gaussian, see (2.7a), we note that this result with $a=0$ is consistent with (3.7) in the limit $\varepsilon \to 0+$.

The FT of the step function. From (2.9) and (3.1) it follows that

$$\begin{aligned}\mathcal{F}[H(x-a)] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} H(x-a)\mathrm{e}^{-\imath kx}\,\mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}} \int_{a}^{\infty} \mathrm{e}^{-\imath kx}\,\mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}} \left[\frac{\mathrm{e}^{-\imath kx}}{-\imath k}\right]_a^{\infty}\end{aligned}$$

[17] This is a little naughty since it takes us into the complex x-plane. However, it can be fixed up once you have done Cauchy's theorem.

There is now a problem, since what is $\lim_{x\to\infty} \mathrm{e}^{-\imath kx}$? For the time being the simplest resolution is, in the spirit of (2.6b) and (2.6c) in § 2.1.4, to find $\mathcal{F}[H(x-a)\mathrm{e}^{-\varepsilon(x-a)}]$ for $\varepsilon > 0$, and then let $\varepsilon \to 0+$. So

$$\begin{aligned}
\mathcal{F}[H(x-a)\mathrm{e}^{-\varepsilon(x-a)}] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} H(x-a)\mathrm{e}^{-\varepsilon(x-a)-\imath kx}\,\mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi}} \left[\frac{\mathrm{e}^{-\varepsilon(x-a)-\imath kx}}{-\varepsilon-\imath k} \right]_a^{\infty} \\
&= \frac{1}{\sqrt{2\pi}} \frac{\mathrm{e}^{-\imath ka}}{\varepsilon+\imath k}\,. \qquad (3.8b)
\end{aligned}$$

On taking the limit $\varepsilon \to 0$ we have that

$$\mathcal{F}[H(x-a)] = \frac{\mathrm{e}^{-\imath ka}}{\sqrt{2\pi}\,\imath k}\,. \qquad (3.8c)$$

Remark. For future reference we observe from a comparison of (3.8a) and (3.8c) that

$$\imath k\mathcal{F}[H(x-a)] = \mathcal{F}[\delta(x-a)]\,. \qquad (3.8d)$$

The FT of the top-hat function. Consider the discontinuous 'top-hat' function $g(x)$ defined by

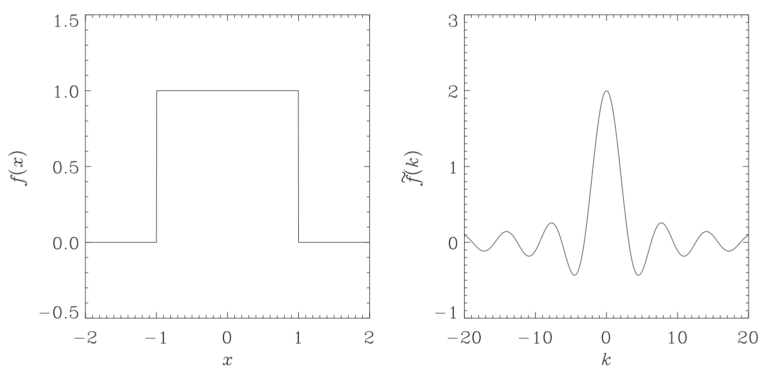
$$g(x) = \begin{cases} c & a < x < b\,, \\ 0 & \text{otherwise}\,. \end{cases} \qquad (3.9a)$$

Then

$$\sqrt{2\pi}\,\widetilde{g}(k) = \int_a^b c\,\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x = \frac{\mathrm{i}c}{k}\left(\mathrm{e}^{-\mathrm{i}kb} - \mathrm{e}^{-\mathrm{i}ka}\right)\,. \qquad (3.9b)$$

For instance, if $a = -1$, $b = 1$ and $c = 1$

$$\sqrt{2\pi}\,\widetilde{g}(k) = \frac{\mathrm{i}}{k}\left(\mathrm{e}^{-\mathrm{i}k} - \mathrm{e}^{\mathrm{i}k}\right) = \frac{2\sin k}{k}\,. \qquad (3.9c)$$



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3.1.3 The Fourier Inversion Theorem

Given a function f we can compute its Fourier transform $\widetilde{f}$ from (3.1). For many functions the converse is also true, i.e. given the Fourier transform $\widetilde{f}$ of a function we can reconstruct the original function f. To see this consider the following calculation (note the use of a dummy variable $\bullet$ to avoid an overabundance of x)

$$\begin{aligned}
\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\imath kx} \widetilde{f}(k)\,\mathrm{d}k &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\imath kx} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath k\bullet} f(\bullet)\,\mathrm{d}\bullet \right) \mathrm{d}k && \text{from definition (3.1)} \\
&= \int_{-\infty}^{\infty} \mathrm{d}\bullet\; f(\bullet) \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k\,\mathrm{e}^{\imath k(x-\bullet)} \right) && \text{swap integration order} \\
&= \int_{-\infty}^{\infty} \mathrm{d}\bullet\; f(\bullet)\,\delta(x-\bullet) && \text{from definition (2.6d)} \\
&= f(x)\,. && \text{from definition (2.5)}
\end{aligned}$$

We thus have the result that if the Fourier transform of $f(x)$ is defined by

$$\widetilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} f(x)\,\mathrm{d}x \equiv \mathcal{F}[f]\,, \tag{3.10a}$$

then the *inverse transform* (note the change of sign in the exponent) acting on $\widetilde{f}(k)$ recovers $f(x)$, i.e.

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\imath kx} \widetilde{f}(k)\,\mathrm{d}k \equiv \mathcal{I}[\widetilde{f}]\,. \tag{3.10b}$$

Note that

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$$\mathcal{I}\left[\mathcal{F}\left[f\right]\right] = f\,, \quad \text{and} \quad \mathcal{F}\left[\mathcal{I}\left[\widetilde{f}\right]\right] = \widetilde{f}\,. \tag{3.10c}$$

Example. Find the Fourier transform of $(x^2+b^2)^{-1}$.

Answer. We start from our earlier result, (3.5), that

$$\mathcal{F}\left[\mathrm{e}^{-b|x|}\right](k) = \frac{1}{\sqrt{2\pi}}\,\frac{2b}{k^2+b^2}\,.$$

Hence from taking the inverse transform and using (3.10c)

$$\sqrt{\frac{\pi}{2b^2}}\,\mathrm{e}^{-b|x|} = \mathcal{I}\left[\frac{1}{k^2+b^2}\right](x)\,,$$

or, after applying the transformation $x \leftrightarrow k$,

$$\mathcal{I}\left[\frac{1}{x^2+b^2}\right](k) = \sqrt{\frac{\pi}{2b^2}}\,\mathrm{e}^{-b|k|}\,. \tag{3.11a}$$

But, from the transformation $x \leftrightarrow k$ in (3.10b) and comparison with (3.10a), we see that

$$\mathcal{F}[f(x)](k) = \mathcal{I}[f(x)](-k)\,. \tag{3.11b}$$

Hence, making the transformation $k \to -k$ in (3.11a), we find that

$$\mathcal{F}\left[\frac{1}{x^2+b^2}\right](k) = \sqrt{\frac{\pi}{2b^2}}\,\mathrm{e}^{-b|k|}\,. \tag{3.11c}$$

Remarks.

(i) The variables are often called t and ω rather than x and k (time $\leftrightarrow$ angular frequency vs. position $\leftrightarrow$ wavenumber).

(ii) It is sometimes useful to consider complex values of k.

(iii) For a rigorous proof, certain technical conditions on $f(x)$ are required. In particular, a necessary condition for $\widetilde{f}(k)$ to exist for all real values of k (in the sense of an ordinary function) is that $f(x) \to 0$ as $x \to \pm\infty$. Otherwise the Fourier integral does not converge (e.g. for $k = 0$).

A set of sufficient conditions for $\widetilde{f}(k)$ to exist is that $f(x)$ have 'bounded variation', have a finite number of discontinuities and be 'absolutely integrable', i.e.

$$\int_{-\infty}^{\infty} |f(x)|\,\mathrm{d}x < \infty.$$

However, we have seen that Fourier transforms can be assigned in a wider sense to some functions that do not satisfy all of these conditions, e.g. $f(x) = 1$.

3.1.4 Properties of Fourier Transforms

Linearity. For constants α and β.

$$\begin{aligned}\mathcal{F}\left[\alpha f(x) + \beta g(x)\right] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} \left(\alpha f(x) + \beta g(x)\right)\,\mathrm{d}x \\ &= \frac{\alpha}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} f\,\mathrm{d}x + \frac{\beta}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} g\,\mathrm{d}x \\ &= \alpha\mathcal{F}\left[f(x)\right] + +\beta\mathcal{F}\left[g(x)\right]\,. \end{aligned} \tag{3.12}$$

Rescaling. Let $g(x) = f(\alpha x)$ for real constant α, then

$$\begin{aligned}\widetilde{g} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} f(\alpha x)\,\mathrm{d}x \\ &= \frac{\operatorname{sgn}\alpha}{\alpha\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath \frac{k}{\alpha} y} f(y)\,\mathrm{d}y \\ &= \frac{1}{|\alpha|} \widetilde{f}\left(\frac{k}{\alpha}\right). \end{aligned} \tag{3.13}$$

Translation. The Fourier transform of $f(x-\alpha)$ for constant α is given by

$$\begin{aligned}\mathcal{F}[f(x-\alpha)] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} f(x-\alpha)\,\mathrm{d}x && \text{from (3.1)} \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath k(y+\alpha)} f(y)\,\mathrm{d}y && x = y+\alpha \\ &= \mathrm{e}^{-\imath k\alpha} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath ky} f(y)\,\mathrm{d}y && \text{rearrange} \\ &= \mathrm{e}^{-\imath k\alpha} \mathcal{F}[f(x)] && \text{from (3.1).} \end{aligned} \tag{3.14}$$

Exponential. Similarly, the Fourier transform of $\mathrm{e}^{\imath\alpha x} f(x)$ for constant α is given by

$$\begin{aligned}\mathcal{F}[\mathrm{e}^{\imath\alpha x} f(x)](k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath(k-\alpha)x} f(x)\,\mathrm{d}x \\ &= \mathcal{F}[f(x)](k-\alpha). \end{aligned} \tag{3.15}$$

Duality. If $g(x) = \widetilde{f}(x)$ then

$$\begin{aligned}\widetilde{g}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} \widetilde{f}(x)\,\mathrm{d}x \\ &= f(-k), \end{aligned} \tag{3.16}$$

i.e. transforming twice returns the reflected function, cf. (3.11b).

Complex conjugation and parity inversion. For real k

$$\begin{aligned}\mathcal{F}[f^*](k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} f^*(x)\,\mathrm{d}x \\ &= \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\imath kx} f(x)\,\mathrm{d}x\right)^* \\ &= \mathcal{F}[f](-k). \end{aligned} \tag{3.17}$$

Symmetry. If $f(-x) = \pm f(x)$, i.e. f is even or odd, then

$$\begin{aligned}\widetilde{f}(-k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\,\mathrm{e}^{+\mathrm{i}kx}\,\mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \pm f(-x)\,\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}x \\ &= \pm\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(y)\,\mathrm{e}^{-\mathrm{i}ky}\,\mathrm{d}y \\ &= \pm\widetilde{f}(k). \end{aligned} \tag{3.18}$$

Differentiation. Recall that if $g(x,k)$ is a function of two variables, then for constants a and b[18]

$$\frac{\mathrm{d}}{\mathrm{d}x}\int_a^b g(x,k)\,\mathrm{d}k = \int_a^b \frac{\partial g(x,k)}{\partial x}\,\mathrm{d}k\,. \tag{3.19}$$

Hence, if we differentiate the inverse Fourier transform (3.10b) with respect to x we obtain

$$\frac{\mathrm{d}f}{\mathrm{d}x}(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{\imath kx}\left(\imath k\widetilde{f}(k)\right)\,\mathrm{d}k = \mathcal{I}\left[\imath k\widetilde{f}\right]\,. \tag{3.20}$$

Now Fourier transform this equation to conclude from using (3.10c) that

$$\mathcal{F}\left[\frac{\mathrm{d}f}{\mathrm{d}x}\right] = \mathcal{F}\left[\mathcal{I}\left[\imath k\widetilde{f}\right]\right] = \imath k\widetilde{f}\,. \tag{3.21a}$$

In other words, each time we differentiate a function we multiply its Fourier transform by $\imath k$. Hence

$$\mathcal{F}\left[\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right] = -k^2\widetilde{f} \quad\text{and}\quad \mathcal{F}\left[\frac{\mathrm{d}^n f}{\mathrm{d}x^n}\right] = (\imath k)^n\widetilde{f}\,. \tag{3.21b}$$

Remark. That Fourier transforms allow a simple representation of derivatives of $f(x)$ in Fourier space has important consequences for solving differential equations.

Alternative proof (unlectured). This does not reply on the use of the inverse Fourier transform:

$$\begin{aligned}\mathcal{F}\left[\frac{\mathrm{d}f}{\mathrm{d}x}\right] &= \int_{-\infty}^{\infty} f'(x)\,\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x \\ &= \left[f(x)\,\mathrm{e}^{-\mathrm{i}kx}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f(x)(-\mathrm{i}k)\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x \\ &= \mathrm{i}k\widetilde{f}(k)\end{aligned} \tag{3.21c}$$

The integrated part vanishes because $f(x)$ must tend to zero as $x\to\pm\infty$ in order to possess a Fourier transform.

Multiplication by x. This time we differentiate (3.10a) with respect to k to obtain

$$\frac{\mathrm{d}\widetilde{f}}{\mathrm{d}k}(k) \quad=\quad \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx}\left(-\imath x f(x)\right)\,\mathrm{d}x\,.$$

Hence, after multiplying by $\imath$, we deduce from (3.1) that (cf. (3.21a))

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$$\imath\,\frac{\mathrm{d}\widetilde{f}}{\mathrm{d}k} \quad=\quad \mathcal{F}\left[xf(x)\right]\,. \tag{3.22}$$

3.1.5 The Relationship to Fourier Series

Suppose that $f(x)$ is a periodic function with period L (so that $f(x+L)=f(x)$). Then f can be represented by a Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} a_n \exp\left(\frac{2\pi\imath nx}{L}\right)\,, \tag{3.23a}$$

where

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$$a_n = \frac{1}{L}\int_{-\frac{1}{2}L}^{\frac{1}{2}L} f(x)\exp\left(-\frac{2\pi\imath nx}{L}\right)\,\mathrm{d}x\,. \tag{3.23b}$$

[18] If this is unfamiliar, work from first principles:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}x}\int_a^b g(x,k)\,\mathrm{d}k &= \lim_{\varepsilon\to 0}\,\frac{1}{\varepsilon}\left(\int_a^b g(x+\varepsilon,k)\,\mathrm{d}k - \int_a^b g(x,k)\,\mathrm{d}k\right) \\ &= \int_a^b \lim_{\varepsilon\to 0}\left(\frac{g(x+\varepsilon,k)-g(x,k)}{\varepsilon}\right)\,\mathrm{d}k \\ &= \int_a^b \frac{\partial g(x,k)}{\partial x}\,\mathrm{d}k\,.\end{aligned}$$

Expression (3.23a) can be viewed as a superposition of an infinite number of waves with wavenumbers $k_n = 2\pi n/L$ ($n = -\infty, \dots, \infty$). We are interested in the limit as the period L tends to infinity. In this limit the increment between successive wavenumbers, i.e. $\Delta k = 2\pi/L$, becomes vanishingly small, and the spectrum of allowed wavenumbers k_n becomes a continuum. Moreover, we recall that an integral can be evaluated as the limit of a sum, e.g.

$$\int_{-\infty}^{\infty} g(k)\,\mathrm{d}k = \lim_{\Delta k \to 0} \sum_{n=-\infty}^{\infty} g(k_n)\Delta k \quad \text{where} \quad k_n = n\Delta k\,. \tag{3.24}$$

Rewrite (3.23a) and (3.23b) as

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \widetilde{f}(k_n) \exp(\imath x k_n)\,\Delta k\,,$$

and

$$\widetilde{f}(k_n) = \frac{1}{\sqrt{2\pi}} \int_{-\frac{1}{2}L}^{\frac{1}{2}L} f(x) \exp(-\imath x k_n)\,\mathrm{d}x\,,$$

where

$$\widetilde{f}(k_n) = \frac{L\,a_n}{\sqrt{2\pi}} \equiv \frac{\sqrt{2\pi}\,a_n}{\Delta k}\,.$$

We then see that in the limit $\Delta k \to 0$, i.e. $L \to \infty$,

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{f}(k) \exp(\imath x k)\,\mathrm{d}k\,, \tag{3.25a}$$

and

$$\widetilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp(-\imath x k)\,\mathrm{d}x\,. \tag{3.25b}$$

These are just our earlier definitions of the inverse Fourier transform (3.10b) and Fourier transform (3.1) respectively.

3.2 The Convolution Theorem

3.2.1 Definition of convolution

The *convolution*, $f * g$, of a function $f(x)$ with a function $g(x)$ is defined by

$$(f * g)(x) = \int_{-\infty}^{\infty} \mathrm{d}y\, f(y)\, g(x-y)\,. \tag{3.26}$$

The convolution expresses the amount of overlap of one function g as it is shifted over another function f.

Property: the convolution operator $*$ is commutative. $f * g = g * f$ since

$$\begin{aligned}
(f * g)(x) &= \int_{-\infty}^{\infty} \mathrm{d}y\, f(y)\, g(x-y) && \text{from (3.26)}\\
&= \int_{\infty}^{-\infty} (-\,\mathrm{d}z)\, f(x-z)\, g(z) && z = x - y\\
&= \int_{-\infty}^{\infty} \mathrm{d}y\, f(x-y)\, g(y) && z \to y\\
&= (g * f)(x) && \text{from (3.26).}
\end{aligned}$$

3.2.2 Interpretation and examples

In statistics, a continuous random variable x (for instance, the height of a person drawn at random from the population) has a *probability distribution* (or *density*) *function* $f(x)$. The probability of x lying in the range $x_0 < x < x_0 + \delta x$ in the limit of small δx is $f(x_0)\delta x$.

If x and y are independent random variables with distribution functions $f(x)$ and $g(y)$, then let the distribution function of their sum, $z = x + y$, be $h(z)$. For the above example, suppose y is the height of a soap box drawn at random; then z would be the height of a random person while standing on the soap box.

For any given value of x, the probability that z lies in the range

$$z_0 < z < z_0 + \delta z\,, \tag{3.27a}$$

is just the probability that y lies in the range

$$z_0 - x < y < z_0 - x + \delta z\,, \tag{3.27b}$$

which is $g(z_0 - x)\delta z$. That's for a fixed x; so the probability that z lies in this same range *for all* x is

$$h(z_0)\delta z = \int_{-\infty}^{\infty} f(x)g(z_0 - x)\delta z\,\mathrm{d}x\,, \tag{3.27c}$$

which implies

$$h = f * g\,. \tag{3.27d}$$

Applications. The effect of measuring, observing or processing scientific data can often be described as a convolution of the data with a certain function. For instance:

(i) When a point source is observed by a telescope, a broadened image is seen, known as the *point spread function* of the telescope. When an extended source is observed, the image that is seen is the convolution of the source with the point spread function.

In this sense convolution corresponds to a broadening or distortion of the original data.

(ii) A point mass M at position $\mathbf{R}$ gives rise to a gravitational potential $\Phi_p(\mathbf{r}) = -GM/|\mathbf{r} - \mathbf{R}|$. A continuous mass density $\rho(\mathbf{r})$ can be thought of as a sum of infinitely many point masses $\rho(\mathbf{R})\,\mathrm{d}^3\mathbf{R}$ at positions $\mathbf{R}$. The resulting gravitational potential is

$$\Phi(\mathbf{r}) = -G \int \frac{\rho(\mathbf{R})}{|\mathbf{r} - \mathbf{R}|}\,\mathrm{d}^3\mathbf{R} \tag{3.28}$$

which is the (3D) convolution of the mass density $\rho(\mathbf{r})$ with the potential of a unit point charge at the origin, $-G/|\mathbf{r}|$.

3.2.3 The convolution theorem

If the functions f and g have Fourier transforms $\mathcal{F}[f]$ and $\mathcal{F}[g]$ respectively, then

$$\mathcal{F}[f * g] = \sqrt{2\pi}\mathcal{F}[f]\mathcal{F}[g]\,. \tag{3.29}$$

Proof.

$$\begin{aligned}
\mathcal{F}[f * g] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x\,\mathrm{e}^{-\imath kx} \left(\int_{-\infty}^{\infty} \mathrm{d}y\, f(y)\, g(x - y) \right) && \text{from (3.1) \& (3.26)} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}y\, f(y) \int_{-\infty}^{\infty} \mathrm{d}x\,\mathrm{e}^{-\imath kx} g(x - y) && \text{swap integration order} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}y\, f(y) \int_{-\infty}^{\infty} \mathrm{d}z\,\mathrm{e}^{-\imath k(z+y)} g(z) && x = z + y \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}y\, f(y)\,\mathrm{e}^{-\imath ky} \int_{-\infty}^{\infty} \mathrm{d}z\,\mathrm{e}^{-\imath kz} g(z) && \text{rearrange} \\
&= \sqrt{2\pi}\,\mathcal{F}[f]\mathcal{F}[g] && \text{from (3.1).}
\end{aligned}$$

Conversely the Fourier transform of the product fg is given by the convolution of the Fourier transforms of f and g divided by $\sqrt{2\pi}$, i.e.

$$\mathcal{F}[fg] = \frac{1}{\sqrt{2\pi}}\,\mathcal{F}[f] * \mathcal{F}[g]\,. \tag{3.30}$$

Proof.

$$\begin{aligned}
\mathcal{F}[fg](k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}x\,\mathrm{e}^{-\imath kx} f(x)g(x) && \text{from (3.1)}\\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}x\,\mathrm{e}^{-\imath kx}\, g(x)\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}\ell\,\mathrm{e}^{\imath\ell x}\widetilde{f}(\ell)\right) && \text{from (3.10b) with } k\to\ell\\
&= \frac{1}{\sqrt{2\pi}}\int_{\infty}^{\infty} \mathrm{d}\ell\,\widetilde{f}(\ell)\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}x\,\mathrm{e}^{-i(k-\ell)x}\, g(x)\right) && \text{swap integration order}\\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}\ell\,\widetilde{f}(\ell)\,\widetilde{g}(k-\ell) && \text{from (3.1)}\\
&= \frac{1}{\sqrt{2\pi}}\,(\widetilde{f} * \widetilde{g})(k) \equiv \frac{1}{\sqrt{2\pi}}\left(\mathcal{F}[f] * \mathcal{F}[g]\right)(k) && \text{from (3.26).}
\end{aligned}$$

Remarks.

(i) Convolution is an operation best carried out as a multiplication in the Fourier domain.

(ii) The Fourier transform of a product is non-trivial.

(iii) Convolution can be undone (*deconvolution*) by a division in the Fourier domain. If g is known and $f * g$ is measured, then f can be obtained, in principle.

Application (unlectured). Suppose a linear 'black box' (e.g. a circuit) has output $G(\omega)\exp(\imath\omega t)$ for a periodic input $\exp(\imath\omega t)$. What is the output $r(t)$ corresponding to input $f(t)$?

Answer. Since the 'black box' is *linear*, changing the input produces a directly proportional change in output. Thus since an input $\exp(\imath\omega t)$ produces an output $G(\omega)\exp(\imath\omega t)$, an input $F(\omega)\exp(\imath\omega t)$ will produce an output $R(\omega)\exp(\imath\omega t) = G(\omega)F(\omega)\exp(\imath\omega t)$.

If we express the input as a Fourier transform, namely,

$$f(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(\omega)\,\mathrm{e}^{\imath\omega t}\,\mathrm{d}\omega\,, \tag{3.31a}$$

then, since the 'black box' is *linear*, we can superpose input to produce the output

$$\begin{aligned}
r(t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} G(\omega)F(\omega)\,\mathrm{e}^{\imath\omega t}\,\mathrm{d}\omega\\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left(\frac{1}{\sqrt{2\pi}}\,\mathcal{F}[f*g]\right)\mathrm{e}^{\imath\omega t}\mathrm{d}\omega && \text{from (3.29)}\\
&= \frac{1}{\sqrt{2\pi}}\,(f*g)(t)\,, && \text{from (3.10b)} \qquad (3.31b)
\end{aligned}$$

where $g(t)$ is the inverse transform of $G(\omega)$, and we have used t and ω, instead of x and k respectively, as the variables in the Fourier transforms and their inverses.

10/02
10/04
Remark. If the know the output of a linear black box for all possible harmonic inputs, then we know everything about the black box.

3.2.4 Correlation

The *correlation* of two functions, $h = f \otimes g$, is defined by

$$h(x) = \int_{-\infty}^{\infty} [f(y)]^* g(x+y)\,\mathrm{d}y\,. \tag{3.32}$$

Correlation is a way of quantifying the relationship between two (typically oscillatory) functions. If two signals (oscillating about an average value of zero) oscillate in phase with each other, their correlation will be positive. If they are out of phase, the correlation will be negative. If they are completely unrelated, their correlation will be zero.

The *Fourier transform of a correlation* is

$$
\begin{aligned}
\tilde{h}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} [f(y)]^* g(x+y)\,\mathrm{d}y \right] \mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [f(y)]^* g(z)\,\mathrm{e}^{\mathrm{i}ky}\,\mathrm{e}^{-\mathrm{i}kz}\,\mathrm{d}z\,\mathrm{d}y \qquad (z = x+y) \\
&= \frac{1}{\sqrt{2\pi}} \left[\int_{-\infty}^{\infty} f(y)\,\mathrm{e}^{-\mathrm{i}ky}\,\mathrm{d}y \right]^* \int_{-\infty}^{\infty} g(z)\,\mathrm{e}^{-\mathrm{i}kz}\,\mathrm{d}z \\
&= \sqrt{2\pi}[\tilde{f}(k)]^* \tilde{g}(k)
\end{aligned} \tag{3.33}
$$

Remarks.

(i) This result (or the special case $g = f$) is the *Wiener–Khinchin theorem.*

(ii) The *autoconvolution* and *autocorrelation* of f are $f * f$ and $f \otimes f$. Their Fourier transforms are $\sqrt{2\pi}\tilde{f}^2$ and $\sqrt{2\pi}|\tilde{f}|^2$, respectively.

3.3 Parseval's theorem

If we apply the inverse transform to the Wiener–Khinchin theorem we find that

$$\int_{-\infty}^{\infty} [f(y)]^* g(x+y)\,\mathrm{d}y = \int_{-\infty}^{\infty} [\tilde{f}(k)]^* \tilde{g}(k)\,\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}k\,. \tag{3.34a}$$

Now set $x = 0$ and relabel $y \mapsto x$ to obtain *Parseval's theorem*

$$\int_{-\infty}^{\infty} [f(x)]^* g(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} [\tilde{f}(k)]^* \tilde{g}(k)\,\mathrm{d}k\,. \tag{3.34b}$$

The special case used most frequently is when $g = f$:

$$\int_{-\infty}^{\infty} |f(x)|^2\,\mathrm{d}x = \int_{-\infty}^{\infty} |\tilde{f}(k)|^2\,\mathrm{d}k\,. \tag{3.34c}$$

Remark. Parseval's theorem means that the Fourier transform is a 'unitary transformation' that preserves the 'inner product' between two functions (see later), in the same way that a rotation preserves lengths and angles.

Alternative derivation using the delta function (unlectured).

$$
\begin{aligned}
\int_{-\infty}^{\infty} \left|f(x)\right|^2 \mathrm{d}x &= \int_{-\infty}^{\infty} \mathrm{d}x\, f(x) f^*(x) \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}x \left[\int_{-\infty}^{\infty} \mathrm{d}k\,\mathrm{e}^{\imath kx} \widetilde{f}(k) \right] \left[\int_{-\infty}^{\infty} \mathrm{d}\ell\,\mathrm{e}^{-\imath \ell x} \widetilde{f}^*(\ell) \right] && \text{from (3.10b) \& (3.10b)}^* \\
&= \int_{-\infty}^{\infty} \mathrm{d}k\, \widetilde{f}(k) \int_{-\infty}^{\infty} \mathrm{d}\ell\, \widetilde{f}^*(\ell) \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}x\,\mathrm{e}^{\imath(k-\ell)x} \right) && \text{swap integration order} \\
&= \int_{-\infty}^{\infty} \mathrm{d}k\, \widetilde{f}(k) \int_{-\infty}^{\infty} \mathrm{d}\ell\, \widetilde{f}^*(\ell)\, \delta(k-\ell) && \text{from (2.6d)} \\
&= \int_{-\infty}^{\infty} \mathrm{d}k\, \widetilde{f}(k) \widetilde{f}^*(k) && \text{from (2.5) \& (2.8a)} \\
&= \int_{-\infty}^{\infty} \left|\widetilde{f}(k)\right|^2 \mathrm{d}k\,.
\end{aligned}
$$

Example. Find the Fourier transform of $x\mathrm{e}^{-|x|}$ and use Parseval's theorem to evaluate the integral

$$\int_{-\infty}^{\infty} \frac{k^2}{(1+k^2)^4}\,\mathrm{d}k\,. \tag{3.35}$$

Answer. From (3.5) with $b = 1$

$$\mathcal{F}\left[\mathrm{e}^{-|x|}\right] = \frac{1}{\sqrt{2\pi}}\frac{2}{1+k^2}\,. \tag{3.36a}$$

Next employ (3.22) to obtain

$$\mathcal{F}\left[x\mathrm{e}^{-|x|}\right] = \imath\,\frac{\partial}{\partial k}\mathcal{F}\left[\mathrm{e}^{-|x|}\right] = -\imath\sqrt{\frac{2}{\pi}}\frac{2k}{(1+k^2)^2}\,. \tag{3.36b}$$

Then from Parseval's theorem (3.34c) and a couple of integrations by parts

$$\int_{-\infty}^{\infty} \frac{k^2}{(1+k^2)^4}\,\mathrm{d}k = \frac{\pi}{8}\int_{-\infty}^{\infty} x^2\mathrm{e}^{-2|x|}\,\mathrm{d}x = \frac{\pi}{4}\int_{0}^{\infty} x^2\mathrm{e}^{-2x}\,\mathrm{d}x = \frac{\pi}{16}\,. \tag{3.36c}$$

9/01

An Application: Heisenberg's Uncertainty Principle (unlectured). Suppose that

$$\psi(x) = \frac{1}{(2\pi\Delta_x^2)^{\frac{1}{4}}}\,\exp\left(-\frac{x^2}{4\Delta_x^2}\right) \tag{3.37}$$

is the [real] wave-function of a particle in quantum mechanics. Then, according to quantum mechanics,

$$|\psi^2(x)| = \frac{1}{\sqrt{2\pi\Delta_x^2}}\,\exp\left(-\frac{x^2}{2\Delta_x^2}\right)\,, \tag{3.38}$$

is the probability of finding the particle at position x, and Δ_x is the root mean square deviation in position.

Remark. There is unit probability of finding the particle somewhere since $|\psi^2|$ is the Gaussian of width Δ_x and

$$\int_{-\infty}^{\infty} |\psi^2(x)|\,\mathrm{d}x = \frac{1}{\sqrt{2\pi\Delta_x^2}}\int_{-\infty}^{\infty}\exp\left(-\frac{x^2}{2\Delta_x^2}\right)\,\mathrm{d}x = 1\,. \tag{3.39}$$

The Fourier transform of $\psi(x)$ follows from (3.7) after the substitution $\varepsilon = \sqrt{2}\,\Delta_x$ and a multiplicative normalisation:

$$\begin{aligned}\widetilde{\psi}(k) &= \left(\frac{2\Delta_x^2}{\pi}\right)^{\frac{1}{4}}\,\exp\left(-\Delta_x^2k^2\right)\\ &= \frac{1}{(2\pi\Delta_k^2)^{\frac{1}{4}}}\,\exp\left(-\frac{k^2}{4\Delta_k^2}\right) \quad \text{where} \quad \Delta_k = \frac{1}{2\Delta_x}\,.\end{aligned} \tag{3.40}$$

Hence $\widetilde{\psi}^2$ is another Gaussian, this time with a root mean square deviation in wavenumber of Δ_k. In agreement with Parseval's theorem

$$\int_{-\infty}^{\infty} |\widetilde{\psi}(k)^2|\,\mathrm{d}k = 1\,. \tag{3.41}$$

In the case of the Gaussian, $\Delta_k\Delta_x = \frac{1}{2}$. More generally, one can show that for *any* (possibly complex) wave-function $\psi(x)$,

$$\Delta_k\Delta_x \geqslant \tfrac{1}{2} \tag{3.42}$$

where Δ_x and Δ_k are, as for the Gaussian, the root mean square deviations of the probability distributions $|\psi(x)|^2$ and $|\widetilde{\psi}(k)|^2$, respectively. An important and well-known result follows from (3.42), since in quantum mechanics the momentum is given by $p = \hbar k$, where $\hbar = h/2\pi$ and h is Planck's constant. Hence if we interpret $\Delta x = \Delta_x$ and $\Delta p = \hbar\Delta_k$ to be the uncertainty in the particle's position and momentum respectively, then *Heisenberg's Uncertainty Principle* follows from (3.42), namely

$$\Delta p\,\Delta x \geqslant \tfrac{1}{2}\hbar\,. \tag{3.43}$$

Remark.

A general property of Fourier transforms that follows from (3.42) is that the smaller the variation in the original function (i.e. the smaller Δ_x), the larger the variation in the transform (i.e. the larger Δ_k), and vice versa. In more prosaic language

a sharp peak in $x \Leftrightarrow$ a broad bulge in k,

and vice versa.

This property has many applications, for instance

- a short pulse of electromagnetic radiation must contain many frequencies;
- a long pulse of electromagnetic radiation (i.e. many wavelengths) is necessary in order to
11/22 obtain an approximately monochromatic signal.

3.4 Power spectra

The quantity

$$\Phi(k) = |\tilde{f}(k)|^2 \tag{3.44}$$

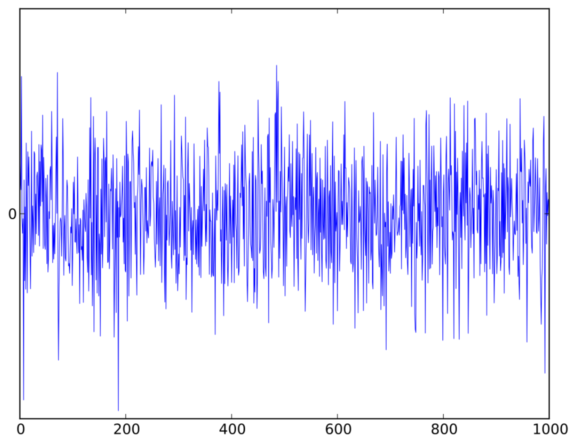
appearing in the Wiener–Khinchin theorem and Parseval's theorem is the *(power) spectrum* or *(power) spectral density* of the function $f(x)$. The Wiener–Khinchin theorem states that the Fourier Transform of the autocorrelation function is the power spectrum.

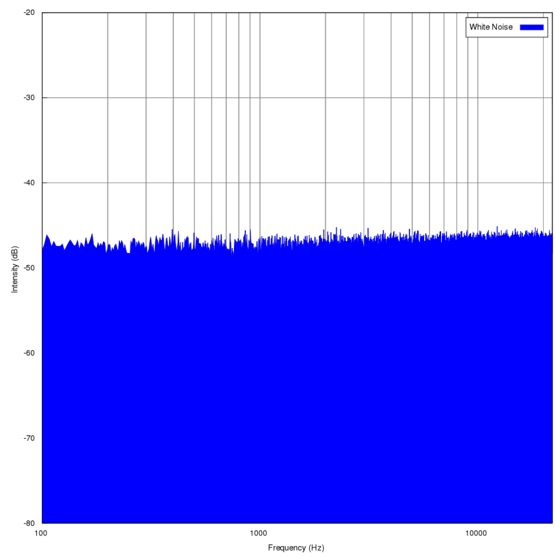
This concept is often used to quantify the spectral content (as a function of angular frequency ω) of a signal $f(t)$.

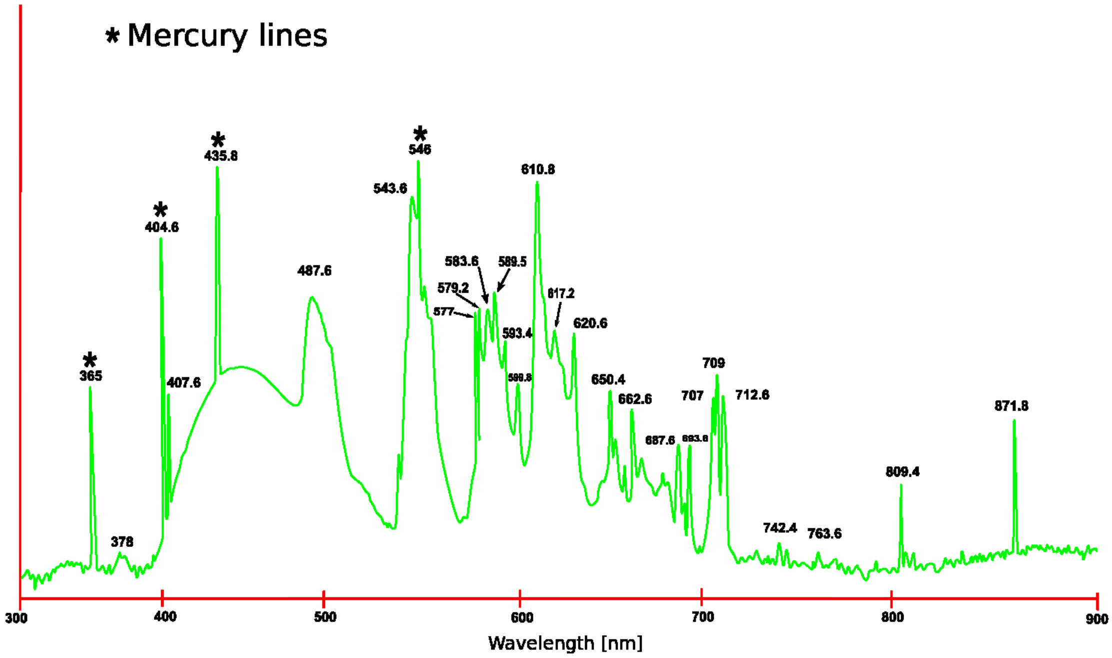
The spectrum of a perfectly periodic signal consists of a series of delta functions at the principal frequency and its harmonics, if present. Its autocorrelation function does not decay as $t \to \infty$.

White noise is an ideal random signal with autocorrelation function proportional to $\delta(t)$: the signal is perfectly decorrelated. It therefore has a flat spectrum ($\Phi = \mathsf{constant}$).

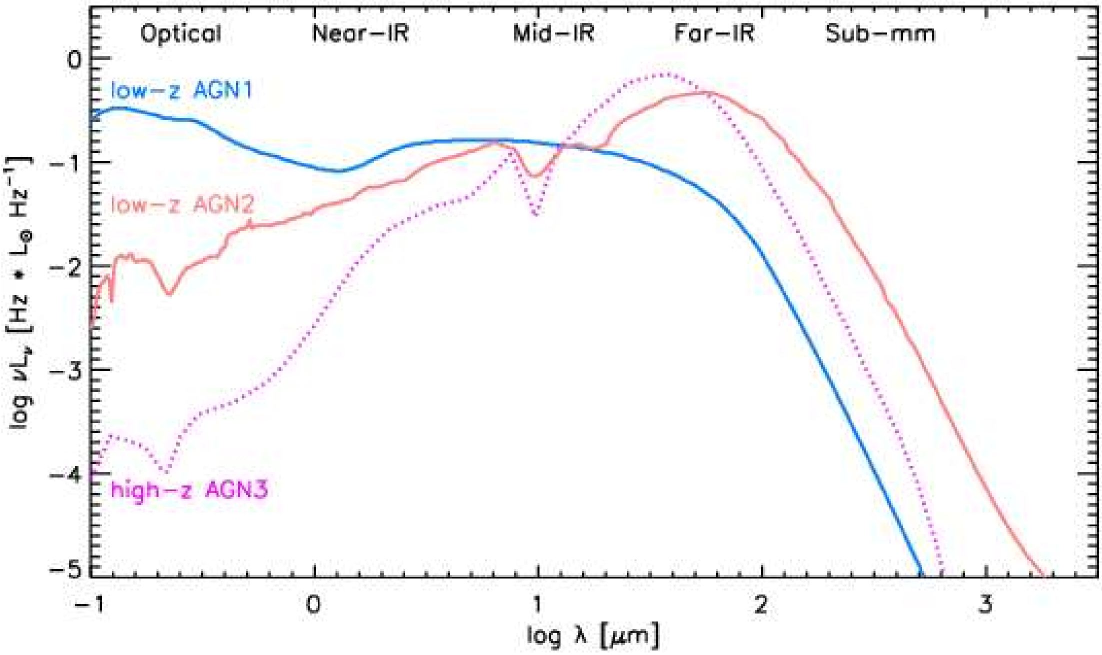
Less idealized signals may have spectra that are peaked at certain frequencies but also contain a general noise component.







Spectrum from a 48" Philips F32T8 natural sunshine fluorescent light



Spectrum of three active galactic nuclei at different red shifts

3.5 Solution of Ordinary Differential Equations using Fourier Transforms

Fourier transforms can be used as a method for solving differential equations. As an exemplar, we consider a simple ordinary differential equation, but similar methods also work for partial differential equations.

Suppose that $\psi(x)$ satisfies

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - a^2\psi = -f(x)\,, \tag{3.45}$$

where a is a constant and f is a known function. Suppose also that ψ satisfies the [two] boundary conditions $|\psi| \to 0$ as $|x| \to \infty$.

If we multiply the left-hand side (3.45) by $\frac{1}{\sqrt{2\pi}} \exp\left(-\imath kx\right)$ and integrate over x, then we obtain

$$\begin{aligned}
\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} \left(\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - a^2\psi \right) \mathrm{d}x &= \mathcal{F}\left(\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} \right) - a^2 \mathcal{F}\left(\psi\right) && \text{from (3.1)} \\
&= -k^2 \mathcal{F}\left(\psi\right) - a^2 \mathcal{F}\left(\psi\right) && \text{from (3.21b).} \qquad (3.46a)
\end{aligned}$$

The same action on the right-hand side yields $-\mathcal{F}(f)$. Hence from taking the Fourier transform of the whole equation we have that

$$-k^2 \mathcal{F}\left(\psi\right) - a^2 \mathcal{F}\left(\psi\right) = -\mathcal{F}\left(f\right) . \tag{3.46b}$$

Rearranging this equation we have that

$$\mathcal{F}\left(\psi\right) = \frac{\mathcal{F}\left(f\right)}{k^2 + a^2} , \tag{3.46c}$$

and so from the inverse transform (3.10b) we have the solution

$$\psi = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\imath kx} \frac{\mathcal{F}\left(f\right)}{k^2 + a^2} \, \mathrm{d}k \, . \tag{3.46d}$$

Remark. The boundary conditions that $|\psi| \to 0$ as $|x| \to \infty$ were implicitly used when we assumed that the Fourier transform of ψ existed. Why?

4 Partial Differential Equations

4.0 Why Study This?

Many scientific phenomena can be described by mathematical equations. Where there is variation in time and space, or more than one spatial coordinate, the governing equations are *partial differential equations* (PDEs).

Many, but not all, of these PDEs are *linear* and classical methods of analysis can be applied. The techniques developed for linear equations are sometimes also useful in the study of nonlinear PDEs.

4.1 Nomenclature

Partial differential equations (PDEs) are equations relating one or more unknown functions, say ψ, (the *dependent variable[s]*) of two or more *independent variables*, say x, y, z and t, with one or more of the functions' partial derivatives with respect to those variables. Hence a partial differential equation is a equation of the form

$$F\left(\psi, \frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial y}, \frac{\partial^2\psi}{\partial x^2}, \frac{\partial^2\psi}{\partial x\partial y}, \frac{\partial^2\psi}{\partial y^2}, \ldots, x, y\right) = 0 \tag{4.1a}$$

involving ψ and any of its derivatives evaluated at the same point, e.g. Schrödinger's equation (1.55b) for the quantum mechanical wave function $\psi(x, y, z, t)$ of a non-relativistic particle:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi + V(\mathbf{r})\psi = \mathrm{i}\hbar\frac{\partial\psi}{\partial t}\,. \tag{4.1b}$$

5/02 *Order.* The power of the highest derivative determines the *order* of the differential equation. Hence (4.1b) is a second-order equation.

Linearity. If the system of differential equations is of the first degree in the dependent variables, then the system is said to be *linear*, i.e. (4.1a) is *linear* if F depends linearly on ψ and its derivatives. Hence Schrödinger's equation is linear; however Euler's equation for an inviscid fluid,

$$\rho\left(\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{u}\right) = -\boldsymbol{\nabla}p\,, \tag{4.2}$$

5/03
5/04 where $\mathbf{u}$ is the velocity, ρ is the density and p is the pressure, is *nonlinear* in $\mathbf{u}$.

4.1.1 Linear Second-Order Partial Differential Equations

The most general linear second-order partial differential equation in two independent variables is

$$L\psi(x, y) = g(x, y)\,, \tag{4.3a}$$

where L is a differential operator such that

$$L\psi \equiv a(x, y)\frac{\partial^2\psi}{\partial x^2} + b(x, y)\frac{\partial^2\psi}{\partial x\partial y} + c(x, y)\frac{\partial^2\psi}{\partial y^2} + d(x, y)\frac{\partial\psi}{\partial x} + e(x, y)\frac{\partial\psi}{\partial y} + f(x, y)\psi\,. \tag{4.3b}$$

Remarks.

(i) If $g = 0$ the equation is said to be *homogeneous*.

(ii) We will concentrate on examples where the coefficients, a, b, c, d, e and f are independent of x and y, in which case the equation is said to have *constant coefficients*.

(iii) These ideas can be generalized to more than two independent variables (e.g. Schrödinger's equation (4.1b) has four independent variables), or to systems of PDEs with more than one dependent variable.

L is a linear operator. L is a *linear operator* since

$$L(\alpha\psi + \beta\varphi) = \alpha L\psi + \beta L\varphi\,, \tag{4.4}$$

where ψ and φ any functions of x and y, and α and β are any constants.

Principle of superposition (again).

(i) If ψ and φ satisfy the homogeneous equation, i.e. $L\psi = L\varphi = 0$, then $\alpha\psi + \beta\varphi$ also satisfies the homogeneous equation.

(ii) If the *particular integral* $\psi_{\rm p}$ satisfies the inhomogeneous equation $L\psi = g$ and the *complementary function* $\psi_{\rm c}$ satisfies the homogeneous equation $L\psi = 0$, then $\psi_{\rm p} + \psi_{\rm c}$ satisfies the inhomogeneous equation:

$$L(\psi_{\rm p} + \psi_{\rm c}) = L\psi_{\rm p} + L\psi_{\rm c} = g + 0 = g \tag{4.5}$$

4.2 Physical Examples and Applications

4.2.1 Waves on a Violin String

Consider *small* displacements on a stretched elastic string of density ρ per unit length (when not displaced). *Assume* that all displacements $y(x,t)$ are vertical (this is a bit of a cheat), and resolve horizontally and vertically to obtain respectively

$$T_2 \cos\theta_2 = T_1 \cos\theta_1 \,, \tag{4.6a}$$

$$\begin{aligned}(\rho\,\mathrm{d}x)\,\frac{\partial^2 y}{\partial t^2} &= T_2 \sin\theta_2 - T_1 \sin\theta_1 \\ &= T_2\cos\theta_2\,(\tan\theta_2 - \tan\theta_1)\,. \end{aligned}\tag{4.6b}$$

In the light of (4.6a) let

$$T = T_j \cos\theta_j \quad (j = 1, 2)\,, \tag{4.7a}$$

and observe that

$$\tan\theta = \frac{\partial y}{\partial x}\,. \tag{4.7b}$$

Then from (4.6b) it follows after use of Taylor's theorem that

$$\begin{aligned}\rho\,\mathrm{d}x\,\frac{\partial^2 y}{\partial t^2} &= T\,(\tan\theta_2 - \tan\theta_1) \\ &= T\left(\frac{\partial}{\partial x}y(x+\mathrm{d}x,t) - \frac{\partial}{\partial x}y(x,t)\right) \\ &= T\frac{\partial^2 y}{\partial x^2}\mathrm{d}x + \ldots\,, \end{aligned}\tag{4.8a}$$

and hence, in the infinitesimal limit, that

$$\frac{\partial^2 y}{\partial t^2} = \frac{T}{\rho}\frac{\partial^2 y}{\partial x^2}\,. \tag{4.8b}$$

This is the *wave equation* with wavespeed $c = \sqrt{\frac{T}{\rho}}$. In general the *one-dimensional wave equation* is

$$\frac{\partial^2 y}{\partial t^2} = c^2\frac{\partial^2 y}{\partial x^2}\,. \tag{4.8c}$$

Typical physical constants. For a violin (D-)string: $T \approx 40\,\mathrm{N}$, and $\rho \approx 1\,\mathrm{g\,m^{-1}}$ so $c \approx 200\,\mathrm{m\,s^{-1}}$.

4.2.2 Electromagnetic Waves (Unlectured)

The theory of electromagnetism is based on Maxwell's equations. These relate the electric field $\mathbf{E}$, the magnetic field $\mathbf{B}$, the charge density ρ and the current density $\mathbf{J}$:

$$\boldsymbol{\nabla}\cdot\mathbf{E} = \frac{\rho}{\epsilon_0}\,, \tag{4.9a}$$

$$\boldsymbol{\nabla}\times\mathbf{E} = -\frac{\partial\mathbf{B}}{\partial t}\,, \tag{4.9b}$$

$$\boldsymbol{\nabla}\times\mathbf{B} = \mu_0\mathbf{J} + \frac{1}{c^2}\frac{\partial\mathbf{E}}{\partial t}\,, \tag{4.9c}$$

$$\boldsymbol{\nabla}\cdot\mathbf{B} = 0\,, \tag{4.9d}$$

where ϵ_0 is the dielectric constant, μ_0 is the magnetic permeability, and $c^2 = (\mu_0\epsilon_0)^{-1}$ is the speed of light ($c \approx 3 \times 10^8\,\mathrm{m\,s^{-1}}$). If there is no charge or current (i.e. $\rho = 0$ and $\mathbf{J} = 0$), then from (4.9a), (4.9b), (4.9c) and the vector identity (1.56a):

$$\begin{aligned}
\frac{1}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} &= \boldsymbol{\nabla} \times \frac{\partial \mathbf{B}}{\partial t} && \text{using (4.9c) with } \mathbf{J} = 0 \\
&= -\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \mathbf{E}) && \text{using (4.9b)} \\
&= \nabla^2 \mathbf{E} - \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \mathbf{E}) && \text{using identity (1.56a)} \\
&= \nabla^2 \mathbf{E}\,. && \text{using (4.9a) with } \rho = 0
\end{aligned} \tag{4.10a}$$

We have therefore recovered the *three-dimensional wave equation* (cf. (4.8c))

$$\frac{\partial^2 \mathbf{E}}{\partial t^2} = c^2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \mathbf{E}\,. \tag{4.10b}$$

Remarks.

(i) $\mathbf{B}$ obeys the same equation.

(ii) The pressure perturbation of a sound waves satisfies the scalar equivalent of this equation, where $c \approx 300\,\mathrm{m\,s^{-1}}$ equals the speed of sound.

4.2.3 Electrostatic Fields

Suppose instead a steady electric field is generated by a known charge density ρ. Then from the second of Maxwell's equations (4.9b)

$$\boldsymbol{\nabla} \times \mathbf{E} = 0\,, \tag{4.11}$$

which implies from (1.51) that there exists an electric potential φ such that

$$\mathbf{E} = -\boldsymbol{\nabla}\varphi\,. \tag{4.12}$$

It then follows from the first of Maxwell's equations, (4.9a), that φ satisfies *Poisson's equation*

$$\nabla^2 \varphi = -\frac{\rho}{\epsilon_0}\,, \tag{4.13a}$$

i.e.

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \varphi = -\frac{\rho}{\epsilon_0}\,. \tag{4.13b}$$

Remark. The vector field $\mathbf{E}$ (and the vector field $\mathbf{g}$ below) is said to be *generated* by the potential φ. A scalar potential is easier to work with because it does not have multiple components and its value is independent of the coordinate system. The potential is also directly related to the energy of the system.

4.2.4 Gravitational Fields (Unlectured)

A Newtonian *gravitational field* $\mathbf{g}$ satisfies

$$\boldsymbol{\nabla} \cdot \mathbf{g} = -4\pi G \rho\,, \tag{4.14a}$$

and

$$\boldsymbol{\nabla} \times \mathbf{g} = 0\,, \tag{4.14b}$$

where G is the gravitational constant and ρ is mass density. From the latter equation and (1.51) it follows that there exists a gravitational potential φ such that

$$\mathbf{g} = -\boldsymbol{\nabla}\varphi\,. \tag{4.15}$$

Thence from (4.14a) we deduce that the gravitational potential satisfies *Poisson's equation*

$$\nabla^2 \varphi = 4\pi G \rho\,. \tag{4.16}$$

5/01 *Remark.* Electrostatic and gravitational fields are similar!

4.2.5 Diffusion of a Passive Tracer

Suppose we want describe how an inert chemical diffuses through a solid or stationary fluid.[19]

Denote the mass concentration of the dissolved chemical per unit volume by $C(\mathbf{r}, t)$, and the material *flux vector* of the chemical by $\mathbf{q}(\mathbf{r}, t)$. Then the amount of chemical crossing a small surface $\mathrm{d}\mathbf{S}$ in time δt is

$$\text{local flux} = (\mathbf{q} \cdot \mathrm{d}\mathbf{S})\, \delta t\,. \tag{4.17a}$$

Hence the flux of chemical out of a closed surface $\mathcal{S}$ enclosing a volume $\mathcal{V}$ in time δt is

$$\text{surface flux} = \left(\iint\limits_{\mathcal{S}} \mathbf{q} \cdot \mathrm{d}\mathbf{S} \right) \delta t\,. \tag{4.17b}$$

Let $Q(\mathbf{r}, t)$ denote any *chemical mass source* per unit time per unit volume of the media. Then if the change of chemical within the volume is to be equal to the flux of the chemical out of the surface in time δt

$$\left(\iint\limits_{\mathcal{S}} \mathbf{q} \cdot \mathrm{d}\mathbf{S} \right) \delta t = -\left(\frac{\mathrm{d}}{\mathrm{d}t} \iiint\limits_{\mathcal{V}} C\, \mathrm{d}V \right) \delta t + \left(\iiint\limits_{\mathcal{V}} Q\, \mathrm{d}V \right) \delta t\,. \tag{4.18a}$$

Hence using the divergence theorem (1.61), and exchanging the order of differentiation and integration,

$$\iiint\limits_{\mathcal{V}} \left(\boldsymbol{\nabla} \cdot \mathbf{q} + \frac{\partial C}{\partial t} - Q \right) \mathrm{d}V = 0\,. \tag{4.18b}$$

But this is true for any volume, and so

$$\frac{\partial C}{\partial t} = -\boldsymbol{\nabla} \cdot \mathbf{q} + Q\,. \tag{4.19}$$

The simplest empirical law relating concentration flux to concentration gradient is *Fick's law*

$$\mathbf{q} = -D \boldsymbol{\nabla} C\,, \tag{4.20}$$

where D is the *diffusion coefficient*; the negative sign is necessary if chemical is to flow from high to low concentrations. If D is constant then the partial differential equation governing the concentration is

$$\frac{\partial C}{\partial t} = D \nabla^2 C + Q\,. \tag{4.21}$$

Diffusion Equation. If there is no chemical source then $Q = 0$, and the governing equation becomes the *diffusion equation*

$$\frac{\partial C}{\partial t} = D \nabla^2 C\,. \tag{4.22}$$

Poisson's Equation. If the system has reached a steady state (i.e. $\partial_t \equiv 0$), then with $f(\mathbf{r}) = Q(\mathbf{r})/D$ the governing equation is *Poisson's equation*

$$\nabla^2 C = -f\,. \tag{4.23}$$

Laplace's Equation. If the system has reached a steady state and there are no chemical sources then the concentration is governed by *Laplace's equation*

$$\nabla^2 C = 0\,. \tag{4.24}$$

[19] Reacting chemicals and moving fluids are slightly more tricky.

4.2.6 Heat Flow (Unlectured)

What governs the flow of heat in a saucepan, an engine block, the earth's core, etc.? Can we write down an equation?

Let $\mathbf{q}(\mathbf{r},t)$ denote the *flux vector for heat flow*. Then the energy in the form of heat (molecular vibrations) flowing out of a closed surface $\mathcal{S}$ enclosing a volume $\mathcal{V}$ in time δt is again (4.17b). Also, let

$E(\mathbf{r},t)$ denote the *internal energy* per unit mass of the solid,
$Q(\mathbf{r},t)$ denote any *heat source* per unit time per unit volume of the solid,
$\rho(\mathbf{r},t)$ denote the *mass density* of the solid (assumed constant here).

The flow of heat in/out of $\mathcal{S}$ must balance the change in internal energy and the heat source over, say, a time δt (cf. (4.18a))

$$\left(\iint_{\mathcal{S}} \mathbf{q}\cdot \mathrm{d}\mathbf{S}\right)\delta t = -\left(\frac{\mathrm{d}}{\mathrm{d}t}\iiint_{\mathcal{V}} \rho E\,\mathrm{d}V\right)\delta t + \left(\iiint_{\mathcal{V}} Q\,\mathrm{d}V\right)\delta t\,.$$

For 'slow' changes at constant pressure (1st and 2nd law of thermodynamics)

$$E(\mathbf{r},t) = c_p\theta(\mathbf{r},t)\,, \tag{4.25}$$

where θ is the *temperature* and c_p is the *specific heat* (assumed constant here). Hence using the divergence theorem (1.61), and exchanging the order of differentiation and integration (cf. (4.18b)),

$$\iiint_{\mathcal{V}} \left(\boldsymbol{\nabla}\cdot\mathbf{q} + \rho c_p\frac{\partial\theta}{\partial t} - Q\right)\mathrm{d}V = 0\,. \tag{4.26}$$

But this is true for any volume, hence

$$\rho c_p\frac{\partial\theta}{\partial t} = -\boldsymbol{\nabla}\cdot\mathbf{q} + Q\,. \tag{4.27}$$

Experience tells us heat flows from hot to cold. The simplest empirical law relating heat flow to temperature gradient is *Fourier's law* (cf. Fick's law (4.20))

$$\mathbf{q} = -k\boldsymbol{\nabla}\theta\,, \tag{4.28}$$

where k is the *heat conductivity*. If k is constant then the partial differential equation governing the temperature is (cf. (4.21))

$$\frac{\partial\theta}{\partial t} = \nu\nabla^2\theta + \frac{Q}{\rho c_p} \tag{4.29}$$

where $\nu = k/(\rho c_p)$ is the *diffusivity* (or coefficient of diffusion).

4.2.7 Other Equations

There are numerous other partial differential equations describing scientific, and non-scientific, phenomena. One equation that you might have heard a lot about is the *Black-Scholes equation* for call option pricing

$$\frac{\partial w}{\partial t} = rw - rx\frac{\partial w}{\partial x} - \tfrac{1}{2}v^2x^2\frac{\partial^2 w}{\partial x^2}\,, \tag{4.30}$$

where $w(x,t)$ is the price of the call option of the stock, x is the variable market price of the stock, t is time, r is a fixed interest rate and v^2 is the variance rate of the stock price.

Also, despite the impression given above where all the equations except (4.2) are linear, many of the most interesting scientific (and non-scientific) equations are *nonlinear*. For instance the nonlinear Schrödinger equation

$$\mathrm{i}\frac{\partial A}{\partial t} + \frac{\partial^2 A}{\partial x^2} = A|A|^2\,, \tag{4.31}$$

where i is the square root of -1, admits *soliton* solutions (which is one of the reasons that optical fibres work).

4.3 Separation of Variables

You may have already met the general idea of 'separability' when solving ordinary differential equations, e.g. when you studied separable equations to the special differential equations that can be written in the form

$$\underbrace{X(x)\mathrm{d}x}_{\text{function of } x} \quad = \quad \underbrace{Y(y)\mathrm{d}y}_{\text{function of } y} \quad = \quad \text{constant}\,. \tag{4.32}$$

Sometimes functions can we written in separable form. For instance,

$$f(x, y) = \cos x\, \exp y = X(x)Y(y)\,, \quad \text{where} \quad X = \cos x \text{ and } Y = \exp y\,, \tag{4.33}$$

is separable in Cartesian coordinates, while

$$g(x, y, z) = \frac{1}{(x^2 + y^2 + z^2)^{\frac{1}{2}}} \tag{4.34}$$

is not separable in Cartesian coordinates, but is separable in spherical polar coordinates since

$$g = R(r)\Theta(\theta)\Phi(\phi) \quad \text{where} \quad R = \tfrac{1}{r}\,,\ \Theta = 1 \text{ and } \Phi = 1\,. \tag{4.35}$$

Solutions to partial differential equations can *sometimes* be found by seeking solutions that can be written in separable form, e.g.

$$\begin{aligned} \text{Time \& 1D Cartesians:} \quad y(x,t) &= X(x)T(t)\,, && (4.36a)\\ \text{2D Cartesians:} \quad \psi(x,y) &= X(x)Y(y)\,, && (4.36b)\\ \text{3D Cartesians:} \quad \psi(x,y,z) &= X(x)Y(y)Z(z)\,, && (4.36c)\\ \text{Cylindrical Polars:} \quad \psi(\rho,\phi,z) &= R(\rho)\Phi(\phi)Z(z)\,, && (4.36d)\\ \text{Spherical Polars:} \quad \psi(r,\theta,\phi) &= R(r)\Theta(\theta)\Phi(\phi)\,. && (4.36e) \end{aligned}$$

12/22 However, we emphasise that *not* all solutions of partial differential equations can be written in this form.

4.4 The One-Dimensional Wave Equation

4.4.1 Separable Solutions

Seek solutions $y(x,t)$ to the one dimensional wave equation (4.8c), i.e.

$$\frac{\partial^2 y}{\partial t^2} = c^2 \frac{\partial^2 y}{\partial x^2}\,, \tag{4.37a}$$

of the form

$$y(x,t) = X(x)T(t)\,. \tag{4.37b}$$

On substituting (4.37b) into (4.37a) we obtain

$$X\,\ddot{T} = c^2\, T\, X''\,, \tag{4.38}$$

where a $\dot{}$ and a $'$ denote differentiation by t and x respectively. After rearrangement we have that

$$\underbrace{\frac{1}{c^2}\frac{\ddot{T}(t)}{T(t)}}_{\text{function of } t} \quad = \quad \underbrace{\frac{X''(x)}{X(x)}}_{\text{function of } x} \quad = \lambda\,, \tag{4.39a}$$

where λ is a constant (the only function of t that equals a function of x). We have therefore split the PDE into two ODEs:

$$\ddot{T} - c^2\lambda T = 0 \qquad \text{and} \qquad X'' - \lambda X = 0\,. \tag{4.39b}$$

There are three cases to consider.

$\lambda = 0$. In this case

$$\ddot{T}(t) = X''(x) = 0 \quad \Rightarrow \quad T = A_0 + B_0 t \quad \text{and} \quad X = C_0 + D_0 x\,, \tag{4.40a}$$

where A_0, B_0, C_0 and D_0 are constants, i.e.

$$y = (A_0 + B_0 t)(C_0 + D_0 x)\,. \tag{4.40b}$$

$\lambda = \sigma^2 > 0$. In this case

$$\ddot{T} - \sigma^2 c^2 T = 0 \quad \text{and} \quad X'' - \sigma^2 X = 0\,. \tag{4.40c}$$

Hence

$$T = A_\sigma e^{\sigma c t} + B_\sigma e^{-\sigma c t} \quad \text{and} \quad X = C_\sigma \cosh \sigma x + D_\sigma \sinh \sigma x\,, \tag{4.40d}$$

where A_σ, B_σ, C_σ and D_σ are constants, i.e.

$$y = \left(A_\sigma e^{\sigma c t} + B_\sigma e^{-\sigma c t}\right)\left(C_\sigma \cosh \sigma x + D_\sigma \sinh \sigma x\right)\,. \tag{4.40e}$$

Alternatively we could express this as

$$y = \left(\tilde{A}_\sigma \cosh \sigma c t + \tilde{B}_\sigma \sinh \sigma c t\right)\left(\tilde{C}_\sigma e^{\sigma x} + \tilde{D}_\sigma e^{-\sigma x}\right)\,, \quad \text{or as} \ldots$$

6/02 where $\tilde{A}_\sigma$, $\tilde{B}_\sigma$, $\tilde{C}_\sigma$ and $\tilde{D}_\sigma$ are constants.

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6/04 $\lambda = -k^2 < 0$. In this case

$$\ddot{T} + k^2 c^2 T = 0 \quad \text{and} \quad X'' + k^2 X = 0\,. \tag{4.40f}$$

Hence

$$T = A_k \cos kct + B_k \sin kct \quad \text{and} \quad X = C_k \cos kx + D_k \sin kx\,, \tag{4.40g}$$

where A_k, B_k, C_k and D_k are constants, i.e.

$$y = \left(A_k \cos kct + B_k \sin kct\right)\left(C_k \cos kx + D_k \sin kx\right)\,. \tag{4.40h}$$

Remark. Without loss of generality we could also impose a normalisation condition, say, $C_j^2 + D_j^2 = 1$.

4.4.2 Boundary and Initial Conditions

Solutions (4.40b), (4.40e) and (4.40h) represent three families of solutions.[20] Although they are based on a special assumption, we shall see that because the wave equation is linear they can represent a wide range of solutions by means of *superposition*. However, before going further it is helpful to remember that when solving a physical problem boundary and initial conditions are also needed.

Boundary Conditions. Suppose that the string considered in § 4.2.1 has ends at $x = 0$ and $x = L$ that are fixed; appropriate *boundary conditions* are then

$$y(0, t) = 0 \quad \text{and} \quad y(L, t) = 0\,. \tag{4.41}$$

It is no coincidence that there are boundary conditions at *two* values of x and the highest derivative in x is *second* order.

Initial Conditions. Suppose also that the initial displacement and initial velocity of the string are known; appropriate *initial conditions* are then

$$y(x, 0) = d(x) \quad \text{and} \quad \frac{\partial y}{\partial t}(x, 0) = v(x)\,. \tag{4.42}$$

Again it is no coincidence that we need two initial conditions and the highest derivative in t is *second* order.

We shall see that the boundary conditions restrict the choice of λ.

[20] Or arguably one family if you wish to nit pick in the complex plane.

4.4.3 Solution

Consider the cases $\lambda = 0$, $\lambda < 0$ and $\lambda > 0$ in turn. These constitute an uncountably infinite number of solutions; our aim is to end up with a countably infinite number of solutions by elimination.

$\lambda = 0$. If the *homogeneous*, i.e. zero, boundary conditions (4.41) are to be satisfied for all time, then in (4.40b) we must have that $C_0 = D_0 = 0$.

$\lambda > 0$. Again if the boundary conditions (4.41) are to be satisfied for all time, then in (4.40e) we must have that $C_\sigma = D_\sigma = 0$.

$\lambda < 0$. Applying the boundary conditions (4.41) to (4.40h) yields

$$C_k = 0 \quad \text{and} \quad D_k \sin kL = 0\,. \tag{4.43}$$

If $D_k = 0$ then the entire solution is trivial (i.e. zero), so the only useful solution has

$$\sin kL = 0 \quad \Rightarrow \quad k = \frac{n\pi}{L}\,, \tag{4.44}$$

where n is a non-zero integer. These special values of k are *eigenvalues* and the corresponding *eigenfunctions*, or *normal modes*, are

$$X_n = D_{\frac{n\pi}{L}} \sin\frac{n\pi x}{L}\,. \tag{4.45}$$

Hence, from (4.40h), solutions to (4.8c) that satisfy the boundary condition (4.41) are

$$y_n(x,t) = \left(\mathcal{A}_n \cos\frac{n\pi ct}{L} + \mathcal{B}_n \sin\frac{n\pi ct}{L}\right)\sin\frac{n\pi x}{L}\,, \tag{4.46}$$

where we have written $\mathcal{A}_n$ for $A_{\frac{n\pi}{L}} D_{\frac{n\pi}{L}}$ and $\mathcal{B}_n$ for $B_{\frac{n\pi}{L}} D_{\frac{n\pi}{L}}$. Since (4.8c) is linear we can superimpose (i.e. add) solutions to get the general solution

$$y(x,t) = \sum_{n=1}^{\infty}\left(\mathcal{A}_n \cos\frac{n\pi ct}{L} + \mathcal{B}_n \sin\frac{n\pi ct}{L}\right)\sin\frac{n\pi x}{L}\,, \tag{4.47}$$

where there is no need to run the sum from $-\infty$ to ∞ because of the symmetry properties of sin and cos. We note that when the solution is viewed as a function of x at fixed t, or as a function of t at fixed x, then
6/01 it has the form of a Fourier series.

The solution (4.47) satisfies the boundary conditions (4.41) by construction. The only thing left to do is to satisfy the initial conditions (4.42), i.e. we require that

$$\begin{aligned} y(x,0) \;&=\; d(x) \;&=\; \sum_{n=1}^{\infty} \mathcal{A}_n \sin\frac{n\pi x}{L}\,, && \text{(4.48a)}\\ \frac{\partial y}{\partial t}(x,0) \;&=\; v(x) \;&=\; \sum_{n=1}^{\infty} \mathcal{B}_n \frac{n\pi c}{L}\sin\frac{n\pi x}{L}\,. && \text{(4.48b)} \end{aligned}$$

$\mathcal{A}_n$ and $\mathcal{B}_n$ can now be found using the orthogonality relations for sin (see (0.12a)), i.e.

$$\int_0^L \sin\frac{n\pi x}{L}\sin\frac{m\pi x}{L}\,\mathrm{d}x = \frac{L}{2}\,\delta_{nm}\,. \tag{4.49}$$

Hence for an integer $m > 0$

$$\begin{aligned} \frac{2}{L}\int_0^L d(x)\sin\frac{m\pi x}{L}\mathrm{d}x &= \frac{2}{L}\int_0^L\left(\sum_{n=1}^{\infty}\mathcal{A}_n\sin\frac{n\pi x}{L}\right)\sin\frac{m\pi x}{L}\mathrm{d}x\\ &= \sum_{n=1}^{\infty}\frac{2\mathcal{A}_n}{L}\int_0^L \sin\frac{n\pi x}{L}\sin\frac{m\pi x}{L}\,\mathrm{d}x\\ &= \sum_{n=1}^{\infty}\frac{2\mathcal{A}_n}{L}\,\frac{L}{2}\,\delta_{nm} && \text{using (4.49)}\\ &= \mathcal{A}_m\,, && \text{using (1.14c)} \qquad \text{(4.50a)} \end{aligned}$$

or alternatively invoke standard results for the coefficients of Fourier series. Similarly

$$\mathcal{B}_m = \frac{2}{m\pi c}\int_0^L v(x)\sin\frac{m\pi x}{L}\,\mathrm{d}x\,. \tag{4.50b}$$

4.5 Poisson's Equation

Suppose we are interested in obtaining solutions to Poisson's equation

$$\nabla^2\theta = -f\,, \tag{4.51a}$$

where, say, θ is a *steady* temperature distribution and $f = Q/(\rho c_p \nu^2)$ is a scaled heat source (see (4.29)). For simplicity let the world be two-dimensional, then (4.51a) becomes

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\theta = -f\,. \tag{4.51b}$$

Suppose we seek a separable solution as before, i.e. $\theta(x,y) = X(x)Y(y)$. Then on substituting into (4.51b) we obtain

$$\frac{X''}{X} = -\frac{Y''}{Y} - \frac{f}{XY}\,. \tag{4.52}$$

It follows that unless we are very fortunate, and $f(x,y)$ has a particular form (e.g. $f=0$), it does not look like we will be able to find separable solutions.

In order to make progress the trick is to first find a[ny] *particular solution*, θ_s, to (4.51b) (cf. finding a particular solution when solving constant coefficient ODEs last year). The function $\varphi = \theta - \theta_s$ then satisfies Laplace's equation

$$\nabla^2\varphi = 0\,. \tag{4.53}$$

This is just Poisson's equation with $f=0$, for which we have just noted that separable solutions exist. To obtain the full solution we need to add these [countably infinite] separable solutions to our particular solution (cf. adding *complementary functions* to a particular solution when solving constant coefficient ODEs last year).

4.5.1 A Particular Solution

We will illustrate the method by considering the particular example where the heating f is uniform, $f=1$ wlog (since the equation is linear), in a semi-infinite rod, $0 \leqslant x$, of unit width, $0 \leqslant y \leqslant 1$.

In order to find a particular solution suppose for the moment that the rod is infinite (or alternatively consider the solution for $x \gg 1$ for a semi-infinite rod, when the rod might look 'infinite' from a local viewpoint).

Then we might expect the particular solution for the temperature θ_s to be independent of x, i.e. $\theta_s \equiv \theta_s(y)$. Poisson's equation (4.51b) then reduces to

$$\frac{\mathrm{d}^2\theta_s}{\mathrm{d}y^2} = -1\,, \tag{4.54a}$$

which has solution

$$\theta_s = a_0 + b_0 y - \tfrac{1}{2}y^2\,, \tag{4.54b}$$

where a_0 and b_0 are constants.

4.5.2 Boundary Conditions

For the rod problem, experience suggests that we need to specify *one* of the following at *all* points on the boundary of the rod:

- the temperature (a *Dirichlet* condition), i.e.

$$\theta = g(\mathbf{r})\,, \tag{4.55a}$$

  where $g(\mathbf{r})$ is a known function;

- the scaled heat flux (a *Neumann* condition), i.e.

$$\frac{\partial\theta}{\partial n} \equiv \widehat{\mathbf{n}}\cdot\boldsymbol{\nabla}\theta = h(\mathbf{r})\,, \tag{4.55b}$$

  where $h(\mathbf{r})$ is a known function;

- a mixed condition, i.e.
$$\alpha(\mathbf{r})\frac{\partial\theta}{\partial n}+\beta(\mathbf{r})\theta=d(\mathbf{r})\,, \tag{4.55c}$$
where $\alpha(\mathbf{r})$, $\beta(\mathbf{r})$ and $d(\mathbf{r})$ are known functions, and $\alpha(\mathbf{r})$ and $\beta(\mathbf{r})$ are not simultaneously zero.

For our rod let us consider the boundary conditions

$$\theta(x,0)=0\,,\qquad \theta(x,1)=0\,,\qquad 0\leqslant x<\infty\,, \tag{4.56a}$$
$$\theta(0,y)=0\,,\qquad \frac{\partial\theta}{\partial x}(x,y)\to 0 \text{ as } x\to\infty\,,\qquad 0\leqslant y\leqslant 1\,. \tag{4.56b}$$

For these conditions it is appropriate to take $a_0=0$ and $b_0=\frac{1}{2}$ in (4.54b) so that
$$\theta_s=\tfrac{1}{2}y(1-y)\geqslant 0\,. \tag{4.57}$$

Let $\varphi=\theta-\theta_s$, then φ satisfies Laplace's equation (4.53) and, from (4.56a), (4.56b) and (4.57), the boundary conditions

$$\varphi(x,0)=0\,,\qquad \varphi(x,1)=0\,,\qquad 0\leqslant x<\infty\,, \tag{4.58a}$$
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$$\varphi(0,y)=-\tfrac{1}{2}y(1-y)\,,\qquad \frac{\partial\varphi}{\partial x}(x,y)\to 0 \text{ as } x\to\infty\,,\qquad 0\leqslant y\leqslant 1\,. \tag{4.58b}$$

4.5.3 Separable Solutions

On writing $\varphi(x,y)=X(x)Y(y)$ and substituting into Laplace's equation (4.53) it follows that (cf. (4.52))
$$\underbrace{\frac{X''(x)}{X(x)}}_{\text{function of } x}\quad=\quad\underbrace{-\frac{Y''(y)}{Y(y)}}_{\text{function of } y}\quad=\lambda\,, \tag{4.59a}$$
so that
$$X''-\lambda X=0\quad\text{and}\quad Y''+\lambda Y=0\,. \tag{4.59b}$$

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We can now consider each of the possibilities $\lambda=0$, $\lambda>0$ and $\lambda<0$ in turn to obtain, cf. (4.40b), (4.40e) and (4.40h),

$\lambda=0.$
$$\varphi=(A_0+B_0x)(C_0+D_0y)\,. \tag{4.60a}$$

$\lambda=\sigma^2>0.$
$$\varphi=\left(A_\sigma \mathrm{e}^{\sigma x}+B_\sigma\mathrm{e}^{-\sigma x}\right)(C_\sigma\cos\sigma y+D_\sigma\sin\sigma y)\,. \tag{4.60b}$$

$\lambda=-k^2<0.$
$$\varphi=(A_k\cos kx+B_k\sin kx)\,(C_k\cosh ky+D_k\sinh ky)\,. \tag{4.60c}$$

The boundary conditions at $y=0$ and $y=1$ in (4.58a) state that $\varphi(x,0)=0$ and $\varphi(x,1)=0$. This implies (cf. the stretched string problem) that solutions proportional to $\sin(n\pi y)$ are appropriate; hence we try $\lambda=n^2\pi^2$ where n is an integer. The eigenfunctions are thus
$$\varphi_n=\left(\mathcal{A}_n\mathrm{e}^{n\pi x}+\mathcal{B}_n\mathrm{e}^{-n\pi x}\right)\sin(n\pi y)\,, \tag{4.61}$$
where $\mathcal{A}_n$ and $\mathcal{B}_n$ are constants and, without loss of generality, $n>0$. However, if the boundary condition in (4.58b) as $x\to\infty$ is to be satisfied then $\mathcal{A}_n=0$. Hence the solution has the form
$$\varphi=\sum_{n=1}^{\infty}\mathcal{B}_n\mathrm{e}^{-n\pi x}\sin(n\pi y)\,. \tag{4.62}$$

The $\mathcal{B}_n$ are fixed by the first boundary condition in (4.58b), i.e. we require that
$$-\tfrac{1}{2}y(1-y)=\sum_{n=1}^{\infty}\mathcal{B}_n\sin(n\pi y)\,. \tag{4.63a}$$

Using the orthogonality relations (4.49) it follows that

$$\mathcal{B}_m = 2\frac{(-1)^m - 1}{m^3\pi^3}\,. \tag{4.63b}$$

and hence that

$$\theta = \tfrac{1}{2}y(1-y) - \sum_{\ell=0}^{\infty} \frac{4}{\pi^3(2\ell+1)^3}\,\sin((2\ell+1)\pi y)\,\mathrm{e}^{-(2\ell+1)\pi x}\,, \tag{4.64a}$$

or equivalently

$$\theta = \sum_{\ell=0}^{\infty} \frac{4}{\pi^3(2\ell+1)^3}\,\sin((2\ell+1)\pi y)\,\left(1 - \mathrm{e}^{-(2\ell+1)\pi x}\right)\,. \tag{4.64b}$$

4.6 The Diffusion Equation

4.6.1 Separable Solutions

Seek solutions $C(x,t)$ to the one dimensional version of the diffusion equation, (4.22), i.e.

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}\,, \tag{4.65}$$

of the form

$$C(x,t) = X(x)T(t)\,. \tag{4.66}$$

On substitution we obtain

$$X\,\dot{T} = D\,T\,X''\,. \tag{4.67}$$

After rearrangement we have that

$$\underbrace{\frac{1}{D}\frac{\dot{T}(t)}{T(t)}}_{\text{function of } t} = \underbrace{\frac{X''(x)}{X(x)}}_{\text{function of } x} = \lambda\,, \tag{4.68a}$$

where λ is again a constant. We have therefore split the PDE into two ODEs:

$$\dot{T} - D\lambda T = 0 \qquad \text{and} \qquad X'' - \lambda X = 0\,. \tag{4.68b}$$

There are again three cases to consider.

$\lambda = 0$. In this case

$$\dot{T}(t) = X''(x) = 0 \quad \Rightarrow \quad T = \alpha_0 \quad \text{and} \quad X = \beta_0 + \gamma_0 x\,, \tag{4.69a}$$

where α_0, β_0 and γ_0 are constants. Combining these results we obtain

$$C = \alpha_0(\beta_0 + \gamma_0 x)\,,$$

or

$$C = \beta_0 + \gamma_0 x\,, \tag{4.69b}$$

since, without loss of generality (wlog), we can take $\alpha_0 = 1$.

$\lambda = \sigma^2 > 0$. In this case

$$\dot{T} - D\sigma^2 T = 0 \quad \text{and} \quad X'' - \sigma^2 X = 0\,. \tag{4.69c}$$

Hence

$$T = \alpha_\sigma \exp(D\sigma^2 t) \quad \text{and} \quad X = \beta_\sigma \cosh\sigma x + \gamma_\sigma \sinh\sigma x\,, \tag{4.69d}$$

where α_σ, β_σ and γ_σ are constants. On taking $\alpha_\sigma = 1$ wlog,

$$C = \exp(D\sigma^2 t)\,(\beta_\sigma \cosh\sigma x + \gamma_\sigma \sinh\sigma x)\;. \tag{4.69e}$$

$\lambda = -k^2 < 0$. In this case

$$\dot{T} + Dk^2 T = 0 \quad \text{and} \quad X'' + k^2 X = 0\,. \tag{4.69f}$$

Hence

$$T = \alpha_k \exp(-Dk^2 t) \quad \text{and} \quad X = \beta_k \cos kx + \gamma_k \sin kx\,, \tag{4.69g}$$

where α_k, β_k and γ_k are constants. On taking $\alpha_k = 1$ wlog,

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$$C = \exp(-Dk^2 t)\,(\beta_k \cos kx + \gamma_k \sin kx)\;. \tag{4.69h}$$

4.6.2 Boundary and Initial Conditions

Consider the problem of a solvent occupying the region between $x = 0$ and $x = L$. Suppose that at $t = 0$ there is no chemical in the solvent, i.e. the initial condition is

$$C(x, 0) = 0\,. \tag{4.70a}$$

Note that here we specify *one* initial condition based on the observation that the highest derivative in t in (4.21) is *first* order.

Suppose also that for $t > 0$ the concentration of the chemical is maintained at C_0 at $x = 0$, and is 0 at $x = L$, i.e.

$$C(0, t) = C_0 \quad \text{and} \quad C(L, t) = 0 \quad \text{for} \quad t > 0\,. \tag{4.70b}$$

Again it is no coincidence that there two boundary conditions and the highest derivative in x is *second* order.

Remark. Equation (4.21) and conditions (4.70a) and (4.70b) are mathematically equivalent to a description of the temperature of a rod of length L which is initially at zero temperature before one of the ends is raised instantaneously to a constant non-dimensional temperature of C_0.

4.6.3 Solution

The trick here is to note that

- the *inhomogeneous* (i.e. non-zero) boundary condition at $x = 0$, i.e $C(0, t) = C_0$, is steady, and
- the separable solutions (4.69e) and (4.69h) depend on time, while (4.69b) does not.

It therefore seems sensible to try and satisfy the the boundary conditions (4.70b) using the solution (4.69b). If we call this part of the total solution $C_\infty(x)$ then, with $\beta_0 = C_0$ and $\gamma_0 = -C_0/L$ in (4.69b),

$$C_\infty(x) = C_0\left(1 - \frac{x}{L}\right), \tag{4.71}$$

which is just a linear variation in C from C_0 at $x = 0$ to 0 at $x = L$. Write

$$C(x, t) = C_\infty(x) + \widetilde{C}(x, t)\,, \tag{4.72}$$

where $\widetilde{C}$ is a sum of the separable time-dependent solutions (4.69e) and (4.69h). Then from the initial condition (4.70a), the boundary conditions (4.70b), and the steady solution (4.71), it follows that

$$\widetilde{C}(x, 0) = -C_0\left(1 - \frac{x}{L}\right), \tag{4.73a}$$

and

$$\widetilde{C}(0, t) = 0 \quad \text{and} \quad \widetilde{C}(L, t) = 0 \quad \text{for} \quad t > 0\,. \tag{4.73b}$$

If the homogeneous boundary conditions (4.73b) are to be satisfied then, as for the wave equation, separable solutions with $\lambda > 0$ are unacceptable, while $\lambda = -k^2 < 0$ is only acceptable if

$$\beta_k = 0 \quad \text{and} \quad \gamma_k \sin kL = 0\,. \tag{4.74a}$$

It follows that if the solution is to be non trivial then

$$k = \frac{n\pi}{L}\,. \tag{4.74b}$$

The eigenfunctions corresponding to (4.74b) are

$$X_n = \Gamma_n \sin\frac{n\pi x}{L}\,, \tag{4.74c}$$

where $\Gamma_n = \gamma_{\frac{n\pi}{L}}$. Again, because (4.21) is a linear equation, we can add individual solutions to get the general solution

$$\widetilde{C}(x, t) = \sum_{n=1}^{\infty} \Gamma_n \exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right) \sin\frac{n\pi x}{L}\,. \tag{4.75}$$

The Γ_n are fixed by the initial condition (4.73b):

$$-C_0\left(1-\frac{x}{L}\right)=\sum_{n=1}^{\infty}\Gamma_n\sin\frac{n\pi x}{L}\,. \tag{4.76a}$$

Hence

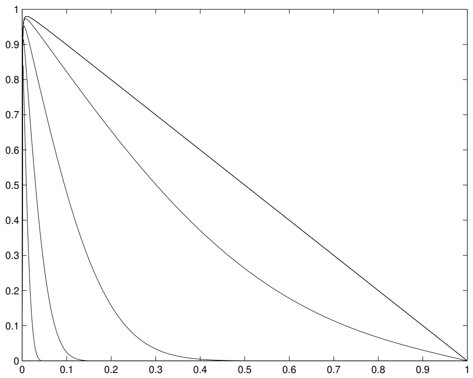
$$\Gamma_m=-\frac{2C_0}{L}\int_0^L\left(1-\frac{x}{L}\right)\sin\frac{m\pi x}{L}\mathrm{d}x=-\frac{2C_0}{m\pi}\,. \tag{4.76b}$$

The solution is thus given by

$$C \;=\; C_0\left(1-\frac{x}{L}\right)-\sum_{n=1}^{\infty}\frac{2C_0}{n\pi}\exp\left(-\frac{n^2\pi^2D\,t}{L^2}\right)\sin\frac{n\pi x}{L}\,. \tag{4.77a}$$

or from using (4.76a)

$$C \;=\; \sum_{n=1}^{\infty}\frac{2C_0}{n\pi}\left(1-\exp\left(-\frac{n^2\pi^2D\,t}{L^2}\right)\right)\sin\frac{n\pi x}{L}\,. \tag{4.77b}$$



The solution (4.77b) with $C_0=1$ and $L=1$, plotted at times $t=0.0001$, $t=0.001$, $t=0.01$, $t=0.1$ and $t=1$ (curves from left to right respectively).

Paradox. $\sin\frac{n\pi x}{L}$ is not a separable solution of the diffusion equation.

Remark. As $t\to\infty$ in (4.77a)

$$C\to C_0\left(1-\frac{x}{L}\right)=C_\infty(x)\,. \tag{4.78}$$

Remark. Solution (4.77b) is odd and has period $2L$. We are in effect solving the $2L$-periodic diffusion problem where C is initially zero. Then, at $t=0+$, C is raised to $+1$ at $2nL+$ and lowered to -1 at $2nL-$ (for integer n), and kept zero everywhere else.

4.6.4 A Rough and Ready Outline Recipe

(i) In the case of an inhomogeneous equation, use the principle of superposition to seek a particular solution to reduce the equation to one that is homogeneous.

(ii) Seek separable solutions to the homogeneous equation.

(iii) In the case of inhomogeneous *boundary* conditions consider seeking a [separable] solution to reduce the boundary conditions to ones that are homogeneous.

(iv) Use the boundary conditions to rule out certain of the separable solutions and to identify eigenvalues.

(v) Using the principle of superposition, seek a solution that is a sum of eigenfunctions.

(vi) Determine unknown constants using the boundary conditions.

4.7 Solution Using Fourier Transforms (Non-examinable & Unlectured)

4.7.1 The diffusion equation as an exemplar

Consider the diffusion equation (see (4.22) or (4.29)) governing the evolution of, say, temperature, $\theta(x,t)$:

$$\frac{\partial\theta}{\partial t} = \nu\frac{\partial^2\theta}{\partial x^2}\,. \tag{4.79}$$

In § 4.6 we have seen how separable solutions and Fourier series can be used to solve (4.79) over finite x-intervals. Fourier transforms can be used to solve (4.79) when the range of x is infinite.[21]

We will assume boundary conditions such as

$$\theta \to \text{constant} \quad \text{and} \quad \frac{\partial\theta}{\partial x} \to 0 \quad \text{as} \quad |x| \to \infty\,, \tag{4.80}$$

so that the Fourier transform of θ exists (at least in a generalised sense):

$$\widetilde{\theta}(k,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx}\,\theta\,\mathrm{d}x\,. \tag{4.81}$$

If we then multiply the left hand side of (4.79) by $\frac{1}{\sqrt{2\pi}}\exp\left(-\imath kx\right)$ and integrate over x we obtain the time derivative of $\widetilde{\theta}$:

$$\begin{aligned}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx}\,\frac{\partial\theta}{\partial t}\,\mathrm{d}x &= \frac{\partial}{\partial t}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx}\,\theta\,\mathrm{d}x\right) && \text{swap differentiation and integration}\\ &= \frac{\partial\widetilde{\theta}}{\partial t} && \text{from (4.81)}\,.\end{aligned}$$

A similar manipulation of the right hand side of (4.79) yields

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx}\left(\nu\frac{\partial^2\theta}{\partial x^2}\right)\mathrm{d}x = -\nu k^2\widetilde{\theta} \qquad \text{from (3.21b).}$$

Putting the left hand side and the right hand side together it follows that $\widetilde{\theta}(k,t)$ satisfies

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$$\frac{\partial\widetilde{\theta}}{\partial t} + \nu k^2\widetilde{\theta} = 0\,. \tag{4.82a}$$

This equation has solution

$$\widetilde{\theta}(k,t) = \gamma(k)\exp(-\nu k^2 t)\,, \tag{4.82b}$$

where $\gamma(k)$ is an unknown function of k (cf. the Γ_n in (4.75)).

Suppose that the temperature distribution is known at a specific time, wlog $t = 0$. Then from evaluating (4.82b) at $t = 0$ we have that

$$\gamma(k) = \widetilde{\theta}(k,0) \quad \text{and so} \quad \widetilde{\theta}(k,t) = \widetilde{\theta}(k,0)\exp(-\nu k^2 t)\,. \tag{4.83}$$

But from definition (3.1)

$$\widetilde{\theta}(k,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{-\imath ky}\theta(y,0)\,\mathrm{d}y\,, \tag{4.84a}$$

and so

$$\widetilde{\theta}(k,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \exp(-\imath ky - \nu k^2 t)\,\theta(y,0)\,\mathrm{d}y\,. \tag{4.84b}$$

We can now use the Fourier inversion formula to find $\theta(x,t)$:

$$\begin{aligned}\theta(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}k\,\mathrm{e}^{\imath kx}\widetilde{\theta}(k,t) && \text{from (3.10b)}\\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}k\,\mathrm{e}^{\imath kx}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \exp(-\imath ky - \nu k^2 t)\,\theta(y,0)\,\mathrm{d}y\right) && \text{from (4.84b)}\\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}y\;\theta(y,0)\int_{-\infty}^{\infty} \mathrm{d}k\;\exp(\imath k(x-y) - \nu k^2 t) && \text{swap integration order.}\end{aligned}$$

[21] Semi-infinite ranges can also be tackled by means of suitable ‘tricks’: see the example sheet.

From completing the square, or alternatively from our earlier calculation of the Fourier transform of a Gaussian (see (3.7) and apply the transformations $\varepsilon \to (2\nu t)^{-\frac{1}{2}}$, $k \to (y-x)$ and $x \to k$), we have that

$$\int_{-\infty}^{\infty} \mathrm{d}k\, \exp\left(\imath k(x-y) - \nu k^2 t\right) = \sqrt{\frac{\pi}{\nu t}}\, \exp\left(-\frac{(x-y)^2}{4\nu t}\right) . \tag{4.85}$$

Substituting into the above expression for $\theta(x,t)$ we obtain a solution to the diffusion equation in terms of the initial condition at $t = 0$:

$$\theta(x,t) = \frac{1}{\sqrt{4\pi\nu t}} \int_{-\infty}^{\infty} \mathrm{d}y\, \theta(y,0) \exp\left(-\frac{(x-y)^2}{4\nu t}\right) . \tag{4.86a}$$

Example. If $\theta(x,0) = \theta_0 \delta(x)$ then we obtain what is sometimes referred to as the fundamental solution of the diffusion equation, namely

$$\theta(x,t) = \frac{\theta_0}{\sqrt{4\pi\nu t}}\, \exp\left(-\frac{x^2}{4\nu t}\right) . \tag{4.86b}$$

Physically this means that if the temperature at one point of an infinite rod is instantaneously raised to ‘infinity’, then the resulting temperature distribution is that of a Gaussian with a maximum temperature decaying like $t^{-\frac{1}{2}}$ and a width increasing like $t^{\frac{1}{2}}$.

5 Matrices

5.0 Why Study This?

A good question since this material is as almost dry as the Sahara (or East Anglia). A general answer is that matrices are essential mathematical tools. You need to know how to manipulate them: the addition and multiplication of scalars, vectors and matrices is referred to as *linear algebra*.

A more specific answer is that many scientific quantities are vectors and a linear relationship between two vectors is described by a *matrix*. This could be either

(i) a *physical* relationship, e.g. that between the angular velocity and angular momentum vectors of a rotating body;

(ii) a relationship between the *components* of (physically) the same vector in different coordinate systems.

However, vectors do not necessarily live in physical space. In some applications (notably quantum mechanics) we have to deal with *complex spaces* of various dimensions.

Inter alia, we will study *eigenvalues* and *eigenvectors*; these are characteristic numbers and directions associated with matrices, which allow them to be expressed in the simplest form. Moreover, the matrices that occur in scientific applications usually have special *symmetries* that impose conditions on their eigenvalues and eigenvectors, e.g. Hermitian matrices (observables in quantum mechanics are Hermitian operators).

5.1 Vector Spaces

The concept of a vector in three-dimensional Euclidean space can be generalised to n dimensions and in a more general (and abstract) way.

5.1.1 Some Notation

First some notation.

Notation	*Meaning*
$\in$	in
$\exists$	there exists
$\forall$	for all

5.1.2 Definition

A set of elements, or 'vectors', are said to form a *complex linear vector space* V if

(i) there exists a *binary operation*, say *addition*, under which the set V is *closed* so that

$$\text{if} \quad \mathbf{u}, \mathbf{v} \in V\,, \quad \text{then} \quad \mathbf{u} + \mathbf{v} \in V\,; \tag{5.1a}$$

(ii) addition is *commutative and associative*, i.e. for all $\mathbf{u}, \mathbf{v}, \mathbf{w} \in V$

$$\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u}\,, \tag{5.1b}$$

$$(\mathbf{u} + \mathbf{v}) + \mathbf{w} = \mathbf{u} + (\mathbf{v} + \mathbf{w})\,; \tag{5.1c}$$

(iii) there exists *closure under multiplication by a complex scalar*, i.e.

$$\text{if} \quad a \in \mathbb{C} \quad \text{and} \quad \mathbf{v} \in V \quad \text{then} \quad a\mathbf{v} \in V\,; \tag{5.1d}$$

(iv) multiplication by a scalar is *distributive and associative*, i.e. for all $a, b \in \mathbb{C}$ and $\mathbf{u}, \mathbf{v} \in V$

$$a(\mathbf{u} + \mathbf{v}) = a\mathbf{u} + a\mathbf{v}\,, \tag{5.1e}$$

$$(a + b)\mathbf{u} = a\mathbf{u} + b\mathbf{u}\,, \tag{5.1f}$$

$$a(b\mathbf{u}) = (ab)\mathbf{u}\,; \tag{5.1g}$$

(v) there exists a *null, or zero, vector* $0 \in V$ such that for all $\mathbf{v} \in V$

$$\mathbf{v} + 0 = \mathbf{v}\,; \tag{5.1h}$$

(vi) for all $\mathbf{v} \in V$ there exists a *negative, or inverse, vector* $(-\mathbf{v}) \in V$ such that

$$\mathbf{v} + (-\mathbf{v}) = 0\,. \tag{5.1i}$$

Remarks.

(i) The existence of a negative/inverse vector (see (5.1i)) allows us to *subtract* as well as add vectors, by defining

$$\mathbf{u} - \mathbf{v} \equiv \mathbf{u} + (-\mathbf{v})\,. \tag{5.2}$$

(ii) Vector multiplication is not defined in general.

(iii) If we restrict all scalars to be real, we have a *real linear vector space*, or a *linear vector space over reals*.

(iv) We will often refer to V as a *vector space*, rather than the more correct *linear vector space*.

The basic example of a vector space is F^n. An element of F^n is a list of n scalars, $(x_1, \ldots, x_n)$, where $x_i \in F$. This is called an *n-tuple*. Vector addition and scalar multiplication are defined component-wise:

$$(x_1, \ldots, x_n) + (y_1, \ldots, y_n) = (x_1 + y_1, \ldots, x_n + y_n) \tag{5.3a}$$
$$\alpha(x_1, \ldots, x_n) = (\alpha x_1, \ldots, \alpha x_n) \tag{5.3b}$$

5.1.3 Span and linear independence

Let $S = \{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_m\}$ be a subset of vectors in V. A *linear combination* of S is any vector of the form

$$a_1\mathbf{u}_1 + a_2\mathbf{u}_2 + \cdots + a_m\mathbf{u}_m = \sum_{i=1}^{m} a_i\mathbf{u}_i = a_i\mathbf{u}_i\,, \tag{5.4}$$

where $a_1, a_2, \ldots, a_m$ are scalars and, henceforth, we will use the summation convention.

Definition: Span. The *span* of S is the set of all vectors that are linear combinations of S. If the span of S is the entire vector space V, then S is said to span V.

Definition: Linear independence. A set of m non-zero vectors $\{\mathbf{u}_1, \mathbf{u}_2, \ldots\ \mathbf{u}_m\}$ is *linearly independent* if

$$a_i\mathbf{u}_i = 0 \quad\Rightarrow\quad a_i = 0 \ \text{ for } \ i = 1, 2, \ldots, m. \qquad \text{(s.c.)} \tag{5.5}$$

Otherwise, the vectors are *linearly dependent*, i.e. there exist scalars a_i, at least one of which is *non-zero*, such that

$$a_i\mathbf{u}_i = 0\,. \qquad \text{(s.c.)}$$

Definition: Dimension of a Vector Space. If a vector space V contains a set of n linearly independent vectors

11/04 but all sets of $n+1$ vectors are linearly dependent, then V is said to be of *dimension n*.

Examples.

(i) Since

$$(a, b, c) = a(1, 0, 0) + b(0, 1, 0) + c(0, 0, 1)\,, \tag{5.6}$$

the vectors $(1, 0, 0)$, $(0, 1, 0)$ and $(0, 0, 1)$ *span* a linear vector space of dimension 3.

(ii) $(1, 0, 0)$, $(0, 1, 0)$ and $(0, 0, 1)$ are linearly independent since

$$a(1, 0, 0) + b(0, 1, 0) + c(0, 0, 1) = (a, b, c) = 0 \quad\Rightarrow\quad a = 0,\ b = 0,\ c = 0\,.$$

(iii) $(1, 0, 0)$, $(0, 1, 0)$ and $(1, 1, 0)$ are linearly dependent since $(1, 1, 0) = (1, 0, 0) + (0, 1, 0)$.

Remarks.

(i) If an additional vector is included in a spanning set, it remains a spanning set.

11/02 (ii) If a vector is removed from a linearly independent set, the set remains linearly independent.

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5.1.4 Basis Vectors

If V is an n-dimensional vector space then *any* set of n linearly independent vectors $\{\mathbf{u}_1, \ldots, \mathbf{u}_n\}$ is a *basis* for V. The are a couple of *key properties* of a basis.

(i) We claim that for all vectors $\mathbf{v} \in V$, there exist scalars v_i such that

$$\mathbf{v} = v_i \mathbf{u}_i \,. \tag{5.7a}$$

The v_i are said to be the components of $\mathbf{v}$ with respect to the basis $\{\mathbf{u}_1, \ldots, \mathbf{u}_n\}$.

Proof (unlectured). To see this we note that since V has dimension n, the set $\{\mathbf{u}_1, \ldots, \mathbf{u}_n, \mathbf{v}\}$ is linearly dependent, i.e. there exist scalars $(a_1, \ldots, a_n, b)$, not all zero, such that

$$a_i \mathbf{u}_i + b\mathbf{v} = 0 \,. \tag{5.7b}$$

If $b = 0$ then the $a_i = 0$ for all i because the $\mathbf{u}_i$ are linear independent, and we have a contradiction; hence $b \neq 0$. Multiplying by b^{-1} we have that

$$\begin{aligned} \mathbf{v} =& - \left(b^{-1} a_i\right) \mathbf{u}_i \\ =& v_i \mathbf{u}_i \,, \end{aligned} \tag{5.7c}$$

where $v_i = -b^{-1} a_i$ $(i = 1, \ldots, n)$. □

(ii) The scalars $v_1, \ldots, v_n$ are *unique*.

Proof (unlectured). Suppose that

$$\mathbf{v} = v_i \mathbf{u}_i \quad \text{and that} \quad \mathbf{v} = w_i \mathbf{u}_i \,. \tag{5.8a}$$

Then, because $\mathbf{v} - \mathbf{v} = 0$,

$$0 = (v_i - w_i)\mathbf{u}_i. \tag{5.8b}$$

But the $\mathbf{u}_i$ $(i = 1, \ldots, n)$ are linearly independent, so the only solution of this equation is $v_i - w_i = 0$ $(i = 1, \ldots n)$. Hence $v_i = w_i$ $(i = 1, \ldots n)$, and we conclude that the two linear combinations (5.8a) are identical. □

Remarks. In (ii) and (i) below, $\{\mathbf{u}_1, \ldots, \mathbf{u}_m\}$ are a set of vectors in an n-dimensional vector space.

(i) If $m < n$ then there exists a vector that cannot be expressed as a linear combination of the $\mathbf{u}_i$.

(ii) If $m > n$ then there exists some vector that, when expressed as a linear combination of the $\mathbf{u}_i$, has non-unique scalar coefficients. This is true whether or not the $\mathbf{u}_i$ span V.

(iii) Vector spaces can have *infinite* dimension, e.g. the set of functions defined on the interval $0 \leqslant x < 2\pi$ and having Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \, \mathrm{e}^{inx} \,. \tag{5.9}$$

14/22 Here $f(x)$ is the 'vector' and f_n are its 'components' with respect to the 'basis' of functions e^{inx}. *Functional analysis* deals with such infinite-dimensional vector spaces.

Examples.

(i) *Three-Dimensional Euclidean Space* $\mathbb{E}^3$. In this case the scalars are real and V is three-dimensional because every vector $\mathbf{v}$ can be written uniquely as (cf. (5.6))

$$\mathbf{v} = v_x \mathbf{e}_x + v_y \mathbf{e}_y + v_z \mathbf{e}_z \tag{5.10a}$$
$$= v_1 \mathbf{u}_1 + v_2 \mathbf{u}_2 + v_3 \mathbf{u}_3 \,, \tag{5.10b}$$

where $\{\mathbf{e}_x = \mathbf{u}_1 = (1, 0, 0), \mathbf{e}_y = \mathbf{u}_2 = (0, 1, 0), \mathbf{e}_3 = \mathbf{u}_1 = (0, 0, 1)\}$ is a basis.

(ii) *The Complex Numbers.* Here we need to be careful what we mean.

Suppose we are considering a complex linear vector space, i.e. a *linear vector space over* $\mathbb{C}$. Then because the scalars are complex, every complex number z can be written uniquely as

$$z = \alpha \cdot 1 \quad \text{where} \quad \alpha \in \mathbb{C}\,, \tag{5.11a}$$

and moreover

$$\alpha \cdot 1 = 0 \quad \Rightarrow \quad \alpha = 0 \quad \text{for} \quad \alpha \in \mathbb{C}\,. \tag{5.11b}$$

We conclude that the single 'vector' $\{1\}$ constitutes a basis for $\mathbb{C}$ when viewed as a linear vector space over $\mathbb{C}$.

However, we might alternatively consider the complex numbers as a *linear vector space over* $\mathbb{R}$, so that the scalars are real. In this case the pair of 'vectors' $\{1, i\}$ constitute a basis because every complex number z can be written uniquely as

$$z = a \cdot 1 + b \cdot \imath \quad \text{where} \quad a, b \in \mathbb{R}\,, \tag{5.12a}$$

and

$$a \cdot 1 + b \cdot \imath = 0 \quad \Rightarrow \quad a = b = 0 \quad \text{if} \quad a, b, \in \mathbb{R}\,. \tag{5.12b}$$

Thus we have that

$$\dim_{\mathbb{C}} \mathbb{C} = 1 \quad \text{but} \quad \dim_{\mathbb{R}} \mathbb{C} = 2\,, \tag{5.13}$$

where the subscript indicates whether the vector space $\mathbb{C}$ is considered over $\mathbb{C}$ or $\mathbb{R}$.

Remarks.

(i) $\mathbb{R}^3$ is not quite the same as physical space because physical space has a rule for the distance between two points (i.e. Pythagoras's theorem, if physical space is approximated as Euclidean)

(ii) $\mathbb{R}^2$ is not quite the same as $\mathbb{C}$ because $\mathbb{C}$ has a rule for multiplication

Worked exercise. Show that 2×2 real symmetric matrices form a real linear vector space under addition. Show that this space has dimension 3 and find a basis.

Answer. Let V be the set of all real symmetric matrices, and let

$$\mathsf{A} = \begin{pmatrix} \alpha_a & \beta_a \\ \beta_a & \gamma_a \end{pmatrix}, \quad \mathsf{B} = \begin{pmatrix} \alpha_b & \beta_b \\ \beta_b & \gamma_b \end{pmatrix}, \quad \mathsf{C} = \begin{pmatrix} \alpha_c & \beta_c \\ \beta_c & \gamma_c \end{pmatrix},$$

be *any* three real symmetric matrices.

(i) We note that addition is closed since $\mathsf{A} + \mathsf{B}$ is a real symmetric matrix.

(ii) Addition is commutative and associative since for all [real symmetric] matrices, $\mathsf{A} + \mathsf{B} = \mathsf{B} + \mathsf{A}$ and $(\mathsf{A} + \mathsf{B}) + \mathsf{C} = \mathsf{A} + (\mathsf{B} + \mathsf{C})$.

(iii) Multiplication by a scalar is closed since if $p \in \mathbb{R}$, then $p\mathsf{A}$ is a real symmetric matrix.

(iv) Multiplication by a scalar is distributive and associative since for all $p, q \in \mathbb{R}$ and for all [real symmetric] matrices, $p(\mathsf{A} + \mathsf{B}) = p\mathsf{A} + p\mathsf{B}$, $(p + q)\mathsf{A} = p\mathsf{A} + q\mathsf{A}$ and $p(q\mathsf{A}) = (pq)\mathsf{A}$.

(v) The zero matrix,

$$0 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix},$$

is real and symmetric (and hence in V), and such that for all [real symmetric] matrices $\mathsf{A} + 0 = \mathsf{A}$.

(vi) For any [real symmetric] matrix there exists a negative matrix, i.e. that matrix with the components reversed in sign. In the case of a real symmetric matrix, the negative matrix is again real and symmetric.

Therefore V is a real linear vector space; the 'vectors' are the 2×2 real symmetric matrices. Moreover, the three 2×2 real symmetric matrices

$$\mathsf{U}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathsf{U}_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \text{and} \quad \mathsf{U}_3 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{5.15}$$

are independent, since for $p, q, r \in \mathbb{R}$

$$p\mathsf{U}_1 + q\mathsf{U}_2 + r\mathsf{U}_3 = \begin{pmatrix} p & q \\ q & r \end{pmatrix} = 0 \quad \Rightarrow \quad p = q = r = 0\,.$$

Further, any 2×2 real symmetric matrix can be expressed as a linear combination of the U_i since

$$\begin{pmatrix} p & q \\ q & r \end{pmatrix} = p\mathsf{U}_1 + q\mathsf{U}_2 + r\mathsf{U}_3\,.$$

We conclude that the 2×2 real symmetric matrices form a three-dimensional real linear vector space
11/01 under addition, and that the 'vectors' U_i defined in (5.15) form a basis.

Exercise. Show that 3×3 symmetric real matrices form a vector space under addition. Show that this space has dimension 6 and find a basis.

5.2 Change of Basis: the Rôle of Matrices

5.2.1 Linear Operators

A *linear operator* $\mathcal{A}$ on a vector space V acts on elements of V to produce other elements of V. The action of $\mathcal{A}$ on $\mathbf{x}$ is written $\mathcal{A}(\mathbf{x})$ or just $\mathcal{A}\mathbf{x}$. The property of linearity means that for scalars α and β

$$\mathcal{A}(\alpha\mathbf{x} + \beta\mathbf{y}) = \alpha\mathcal{A}\mathbf{x} + \beta\mathcal{A}\mathbf{y}\,. \tag{5.16}$$

Remarks.

(i) A linear operator has an existence without reference to any basis.

(ii) The operation can be thought of as a *linear transformation* or *mapping* of the space V (a simple example is a rotation of three-dimensional space).

(iii) A more general idea, not considered here, is that a linear operator can act on vectors of one space V to produce vectors of another space V', possibly of a different dimension.

The components of $\mathcal{A}$ with respect to a basis $\{\mathbf{e}_i\}$ are defined by the action of $\mathcal{A}$ on those basis vectors:

$$\mathcal{A}\mathbf{e}_j = \mathbf{e}_i A_{ij}\,. \qquad \text{(s.c.)} \tag{5.17}$$

The components, A_{ij}, form a square matrix A, where $(\mathsf{A})_{ij} = A_{ij}$.

Since $\mathcal{A}$ is a linear operator, a knowledge of its action on a basis is sufficient to determine its action on any vector $\mathbf{x}$ since, from (5.16),

$$\mathcal{A}\mathbf{x} = \mathcal{A}(\mathbf{e}_j x_j) = x_j(\mathcal{A}\mathbf{e}_j) = x_j(\mathbf{e}_i A_{ij}) = \mathbf{e}_i A_{ij} x_j\,, \tag{5.18a}$$

or

$$(\mathcal{A}\mathbf{x})_i = A_{ij} x_j\,. \tag{5.18b}$$

This corresponds to the rule for multiplying a matrix by a vector.

The sum of two linear operators is defined by

$$(\mathcal{A} + \mathcal{B})\mathbf{x} = \mathcal{A}\mathbf{x} + \mathcal{B}\mathbf{x} = \mathbf{e}_i(A_{ij} + B_{ij})x_j\,. \tag{5.19a}$$

The product, or composition, of two linear operators has the action

$$(\mathcal{A}\mathcal{B})\mathbf{x} = \mathcal{A}(\mathcal{B}\mathbf{x}) = \mathcal{A}(\mathbf{e}_k B_{kj} x_j) = (\mathcal{A}\mathbf{e}_k)B_{kj}x_j = \mathbf{e}_i A_{ik} B_{kj} x_j\,. \tag{5.19b}$$

The components therefore satisfy the rules of matrix addition and multiplication:

$$(\mathsf{A} + \mathsf{B})_{ij} = A_{ij} + B_{ij}\,, \qquad (\mathsf{A}\mathsf{B})_{ij} = A_{ik} B_{kj}\,. \tag{5.19c}$$

Recall that matrix multiplication is not commutative, so $\mathcal{B}\mathcal{A} \neq \mathcal{A}\mathcal{B}$ in general.

Therefore a matrix can be thought of as the components of a linear operator with respect to a given basis, just as a column matrix or n-tuple can be thought of as the components of a vector with respect to a given basis.

5.2.2 Transformation Matrices

Let $\{\mathbf{u}_i : i = 1, \ldots, n\}$ and $\{\mathbf{u}'_i : i = 1, \ldots, n\}$ be two sets of basis vectors for an n-dimensional vector space V. Since the $\{\mathbf{u}_i : i = 1, \ldots, n\}$ is a basis, the individual basis vectors of the basis $\{\mathbf{u}'_i : i = 1, \ldots, n\}$ can be written as

$$\mathbf{u}'_j = \mathbf{u}_i \, A_{ij} \quad (j = 1, \ldots, n) , \tag{5.20a}$$

for some numbers A_{ij}. From (5.7a) we see that A_{ij} is the ith component of the vector $\mathbf{u}'_j$ in the basis $\{\mathbf{u}_i : i = 1, \ldots, n\}$. Hence, the numbers A_{ij} can be represented by a square $n \times n$ *transformation matrix* A

$$\mathsf{A} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{pmatrix} , \tag{5.20b}$$

where the j^{th} column of A consists of the components of $\mathbf{u}'_j$ in terms of the $\{\mathbf{u}_i : i = 1, \ldots, n\}$ basis.

Similarly, since the $\{\mathbf{u}'_i : i = 1, \ldots, n\}$ is a basis, the individual basis vectors of the basis $\{\mathbf{u}_i : i = 1, \ldots, n\}$ can be written as

$$\mathbf{u}_i = \mathbf{u}'_k B_{ki} \quad (i = 1, 2, \ldots, n) , \tag{5.21a}$$

for some numbers B_{ki}. Here B_{ki} is the kth component of the vector $\mathbf{u}_i$ in the basis $\{\mathbf{u}'_k : k = 1, \ldots, n\}$. Again the B_{ki} can be viewed as the entries of a matrix B

$$\mathsf{B} = \begin{pmatrix} B_{11} & B_{12} & \cdots & B_{1n} \\ B_{21} & B_{22} & \cdots & B_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ B_{n1} & B_{n2} & \cdots & B_{nn} \end{pmatrix} . \tag{5.21b}$$

5.2.3 Properties of Transformation Matrices

From substituting (5.21a) into (5.20a) we have that

$$\mathbf{u}'_j = \left(\mathbf{u}'_k B_{ki}\right) A_{ij} = \mathbf{u}'_k \left(B_{ki} A_{ij}\right) . \tag{5.22a}$$

However, because of the uniqueness of a basis representation and the fact that

$$\mathbf{u}'_j = \mathbf{u}'_k \, \delta_{kj} , \tag{5.22b}$$

it follows that

$$B_{ki} A_{ij} = \delta_{kj} . \tag{5.22c}$$

Hence in matrix notation, $\mathsf{BA} = \mathsf{I}$, where I is the identity matrix. Conversely, substituting (5.20a) into (5.21a) leads to the conclusion that $\mathsf{AB} = \mathsf{I}$ (alternatively argue by a relabeling symmetry). Thus

$$\mathsf{B} = \mathsf{A}^{-1} , \tag{5.23a}$$

and

$$\det \mathsf{A} \neq 0 \quad \text{and} \quad \det \mathsf{B} \neq 0 . \tag{5.23b}$$

5.2.4 Transformation Law for Vector Components

Consider a vector $\mathbf{v}$, then in the $\{\mathbf{u}_i : i = 1, \ldots, n\}$ basis we have from (5.7a)

$$\mathbf{v} = v_i \mathbf{u}_i . \tag{5.24}$$

Similarly, in the $\{\mathbf{u}'_i : i = 1, \ldots, n\}$ basis we can write

$$\begin{aligned} \mathbf{v} &= v'_j \mathbf{u}'_j && \\ &= v'_j \mathbf{u}_i A_{ij} && \text{from (5.20a)} \\ &= \mathbf{u}_i (A_{ij} v'_j) && \textit{de facto} \text{ swap summation order.} \end{aligned} \tag{5.25}$$

Since a basis representation is unique it follows from (5.7a) that

$$v_i = A_{ij} v'_j , \tag{5.26}$$

which relates the components of $\mathbf{v}$ in the basis $\{\mathbf{u}_i : i = 1, \ldots, n\}$ to those in the basis $\{\mathbf{u}'_i : i = 1, \ldots, n\}$.

Some Notation. Let v and v' be the column matrices

$$\mathsf{v} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} \quad \text{and} \quad \mathsf{v}' = \begin{pmatrix} v_1' \\ v_2' \\ \vdots \\ v_n' \end{pmatrix} \quad \text{respectively.} \tag{5.27}$$

Note that we now have **bold v** denoting a vector, *italic* v_i denoting a component of a vector, and sans serif v denoting a column matrix of components. Then (5.26) can be expressed as

$$\mathsf{v} = \mathsf{A}\mathsf{v}', \tag{5.28a}$$

and hence, from applying A^{-1} to either side of (5.28a),

$$\mathsf{v}' = \mathsf{A}^{-1}\mathsf{v}. \tag{5.28b}$$

Remark. In matrix notation (5.20a) can be expressed as

$$\mathsf{u}' = \mathsf{u}\mathsf{A}. \tag{5.28c}$$

From a comparison between (5.28b) and (5.28c) we see that the *components* of $\mathbf{v}$ transform *inversely* to the way that the basis vectors transform. This is so that the vector $\mathbf{v}$ is unchanged:

$$\begin{aligned}
\mathbf{v} &= v_j'\mathbf{u}_j' && \text{from (5.25)} \\
&= \left((\mathsf{A}^{-1})_{jk}v_k\right)(\mathbf{u}_i A_{ij}) && \text{from (5.28b) and (5.20a)} \\
&= \mathbf{u}_i \left(v_k \left(A_{ij}(\mathsf{A}^{-1})_{jk}\right)\right) && \textit{de facto} \text{ swap summation order} \\
&= \mathbf{u}_i \left(v_k \delta_{ik}\right) && \mathsf{A}\mathsf{A}^{-1} = \mathsf{I} \\
&= v_i \mathbf{u}_i\,. && \text{contract using (1.14c)}
\end{aligned}$$

Worked example. Let $\{\mathbf{u}_1 = (1,0), \mathbf{u}_2 = (0,1)\}$ and $\{\mathbf{u}_1' = (1,1), \mathbf{u}_2' = (-1,1)\}$ be two sets of basis vectors in $\mathbb{R}^2$. Find the transformation matrix A_{ij} that connects them. Verify the transformation law for the components of an arbitrary vector $\mathbf{v}$ in the two coordinate systems.

Answer. We have from direct substitution and using (5.20a) that

$$\begin{aligned}
\mathbf{u}_1' &= (\ \ 1,1) = \qquad (1,0) + (0,1) = \ \ \mathbf{u}_1 + \mathbf{u}_2 = \mathbf{u}_j A_{ji}\,, \\
\mathbf{u}_2' &= (-1,1) = -1 \cdot (1,0) + (0,1) = -\mathbf{u}_1 + \mathbf{u}_2 = \mathbf{u}_j A_{j2}\,.
\end{aligned}$$

Hence

$$A_{11} = 1\,, \quad A_{21} = 1\,, \quad A_{12} = -1 \quad \text{and} \quad A_{22} = 1\,,$$

i.e.

$$\mathsf{A} = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad \text{with inverse} \quad \mathsf{A}^{-1} = \tfrac{1}{2}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}.$$

First Check. Note that A^{-1} is consistent with (5.21a), (5.23a) and the observation that

$$\begin{aligned}
\mathbf{u}_1 &= (1,0) = \tfrac{1}{2}(\ (1,1) - (-1,1)\ ) = \tfrac{1}{2}(\mathbf{u}_1' - \mathbf{u}_2') = \mathbf{u}_j' A^{-1}_{ji}\,, \\
\mathbf{u}_2 &= (0,1) = \tfrac{1}{2}(\ (1,1) + (-1,1)\ ) = \tfrac{1}{2}(\mathbf{u}_1' + \mathbf{u}_2') = \mathbf{u}_j' A^{-1}_{j2}\,.
\end{aligned}$$

Second Check. Consider an arbitrary vector $\mathbf{v}$, then from direct substitution

$$\begin{aligned}
\mathbf{v} &= v_1\mathbf{u}_1 + v_2\mathbf{u}_2 \\
&= \tfrac{1}{2}v_1(\mathbf{u}_1' - \mathbf{u}_2') + \tfrac{1}{2}v_2(\mathbf{u}_1' + \mathbf{u}_2') \\
&= \tfrac{1}{2}(v_1 + v_2)\mathbf{u}_1' - \tfrac{1}{2}(v_1 - v_2)\mathbf{u}_2'\,.
\end{aligned}$$

Thus

$$v_1' = \tfrac{1}{2}(v_1 + v_2) \quad \text{and} \quad v_2' = -\tfrac{1}{2}(v_1 - v_2)\,.$$

This is consistent with the result obtained using (5.28b), viz.

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$$\mathsf{v}' = \mathsf{A}^{-1}\mathsf{v} = \tfrac{1}{2}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} v_1 + v_2 \\ -v_1 + v_2 \end{pmatrix}.$$

5.3 Some Definitions of Special Matrices

From last year you should be familiar with the following definitions.

Symmetric Matrix. A square $n \times n$ matrix is *symmetric* if it is equal to its transpose:

$$\mathsf{A}^{\mathrm{T}} = \mathsf{A} \qquad \text{or} \qquad A_{ji} = A_{ij}\,. \tag{5.29a}$$

Antisymmetric matrix. A square $n \times n$ matrix is *antisymmetric* (or *skew-symmetric*) if it is equal to the negative of its transpose:

$$\mathsf{A}^{\mathrm{T}} = -\mathsf{A} \qquad \text{or} \qquad A_{ji} = -A_{ij}\,. \tag{5.29b}$$

Orthogonal matrix. A square $n \times n$ matrix is *orthogonal* if its transpose is equal to its inverse:

$$\mathsf{A}^{\mathrm{T}} = \mathsf{A}^{-1} \qquad \text{or} \qquad \mathsf{A}\mathsf{A}^{\mathrm{T}} = \mathsf{A}^{\mathrm{T}}\mathsf{A} = 1\,. \tag{5.29c}$$

These ideas can be generalized to a complex vector space; however, first we need a definition.

Hermitian conjugate. The *Hermitian conjugate* of a matrix A is defined to be the complex conjugate (denoted by *) of its transpose, i.e.

$$\mathsf{A}^{\dagger} = (\mathsf{A}^{\mathrm{T}})^* = (\mathsf{A}^*)^{\mathrm{T}} \qquad \text{or equivalently} \qquad (\mathsf{A}^{\dagger})_{ij} = A^*_{ji}\,. \tag{5.30}$$

For example

$$\text{if} \quad \mathsf{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \end{pmatrix} \quad \text{then} \quad \mathsf{A}^{\dagger} = \begin{pmatrix} A^*_{11} & A^*_{21} \\ A^*_{12} & A^*_{22} \\ A^*_{13} & A^*_{23} \end{pmatrix}. \tag{5.31a}$$

Similarly, the Hermitian conjugate of a column matrix x is a row matrix, e.g.

$$\mathsf{x}^{\dagger} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}^{\dagger} = \begin{pmatrix} x^*_1 & x^*_2 & \cdots & x^*_n \end{pmatrix}. \tag{5.31b}$$

The Hermitian conjugate of a Hermitian conjugate. From (5.30)

$$\mathsf{A}^{\dagger\dagger} = \left(\mathsf{A}^{*\mathrm{T}}\right)^{\mathrm{T}*} = \mathsf{A}\,. \tag{5.32a}$$

The Hermitian conjugate of a product of matrices. For matrices A and B recall that $(\mathsf{AB})^{\mathrm{T}} = \mathsf{B}^{\mathrm{T}}\mathsf{A}^{\mathrm{T}}$. Hence $(\mathsf{AB})^{\mathrm{T}*} = \mathsf{B}^{\mathrm{T}*}\mathsf{A}^{\mathrm{T}*}$, and so

$$(\mathsf{AB})^{\dagger} \quad = \quad \mathsf{B}^{\dagger}\mathsf{A}^{\dagger}\,. \tag{5.32b}$$

This result extends to arbitrary products of matrices and vectors, e.g.

$$(\mathsf{ABCx})^{\dagger} = \mathsf{x}^{\dagger}\mathsf{C}^{\dagger}\mathsf{B}^{\dagger}\mathsf{A}^{\dagger}\,, \tag{5.32c}$$

$$(\mathsf{x}^{\dagger}\mathsf{Ay})^{\dagger} = \mathsf{y}^{\dagger}\mathsf{A}^{\dagger}\mathsf{x}\,. \tag{5.32d}$$

In the latter example, if x and y are column matrices, each side of the equation is a scalar (a complex number). The Hermitian conjugate of a scalar is just the complex conjugate.

Positive definiteness. A square $n \times n$ matrix A is said to be *positive definite* if for all column matrices v of length n

$$\mathsf{v}^{\dagger}\mathsf{A}\mathsf{v} \geqslant 0\,, \text{ with equality iff } \mathsf{v} = 0\,, \tag{5.33a}$$

where 'iff' means *if and only if.*

15/22 *Remark.* If equality to zero were possible in (5.33a) for non-zero v, then A would said to be *positive* rather than *positive definite.*

Hermitian matrix. A square $n \times n$ matrix is *Hermitian* if it is equal to its Hermitian conjugate:

$$\mathsf{A}^{\dagger} = \mathsf{A} \qquad \text{or} \qquad A^*_{ji} = A_{ij} \tag{5.33b}$$

Anti-Hermitian matrix. A square $n \times n$ matrix is *anti-Hermitian* (or *skew-Hermitian*) if it is equal to the negative of its Hermitian conjugate:

$$\mathsf{A}^{\dagger} = -\mathsf{A} \qquad \text{or} \qquad A^{*}_{ji} = -A_{ij} \,. \tag{5.33c}$$

Unitary matrix. A square $n \times n$ matrix is *unitary* if its Hermitian conjugate is equal to its inverse:

$$\mathsf{A}^{\dagger} = \mathsf{A}^{-1} \qquad \text{or} \qquad \mathsf{A}\mathsf{A}^{\dagger} = \mathsf{A}^{\dagger}\mathsf{A} = 1 \,. \tag{5.33d}$$

Normal matrix. A square $n \times n$ matrix is *normal* if it commutes with its Hermitian conjugate:

$$\mathsf{A}\mathsf{A}^{\dagger} = \mathsf{A}^{\dagger}\mathsf{A} \,. \tag{5.33e}$$

Exercise. Verify that Hermitian, anti-Hermitian and unitary matrices are all normal.

5.4 Scalar Product (Inner Product)

5.4.1 Definition of a Scalar Product

The prototype linear vector space $V = \mathbb{E}^3$ has the additional property that any two vectors $\mathbf{u}$ and $\mathbf{v}$ can be combined to form a *scalar* $\mathbf{u} \cdot \mathbf{v}$. This can be generalised to an n-dimensional vector space V over $\mathbb{C}$ by assigning, for every pair of vectors $\mathbf{u}$, $\mathbf{v} \in V$, a *scalar product* $\mathbf{u} \cdot \mathbf{v} \in \mathbb{C}$ with the following properties.

(i) The scalar product should be *linear in its second argument*, i.e. for $a, b \in \mathbb{C}$

$$\mathbf{u} \cdot (a\mathbf{v}_1 + b\mathbf{v}_2) = a\,\mathbf{u} \cdot \mathbf{v}_1 + b\,\mathbf{u} \cdot \mathbf{v}_2 \,. \tag{5.34a}$$

(ii) The scalar product should have *Hermitian symmetry*, i.e.

$$\mathbf{u} \cdot \mathbf{v} = (\mathbf{v} \cdot \mathbf{u})^{*} \,, \tag{5.34b}$$

where we again denote a complex conjugate with *. Implicit in this equation is the conclusion that for a complex vector space the *ordering* of the vectors in the scalar product is important (whereas for $\mathbb{E}^3$ this is not important). Further, if we let $\mathbf{u} = \mathbf{v}$, then this implies that

$$\mathbf{v} \cdot \mathbf{v} = (\mathbf{v} \cdot \mathbf{v})^{*} \,, \tag{5.34c}$$

i.e. $\mathbf{v} \cdot \mathbf{v}$ is *real*.

(iii) The scalar product of a vector with itself should be *positive*, i.e.

$$\mathbf{v} \cdot \mathbf{v} \geqslant 0 \,. \tag{5.34d}$$

This allows us to write $\mathbf{v} \cdot \mathbf{v} = |\mathbf{v}|^2$, where the real positive number $|\mathbf{v}|$ is the *norm* (cf. length) of the vector $\mathbf{v}$.

(iv) Further, the scalar product should be *positive definite*, i.e. the only vector of zero norm should be the zero vector:

$$|\mathbf{v}| = 0 \quad \Rightarrow \quad \mathbf{v} = 0 \,. \tag{5.34e}$$

Remarks.

(i) A scalar/inner product has existence without reference to any basis.

(ii) Properties (5.34a) and (5.34b) imply that for $a, b \in \mathbb{C}$

$$\begin{aligned}
(a\mathbf{u}_1 + b\mathbf{u}_2) \cdot \mathbf{v} &= (\mathbf{v} \cdot (a\mathbf{u}_1 + b\mathbf{u}_2))^{*} \\
&= (a\mathbf{v} \cdot \mathbf{u}_1 + b\mathbf{v} \cdot \mathbf{u}_2)^{*} \\
&= a^{*}\,(\mathbf{v} \cdot \mathbf{u}_1)^{*} + b^{*}\,(\mathbf{v} \cdot \mathbf{u}_2)^{*} \\
&= a^{*}\,(\mathbf{u}_1 \cdot \mathbf{v}) + b^{*}\,(\mathbf{u}_2 \cdot \mathbf{v}) \,,
\end{aligned} \tag{5.35}$$

i.e. the scalar product is *'anti-linear' in the first argument.*

Failure to remember this is a common cause of error.

However, if $a, b \in \mathbb{R}$ then (5.35) reduces to linearity in *both* arguments.

Alternative notation. An alternative notation for the scalar product and associated norm is

$$\langle\, \mathbf{u} \mid \mathbf{v} \,\rangle \equiv \mathbf{u} \cdot \mathbf{v} \,, \tag{5.36a}$$

$$\|\mathbf{v}\| \equiv |\mathbf{v}| = (\mathbf{v} \cdot \mathbf{v})^{\frac{1}{2}} \,. \tag{5.36b}$$

5.4.2 Worked Example

Question. Identify an inner product for the vector space of real symmetric 2×2 matrices under addition.

Answer. We have already seen that the real symmetric 2×2 matrices form a vector space. In defining an inner product a key point to remember is that we need property (5.45a), i.e. that the scalar product of a vector with itself is zero only if the vector is zero. One way to do this is to spot that the vector space of real symmetric 2×2 matrices is really the 4-tuple $(A_{11}, A_{12}, A_{21}, A_{22})$, with $A_{12} = A_{21}$, in disguise. Hence, one way forward is to consider the inner product defined for matrices A and B by

$$\begin{aligned} \langle\, \mathsf{A} \mid \mathsf{B} \,\rangle &= A_{ij}^* B_{ij} && (5.37a)\\ &= A_{11}^* B_{11} + A_{12}^* B_{12} + A_{21}^* B_{21} + A_{22}^* B_{22} \,, && (5.37b) \end{aligned}$$

where we are using the alternative notation (5.36a) for the inner product. For this definition of inner product we have for real symmetric 2×2 matrices A, B and C, and $a, b \in \mathbb{C}$:

(i) as in (5.34a)

$$\begin{aligned} \langle\, \mathsf{A} \mid (\beta \mathsf{B} + \gamma \mathsf{C}) \,\rangle &= A_{ij}^* (\beta B_{ij} + \gamma C_{ij}) \\ &= \beta A_{ij}^* B_{ij} + \gamma A_{ij}^* C_{ij} \\ &= \beta \,\langle\, \mathsf{A} \mid \mathsf{B} \,\rangle + \gamma \,\langle\, \mathsf{A} \mid \mathsf{C} \,\rangle \,; \end{aligned}$$

(ii) as in (5.34b)

$$\langle\, \mathsf{B} \mid \mathsf{A} \,\rangle = B_{ij}^* A_{ij} = \langle\, \mathsf{A} \mid \mathsf{B} \,\rangle^* \,;$$

(iii) as in (5.34d) and (5.34e)

$$\begin{aligned} &\langle\, \mathsf{A} \mid \mathsf{A} \,\rangle = A_{ij}^* A_{ij} = \sum_{i,j=1}^{n} |A_{ij}|^2 \geqslant 0 \,; \\ &\langle\, \mathsf{A} \mid \mathsf{A} \,\rangle = 0 \quad \Rightarrow \quad \mathsf{A} = 0 \,. \end{aligned}$$

Hence we have a well defined inner product.

5.4.3 Some Inequalities

Schwarz's Inequality. This states that

$$|\langle\, \mathbf{u} \mid \mathbf{v} \,\rangle| \leqslant \|\mathbf{u}\| \, \|\mathbf{v}\| \,, \tag{5.38}$$

with equality only when $\mathbf{u}$ is a scalar multiple of $\mathbf{v}$.

Proof. Write $\langle\, \mathbf{u} \mid \mathbf{v} \,\rangle = |\langle\, \mathbf{u} \mid \mathbf{v} \,\rangle| \mathrm{e}^{\imath\alpha}$, and for $\lambda \in \mathbb{C}$ consider

$$\begin{aligned} \|\mathbf{u} + \lambda \mathbf{v}\|^2 &= \langle\, \mathbf{u} + \lambda \mathbf{v} \mid \mathbf{u} + \lambda \mathbf{v} \,\rangle && \text{from (5.36b)} \\ &= \langle\, \mathbf{u} \mid \mathbf{u} \,\rangle + \lambda \langle\, \mathbf{u} \mid \mathbf{v} \,\rangle + \lambda^* \langle\, \mathbf{v} \mid \mathbf{u} \,\rangle + |\lambda|^2 \langle\, \mathbf{v} \mid \mathbf{v} \,\rangle && \text{from (5.34a) and (5.35)} \\ &= \langle\, \mathbf{u} \mid \mathbf{u} \,\rangle + (\lambda \mathrm{e}^{\imath\alpha} + \lambda^* \mathrm{e}^{-\imath\alpha}) |\langle\, \mathbf{u} \mid \mathbf{v} \,\rangle| + |\lambda|^2 \langle\, \mathbf{v} \mid \mathbf{v} \,\rangle && \text{from (5.34b).} \end{aligned}$$

First, suppose that $\mathbf{v} = 0$. The right-hand-side then simplifies from a quadratic in λ to an expression that is linear in λ. If $\langle\, \mathbf{u} \mid \mathbf{v} \,\rangle \neq 0$ we then have a contradiction since for certain choices of λ this simplified expression can be negative. Hence we conclude that

$$\langle\, \mathbf{u} \mid \mathbf{v} \,\rangle = 0 \quad \text{if} \quad \mathbf{v} = 0 \,,$$

in which case (5.38) is satisfied as an equality. Next suppose that $\mathbf{v} \neq 0$ and choose $\lambda = r\mathrm{e}^{-\imath\alpha}$ so that from (5.34d)

$$0 \leqslant \|\mathbf{u} + \lambda \mathbf{v}\|^2 = \|\mathbf{u}\|^2 + 2r |\langle\, \mathbf{u} \mid \mathbf{v} \,\rangle| + r^2 \|\mathbf{v}\|^2 \,.$$

The right-hand-side is a quadratic in r that has a minimum when $r\|\mathbf{v}\|^2 = -|\langle\, \mathbf{u} \mid \mathbf{v} \,\rangle|$. Schwarz's inequality follows on substituting this value of r, with equality if $\mathbf{u} = -\lambda \mathbf{v}$. □

The Triangle Inequality. This states that

$$\|\mathbf{u}+\mathbf{v}\| \leqslant \|\mathbf{u}\| + \|\mathbf{v}\| \,. \tag{5.39}$$

Proof. This follows from taking square roots of the following inequality:

$$\begin{aligned}
\|\mathbf{u}+\mathbf{v}\|^2 &= \langle\, \mathbf{u} \mid \mathbf{u}\,\rangle + \langle\, \mathbf{u} \mid \mathbf{v}\,\rangle + \langle\, \mathbf{u} \mid \mathbf{v}\,\rangle^* + \langle\, \mathbf{v} \mid \mathbf{v}\,\rangle && \text{from above with } \lambda = 1\\
&= \|\mathbf{u}\|^2 + 2\,\mathrm{Re}\,\langle\, \mathbf{u} \mid \mathbf{v}\,\rangle + \|\mathbf{v}\|^2 && \text{from (5.34b)}\\
&\leqslant \|\mathbf{u}\|^2 + 2|\langle\, \mathbf{u} \mid \mathbf{v}\,\rangle| + \|\mathbf{v}\|^2 && \\
&\leqslant \|\mathbf{u}\|^2 + 2\|\mathbf{u}\|\,\|\mathbf{v}\| + \|\mathbf{v}\|^2 && \text{from (5.38)}\\
&\leqslant (\|\mathbf{u}\| + \|\mathbf{v}\|)^2 \,.
\end{aligned}$$

5.4.4 The Scalar Product in Terms of Components

Suppose that we have a scalar product defined on a vector space with a given basis $\{\mathbf{u}_i : i = 1, \ldots, n\}$. We will next show that the scalar product is in some sense determined for all pairs of vectors by its values for all pairs of basis vectors. To start, define the complex numbers G_{ij} by

$$G_{ij} = \mathbf{u}_i \cdot \mathbf{u}_j \quad (i, j = 1, \ldots, n)\,. \tag{5.40}$$

Then, for *any* two vectors

$$\mathbf{v} = v_i \mathbf{u}_i \quad \text{and} \quad \mathbf{w} = w_j \mathbf{u}_j\,, \tag{5.41}$$

we have that

$$\begin{aligned}
\mathbf{v}\cdot\mathbf{w} &= (v_i\mathbf{u}_i)\cdot(w_j\mathbf{u}_j)\\
&= v_i^* w_j\, \mathbf{u}_i\cdot\mathbf{u}_j && \text{from (5.34a) and (5.35)}\\
&= v_i^* G_{ij} w_j\,. && (5.42)
\end{aligned}$$

In matrix notation the scalar product (5.42) can be written as

$$\mathbf{v}\cdot\mathbf{w} = \mathsf{v}^\dagger \mathsf{G}\,\mathsf{w}\,, \tag{5.43}$$

where G is the matrix, or *metric*, with entries G_{ij} (metrics are a key ingredient of General Relativity).

5.4.5 Properties of the Metric

Property: a metric is Hermitian. The elements of the Hermitian conjugate of the metric G are the complex numbers

$$\begin{aligned}
(\mathsf{G}^\dagger)_{ij} \equiv G^\dagger_{ij} &= (G_{ji})^* && \text{from (5.30)} && (5.44a)\\
&= (\mathbf{u}_j\cdot\mathbf{u}_i)^* && \text{from (5.40)}\\
&= \mathbf{u}_i\cdot\mathbf{u}_j && \text{from (5.34b)}\\
&= G_{ij}\,. && \text{from (5.40)} && (5.44b)
\end{aligned}$$

Hence G is Hermitian, i.e.

$$\mathsf{G}^\dagger = \mathsf{G}\,. \tag{5.44c}$$

Remark (unlectured). That G is Hermitian is consistent with the requirement (5.34c) that $|\mathbf{v}|^2 = \mathbf{v}\cdot\mathbf{v}$ is real, since

$$\begin{aligned}
(\mathbf{v}\cdot\mathbf{v})^* &= ((\mathbf{v}\cdot\mathbf{v})^*)^{\mathrm{T}} && \text{since a scalar is its own transpose}\\
&= (\mathbf{v}\cdot\mathbf{v})^\dagger && \text{from definition (5.30)}\\
&= (\mathsf{v}^\dagger\,\mathsf{G}\,\mathsf{v})^\dagger && \text{from (5.43)}\\
&= \mathsf{v}^\dagger\,\mathsf{G}^\dagger\,\mathsf{v} && \text{from (5.32b) and (5.32a)}\\
&= \mathsf{v}^\dagger\,\mathsf{G}\,\mathsf{v} && \text{from (5.44c)}\\
&= \mathbf{v}\cdot\mathbf{v}\,. && \text{from (5.43)}
\end{aligned}$$

Property: a metric is positive definite. From (5.34d) and (5.34e) we have from the properties of a scalar product that for any $\mathbf{v}$

$$|\mathbf{v}|^2 \geqslant 0 \quad \text{with equality iff} \quad \mathbf{v} = 0\,. \tag{5.45a}$$

Hence, from (5.43), for any $\mathbf{v}$

$$\mathsf{v}^\dagger \mathsf{G} \mathsf{v} \geqslant 0 \quad \text{with equality iff} \quad \mathsf{v} = 0\,. \tag{5.45b}$$

13/01 It follows from definition (5.33a) that G is *positive definite*.

5.5 Eigenvalues, Eigenvectors and Diagonalization

Suppose that M is a square $n \times n$ matrix. Then a *non-zero* column vector x such that

$$\mathsf{M}\mathsf{x} = \lambda \mathsf{x}\,, \tag{5.46a}$$

where $\lambda \in \mathbb{C}$, is said to be an eigenvector of the matrix M with eigenvalue λ. If we rewrite this equation as

$$(\mathsf{M} - \lambda \mathsf{I})\mathsf{x} = 0\,, \tag{5.46b}$$

then, since x is non-zero, we conclude that a a non-trivial linear combination of the columns of the matrix $(\mathsf{M} - \lambda \mathsf{I})$ is equal to zero, i.e. that the columns of the matrix are linearly dependent. This statement is also equivalent to the requirement

$$\det(\mathsf{M} - \lambda \mathsf{I}) = 0\,, \tag{5.47}$$

which is called the *characteristic equation* of the matrix M. The left-hand-side of (5.47) is an nth order polynomial in λ called the *characteristic polynomial* of M.

The roots of the characteristic polynomial are the eigenvalues of M, and since an nth order polynomial has exactly n, possibly complex, roots (counting multiplicities in the case of repeated roots), there are always n eigenvalues.

Examples.

(i) Find the eigenvalues and eigenvectors of

$$\mathsf{M} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{5.48a}$$

Answer. From (5.47)

$$0 = \det(\mathsf{M} - \lambda \mathsf{I}) = \begin{Vmatrix} -\lambda & 1 \\ -1 & -\lambda \end{Vmatrix} = \lambda^2 + 1 = (\lambda - \imath)(\lambda + \imath)\,, \tag{5.48b}$$

and so the eigenvalues of M are $\pm\imath$. The eigenvectors are the non-zero solutions to

$$\begin{pmatrix} \mp\imath & 1 \\ -1 & \mp\imath \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}\,. \tag{5.48c}$$

Hence there are two linearly independent eigenvectors

$$\alpha \begin{pmatrix} 1 \\ \imath \end{pmatrix} \quad \text{and} \quad \beta \begin{pmatrix} 1 \\ -\imath \end{pmatrix}\,, \tag{5.48d}$$

where α and β are any non-zero constants.

(ii) Find the eigenvalues and eigenvectors of

$$\mathsf{M} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{5.49a}$$

Answer. From (5.47)

$$0 = \det(\mathsf{M} - \lambda \mathsf{I}) = \begin{Vmatrix} -\lambda & 1 \\ 0 & -\lambda \end{Vmatrix} = \lambda^2\,, \tag{5.49b}$$

and so the eigenvalues of M are 0 and 0. The eigenvectors are the non-zero solutions to

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}\,. \tag{5.49c}$$

Hence there is only one linearly independent eigenvector, namely any non-zero multiple of

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}\,. \tag{5.49d}$$

Degeneracy. If the n eigenvalues are distinct, then there are n linearly independent eigenvectors, each of which is determined uniquely up to an arbitrary multiplicative constant.

If the eigenvalues are not all distinct, the repeated eigenvalues are said to be *degenerate*. If an eigenvalue λ occurs m times, there may be any number between 1 and m of linearly independent eigenvectors corresponding to it. Any linear combination of these is also an eigenvector and the space spanned by such vectors is called an *eigenspace*.

Diagonalization. Denote the n, not necessarily distinct, eigenvalues by $\lambda_i, i = 1, 2, \dots, n$, and let x^i be the respective eigenvectors; so

$$\mathsf{M}\mathsf{x}^i = \lambda_i \mathsf{x}^i \,, \qquad (i = 1, 2, \dots, n, \text{ no s.c.}) \tag{5.50a}$$

or in component notation for the j^{th} component

$$\sum_{k=1}^{n} M_{jk} x_k^i = \lambda_i x_j^i \,. \tag{5.50b}$$

Let X be the $n \times n$ matrix whose columns are the eigenvectors of M, then

$$(\mathsf{X})_{ij} \equiv X_{ij} = x_i^j \,, \tag{5.51a}$$

i.e.

$$\mathsf{X} = \begin{pmatrix} x_1^1 & x_1^2 & \cdots & x_1^n \\ x_2^1 & x_2^2 & \cdots & x_2^n \\ \vdots & \vdots & \ddots & \vdots \\ x_n^1 & x_n^2 & \cdots & x_n^n \end{pmatrix} . \tag{5.51b}$$

in which case (5.50b) can be rewritten as

$$\sum_{k=1}^{n} M_{jk} X_{ki} = \lambda_i X_{ji} = \sum_{k=1}^{n} X_{jk}\, \delta_{ki} \lambda_i \tag{5.52a}$$

or, in matrix notation, as

$$\mathsf{M}\mathsf{X} = \mathsf{X}\Lambda \,, \tag{5.52b}$$

where Λ is the diagonal matrix

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} . \tag{5.52c}$$

If X has an inverse, X^{-1}, then

$$\mathsf{X}^{-1}\mathsf{M}\mathsf{X} = \Lambda \,, \tag{5.53}$$

i.e. X diagonalizes M. But for X^{-1} to exist we require that $\det \mathsf{X} \neq 0$; this is equivalent to the requirement that the columns of X are linearly independent. These columns are just the eigenvectors of M, so

an $n \times n$ matrix is diagonalizable if and only if it has n linearly-independent eigenvectors.

5.6 Eigenvalues and Eigenvectors of Hermitian Matrices

In order to determine whether a metric is diagonalizable, we conclude from the above considerations that we need to determine whether the metric has n linearly-independent eigenvectors. To this end we shall determine two important properties of Hermitian matrices.

5.6.1 Properties of the Eigenvalues and Eigenvectors of an Hermitian Matrix

Let H be an Hermitian matrix, and consider two eigenvectors x and y corresponding to eigenvalues λ and μ:

$$\mathsf{H}\mathsf{x} = \lambda \mathsf{x} \,, \tag{5.54a}$$

$$\mathsf{H}\mathsf{y} = \mu \mathsf{y} \,. \tag{5.54b}$$

The Hermitian conjugate of (5.54b) is, since $\mathsf{H}^\dagger = \mathsf{H}$,

$$\mathsf{y}^\dagger \mathsf{H} = \mu^* \mathsf{y}^\dagger \,. \tag{5.54c}$$

Using (5.54a) and (5.54c) we can construct two expressions for $\mathsf{y}^\dagger\mathsf{H}\mathsf{x}$:

$$\mathsf{y}^\dagger\mathsf{H}\mathsf{x} = \lambda \mathsf{y}^\dagger \mathsf{x} = \mu^* \mathsf{y}^\dagger \mathsf{x} \,, \tag{5.55a}$$

and hence

$$(\lambda - \mu^*)\mathsf{y}^\dagger \mathsf{x} = 0 \,. \tag{5.55b}$$

The eigenvalues of an Hermitian matrix are real. Suppose that x and y are the *same* eigenvector. Then $\mathsf{y} = \mathsf{x}$ and $\mu = \lambda$, so (5.55b) becomes

$$(\lambda - \lambda^*)\mathsf{x}^\dagger\mathsf{x} = 0 \tag{5.56}$$

Since $\mathsf{x} \neq 0$, $\mathsf{x}^\dagger\mathsf{x} = x_i^* x_i = |\mathbf{x}|^2 \neq 0$,and so $\lambda^* = \lambda$. Therefore

the eigenvalues of an Hermitian matrix are real.

The eigenvectors of an Hermitian matrix with distinct eigenvalues are orthogonal. Knowing that the eigenvalues of an Hermitian matrix are real allows us to simplify (5.55b) to

$$(\lambda - \mu)\mathsf{y}^\dagger\mathsf{x} = 0\,. \tag{5.57}$$

If x and y are now *different* eigenvectors, we deduce that $\mathsf{y}^\dagger\mathsf{x} = 0$, provided that $\mu \neq \lambda$. Therefore, (in the standard inner product on $\mathbb{C}^n$,

16/22 *the eigenvectors of an Hermitian matrix corresponding to distinct eigenvalues are orthogonal.*

Degenerate eigenvalues. The case when there is a repeated eigenvalue is more difficult. However with sufficient mathematical effort it can still be proved that orthogonal eigenvectors exist for the repeated eigenvalue. Instead of adopting this approach we appeal to arm-waving arguments.

An 'experimental' approach. First adopt an 'experimental' approach. In real life it is highly unlikely that two eigenvalues will be exactly equal (because of experimental error, etc.). Hence this case never arises and we can assume that we have n orthogonal eigenvectors. ☹

A perturbation approach. Alternatively suppose that in the real problem two eigenvalues are exactly equal. Introduce a specific, but small, perturbation of size ε (cf. the ε introduced in (3.8b) when calculating the Fourier transform of the Heaviside step function) such that the perturbed problem has unequal eigenvalues (this is highly likely to be possible because the problem with equal eigenvalues is likely to be 'structurally unstable'). Now let $\varepsilon \to 0$. For all non-zero values of ε (both positive and negative) there will be n orthogonal eigenvectors. On appealing to a continuity argument
14/02 there will be n orthogonal eigenvectors for the specific case $\varepsilon = 0$.

14/04 *An Hermitian matrix has n orthogonal linearly independent eigenvectors.* We have already concluded that the eigenvectors of an Hermitian matrix are orthogonal, we now need to prove that two orthogonal [eigen]vectors are linearly independent.

Proof. Suppose there exist α and β such that

$$\alpha\mathsf{x} + \beta\mathsf{y} = 0\,. \tag{5.58a}$$

Then from pre-multiplying (5.58a) by $\mathsf{y}^\dagger$ and using the orthogonality of x and y, i.e. $\mathsf{y}^\dagger\mathsf{x} = 0$, it follows that

$$0 = \beta\mathsf{y}^\dagger\mathsf{y} = \beta\mathsf{y}_k^*\mathsf{y}_k\,. \tag{5.58b}$$

Since y is non-zero it follows that $\beta = 0$. By the relabeling symmetry, or from pre-multiplying (5.58a) by $\mathsf{x}^\dagger$, it similarly follows that $\alpha = 0$. □

We conclude that, whether or not two or more eigenvalues are equal,

an n-dimensional Hermitian matrix has n orthogonal eigenvectors that are linearly independent.

An Hermitian matrix has n orthonormal eigenvectors. We can tighten this result a little further by noting that, for any $\mu \in \mathbb{C}$,

$$\text{if} \quad \mathsf{Hx} = \lambda\mathsf{x}\,, \quad \text{then} \quad \mathsf{H}(\mu\mathsf{x}) = \lambda(\mu\mathsf{x})\,. \tag{5.59a}$$

This allows us to normalise the eigenvectors so that

$$\mathsf{x}^\dagger\,\mathsf{x} = 1\,. \tag{5.59b}$$

Hence for Hermitian matrices it is always possible to find n *orthonormal* eigenvectors that are linearly
14/03 independent.

Anti-Hermitian and Unitary Matrices. The eigenvalues of anti-Hermitian and unitary matrices are imaginary and of unit modulus, respectively. These results can be proved using a similar approach to that leading to (5.56) for proving that the eigenvalues for Hermitian matrices are real.

Normal matrices. It can be shown that the eigenvectors of normal matrices corresponding to distinct eigenvalues are orthogonal. Moreover, if a repeated eigenvalue λ occurs m times, it can be shown (with some difficulty) that there are exactly m corresponding linearly independent eigenvectors.

Construction of orthogonal eigenvectors. If the multiplicity of an eigenvalue, say m, matches the number of its linearly independent eigenvectors, then the eigenvalue is said to have no *defect*. In this case it is always possible to construct an orthogonal basis within the m-dimensional eigenspace, e.g. by the Gram–Schmidt procedure (see Example Sheet 3, Question 2). Therefore, even if the eigenvalues are degenerate, it is possible to find n mutually orthogonal eigenvectors, which form a basis for the vector space.

5.6.2 Diagonalization of Hermitian Matrices

It follows from the above result, (5.51b) and (5.53), that an Hermitian matrix H can be 'diagonalized' to the matrix Λ by means of the transformation $\mathsf{X}^{-1}\mathsf{H}\,\mathsf{X}$, where the columns of X are the eigenvectors of H:

$$\mathsf{X} = \begin{pmatrix} x_1^1 & x_1^2 & \cdots & x_1^n \\ x_2^1 & x_2^2 & \cdots & x_2^n \\ \vdots & \vdots & \ddots & \vdots \\ x_n^1 & x_n^2 & \cdots & x_n^n \end{pmatrix}. \tag{5.60}$$

Orthonormal eigenvectors. If the x^i are orthonormal eigenvectors of H then X is a *unitary* matrix since

$$(\mathsf{X}^\dagger\,\mathsf{X})_{ij} = (\mathsf{X}^\dagger)_{ik}(\mathsf{X})_{kj} = (x_k^i)^* x_k^j = \mathsf{x}^{i\,\dagger}\,\mathsf{x}^j = \delta_{ij} \qquad \text{by orthonormality,} \tag{5.61a}$$

or, in matrix notation,

$$\mathsf{X}^\dagger\,\mathsf{X} = \mathsf{I}\,. \tag{5.61b}$$

Hence X is a unitary matrix, and we deduce that every Hermitian matrix, H, is diagonalizable by a transformation

$$\mathsf{X}^\dagger\mathsf{H}\mathsf{X} = \Lambda\,, \tag{5.62}$$

where X is a unitary matrix.

In the case when we restrict ourselves to real matrices, we conclude that every real symmetric matrix, S, is diagonalizable by a transformation $\mathsf{R}^{\mathrm{T}}\mathsf{S}\,\mathsf{R}$, where R is an orthogonal matrix.

Example. Find the orthogonal matrix that diagonalizes the real symmetric matrix

$$\mathsf{S} = \begin{pmatrix} 1 & \beta \\ \beta & 1 \end{pmatrix} \quad \text{where } \beta \text{ is real.} \tag{5.63}$$

Answer. The characteristic equation is

$$0 = \left\| \begin{matrix} 1-\lambda & \beta \\ \beta & 1-\lambda \end{matrix} \right\| = (1-\lambda)^2 - \beta^2\,. \tag{5.64}$$

The solutions to (5.64) are

$$\lambda = \begin{cases} \lambda_+ = 1+\beta \\ \lambda_- = 1-\beta \end{cases}. \tag{5.65}$$

The corresponding eigenvectors $\mathsf{x}^{(\pm)}$ are found by solving $\mathsf{S}\mathsf{x}^{(\pm)} = \lambda_\pm \mathsf{x}^{(\pm)}$, i.e.

$$\begin{pmatrix} 1-\lambda_\pm & \beta \\ \beta & 1-\lambda_\pm \end{pmatrix} \begin{pmatrix} x_1^{(\pm)} \\ x_2^{(\pm)} \end{pmatrix} = 0\,, \tag{5.66a}$$

or

$$\beta \begin{pmatrix} \mp 1 & 1 \\ 1 & \mp 1 \end{pmatrix} \begin{pmatrix} x_1^{(\pm)} \\ x_2^{(\pm)} \end{pmatrix} = 0\,. \tag{5.66b}$$

$\beta \neq 0$**.** If $\beta \neq 0$ (in which case $\lambda_+ \neq \lambda_-$) we have that
$$x_2^{(\pm)} = \pm\, x_1^{(\pm)}\,. \tag{5.67a}$$
On normalising $\mathsf{x}^{(\pm)}$ so that $\mathsf{x}^{(\pm)\dagger}\,\mathsf{x}^{(\pm)} = 1$, it follows that
$$\mathsf{x}^{(+)} = \pm\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \mathsf{x}^{(-)} = \pm\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{5.67b}$$
Note that $\mathsf{x}^{+\dagger}\,\mathsf{x}^{-} = 0$, as proved earlier.

$\beta = 0$**.** If $\beta = 0$, then $\mathsf{S} = \mathsf{I}$, and so any non-zero vector is an eigenvector with eigenvalue 1. In agreement with the result stated earlier, two linearly-independent eigenvectors can still be found, and we can choose them to be orthonormal, e.g. x^{+} and x^{-} as above (if fact there is an uncountable choice of orthonormal eigenvectors in this very special case).

To diagonalize S when $\beta \neq 0$ (it already is diagonal if $\beta = 0$) we construct an orthogonal matrix R using (5.60):
$$\mathsf{R} \equiv \mathsf{X} = \begin{pmatrix} x_1^{(+)} & x_1^{(-)} \\ x_2^{(+)} & x_2^{(-)} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{5.68}$$
As a check we note that
$$\mathsf{R}^{\mathrm{T}}\mathsf{R} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{5.69}$$
and that
$$\begin{aligned} \mathsf{R}^{\mathrm{T}}\mathsf{S}\,\mathsf{R} &= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & \beta \\ \beta & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1+\beta & 1-\beta \\ 1+\beta & -1+\beta \end{pmatrix} \\ &= \begin{pmatrix} 1+\beta & 0 \\ 0 & 1-\beta \end{pmatrix} \\ &= \Lambda\,. \end{aligned} \tag{5.70}$$

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5.6.3 Diagonalization of Matrices

For a general $n \times n$ matrix M with n *distinct* eigenvalues λ_i, $(i = 1, \dots, n)$, it is possible to show (but not here) that there are n linearly independent eigenvectors x^i. It then follows from (5.53) M is diagonalized by the matrix
$$\mathsf{X} = \begin{pmatrix} x_1^1 & x_1^2 & \cdots & x_1^n \\ x_2^1 & x_2^2 & \cdots & x_2^n \\ \vdots & \vdots & \ddots & \vdots \\ x_n^1 & x_n^2 & \cdots & x_n^n \end{pmatrix}. \tag{5.71}$$

Remark. If M has two or more equal eigenvalues it *may or may not* have n linearly independent eigenvectors. If it does not have n linearly independent eigenvectors then it is *not* diagonalizable. As an example recall matrix (5.49a), i.e.
$$\mathsf{M} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \tag{5.72a}$$
which was shown to have only one linearly independent eigenvector, namely (5.49d):
$$\mathsf{x} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{5.72b}$$
Hence M is *not* diagonalizable.

Normal Matrices. As noted above, *normal matrices* always have n linearly independent eigenvectors, and hence can always be diagonalized. So, in addition to Hermitian matrices, skew-symmetric Hermitian matrices and unitary matrices (and their real restrictions) can always be diagonalized.

5.7 Applications of Diagonalization

The first application of diagonalization we consider concerns changes of basis.

5.7.1 Transformation Law for Metrics

In §5.2 we determined how vector components transform under a change of basis from $\{\mathbf{u}_i : i = 1, \dots, n\}$ to $\{\mathbf{u}'_i : i = 1, \dots, n\}$, while in §5.4 we introduced inner products and defined the metric associated with a given basis. We next consider how a metric transforms under a change of basis.

First we recall from (5.28a) that for an arbitrary vector $\mathbf{v}$, its components in the two bases transform according to $\mathsf{v} = \mathsf{A}\mathsf{v}'$, where v and v' are column vectors containing the components. From taking the Hermitian conjugate of this expression, we also have that

$$\mathsf{v}^\dagger = \mathsf{v}'^\dagger \mathsf{A}^\dagger \,. \tag{5.73}$$

Hence for arbitrary vectors $\mathbf{v}$ and $\mathbf{w}$

$$\begin{aligned} \mathbf{v} \cdot \mathbf{w} &= \mathsf{v}^\dagger \mathsf{G}\, \mathsf{w} && \text{from (5.43)} \\ &= \mathsf{v}'^\dagger \mathsf{A}^\dagger \mathsf{G}\, \mathsf{A} \mathsf{w}' && \text{from (5.28a) and (5.73).} \end{aligned}$$

But from (5.43) we must also have that in terms of the new basis

$$\mathbf{v} \cdot \mathbf{w} = \mathsf{v}'^\dagger \mathsf{G}' \mathsf{w}' \,, \tag{5.74}$$

where G' is the metric in the new $\{\mathbf{u}'_i : i = 1, \dots, n\}$ basis. Since $\mathbf{v}$ and $\mathbf{w}$ are arbitrary we conclude that the metric in the new basis is given in terms of the metric in the old basis by

$$\mathsf{G}' = \mathsf{A}^\dagger \mathsf{G} \mathsf{A} \,. \tag{5.75}$$

Alternative derivation (unlectured). (5.75) can also be derived from the definition of the metric since

$$\begin{aligned} (\mathsf{G}')_{ij} \equiv G'_{ij} &= \mathbf{u}'_i \cdot \mathbf{u}'_j && \text{from (5.40)} \\ &= (\mathbf{u}_k A_{ki}) \cdot (\mathbf{u}_\ell \, A_{\ell j}) && \text{from (5.20a)} \\ &= A^*_{ki} (\mathbf{u}_k \cdot \mathbf{u}_\ell)\, A_{\ell j} && \text{from (5.34a) and (5.35)} \\ &= A^\dagger_{ik} G_{k\ell} A_{\ell j} && \text{from (5.40) and (5.44a)} \\ &= (\mathsf{A}^\dagger \mathsf{G} \mathsf{A})_{ij} \,. \end{aligned} \tag{5.76}$$

Remark. As a check we observe that

$$(\mathsf{G}')^\dagger = (\mathsf{A}^\dagger \mathsf{G} \mathsf{A})^\dagger = \mathsf{A}^\dagger \mathsf{G}^\dagger (\mathsf{A}^\dagger)^\dagger = \mathsf{A}^\dagger \mathsf{G} \mathsf{A} = \mathsf{G}' \,. \tag{5.77}$$

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Thus G' is confirmed to be Hermitian.

5.7.2 Diagonalization of the Metric

If in (5.75) we identify A with X, the matrix with columns consisting of the orthonormal eigenvectors of G, then from (5.51a), (5.51b), (5.53) and § 5.6.2,

$$\mathsf{G}' = \mathsf{X}^\dagger \mathsf{G} \mathsf{X} = \mathsf{\Lambda} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} , \tag{5.78}$$

where the λ_i are the real eigenvalues of the Hermitian matrix G.

Property: the eigenvalues of a metric are strictly positive. From (5.45b), (5.78) and writing $\Lambda_{ij} = \lambda_i \delta_{ij}$, we have that

$$0 \leqslant \mathsf{v}'^\dagger \mathsf{G}' \mathsf{v}' = \sum_{i,j=1}^{n} v'^*_i \lambda_i \delta_{ij} v'_j = \sum_{i=1}^{n} \lambda_i |v'_i|^2 \,, \tag{5.79a}$$

with equality only if $\mathbf{v}' = 0$. This can only be true for all vectors $\mathbf{v}'$ if

$$\lambda_i > 0 \quad \text{for} \quad i = 1, \dots, n \,, \tag{5.79b}$$

i.e. if the diagonal entries λ_i are *strictly positive*.

5.7.3 Orthonormal Bases

For a diagonalized metric, the new basis vectors $\{\mathbf{u}'_i : i = 1, \ldots, n\}$ are the eigenvectors of G since

$$\mathbf{u}'_j = \mathbf{u}_i \, X_{ij} = \mathbf{u}_i \, x_i^j \quad (j = 1, \ldots, n) \,. \tag{5.80a}$$

Hence the new basis vectors are orthogonal; further, from (5.40) and (5.78),

$$\mathbf{u}'_i \cdot \mathbf{u}'_j = G'_{ij} = \Lambda_{ij} = \lambda_i \delta_{ij} \,. \tag{5.80b}$$

Hence, because the λ_i are strictly positive, we can normalise the basis, viz.

$$\mathbf{e}_i = \frac{1}{\sqrt{\lambda_i}} \mathbf{u}'_i \,, \tag{5.81a}$$

so that

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \,. \tag{5.81b}$$

The $\{\mathbf{e}_i : i = 1, \ldots, n\}$ are thus an *orthonormal basis*. We conclude that:

any vector space with a scalar product has an orthonormal basis.

Since from (5.40) the elements of the metric are just $\mathbf{e}_i \cdot \mathbf{e}_j$, the metric for an orthonormal basis is the identity matrix I.

The scalar product in orthonormal bases. Let the column vectors v and w contain the components of two vectors $\mathbf{v}$ and $\mathbf{w}$, respectively, in an orthonormal basis $\{\mathbf{e}_i : i = 1, \ldots, n\}$. Then from (5.43)

$$\mathbf{v} \cdot \mathbf{w} = \mathsf{v}^\dagger \mathsf{I} \, \mathsf{w} = \mathsf{v}^\dagger \, \mathsf{w} \,. \tag{5.82}$$

This is consistent with the definition of the scalar product from last year.

Orthogonality in orthonormal bases. If the vectors $\mathbf{v}$ and $\mathbf{w}$ are orthogonal, i.e. $\mathbf{v} \cdot \mathbf{w} = 0$, then the components in an orthonormal basis are such that

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$$\mathsf{v}^\dagger \mathsf{w} = 0 \,. \tag{5.83}$$

5.7.4 Transformations Between Orthonormal Bases

Given an orthonormal basis, a question that arises is what changes of basis maintain orthonormality. Suppose that $\{\mathbf{e}'_i : i = 1, \ldots, n\}$ is a new orthonormal basis, and suppose that in terms of the original orthonormal basis

$$\mathbf{e}'_i = \mathbf{e}_k \, U_{ki} \,, \qquad \text{(s.c.)} \tag{5.84}$$

where U is the transformation matrix (cf. (5.20a)). Then from (5.75) the metric for the new basis is given by

$$\mathsf{G}' = \mathsf{U}^\dagger \mathsf{I} \, \mathsf{U} = \mathsf{U}^\dagger \mathsf{U} \,. \tag{5.85a}$$

For the new basis to be orthonormal we require that the new metric to be the identity matrix, i.e. we require that

$$\mathsf{U}^\dagger \mathsf{U} = \mathsf{I} \,. \tag{5.85b}$$

Since $\det \mathsf{U} \neq 0$, the inverse U^{-1} exists and hence U must be unitary:

$$\mathsf{U}^\dagger = \mathsf{U}^{-1} \,. \tag{5.86}$$

Vector spaces over $\mathbb{R}$. An analogous result applies to vector spaces over $\mathbb{R}$. Then, because the transformation matrix, say $\mathsf{U} = \mathsf{R}$, is *real*,

$$\mathsf{U}^\dagger = \mathsf{R}^{\mathrm{T}} \,,$$

and so R must the orthogonal:

$$\mathsf{R}^{\mathrm{T}} = \mathsf{R}^{-1} \,. \tag{5.87}$$

Example. An example of an orthogonal matrix is the 3×3 rotation matrix R that determines the new components, $\mathsf{v}' = \mathsf{R}^{\mathrm{T}} \mathsf{v}$, of a three-dimensional vector $\mathbf{v}$ after a rotation of the axes (note that under a rotation orthogonal axes remain orthogonal and unit vectors remain unit vectors).

5.7.5 Worked example (unlectured)

By finding an orthonormal set of eigenvectors, diagonalize the Hermitian matrix

$$\mathsf{H} = \begin{pmatrix} 0 & \mathrm{i} & 0 \\ -\mathrm{i} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The characteristic equation is

$$\begin{aligned} 0 &= \begin{vmatrix} -\lambda & \mathrm{i} & 0 \\ -\mathrm{i} & -\lambda & 0 \\ 0 & 0 & 1-\lambda \end{vmatrix} \\ &= (\lambda^2 - 1)(1-\lambda)\,, \end{aligned} \tag{5.88a}$$

with solutions

$$\lambda = 1, -1, 1\,. \tag{5.88b}$$

Eigenvector, $\mathsf{x}^{(-1)}$*, for* $\lambda = -1$. We require

$$\begin{pmatrix} 1 & \mathrm{i} & 0 \\ -\mathrm{i} & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \tag{5.89a}$$

and hence

$$\mathsf{x}^{(-1)} = \begin{pmatrix} x \\ ix \\ 0 \end{pmatrix}. \tag{5.89b}$$

The normalized eigenvector, $\mathsf{e}^{(-1)}$, is thus, for α real,

$$\mathsf{e}^{(-1)} = \frac{e^{i\alpha}}{\sqrt{2}} \begin{pmatrix} 1 \\ \mathrm{i} \\ 0 \end{pmatrix}. \tag{5.89c}$$

Eigenvectors, $\mathsf{x}^{(1)}$*, for* $\lambda = 1$. We require

$$\begin{pmatrix} -1 & \mathrm{i} & 0 \\ -\mathrm{i} & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \tag{5.90a}$$

and hence

$$\mathsf{x}^{(1)} = \begin{pmatrix} x \\ -ix \\ z \end{pmatrix}. \tag{5.90b}$$

The two independent variables x and z allow for a wide choice of eigenvectors, $\mathsf{e}^{(1)}$. Two normalised orthogonal eigenvectors are, for β and γ real,

$$\mathsf{e}^{(1)} = \frac{e^{i\beta}}{\sqrt{2}} \begin{pmatrix} 1 \\ -\mathrm{i} \\ 0 \end{pmatrix}, \quad e^{i\gamma} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{5.90c}$$

Remark. All three eigenvectors given in (5.89c) and (5.90c) can be confirmed to be orthonormal.

Diagonalisation of H. Using (5.62), (5.89c) and (5.90c), with the choices $\alpha = \beta = \gamma = 0$, it follows that

$$\begin{pmatrix} 1/\sqrt{2} & -\mathrm{i}/\sqrt{2} & 0 \\ 1/\sqrt{2} & \mathrm{i}/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & \mathrm{i} & 0 \\ -\mathrm{i} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ \mathrm{i}/\sqrt{2} & -\mathrm{i}/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

5.7.6 Uses of diagonalization

Because diagonal matrices can be multiplied easily (i.e. component-wise), certain operations on diagonalizable matrices are more easily carried out using the representation (5.53):

$$\mathsf{X}^{-1}\mathsf{M}\mathsf{X} = \Lambda \qquad \text{or} \qquad \mathsf{M} = \mathsf{X}\Lambda\mathsf{X}^{-1}\,, \tag{5.91}$$

Examples.

$$\begin{aligned}
\mathsf{M}^n &= \left(\mathsf{X}\Lambda\mathsf{X}^{-1}\right)\left(\mathsf{X}\Lambda\mathsf{X}^{-1}\right)\dots\left(\mathsf{X}\Lambda\mathsf{X}^{-1}\right)\\
&= \mathsf{X}\Lambda^n\mathsf{X}^{-1}\,, && (5.92\text{a})\\
\det(\mathsf{M}) &= \det\left(\mathsf{X}\Lambda\mathsf{X}^{-1}\right)\\
&= \det(\mathsf{X})\det(\Lambda)\det(\mathsf{X}^{-1}) && \text{using } \det(\mathsf{AB}) = \det(\mathsf{A})\det(\mathsf{B})\\
&= \det(\Lambda) = \prod_{i=1}^{n}\lambda_i\,, && (5.92\text{b})\\
\operatorname{tr}(\mathsf{M}) &= \operatorname{tr}\left(\mathsf{X}\Lambda\mathsf{X}^{-1}\right)\\
&= \operatorname{tr}\left(\Lambda\mathsf{X}^{-1}\mathsf{X}\right) && \text{using } \operatorname{tr}(\mathsf{AB}) = \mathsf{A}_{ij}\mathsf{B}_{ji} = \mathsf{B}_{ji}\mathsf{A}_{ij} = \operatorname{tr}(\mathsf{BA})\\
&= \operatorname{tr}(\Lambda) = \sum_{i=1}^{n}\lambda_i\,, && (5.92\text{c})\\
\operatorname{tr}(\mathsf{M}^n) &= \operatorname{tr}\left(\mathsf{X}\Lambda^n\mathsf{X}^{-1}\right)\\
&= \operatorname{tr}\left(\Lambda^n\mathsf{X}^{-1}\mathsf{X}\right) = \operatorname{tr}(\Lambda^n)\,. && (5.92\text{d})
\end{aligned}$$

Remark. (5.92b) and (5.92c) are in fact true for all matrices (whether or not they are diagonalizable), as follows from the product and sum of roots in the characteristic equation

$$\det(\mathsf{A} - \lambda 1) = \det(\mathsf{A}) + \dots + \operatorname{tr}(\mathsf{A})(-\lambda)^{n-1} + (-\lambda)^n = 0\,. \tag{5.93}$$

5.8 Forms

Definition: form. A map $\mathcal{F}(\mathbf{x})$

$$\mathcal{F}(\mathbf{x}) = \mathsf{x}^\dagger\mathsf{A}\mathsf{x} = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i^* A_{ij} x_j\,, \tag{5.94a}$$

is called a *[sesquilinear] form*; A is called its *coefficient matrix*.

Definition: Hermitian form. If $\mathsf{A} = \mathsf{H}$ is an Hermitian matrix, the map $\mathcal{F}(\mathbf{x}) : \mathbb{C}^n \mapsto \mathbb{C}$, where

$$\mathcal{F}(\mathbf{x}) = \mathsf{x}^\dagger\mathsf{H}\mathsf{x} = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i^* H_{ij} x_j\,, \tag{5.94b}$$

is referred to as an *Hermitian form* on $\mathbb{C}^n$.

Hermitian forms are real. An Hermitian form is real since

$$\begin{aligned}
(\mathsf{x}^\dagger\mathsf{H}\mathsf{x})^* &= (\mathsf{x}^\dagger\mathsf{H}\mathsf{x})^\dagger && \text{since a scalar is its own transpose}\\
&= \mathsf{x}^\dagger\mathsf{H}^\dagger\mathsf{x} && \text{since } (\mathsf{AB})^\dagger = \mathsf{B}^\dagger\mathsf{A}^\dagger\\
&= \mathsf{x}^\dagger\mathsf{H}\mathsf{x}\,. && \text{since } \mathsf{H} \text{ is Hermitian}
\end{aligned}$$

Definition: quadratic form. An important special case is obtained by restriction to *real vector spaces*; then x and H are real. It follows that $\mathsf{H}^{\mathrm{T}} = \mathsf{H}$, i.e. H is a real symmetric matrix; let us denote such a matrix by S. In this case

$$\mathcal{F}(\mathbf{x}) = \mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i S_{ij} x_j\,. \tag{5.94c}$$

When considered as a function of the real variables $x_1, x_2, \dots, x_n$, this expression is referred to as a *quadratic form* on $\mathbb{R}^n$.

5.8.1 Eigenvectors and Principal Axes

From (5.62) the coefficient matrix, H, of a Hermitian form can be written as

$$\mathsf{H} = \mathsf{U}\Lambda\mathsf{U}^\dagger\,, \tag{5.95a}$$

where U is unitary and Λ is a diagonal matrix of eigenvalues. Let

$$\mathsf{x}' = \mathsf{U}^\dagger\mathsf{x}\,, \tag{5.95b}$$

then (5.94b) can be written as

$$\begin{aligned}\mathcal{F}(\mathbf{x}) &= \mathsf{x}^\dagger\mathsf{U}\Lambda\mathsf{U}^\dagger\mathsf{x}\\ &= \mathsf{x}'^\dagger\Lambda\mathsf{x}' &\text{(5.95c)}\\ &= \sum_{i=1}^{n}\lambda_i|x_i'|^2\,. &\text{(5.95d)}\end{aligned}$$

Transforming to a basis of orthonormal eigenvectors transforms the Hermitian form to a standard form with no 'off-diagonal' terms. The orthonormal basis vectors that coincide with the eigenvectors of the coefficient matrix, and which lead to the simplified version of the form, are known as *principal axes*.

Example. Let $\mathcal{F}(\mathbf{x})$ be the quadratic form

$$\mathcal{F}(\mathbf{x}) = 2x^2 - 4xy + 5y^2 = \mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}\,, \tag{5.96a}$$

where, by splitting the xy term equally between the off-diagonal matrix elements,

$$\mathsf{x} = \begin{pmatrix} x\\ y\end{pmatrix} \qquad\text{and}\qquad \mathsf{S} = \begin{pmatrix} 2 & -2\\ -2 & 5\end{pmatrix}\,. \tag{5.96b}$$

What surface is described by $\mathcal{F}(\mathbf{x}) = \text{constant}$?

Solution. The eigenvalues of the real symmetric matrix S are $\lambda_1 = 1$ and $\lambda_2 = 6$, with corresponding unit eigenvectors

$$\mathsf{u}_1 = \frac{1}{\sqrt{5}}\begin{pmatrix} 2\\ 1\end{pmatrix} \qquad\text{and}\qquad \mathsf{u}_2 = \frac{1}{\sqrt{5}}\begin{pmatrix} 1\\ -2\end{pmatrix}\,. \tag{5.96c}$$

The orthogonal matrix

$$\mathsf{Q} = \frac{1}{\sqrt{5}}\begin{pmatrix} 2 & 1\\ 1 & -2\end{pmatrix} \tag{5.96d}$$

transforms the original orthonormal basis to a basis of principal axes. Hence $\mathsf{S} = \mathsf{Q}\Lambda\mathsf{Q}^{\mathrm{T}}$, where Λ is a diagonal matrix of eigenvalues. It follows that $\mathcal{F}$ can be rewritten in the normalised form

$$\mathcal{F} = \mathsf{x}^{\mathrm{T}}\mathsf{Q}\Lambda\mathsf{Q}^{\mathrm{T}}\mathsf{x} = \mathsf{x}'^{\mathrm{T}}\Lambda\mathsf{x}' = x'^2 + 6y'^2\,, \tag{5.96e}$$

where

$$\mathsf{x}' = \mathsf{Q}^{\mathrm{T}}\mathsf{x}\,,\quad\text{i.e.}\quad \begin{pmatrix} x'\\ y'\end{pmatrix} = \frac{1}{\sqrt{5}}\begin{pmatrix} 2 & 1\\ 1 & -2\end{pmatrix}\begin{pmatrix} x\\ y\end{pmatrix}\,. \tag{5.96f}$$

The surface $\mathcal{F}(\mathbf{x}) = \text{constant}$ is thus an ellipse.

Remark. In diagonalizing S by transforming to its eigenvector basis, we are rotating the coordinates to reduce the quadratic form to its simplest form.

5.8.2 Quadrics and conics

A *quadric*, or *quadric surface*, is the n-dimensional hypersurface defined by the zeros of a real quadratic polynomial. For co-ordinates $(x_1, \ldots, x_n)$ the general quadric is defined by

$$x_iA_{ij}x_j + b_ix_i + c \equiv \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x} + \mathsf{b}^{\mathrm{T}}\mathsf{x} + c = 0\,, \qquad\text{(s.c.)}\quad \text{(5.97a)}$$

or equivalently

$$x_jA_{ij}x_i + b_ix_i + c \equiv \mathsf{x}^{\mathrm{T}}\mathsf{A}^{\mathrm{T}}\mathsf{x} + \mathsf{b}^{\mathrm{T}}\mathsf{x} + c = 0\,, \qquad\text{(s.c.)}\quad \text{(5.97b)}$$

where A is a $n\times n$ matrix, b is a $n\times 1$ column vector and c is a constant. Let

$$\mathsf{S} = \tfrac{1}{2}\left(\mathsf{A} + \mathsf{A}^{\mathrm{T}}\right)\,, \tag{5.97c}$$

then from (5.97a) and (5.97b)

$$\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + \mathsf{b}^{\mathrm{T}}\mathsf{x} + c = 0\,. \tag{5.97d}$$

By taking the principal axes as basis vectors it follows that

$$\mathsf{x}'^{\mathrm{T}}\Lambda\mathsf{x}' + \mathsf{b}'^{\mathrm{T}}\mathsf{x}' + c = 0\,. \tag{5.97e}$$

where $\Lambda = \mathsf{Q}^{\mathrm{T}}\mathsf{S}\mathsf{Q}$, $\mathsf{b}' = \mathsf{Q}^{\mathrm{T}}\mathsf{b}$ and $\mathsf{x}' = \mathsf{Q}^{\mathrm{T}}\mathsf{x}$. If Λ does not have a zero eigenvalue, then it is invertible and (5.97e) can be simplified further by a translation of the origin

$$\mathsf{x}' \to \mathsf{x}' - \tfrac{1}{2}\Lambda^{-1}\mathsf{b}'\,, \tag{5.97f}$$

to obtain

$$\mathsf{x}'^{\mathrm{T}}\Lambda\mathsf{x}' = k\,. \tag{5.97g}$$

where k is a constant.

Conic Sections. First suppose that $n = 2$ and that Λ (or equivalently S) does not have a zero eigenvalue, then with

$$\mathsf{x}' = \begin{pmatrix} x' \\ y' \end{pmatrix} \quad \text{and} \quad \Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}\,, \tag{5.98a}$$

(5.97g) becomes

$$\lambda_1 x'^2 + \lambda_2 y'^2 = k\,, \tag{5.98b}$$

which is the normalised equation of a *conic section*.

$\lambda_1\lambda_2 > 0$. If $\lambda_1\lambda_2 > 0$, then k must have the same sign as the λ_j $(j = 1, 2)$, and (5.98b) is the equation of an *ellipse* with principal axes coinciding with the x' and y' axes.

Scale. The *scale* of the ellipse is determined by k.

Shape. The *shape* of the ellipse is determined by the ratio of eigenvalues λ_1 and λ_2.

Orientation. The *orientation* of the ellipse in the original basis is determined by the eigenvectors of S.

In the *degenerate case*, $\lambda_1 = \lambda_2$, the ellipse becomes a circle with no preferred principal axes. Any two orthogonal (and hence linearly independent) vectors may be chosen as the principal axes.

$\lambda_1\lambda_2 < 0$. If $\lambda_1\lambda_2 < 0$ then (5.98b) is the equation for a *hyperbola* with principal axes coinciding with the x' and y' axes. Similar results to above hold for the scale, shape and orientation.

$\lambda_1\lambda_2 = 0$. If $\lambda_1 = \lambda_2 = 0$, then there is no quadratic term, so assume that only one eigenvalue is zero; wlog $\lambda_2 = 0$. Then instead of (5.97f), translate the origin according to

$$x' \to x' - \frac{b_1'}{2\lambda_1}\,, \quad y' \to y' - \frac{c}{b_2'} + \frac{b_1'^2}{4\lambda_1 b_2'}\,, \tag{5.99}$$

assuming $b_2' \neq 0$, to obtain instead of (5.98b)

$$\lambda_1 {x'}^2 + b_2' y' = 0\,. \tag{5.100}$$

This is the equation of a *parabola* with principal axes coinciding with the x' and y' axes. Similar results to above hold for the scale, shape and orientation.

Remark. If $b_2' = 0$, the equation for the conic section can be reduced (after a translation) to $\lambda_1 x'^2 = k$ (cf. (5.98b)), with possible solutions of zero ($\lambda_1 k < 0$), one ($k = 0$) or two ($\lambda_1 k > 0$) lines.

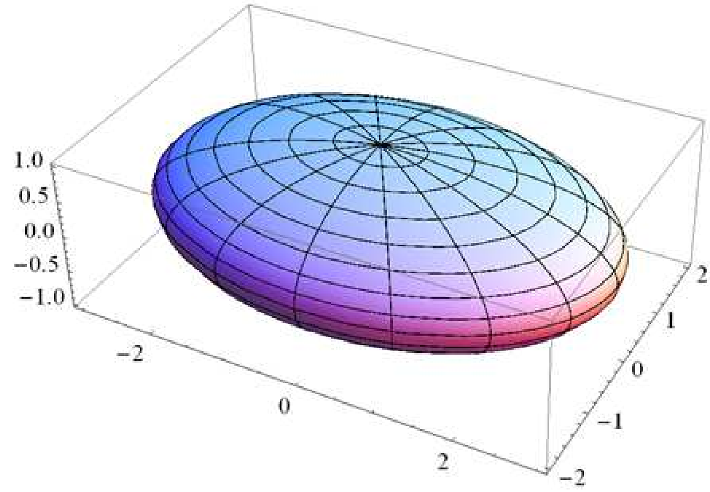

Figure 5.1: Ellipsoid ($\lambda_1 > 0$, $\lambda_2 > 0$, $\lambda_3 > 0$, $k > 0$); *Wikipedia.*

Three Dimensions. If $n = 3$ and Λ does not have a zero eigenvalue, then with

$$\mathsf{x}' = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} \quad \text{and} \quad \Lambda = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}, \tag{5.101a}$$

(5.97g) becomes

$$\lambda_1 x'^2 + \lambda_2 y'^2 + \lambda_3 z'^2 = k\,. \tag{5.101b}$$

When $\lambda_i k > 0$,

$$\text{the distance to surface along the } i\text{th principal axes} = \sqrt{\frac{k}{\lambda_i}}\,. \tag{5.101c}$$

Analogously to the case of two dimensions, this equation describes a number of characteristic surfaces.

Coefficients	**Quadric Surface**
$\lambda_1 > 0,\ \lambda_2 > 0,\ \lambda_3 > 0,\ k > 0.$	*Ellipsoid*: this includes the case of metric matrices, since S is then positive definite and the λ_i are all positive.
$\lambda_1 = \lambda_2.$	*Surface of revolution* about the z' axis.
$\lambda_1 = \lambda_2 > 0,\ \lambda_3 > 0,\ k > 0.$	*Spheroid*: the surface is a *prolate spheroid* if $\lambda_1 = \lambda_2 > \lambda_3$ and an *oblate spheroid* if $\lambda_1 = \lambda_2 < \lambda_3$.
$\lambda_1 = \lambda_2 = \lambda_3 > 0,\ k > 0.$	*Sphere.*
$\lambda_3 = 0.$	*Cylinder.*
$\lambda_1 > 0,\ \lambda_2 > 0,\ \lambda_3 = 0,\ k > 0.$	*Elliptic cylinder.*
$\lambda_1 > 0,\ \lambda_2 > 0,\ \lambda_3 < 0,\ k > 0.$	*Hyperboloid of one sheet.*
$\lambda_1 > 0,\ \lambda_2 > 0,\ \lambda_3 < 0,\ k = 0.$	*Elliptical conical surface.*
$\lambda_1 > 0,\ \lambda_2 < 0,\ \lambda_3 < 0,\ k > 0.$	*Hyperboloid of two sheets.*
15/02 $\lambda_1 > 0,\ \lambda_2 = \lambda_3 = 0,\ \lambda_1 k \geqslant 0.$	Planes $x' = \pm\sqrt{\frac{k}{\lambda_1}}$.

5.8.3 The Stationary Properties of the Eigenvalues

Suppose that we have an orthonormal basis, and let x be a point on $\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} = k$ where k is a constant. Then from (5.82) the distance squared from the origin to the quadric surface is $\mathsf{x}^{\mathrm{T}}\mathsf{x}$. This distance naturally depends on the value of k, i.e. the scale of the surface. This dependence on k can be removed by considering the square of the *relative* distance to the surface, i.e.

$$(\text{relative distance to surface})^2 = \frac{\mathsf{x}^{\mathrm{T}}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}}\,. \tag{5.102}$$

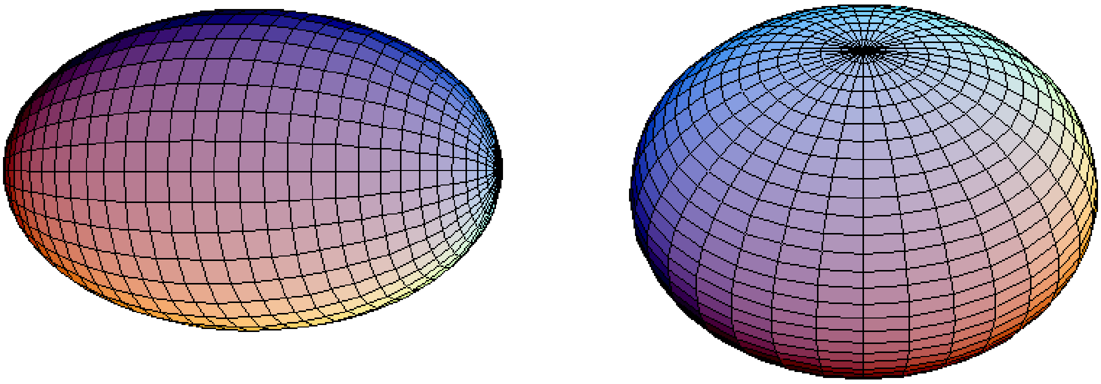

Figure 5.2: Prolate spheroid ($\lambda_1 = \lambda_2 > \lambda_3 > 0$, $k > 0$) and oblate spheroid ($0 < \lambda_1 = \lambda_2 < \lambda_3$, $k > 0$); *Wikipedia.*

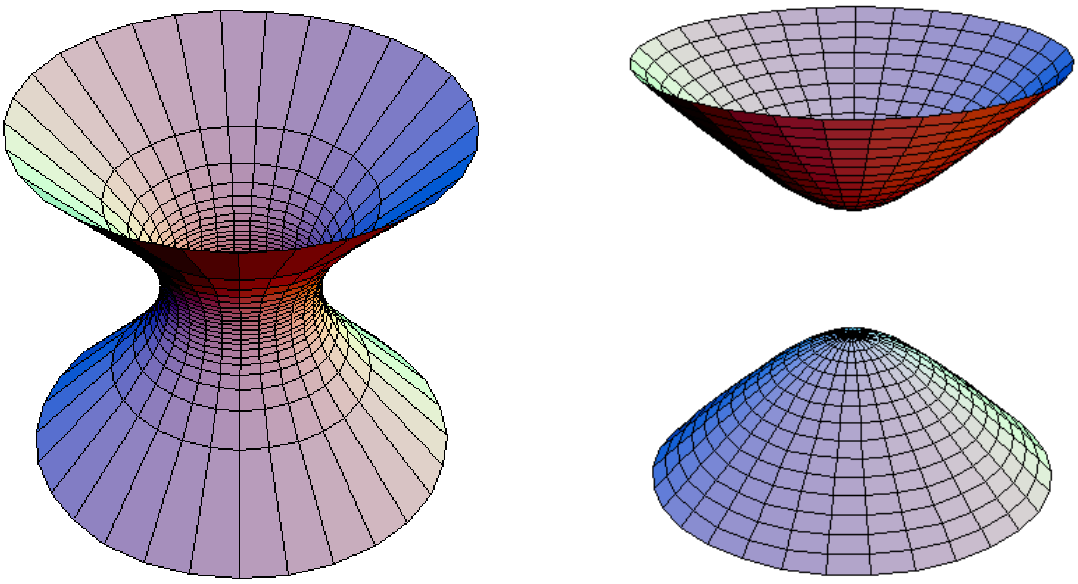

Figure 5.3: Hyperboloid of one sheet ($\lambda_1 > 0$, $\lambda_2 > 0$, $\lambda_3 < 0$, $k > 0$) and hyperboloid of two sheets ($\lambda_1 > 0$, $\lambda_2 < 0$, $\lambda_3 < 0$, $k > 0$); *Wikipedia.*

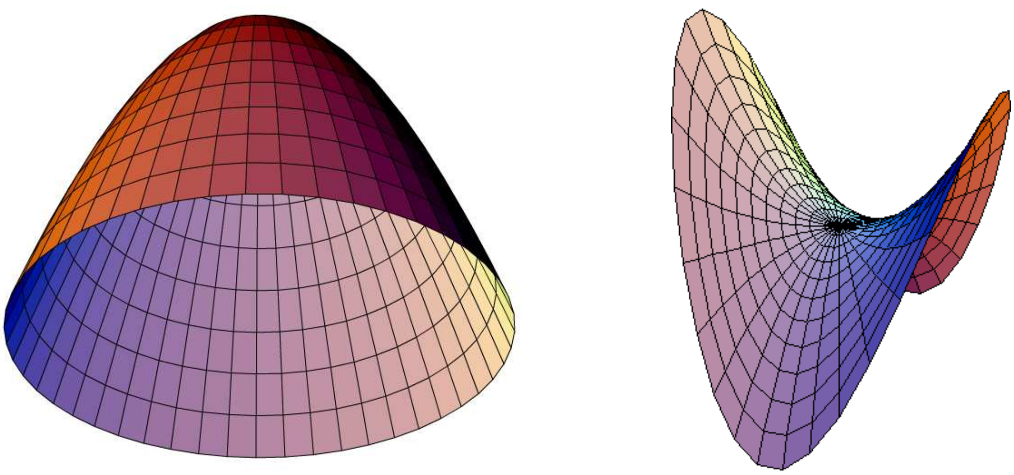

Figure 5.4: Paraboloid of revolution ($\lambda_1 x'^2 + \lambda_2 y'^2 + z' = 0$, $\lambda_1 > 0$, $\lambda_2 > 0$) and hyperbolic paraboloid ($\lambda_1 x'^2 + \lambda_2 y'^2 + z' = 0$, $\lambda_1 < 0$, $\lambda_2 > 0$); *Wikipedia.*

Let us consider the directions for which this relative distance, or equivalently its inverse (referred to as the *Rayleigh quotient*)

$$\lambda(\mathsf{x}) = \frac{\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\,, \tag{5.103}$$

is *stationary*. We can find the so-called *first variation* in $\lambda(\mathsf{x})$ by letting

$$\mathsf{x} \to \mathsf{x} + \delta\mathsf{x} \quad \text{and} \quad \mathsf{x}^{\mathrm{T}} \to \mathsf{x}^{\mathrm{T}} + \delta\mathsf{x}^{\mathrm{T}}\,, \tag{5.104}$$

by performing a Taylor expansion, and by ignoring terms quadratic or higher in $|\delta\mathsf{x}|$. First note that

$$\begin{aligned}(\mathsf{x}^{\mathrm{T}} + \delta\mathsf{x}^{\mathrm{T}})(\mathsf{x} + \delta\mathsf{x}) &= \mathsf{x}^{\mathrm{T}}\mathsf{x} + \mathsf{x}^{\mathrm{T}}\delta\mathsf{x} + \delta\mathsf{x}^{\mathrm{T}}\mathsf{x} + \dots \\ &= \mathsf{x}^{\mathrm{T}}\mathsf{x} + 2\delta\mathsf{x}^{\mathrm{T}}\mathsf{x} + \dots\,. \qquad \text{since the transpose of a scalar is itself}\end{aligned}$$

Hence

$$\begin{aligned}\frac{1}{(\mathsf{x}^{\mathrm{T}} + \delta\mathsf{x}^{\mathrm{T}})(\mathsf{x} + \delta\mathsf{x})} &= \frac{1}{\mathsf{x}^{\mathrm{T}}\mathsf{x} + 2\delta\mathsf{x}^{\mathrm{T}}\mathsf{x} + \dots} \\ &= \frac{1}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\left(1 + \frac{2\delta\mathsf{x}^{\mathrm{T}}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} + \dots\right)^{-1} \\ &= \frac{1}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\left(1 - \frac{2\delta\mathsf{x}^{\mathrm{T}}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} + \dots\right)\,.\end{aligned}$$

Similarly

$$\begin{aligned}(\mathsf{x}^{\mathrm{T}} + \delta\mathsf{x}^{\mathrm{T}})\mathsf{S}(\mathsf{x} + \delta\mathsf{x}) &= \mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + \mathsf{x}^{\mathrm{T}}\mathsf{S}\delta\mathsf{x} + \delta\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + \dots \\ &= \mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + 2\delta\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + \dots\,. \qquad \text{since } \mathsf{S}^{\mathrm{T}} = \mathsf{S}\end{aligned}$$

Putting the above results together we have that

$$\begin{aligned}\delta\lambda(\mathsf{x}) \equiv \lambda(\mathsf{x} + \delta\mathsf{x}) - \lambda(\mathsf{x}) &= \frac{(\mathsf{x}^{\mathrm{T}} + \delta\mathsf{x}^{\mathrm{T}})\mathsf{S}(\mathsf{x} + \delta\mathsf{x})}{(\mathsf{x}^{\mathrm{T}} + \delta\mathsf{x}^{\mathrm{T}})(\mathsf{x} + \delta\mathsf{x})} - \frac{\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} \\ &= \frac{\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + 2\delta\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + \dots}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\left(1 - \frac{2\delta\mathsf{x}^{\mathrm{T}}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} + \dots\right) - \frac{\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} \\ &= \frac{2\delta\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} - \frac{\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\,\frac{2\delta\mathsf{x}^{\mathrm{T}}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} + \dots \\ &= \frac{2}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\left(\delta\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} - \lambda(\mathsf{x})\delta\mathsf{x}^{\mathrm{T}}\mathsf{x}\right) \\ &= \frac{2}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\,\delta\mathsf{x}^{\mathrm{T}}\left(\mathsf{S}\mathsf{x} - \lambda(\mathsf{x})\mathsf{x}\right)\,.\end{aligned} \tag{5.105}$$

The Rayleigh-Ritz variational principle. Hence the first variation of $\lambda(\mathsf{x})$ is zero for all possible $\delta\mathsf{x}$ when

$$\mathsf{S}\mathsf{x} = \lambda(\mathsf{x})\mathsf{x}\,, \tag{5.106}$$

i.e. when x is an eigenvector of S and λ is the associated eigenvalue. So the eigenvectors of S are the directions which make the relative distance (5.102) stationary, and the eigenvalues are the values of (5.103) at the stationary points.

By a similar argument one can show that the eigenvalues of an Hermitian matrix, H, are the values of the function

$$\lambda(\mathsf{x}) = \frac{\mathsf{x}^{\dagger}\mathsf{H}\mathsf{x}}{\mathsf{x}^{\dagger}\mathsf{x}} \tag{5.107}$$

18/22 at its stationary points.

6 Elementary Analysis

6.0 Why Study This?

Analysis is one of the foundations upon which mathematics is built. It is the careful study of infinite processes such as limits, convergence, continuity, differential and integral calculus. This section covers some of the basic concepts including the important problem of the convergence of infinite series, since you need to have an idea of when, and when not, you can sum a series, e.g. a Fourier series.

We also discuss the remarkable properties of analytic functions of a complex variable.

6.1 Sequences and Limits

6.1.1 Sequences

A *sequence* is a set of of real or complex numbers, s_n, defined for all integers $n \geqslant n_0$ and occurring in order. If the sequence is unending we have an *infinite sequence*.

Example. If the nth term of a sequence is $s_n = \frac{1}{n}$, the sequence is

$$1, \tfrac{1}{2}, \tfrac{1}{3}, \tfrac{1}{4}, \ldots . \tag{6.1}$$

6.1.2 Sequences tending to a limit, or not.

Possible behaviours of the s_n as n increases are:

(i) s_n tends towards a particular value;

(ii) s_n does not tend to any value but remains limited in magnitude;

(iii) s_n is unlimited in magnitude.

Sequences tending to a finite limit. A sequence, s_n, is said to tend to the *limit* s if, given any positive ε, there exists $N \equiv N(\varepsilon)$ such that

$$|s_n - s| < \varepsilon \quad \text{for all} \quad n > N\,. \tag{6.2a}$$

In other words *the members of the sequence are eventually contained within an arbitrarily small disk centred on s*. We write this as

$$\lim_{n\to\infty} s_n = s \qquad \text{or as} \qquad s_n \to s \quad \text{as } n \to \infty \tag{6.2b}$$

Examples.

(i) Suppose $s_n = n^{-\alpha}$ for any $\alpha > 0$. Given $0 < \varepsilon < 1$ it follows that

$$|n^{-\alpha} - 0| < \varepsilon \qquad \text{for all} \qquad n > N(\varepsilon) = \left(\frac{1}{\varepsilon}\right)^{\frac{1}{\alpha}}. \tag{6.3a}$$

Hence

$$\lim_{n\to\infty} n^{-\alpha} = 0 \qquad \text{for any } \alpha > 0. \tag{6.3b}$$

(ii) Suppose $s_n = x^n$ with $|x| < 1$. Given $0 < \varepsilon < 1$ let $N(\varepsilon)$ be the smallest integer such that, for a given x,

$$N > \frac{\log 1/\varepsilon}{\log 1/|x|}\,. \tag{6.4a}$$

Then, if $n > N$,

$$|s_n - 0| = |x|^n < |x|^N < \varepsilon\,. \tag{6.4b}$$

Hence

$$\lim_{n\to\infty} x^n = 0\,. \tag{6.4c}$$

Cauchy's principle of convergence. A necessary and sufficient condition for the sequence s_n to converge is that, for any positive number ε, $|s_{n+m} - s_n| < \varepsilon$ for all positive integers m, for sufficiently large n. This condition does not require a knowledge of the value of the limit s.

Bounded sequences. If s_n does not tend to a limit it may nevertheless be *bounded*.

Definition. The sequence s_n is bounded as $n \to \infty$ if there exists a positive number K such that $|s_n| < K$ for sufficiently large n.

Example. Suppose

$$s_n = \left(\frac{n+1}{n}\right) \mathrm{e}^{in\alpha} . \tag{6.5a}$$

Then for all $n \geqslant 2$

$$|s_n| = \frac{n+1}{n} < 2 . \tag{6.5b}$$

We conclude that the sequence s_n is bounded.

Property. An increasing sequence tends either to a limit or to $+\infty$. Hence a bounded increasing sequence tends to a limit, i.e. if

$$s_{n+1} > s_n \,, \quad \text{and} \quad s_n < \mathcal{K} \in \mathbb{R} \quad \text{for all } n \text{, then} \quad s = \lim_{n\to\infty} s_n \quad \text{exists.} \tag{6.6}$$

Remark. You really ought to have a proof of this property, but I do not have time.[22]

Sequences tending to infinity. A sequence, s_n, is said to tend to infinity if given any A (however large), there exists $N \equiv N(A)$ such that

$$s_n > A \quad \text{for all} \quad n > N . \tag{6.7a}$$

We then write

$$s_n \to \infty \quad \text{as} \quad n \to \infty . \tag{6.7b}$$

Similarly we say that $s_n \to -\infty$ as $n \to \infty$ if given any A (however large), there exists $N \equiv N(A)$ such that

$$s_n < -A \quad \text{for all} \quad n > N . \tag{6.7c}$$

Oscillating sequences. If a sequence does not tend to a limit or $\pm\infty$, then s_n is said to *oscillate*. If s_n oscillates and is bounded, it *oscillates finitely*, otherwise it *oscillates infinitely*.

6.2 Convergence of Infinite Series

6.2.1 Convergent and divergent series

The section is concerned with the meaning of an infinite series such as

$$\sum_{r=r_0}^{\infty} u_r \tag{6.8}$$

involving the addition of an infinite number of terms.

Definition: Partial sum. Given an infinite sequence of numbers $u_1, u_2, \ldots$, define the *partial sum* s_n by

$$s_n = \sum_{r=r_0}^{n} u_r . \tag{6.9}$$

Definition: Convergent series. If as $n \to \infty$, s_n tends to a finite limit, s, then we say that the infinite series

$$\sum_{r=r_0}^{\infty} u_r \,, \tag{6.10}$$

converges (or is convergent), and that s is its sum.

[22] Alternatively you can view this property as an axiom that specifies the real numbers $\mathbb{R}$ essentially uniquely.

Definition: Divergent series. An infinite series which is not convergent is called *divergent*.

Remarks.

(i) Whether a series converges or diverges does not depend on the value of r_0 (i.e. on when the series begins) but only on the behaviour of the terms for large r.

(ii) According to Cauchy's principle of convergence, a necessary and sufficient condition for $\sum u_r$ to converge is that, for any positive number ε,

$$|s_{n+m} - s_n| = |u_{n+1} + u_{n+2} + \cdots + u_{n+m}| < \varepsilon \tag{6.11}$$

for all positive integers m, for sufficiently large n.

Example: the convergence of a geometric series. The series

$$\sum_{r=0}^{\infty} z^r = 1 + z + z^2 + z^3 + \dots\,, \tag{6.12a}$$

converges to $(1-z)^{-1}$ provided that $|z| < 1$.

Proof. Consider the partial sum

$$s_n = 1 + z + \cdots + z^{n-1} = \frac{1-z^n}{1-z}\,. \tag{6.12b}$$

If $|z| < 1$, then from (6.4c) we have that $z^n \to 0$ as $n \to \infty$, and hence

$$s = \lim_{n\to\infty} s_n = \frac{1}{1-z} \quad \text{for } |z| < 1. \tag{6.12c}$$

However if $|z| \geqslant 1$ the series diverges.

Example: the divergence of the harmonic series. The *harmonic series*, for which $u_r = r^{-1}$, diverges.

Proof. Consider the partial sum

$$s_n = \sum_{r=1}^{n} \frac{1}{r} = 1 + \tfrac{1}{2} + \tfrac{1}{3} \cdots + \tfrac{1}{n}\,. \tag{6.13a}$$

Then

$$s_n > \int_1^{n+1} \frac{\mathrm{d}x}{x} = \ln(n+1)\,. \tag{6.13b}$$

Therefore s_n increases without bound and does not tend to a limit as $n \to \infty$.

Alternative Proof. Consider s_{2^m} where m is an integer. First we note that

$$\begin{aligned}
m = 1: &\quad s_2 = 1 + \tfrac{1}{2} \\
m = 2: &\quad s_4 = s_2 + \tfrac{1}{3} + \tfrac{1}{4} > s_2 + \tfrac{1}{4} + \tfrac{1}{4} = 1 + \tfrac{1}{2} + \tfrac{1}{2} \\
m = 3: &\quad s_8 = s_4 + \tfrac{1}{5} + \tfrac{1}{6} + \tfrac{1}{7} + \tfrac{1}{8} > s_4 + \tfrac{1}{8} + \tfrac{1}{8} + \tfrac{1}{8} + \tfrac{1}{8} > 1 + \tfrac{1}{2} + \tfrac{1}{2} + \tfrac{1}{2}\,.
\end{aligned}$$

Similarly we can show that (e.g. by induction)

$$s_{2^m} > 1 + \tfrac{m}{2}\,, \tag{6.13c}$$

and hence the series is divergent.

6.2.2 A necessary condition for convergence

A *necessary* condition for s to converge is that $u_r \to 0$ as $r \to \infty$.

Proof. Using the fact that $u_r = s_r - s_{r-1}$ we have that

$$\lim_{r\to\infty} u_r = \lim_{r\to\infty} (s_r - s_{r-1}) = \lim_{r\to\infty} s_r - \lim_{r\to\infty} s_{r-1} = s - s = 0\,. \tag{6.14}$$

Remark. However, as illustrated by the harmonic series (see (6.13a), (6.13b) and (6.13c)), $u_r \to 0$ as $r \to \infty$ is *not* a sufficient condition for convergence.

6.2.3 Absolute and conditional convergence

Definition: Absolute convergence. A series $\sum u_r$ is said to *converge absolutely* if

$$\sum_{r=1}^{\infty} |u_r| \tag{6.15}$$

converges.

Property. If $\sum |u_r|$ converges, then $\sum u_r$ also converges.

Proof. If $\sum |u_r|$ converges then, for any positive number ε,

$$|u_{n+1}| + |u_{n+2}| + \cdots + |u_{n+m}| < \varepsilon \tag{6.16a}$$

for all positive integers m, for sufficiently large n. But then

$$\begin{aligned} |u_{n+1} + u_{n+2} + \cdots + u_{n+m}| &\leqslant |u_{n+1}| + |u_{n+2}| + \cdots + |u_{n+m}| \\ &< \varepsilon\,, \end{aligned} \tag{6.16b}$$

and so $\sum u_r$ also converges.

Definition: Conditional convergence. If $\sum |u_r|$ diverges, then $\sum u_r$ may or may not converge. If $\sum u_r$ does converge, it is said to converge *conditionally.*

Example. Suppose that

$$u_r = (-1)^{r-1}\frac{1}{r} \quad \text{so that} \quad s_n = \sum_{r=1}^{n} (-1)^{r-1}\frac{1}{r} = 1 - \tfrac{1}{2} + \tfrac{1}{3} \cdots + (-1)^{n-1}\tfrac{1}{n}\,. \tag{6.17a}$$

Then, from the Taylor expansion

$$\log(1+x) = -\sum_{r=1}^{\infty} \frac{(-x)^r}{r}\,, \tag{6.17b}$$

we spot that $s = \lim_{n\to\infty} s_n = \log 2$; hence $\sum_{r=1}^{\infty} u_r$ converges. However, from (6.13a), (6.13b) and (6.13c) we already know that $\sum_{r=1}^{\infty} |u_r|$ diverges. Hence $\sum_{r=1}^{\infty} u_r$ is conditionally convergent.

6.3 Tests of Convergence

6.3.1 The comparison test

This test applies to series of non-negative real numbers.

Statement. Suppose that we are given that $v_r > 0$ and that $S = \sum_{r=1}^{\infty} v_r$ is convergent. Suppose also that

$$0 < u_r < \mathcal{K} v_r \tag{6.18a}$$

for some $\mathcal{K}$ independent of r. Then the infinite series

$$\sum_{r=1}^{\infty} u_r \tag{6.18b}$$

is also convergent.

Proof. Since $u_r > 0$, $s_n = \sum_{r=1}^{n} u_r$ is an increasing sequence. Further

$$s_n = \sum_{r=1}^{n} u_r < \mathcal{K} \sum_{r=1}^{n} v_r\,, \tag{6.19a}$$

and thus

$$\lim_{n\to\infty} s_n < \mathcal{K} \sum_{r=1}^{\infty} v_r = \mathcal{K}\, S\,, \tag{6.19b}$$

16/01 16/02 i.e. s_n is an increasing bounded sequence. Thence from (6.6), $\sum_{r=1}^{\infty} u_r$ is convergent.

16/03 16/04 *Remark.* Similarly if $\sum_{r=1}^{\infty} v_r$ diverges, $v_r > 0$ and $u_r > \mathcal{K} v_r$ for some $\mathcal{K}$ independent of r, then $\sum_{r=1}^{\infty} u_r$ diverges.

6.3.2 D'Alembert's ratio test

This uses a comparison between a given series $\sum u_r$ of complex terms and a geometric series $\sum v_r = \sum \varrho^r$, where $\varrho > 0$.

D'Alembert's ratio test. We start by supposing that the u_r are real and positive, i.e. $u_r > 0$. Define the *ratio of successive terms* to be

$$\varrho_r = \frac{u_{r+1}}{u_r}\,, \tag{6.20a}$$

and suppose that ϱ_r tends to a limit ϱ as $r \to \infty$, i.e.

$$\lim_{r\to\infty} \frac{u_{r+1}}{u_r} = \varrho\,. \tag{6.20b}$$

Then $\sum u_r$ converges if $\varrho < 1$ and diverges if $\varrho > 1$.

Proof.

$\varrho < 1$. For the case $\varrho < 1$, choose σ with $\varrho < \sigma < 1$. Then there exists $N \equiv N(\sigma)$ such that

$$\frac{u_{r+1}}{u_r} < \sigma \quad \text{for all} \quad r > N\,. \tag{6.21a}$$

It follows that

$$\begin{aligned}
\sum_{r=1}^{\infty} u_r &= \sum_{r=1}^{N} u_r + u_{N+1}\left\{1 + \frac{u_{N+2}}{u_{N+1}} + \frac{u_{N+2}}{u_{N+1}}\frac{u_{N+3}}{u_{N+2}} + \dots\right\} \\
&< \sum_{r=1}^{N} u_r + u_{N+1}(1 + \sigma + \sigma^2 + \dots) && \text{by hypothesis} \\
&< \sum_{r=1}^{N} u_r + \frac{u_{N+1}}{1-\sigma} && \text{by (6.12c) since } \sigma < 1.
\end{aligned} \tag{6.21b}$$

We conclude that $\sum_{r=1}^{\infty} u_r$ is bounded. Thence, since $s_n = \sum_{r=1}^{n} u_r$ is an increasing sequence, it follows from (6.6) that $\sum u_r$ converges.

$\varrho > 1$. For the case $\varrho > 1$, choose τ with $1 < \tau < \varrho$. Then there exists $M \equiv M(\tau)$ such that

$$\frac{u_{r+1}}{u_r} > \tau > 1 \quad \text{for all} \quad r > M\,, \tag{6.22a}$$

and hence

$$\frac{u_r}{u_M} > \tau^{r-M} > 1 \quad \text{for all} \quad r > M\,. \tag{6.22b}$$

Thus, since $u_r \not\to 0$ as $r \to \infty$, we conclude that $\sum u_r$ diverges.

Corollary. A series $\sum u_r$ of complex terms converges if the limit of the *absolute ratio of successive terms* is less than one, i.e. if

$$\lim_{r\to\infty} \left|\frac{u_{r+1}}{u_r}\right| = \varrho < 1\,. \tag{6.23}$$

Proof. D'Alembert's ratio test shows that $\sum u_r$ converges absolutely, thence from § 6.2.3 we conclude that $\sum u_r$ converges.

Example. For the harmonic series $\sum r^{-1}$,

$$\varrho_r = \frac{r}{r+1} \to 1 \quad \text{as } r \to \infty\,, \tag{6.24}$$

from which nothing can be concluded. A different test is required, such as the integral comparison test.

Remark. The ratio test can not be used for series in which some of the terms are zero. However, it can
19/22 sometimes be adapted by relabelling the series to remove the vanishing terms.

6.3.3 Cauchy's test

Suppose that $u_r > 0$ and that

$$\lim_{r\to\infty} u_r^{1/r} = \varrho\,. \tag{6.25}$$

Then $\sum u_r$ converges if $\varrho < 1$, while $\sum u_r$ diverges if $\varrho > 1$.

Proof. First suppose that $\varrho < 1$. Choose σ with $\varrho < \sigma < 1$. Then there exists $N \equiv N(\sigma)$ such that

$$u_r^{1/r} < \sigma\,, \quad \text{i.e.} \quad u_r < \sigma^r \quad \text{for all} \quad r > N\,. \tag{6.26a}$$

It follows that

$$\sum_{r=1}^{\infty} u_r < \sum_{r=1}^{N} u_r + \sum_{r=N+1}^{\infty} \sigma^r\,. \tag{6.26b}$$

We conclude that $\sum_{r=1}^{\infty} u_r$ is bounded (since $\sigma < 1$). Moreover $s_n = \sum_{r=1}^{n} u_r$ is an increasing sequence, and hence from (6.6) we conclude that $\sum u_r$ converges.

Next suppose that $\varrho > 1$. Choose τ with $1 < \tau < \varrho$. Then there exists $M \equiv M(\tau)$ such that

$$u_r^{1/r} > \tau > 1\,, \quad \text{i.e.} \quad u_r > \tau^r > 1\,, \quad \text{for all} \quad r > M\,. \tag{6.26c}$$

Thus, since $u_r \not\to 0$ as $r \to \infty$, $\sum u_r$ must diverge.

6.4 Functions of a Continuous Variable

6.4.1 Limits and continuity

Building on the ideas introduced in § 6.1.2 on sequences tending to a limit, in this section we consider how a real or complex function $f(z)$ of a real or complex variable z behaves near a point z_0.

Definition: Limit at a point $z = z_0$. The function $f(z)$ tends to the limit L as $z \to z_0$ if, for any positive number ε, there exists a positive number δ, depending on ε, such that $|f(z) - L| < \varepsilon$ for all z such that $|z - z_0| < \delta$.

We write this as

$$\lim_{z\to z_0} f(z) = L \qquad \text{or} \qquad f(z) \to L \quad \text{as } z \to z_0\,. \tag{6.27a}$$

Remark. The value of L would normally be $f(z_0)$. However, cases such as

$$\lim_{z\to 0} \frac{\sin z}{z} = 1\,. \tag{6.27b}$$

must be expressed as limits because $\sin 0/0 = 0/0$ is indeterminate.

Definition: Continuity at a point $z = z_0$. The function $f(z)$ is continuous at the point $z = z_0$ if $f(z) \to f(z_0)$ as $z \to z_0$.

Definition: Bounded at a point $z = z_0$. The function $f(z)$ is bounded as $z \to z_0$ if there exist positive numbers $\mathcal{K}$ and δ such that $|f(z)| < \mathcal{K}$ for all z with $|z - z_0| < \delta$.

Definition: Limit as $z \to \infty$. The function $f(z)$ tends to the limit L as $z \to \infty$ if, for any positive number ε, there exists a positive number R, depending on ε, such that $|f(z) - L| < \varepsilon$ for all z with $|z| > R$. We write this as

$$\lim_{z\to\infty} f(z) = L \qquad \text{or} \qquad f(z) \to L \quad \text{as } z \to \infty\,. \tag{6.28}$$

Definition: Bounded as $z \to \infty$. The function $f(z)$ is bounded as $z \to \infty$ if there exist positive numbers $\mathcal{K}$ and R such that $|f(z)| < \mathcal{K}$ for all z with $|z| > R$.

Warning: approaches to a point. There are different ways in which z can approach z_0 or ∞, especially in the complex plane. Sometimes the limit or bound applies only if the point is approached in a particular way. For example, consider $\tanh(z)$ as $|z| \to \infty$ for z real:

$$\lim_{z\to+\infty} \tanh z = 1, \qquad \lim_{z\to-\infty} \tanh z = -1 \tag{6.29a}$$

This notation implies that z is approaching positive or negative real infinity along the real axis. But if z approaches infinity along the imaginary axis, i.e. $z \to \pm i\infty$, the limit of tanh is not defined.

Remark. In the context of real variables, $x \to \infty$ usually means specifically $x \to +\infty$. A related notation for one-sided limits is exemplified by

$$\lim_{x\to 0^+} \frac{x(1+x)}{|x|} = 1, \qquad \lim_{x\to 0^-} \frac{x(1+x)}{|x|} = -1 \tag{6.29b}$$

6.4.2 The O notation

The symbols O, o and $\sim$ are often used to compare the rates of growth or decay of different functions.

Suppose that $f(z)$ and $g(z)$ are functions of z, then

(i) if $\dfrac{f(z)}{g(z)}$ is bounded as $z \to z_0$, we say that $f(z) = O(g(z))$ as $z \to z_0$;

(ii) if $\dfrac{f(z)}{g(z)} \to 0$ as $z \to z_0$, we say that $f(z) = o(g(z))$ as $z \to z_0$;

(iii) if $\dfrac{f(z)}{g(z)} \to 1$ as $z \to z_0$, we say that $f(z) \sim g(z)$ as $z \to z_0$.

Remarks.

(i) These definitions continue to apply when $z_0 = \infty$.

(ii) $f(z) = O(1)$ means that $f(z)$ is bounded.

(iii) Either $f(z) = o(g(z))$ or $f(z) \sim g(z)$ implies $f(z) = O(g(z))$.

(iv) Only $f(z) \sim g(z)$ is a symmetric relation (so should *not* be written as $f(z) \to g(z)$).

(v) If $f(z) \sim g(z)$ we say that f is *asymptotically equal* to g.

(vi) The O notation is often used in conjunction with truncated Taylor series, e.g. for small $(z - z_0)$

$$f(z) = f(z_0) + (z - z_0)f'(z_0) + \tfrac{1}{2}(z - z_0)^2 f''(z_0) + O((z - z_0)^3)\,. \tag{6.30}$$

Examples.

(i) As $z \to 0$ we have that

$$\begin{aligned}
2\sin z &= O(1) && \text{since } 2\sin z/1 \text{ is bounded as } z \to 0;\\
2\sin z &= o(1) && \text{since } 2\sin z/1 \to 0 \text{ as } z \to 0;\\
2\sin z &= O(z) && \text{since } 2\sin z/z \text{ is bounded as } z \to 0;\\
\sin z &\sim z && \text{since } \sin z/z \to 1 \text{ as } z \to 0.
\end{aligned}$$

(ii) As $x \to +\infty$ we have that

$$\begin{aligned}
\ln x &= o(x) && \text{since } \ln x/x \to 0 \text{ as } x \to +\infty;\\
\cosh x &\sim \tfrac{1}{2}\mathrm{e}^x && \text{since } 2\cosh x/\mathrm{e}^x \to 1 \text{ as } x \to +\infty.
\end{aligned}$$

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6.5 Taylor's Theorem for Functions of a Real Variable

Let $f(x)$ be a (real or complex) function of a real variable x, which is differentiable at least n times in the interval $x_0 \leqslant x \leqslant x_0 + h$. Then the *Taylor series* of $f(x_0 + h)$ is given by

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \ldots + \frac{h^{n-1}}{(n-1)!}f^{(n-1)}(x_0) + R_n\,, \tag{6.31a}$$

where the remainder after n terms, R_n, can be shewn to be (by integrating by parts)

$$R_n = \int_{x_0}^{x_0+h} \frac{(x_0 + h - x)^{n-1}}{(n-1)!} f^{(n)}(x)\,\mathrm{d}x\,. \tag{6.31b}$$

Alternative forms of the remainder. The remainder term can be expressed in alternative ways. Lagrange's expression for the remainder is

$$R_n = \frac{h^n}{n!} f^{(n)}(\xi) \tag{6.32a}$$

where ξ is an unknown number in the interval $x_0 < \xi < x_0 + h$. It follows that

$$R_n = O(h^n)\,. \tag{6.32b}$$

Smooth functions. If $f(x)$ is a *smooth* function, i.e. if $f(x)$ is infinitely differentiable in $x_0 \leqslant x \leqslant x_0 + h$, we can write (6.31a) as an infinite Taylor series:

$$f(x_0 + h) = \sum_{n=0}^{\infty} \frac{h^n}{n!} f^{(n)}(x_0)\,. \tag{6.33}$$

This *power series* in h converges for sufficiently small h (see § 6.8)

6.6 Analytic Functions of a Complex Variable

6.6.1 Complex differentiability

Definition: Complex differentiability. The complex derivative of the function $f(z)$ at the point $z = z_0$ is defined as

$$f'(z_0) = \lim_{z \to z_0} \frac{f(z) - f(z_0)}{z - z_0}\,, \tag{6.34a}$$

where the same limit must be obtained for any sequence of complex values for z that tends to z_0. If this same limit exists, the function $f(z)$ is said to be complex differentiable at $z = z_0$.

Alternative expression. Another way to write this is

$$\frac{df}{dz} \equiv f'(z) = \lim_{\delta z \to 0} \frac{f(z + \delta z) - f(z)}{\delta z}\,, \tag{6.34b}$$

where the limit must be the same when $\delta z \to 0$ by any route/direction in the complex plane.

Remark. Requiring a function of a *complex* variable to be differentiable is a surprisingly strong constraint.

6.6.2 The Cauchy–Riemann equations

Express $f = u + \mathrm{i}v$ and $z = x + \mathrm{i}y$ in terms of their real and imaginary parts:

$$f(z) = u(x, y) + \mathrm{i}v(x, y) \tag{6.35}$$

If $f'(z)$ exists we can calculate it by assuming that $\delta z = \delta x + \mathrm{i}\,\delta y$ approaches 0 along the real axis, i.e. by taking $\delta y = 0$; then

$$\begin{aligned} f'(z) &= \lim_{\delta x \to 0} \frac{f(z + \delta x) - f(z)}{\delta x} \\ &= \lim_{\delta x \to 0} \frac{u(x + \delta x, y) + \mathrm{i}v(x + \delta x, y) - u(x, y) - \mathrm{i}v(x, y)}{\delta x} \\ &= \lim_{\delta x \to 0} \frac{u(x + \delta x, y) - u(x, y)}{\delta x} + \mathrm{i} \lim_{\delta x \to 0} \frac{v(x + \delta x, y) - v(x, y)}{\delta x} \\ &= \frac{\partial u}{\partial x} + \mathrm{i}\,\frac{\partial v}{\partial x}\,. \end{aligned} \tag{6.36a}$$

However, from definition (6.34a), the derivative must have the same value if δz approaches 0 along the imaginary axis, i.e. by taking $\delta x = 0$; then

$$\begin{aligned} f'(z) &= \lim_{\delta y \to 0} \frac{f(z + \mathrm{i}\,\delta y) - f(z)}{\mathrm{i}\,\delta y} \\ &= \lim_{\delta y \to 0} \frac{u(x, y + \delta y) + \mathrm{i}v(x, y + \delta y) - u(x, y) - \mathrm{i}v(x, y)}{\mathrm{i}\,\delta y} \\ &= -\mathrm{i} \lim_{\delta y \to 0} \frac{u(x, y + \delta y) - u(x, y)}{\delta y} + \lim_{\delta y \to 0} \frac{v(x, y + \delta y) - v(x, y)}{\delta y} \\ &= -\mathrm{i}\,\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}\,. \end{aligned} \tag{6.36b}$$

Comparing the real and imaginary parts of (6.36a) and (6.36b), we deduce the *Cauchy–Riemann equations*

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \qquad \frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y}\,. \tag{6.37}$$

These are necessary conditions for $f(z)$ to have a complex derivative. They are also sufficient conditions, provided that the partial derivatives are also continuous.

6.6.3 Analytic functions

Definition: Analytic function. If a function $f(z)$ has a complex derivative at every point z in a region $\mathcal{R}$ of the complex plane, it is said to be *analytic* in $\mathcal{R}$.[23]

Remark. To be analytic at a point $z = z_0$, $f(z)$ must be differentiable throughout some neighbourhood $|z - z_0| < \varepsilon$ of that point.

Definition: Entire function. An *entire function* is one that is analytic in the whole complex plane.

Examples of entire functions. Each of the following can be confirmed to satisfy the the Cauchy-Riemann equations (6.37) in the whole complex plane.

(i) $f(z) = c$: a complex constant.

(ii) $f(z) = z$: for which $u = x$ and $v = y$.

(iii) $f(z) = \exp(z)$: for which

$$f(z) = \mathrm{e}^z = \mathrm{e}^x\mathrm{e}^{\mathrm{i}y} = \mathrm{e}^x\cos y + \mathrm{i}\,\mathrm{e}^x \sin y = u + \mathrm{i}v\,. \tag{6.38a}$$

The Cauchy–Riemann equations are satisfied for all x and y since

$$\frac{\partial u}{\partial x} = \mathrm{e}^x\cos y = \frac{\partial v}{\partial y} \qquad \text{and} \qquad \frac{\partial v}{\partial x} = \mathrm{e}^x \sin y = -\frac{\partial u}{\partial y}\,. \tag{6.38b}$$

As expected the derivative of the exponential function is

$$f'(z) = \frac{\partial u}{\partial x} + \mathrm{i}\,\frac{\partial v}{\partial x} = \mathrm{e}^x\cos y + \mathrm{i}\,\mathrm{e}^x\sin y = \mathrm{e}^z\,. \tag{6.38c}$$

(iv) $f(z) = z^n$, where n is a positive integer: for which

$$x = r\cos\theta, \quad y = r\sin\theta, \quad u = r^n\cos n\theta \quad \text{and} \quad v = r^n \sin n\theta. \tag{6.39}$$

Properties.

(i) Sums, products and compositions of analytic functions are also analytic, e.g.

(a) $$f(z) = P(z) = c_n z^n + c_{n-1}z^{n-1} + \cdots + c_0 \qquad \text{where } c_r \in \mathbb{C}, \tag{6.40a}$$

(b) $$f(z) = z\exp(\mathrm{i}z^2) + z^3. \tag{6.40b}$$

(ii) The usual product, quotient and chain rules apply to complex derivatives of analytic functions, e.g.

$$\frac{\mathrm{d}}{\mathrm{d}z}z^n = nz^{n-1}, \qquad \frac{\mathrm{d}}{\mathrm{d}z}\sin z = \cos z, \qquad \frac{\mathrm{d}}{\mathrm{d}z}\cosh z = \sinh z\,. \tag{6.40c}$$

Definition: Singular points. Many complex functions are analytic everywhere in the complex plane except at isolated points, which are called the *singular points* or *singularities* of the function.

Examples.

(i) $f(z) = P(z)/Q(z)$, where $P(z)$ and $Q(z)$ are polynomials. This is called a *rational function* and is analytic *except* at points where $Q(z) = 0$.

(ii) $f(z) = z^c$ is analytic *except* at $z = 0$ if c is a complex constant which is not a positive integer (see (6.39) for the case when c is a positive integer).

(iii) $f(z) = \ln z$ is analytic *except* at $z = 0$.

The last two examples are in fact *multiple-valued functions*, which require special treatment (see next term).

[23] Some use this definition for *holomorphic* functions and use *analytic* for functions with a convergent power series. However, in complex analysis holomorphic functions are analytic and vice versa.

Examples of non-analytic functions.

(i) $f(z) = \operatorname{Re}(z)$, for which $u = x$ and $v = 0$, so the Cauchy–Riemann equations are not satisfied anywhere.

(ii) $f(z) = z^*$, for which $u = x$ and $v = -y$.

(iii) $f(z) = |z|$, for which $u = (x^2 + y^2)^{1/2}$ and $v = 0$.

(iv) $f(z) = |z|^2$, for which $u = x^2 + y^2$ and $v = 0$.

Remark. In this case the Cauchy–Riemann equations are satisfied only at $x = y = 0$ and we can say that $f'(0) = 0$. However, $f(z)$ is not analytic even at $z = 0$ because it is not differentiable throughout any neighbourhood $|z| < \varepsilon$ of 0.

6.6.4 Consequences of the Cauchy–Riemann equations

If we know the real part of an analytic function in some region, we can find its imaginary part (or vice versa) up to an additive constant by integrating the Cauchy–Riemann equations.

Example. Suppose that you are given $u(x,y) = x^2 - y^2$, then what is the analytic function? From (6.37)

$$\frac{\partial v}{\partial y} = \frac{\partial u}{\partial x} = 2x \quad \Rightarrow \quad v = 2xy + g(x)\,, \tag{6.41a}$$

$$\frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y} = 2y \quad \Rightarrow \quad 2y + g'(x) = 2y \quad \Rightarrow \quad g'(x) = 0\,. \tag{6.41b}$$

Therefore $v(x,y) = 2xy + c$, where c is a real constant, and we find that

$$f(z) = x^2 - y^2 + \mathrm{i}(2xy + c) = (x + \mathrm{i}y)^2 + \mathrm{i}c = z^2 + \mathrm{i}c\,. \tag{6.41c}$$

Property: u and v are harmonic functions. The real and imaginary parts of an analytic function satisfy Laplace's equation (they are *harmonic functions*):

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} &= \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\partial u}{\partial y}\right)\\ &= \frac{\partial}{\partial x}\left(\frac{\partial v}{\partial y}\right) + \frac{\partial}{\partial y}\left(-\frac{\partial v}{\partial x}\right)\\ &= 0\end{aligned} \tag{6.42}$$

The proof that $\nabla^2 v = 0$ is similar.

Remark. This property provides a useful method for solving Laplace's equation in two dimensions: one "just" needs to find an analytic function that satisfies the boundary conditions.

Property: u and v are conjugate harmonic functions. Using the Cauchy–Riemann equations (6.37), we see that

$$\begin{aligned}\nabla u \cdot \nabla v &= \frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial v}{\partial y}\\ &= \frac{\partial v}{\partial y}\frac{\partial v}{\partial x} - \frac{\partial v}{\partial x}\frac{\partial v}{\partial y}\\ &= 0\,.\end{aligned} \tag{6.43}$$

20/22 Hence the curves of constant u and those of constant v are orthogonal: u and v are said to be *conjugate harmonic functions.*

6.6.5 Taylor series for analytic functions

If a function of a complex variable is analytic in a region $\mathcal{R}$ of the complex plane, not only is it differentiable everywhere in $\mathcal{R}$, it is also differentiable any number of times. It follows that if $f(z)$ is analytic at $z = z_0$, it has an infinite Taylor series

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n, \quad \text{where} \quad a_n = \frac{1}{n!} f^{(n)}(z_0) \equiv \frac{1}{n!}\frac{\mathrm{d}^n f}{\mathrm{d}z^n}(z_0)\,. \tag{6.44}$$

As discussed in § 6.8, this series converges within some neighbourhood of z_0.

Alternative definition of analyticity. An alternative definition of the analyticity of a function $f(z)$ at $z = z_0$ is that $f(z)$ has a Taylor series expansion about $z = z_0$ with a *non-zero radius of convergence.*

6.7 Zeros, Poles and Essential Singularities

6.7.1 Zeros of complex functions

Definition: Order. The zeros of $f(z)$ are the points $z = z_0$ in the complex plane where $f(z_0) = 0$. A zero is of order N if

$$f(z_0) = f'(z_0) = f''(z_0) = \cdots = f^{(N-1)}(z_0) = 0 \qquad \text{but} \quad f^{(N)}(z_0) \neq 0 \tag{6.45a}$$

The first non-zero term in the Taylor series of $f(z)$ about $z = z_0$ is then proportional to $(z - z_0)^N$. Indeed

$$f(z) \sim a_N (z - z_0)^N \qquad \text{as} \quad z \to z_0 \tag{6.45b}$$

A *simple zero* is a zero of order 1. A *double zero* is one of order 2, etc.

Examples.

(i) $f(z) = z$ has a simple zero at $z = 0$.

(ii) $f(z) = (z - \mathrm{i})^2$ has a double zero at $z = \mathrm{i}$.

(iii) $f(z) = z^2 - 1 = (z - 1)(z + 1)$ has simple zeros at $z = \pm 1$.

Worked exercise. Find and classify the zeros of $f(z) = \sinh z$.

Answer.

$$\sinh z = \tfrac{1}{2}(\mathrm{e}^z - \mathrm{e}^{-z}) = 0$$

if

$$\mathrm{e}^z = \mathrm{e}^{-z} \quad \Rightarrow \quad \mathrm{e}^{2z} = 1 \quad \Rightarrow \quad z = n\pi\mathrm{i}, \quad n \in \mathbb{Z}\,.$$

Since $f'(z) = \cosh z = \cos(n\pi) \neq 0$ at these points, all the zeros are simple zeros.

6.7.2 Poles of complex functions

Definition: Order. Suppose $g(z)$ is analytic and non-zero at $z = z_0$. Consider the function

$$f(z) = (z - z_0)^{-N} g(z)\,, \tag{6.46a}$$

in which case

$$f(z) \sim g(z_0)(z - z_0)^{-N} \qquad \text{as} \quad z \to z_0\,. \tag{6.46b}$$

$f(z)$ is not analytic at $z = z_0$, and we say that $f(z)$ has a *pole of order* N. We refer to a pole of order 1 as a *simple pole*, a pole of order 2 as a *double pole*, etc.

Expansion of $f(z)$ near a pole. Because $g(z)$ is analytic, from (6.44) it has a Taylor series expansion at z_0:

$$g(z) = \sum_{n=0}^{\infty} b_n (z - z_0)^n \qquad \text{with} \quad b_0 \neq 0\,. \tag{6.47a}$$

Hence

$$f(z) = (z - z_0)^{-N} g(z) = \sum_{n=-N}^{\infty} a_n (z - z_0)^n\,, \tag{6.47b}$$

with $a_n = b_{n+N}$, and $a_{-N} \neq 0$. This is not a Taylor series because it includes negative powers of $z - z_0$, and $f(z)$ is not analytic at $z = z_0$.

Remarks.

(i) If $f(z)$ has a zero of order N at $z = z_0$, then $1/f(z)$ has a pole of order N there, and vice versa.

(ii) If $f(z)$ is analytic and non-zero at $z = z_0$ and $g(z)$ has a zero of order N there, then $f(z)/g(z)$ has a pole of order N there.

Worked exercise. Find and characterise the poles of

$$f(z) = \frac{2z}{(z + 1)(z - \mathrm{i})^2}\,. \tag{6.48a}$$

Answer. $f(z)$ has a simple pole at $z = -1$ and a double pole at $z = \mathrm{i}$ (as well as a simple zero at $z = 0$). To expand about the double pole let $z = \mathrm{i} + w$ and expand in w:

$$\begin{aligned}
f(z) &= \frac{2(\mathrm{i}+w)}{(\mathrm{i}+w+1)w^2} \\
&= \frac{2\mathrm{i}(1-\mathrm{i}w)}{(\mathrm{i}+1)\left(1+\frac{1}{2}(1-\mathrm{i})w\right)w^2} \\
&= \frac{2\mathrm{i}}{(\mathrm{i}+1)w^2}(1-\mathrm{i}w)\left(1-\tfrac{1}{2}(1-\mathrm{i})w+O(w^2)\right) \\
&= (1+\mathrm{i})w^{-2}\left(1-\tfrac{1}{2}(1+\mathrm{i})w+O(w^2)\right) \\
&= (1+\mathrm{i})(z-\mathrm{i})^{-2} - \mathrm{i}(z-\mathrm{i})^{-1} + O(1) \qquad \text{as} \quad z \to \mathrm{i}\,. \qquad (6.48\text{b})
\end{aligned}$$

6.7.3 Laurent series and essential singularities

Definition: Laurent series. It can be shown that any function that is analytic (and single-valued) throughout an annulus $\alpha < |z - z_0| < \beta$ centred on a point $z = z_0$ has a unique *Laurent series*,

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z-z_0)^n\,, \qquad (6.49)$$

which converges for all values of z within the annulus.

If $\alpha = 0$, then $f(z)$ is analytic throughout the disk $|z - z_0| < \beta$ except possibly at $z = z_0$ itself, and the Laurent series determines the behaviour of $f(z)$ near $z = z_0$. There are three possibilities:

(i) If the first non-zero term in the Laurent series has $n \geqslant 0$, then $f(z)$ is analytic at $z = z_0$ and the series is just a Taylor series.

(ii) If the first non-zero term in the Laurent series has $n = -N < 0$, then $f(z)$ has a pole of order N at $z = z_0$.

(iii) Otherwise, if the Laurent series involves an infinite number of terms with $n < 0$, then $f(z)$ has an *essential singularity* at $z = z_0$.

Example of a essential singularity. An example of an essential singularity is $f(z) = \mathrm{e}^{1/z}$ at $z = 0$, where the Laurent series can be generated from a Taylor series in $1/z$:

$$\mathrm{e}^{1/z} = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{1}{z}\right)^n = \sum_{n=-\infty}^{0} \frac{1}{(-n)!} z^n \qquad (6.50)$$

Remark. The behaviour of a function near an essential singularity is remarkably complicated. *Picard's theorem* states that, in any neighbourhood of an essential singularity, the function takes all possible complex values (possibly with one exception) at infinitely many points. In the case of $f(z) = \mathrm{e}^{1/z}$, the exceptional value 0 is never attained.

6.7.4 Behaviour at infinity

We can examine the behaviour of a function $f(z)$ as $z \to \infty$ by defining a new variable $\zeta = 1/z$ and a new function $g(\zeta) = f(z)$. Then $z = \infty$ maps to a single point $\zeta = 0$, the *point at infinity.*

If $g(\zeta)$ has a zero, pole or essential singularity at $\zeta = 0$, then we can say that $f(z)$ has the corresponding property at $z = \infty$.

Examples.

(i)
$$f_1(z) = \mathrm{e}^z = \mathrm{e}^{1/\zeta} = g_1(\zeta) \qquad (6.51\text{a})$$

has an essential singularity at $z = \infty$.

(ii)
$$f_2(z) = z^2 = 1/\zeta^2 = g_2(\zeta) \tag{6.51b}$$
has a double pole at $z = \infty$.

(iii)
$$f_3(z) = e^{1/z} = e^{\zeta} = g_3(\zeta) \tag{6.51c}$$
is analytic at $z = \infty$.

Remark. It can be shewn that all entire functions $f(z)$ have essential singularities at $z = \infty$ unless they are polynomials, and all polynomials have poles at $z = \infty$ unless they are constant.

6.8 Power Series of a Complex Variable

6.8.1 Convergence of Power Series

A power series about $z = z_0$ of a complex variable has the form

$$f(z) = \sum_{r=0}^{\infty} a_r (z - z_0)^r \quad \text{where} \quad a_r \in \mathbb{C}\,. \tag{6.52}$$

Hence the Taylor series for an analytic function, (6.44), is a power series.

Many of the tests of convergence for real series discussed in § 6.3 can be generalised for complex series. Indeed, we have already noted that if the sum of the absolute values of a complex series converges, i.e. if $\sum |u_r|$ converges, then so does the series, i.e. $\sum u_r$. Hence if $\sum |a_r(z - z_0)^r|$ converges, so does $\sum a_r(z - z_0)^r$.

6.8.2 Radius of convergence

If the power series (6.52) converges for $z = z_1$, then the series converges absolutely for all z such that $|z - z_0| < |z_1 - z_0|$.

Proof. Since $\sum a_r(z_1 - z_0)^r$ converges, then from the necessary condition for convergence in § 6.2.2,

$$\lim_{r\to\infty} a_r(z_1 - z_0)^r = 0\,. \tag{6.53a}$$

Hence for a given ε there exists $N \equiv N(\varepsilon)$ such that if $r > N$ then

$$|a_r(z_1 - z_0)^r| < \varepsilon\,. \tag{6.53b}$$

Thus for $r > N$

$$\begin{aligned} |a_r(z - z_0)^r| &= |a_r(z_1 - z_0)^r| \left| \frac{z - z_0}{z_1 - z_0} \right|^r \\ &< \varepsilon \varrho^r \quad \text{where} \quad \varrho = \left| \frac{z - z_0}{z_1 - z_0} \right|. \end{aligned} \tag{6.53c}$$

Thus, by means of a comparison with a geometric series, $\sum a_r(z - z_0)^r$ converges for $\varrho < 1$, i.e. for $|z - z_0| < |z_1 - z_0|$.

Corollary. If the sum diverges for $z = z_1$ then it diverges for all z such that $|z - z_0| > |z_1 - z_0|$. For suppose that it were to converge for some such $z = z_2$ with $|z_2 - z_0| > |z_1 - z_0|$, then it would converge for $z = z_1$ by the above result; this is in contradiction to the hypothesis.

Definition: Radius and circle of convergence. These results imply there must exist a real, non-negative number R such that

$$\begin{array}{c} \sum a_r(z - z_0)^r \text{ converges for } |z - z_0| < R \\ \sum a_r(z - z_0)^r \text{ diverges for } |z - z_0| > R \end{array}\,. \tag{6.54}$$

R is called the *radius of convergence*, and $|z - z_0| = R$ is called the *circle of convergence*, within which the series converges and outside of which it diverges.

Remarks.

(i) The radius of convergence may be be zero (exceptionally), positive or infinite.

(ii) On the circle of convergence, the series may either converge or diverge.

(iii) The radius of convergence of the Taylor series of a function $f(z)$ about the point $z = z_0$ is equal to the distance of the nearest singular point of the function $f(z)$ from z_0. Since a convergent power series defines an analytic function, no singularity can lie inside the circle of convergence.

6.8.3 Determination of the radius of convergence

Without loss of generality take $z_0 = 0$, so that (6.52) becomes

$$f(z) = \sum_{r=0}^{\infty} u_r \quad \text{where} \quad u_r = a_r z^r\,. \tag{6.55}$$

Use D'Alembert's ratio test. If the limit exists, then

$$\lim_{r\to\infty} \left| \frac{a_{r+1}}{a_r} \right| = \frac{1}{R}\,. \tag{6.56a}$$

Proof. We have that

$$\lim_{r\to\infty} \left| \frac{u_{r+1}}{u_r} \right| = \lim_{r\to\infty} \left| \frac{a_{r+1}}{a_r} \right| |z| = \frac{|z|}{R} \quad \text{by hypothesis (6.56a).}$$

Hence the series converges absolutely by D'Alembert's ratio test if $|z| < R$. On the other hand if $|z| > R$, then

$$\lim_{r\to\infty} \left| \frac{u_{r+1}}{u_r} \right| = \frac{|z|}{R} > 1\,. \tag{6.56b}$$

Hence $u_r \not\to 0$ as $r \to \infty$, and so the series does not converge. It follows that R is the radius of convergence.

Remark. The limit (6.56a) may not exist, e.g. if $a_r = 0$ for r odd then $\left| \dfrac{a_{r+1}}{a_r} \right|$ is alternately 0 or ∞.

Use Cauchy's test (unlectured). If the limit exists, then

$$\lim_{r\to\infty} |a_r|^{1/r} = \frac{1}{R}\,. \tag{6.57a}$$

Proof. We have that

$$\lim_{r\to\infty} |u_r|^{1/r} = \lim_{r\to\infty} |a_r|^{1/r} |z| = \frac{|z|}{R} \quad \text{by hypothesis.} \tag{6.57b}$$

Hence the series converges absolutely by Cauchy's test if $|z| < R$.
On the other hand if $|z| > R$, choose τ with $1 < \tau < |z|/R$. Then there exists $M \equiv M(\tau)$ such that

$$|u_r|^{1/r} > \tau > 1\,, \quad \text{i.e.} \quad |u_r| > \tau^r > 1\,, \quad \text{for all} \quad r > M\,.$$

21/22 Thus, since $u_r \not\to 0$ as $r \to \infty$, $\sum u_r$ must diverge. It follows that R is the radius of convergence.

6.8.4 Examples

(i) Suppose that $a_r = 1$ for all r, then $f(z)$ is the geometric series

$$f(z) = \sum_{r=0}^{\infty} z^r\,. \tag{6.58a}$$

Both D'Alembert's ratio test, (6.56a), and Cauchy's test, (6.57a), give $R = 1$:

$$\left| \frac{a_{r+1}}{a_r} \right| = 1 \quad \text{and} \quad |a_r|^{1/r} = 1 \quad \text{for all } r. \tag{6.58b}$$

Hence the series converges for $|z| < 1$. In fact

$$f(z) = \frac{1}{1-z}\,, \tag{6.58c}$$

where we note that it is the *singularity* at $z = 1$ which determines the radius of convergence.

(ii) Suppose next that $a_r = (-1)^{r-1}/r$ for all r, then $f(z)$ is the geometric series

$$f(z) = -\sum_{r=1}^{\infty} \frac{(-z)^r}{r} = z - \frac{z^2}{2} + \frac{z^3}{3} - \cdots . \tag{6.59a}$$

D'Alembert's ratio test gives

$$\frac{1}{R} = \lim_{r\to\infty} \left| \frac{a_{r+1}}{a_r} \right| = \lim_{r\to\infty} \frac{r}{r+1} = 1 . \tag{6.59b}$$

For Cauchy's test, we first note that

$$\lim_{r\to\infty} \log |a_r|^{\frac{1}{r}} = \lim_{r\to\infty} \frac{1}{r} \log \frac{1}{r} = 0 , \tag{6.59c}$$

and thence, as for D'Alembert's ratio test,

$$\frac{1}{R} = \lim_{r\to\infty} |a_r|^{1/r} = 1 . \tag{6.59d}$$

Remark. The series converges to $\log(1+z)$ for $|z| < 1$, where the singularity at $z = -1$ limits the radius of convergence. In fact it can be shewn that the series converges on the circle $|z| = 1$ except at the point $z = -1$.

(iii) If $a_r = \frac{1}{r!}$ for all r, then $f(z)$ is the series

$$f(z) = \sum_{r=0}^{\infty} \frac{z^r}{r!} . \tag{6.60a}$$

D'Alembert's ratio test gives an infinite radius of convergence:

$$\frac{1}{R} = \lim_{r\to\infty} \left| \frac{a_{r+1}}{a_r} \right| = \lim_{r\to\infty} \frac{1}{r+1} = 0 . \tag{6.60b}$$

For Cauchy's test, we first note, using Stirling's formula,[24] that

$$\log |a_r|^{\frac{1}{r}} = -\frac{1}{r} \log r! \sim -\log r \quad \text{as} \quad r \to \infty , \tag{6.60c}$$

and thence we confirm an infinite radius of convergence:

$$\frac{1}{R} = \lim_{r\to\infty} |a_r|^{1/r} = 0 . \tag{6.60d}$$

The series converges to e^z for all finite z, which is an entire function.

(iv) Instead consider $a_r = r!$. This has *zero radius of convergence* since by D'Alembert's ratio test

$$\frac{a_{r+1}}{a_r} = r + 1 \to \infty \quad \text{as} \quad r \to \infty . \tag{6.61}$$

This conclusion can be confirmed using Cauchy's test. The series $\sum_{r=0}^{\infty} r! z^r$ fails to define a function since it does not converge for any non-zero z.

(v) Finally consider

$$z \sum_{r=0}^{\infty} \frac{1}{2r+1} (-z^2)^r = z - \frac{z^3}{3} + \frac{z^5}{5} - \frac{z^7}{7} + \cdots = \arctan z . \tag{6.62}$$

Thought of as a power series in $(-z^2)$, this has $|a_{r+1}/a_r| = (2r+1)/(2r+3) \to 1$ as $r \to \infty$. Therefore $R = 1$ in terms of $(-z^2)$. But since $|-z^2| = 1$ is equivalent to $|z| = 1$, the series converges for $|z| < 1$ and diverges for $|z| > 1$.

[24] Stirling's formula states that

$$\log r! \sim r \log r - r + \tfrac{1}{2} \log(2\pi r) \quad \text{as} \quad r \to \infty .$$

7 Series Solutions of Ordinary Differential Equations

7.0 Why Study This?

Numerous scientific phenomena are described by differential equations. Even if these are partial differential equations, they can often be reduced to ordinary differential equations (ODEs), e.g. by the method of separation of variables. This section is about extending your armoury for solving ordinary differential equations, such as those that arise in quantum mechanics and electrodynamics.

The ordinary differential equations encountered are often linear and of either first or second order. In particular, second-order equations can describe oscillatory phenomena.

7.1 Classification

7.1.1 First-order linear ordinary differential equations

The general *linear first-order* inhomogeneous ODE,

$$y'(x) + p(x)y(x) = f(x)\,, \tag{7.1a}$$

can be solved using the integrating factor

$$g = \exp \int p(x)\,\mathrm{d}x\,, \tag{7.1b}$$

to obtain the general solution

$$y = \frac{1}{g}\left(\int gf\,\mathrm{d}x + \text{constant}\right)\,. \tag{7.1c}$$

Provided that the integrals can be evaluated, the problem is completely solved. An equivalent method does not exist for second-order ODEs, but an extensive theory can still be developed.

7.1.2 Second-order ordinary differential equations

The general second-order ODE is an equation of the form

$$F(y'', y', y, x) = 0\,, \tag{7.2}$$

for an unknown function $y(x)$, where $y' = \mathrm{d}y/\mathrm{d}x$, $y'' = \mathrm{d}^2y/\mathrm{d}x^2$ and F is a known function.

7.1.3 Second-order linear ordinary differential equations

The general *linear second-order* ordinary differential equation for $y(x)$ has the form

$$Ly(x) = g(x)\,, \tag{7.3a}$$

where L is a linear operator such that

$$Ly(x) = a(x)y'' + b(x)y' + c(x)y\,. \tag{7.3b}$$

We recover the standard form (2.12a) by dividing through by the coefficient of y'' to obtain

$$y''(x) + p(x)y'(x) + q(x)y(x) = f(x)\,. \tag{7.3c}$$

Recall from § 2.2 that if $f(x) = 0$ the equation is said to be *homogeneous*, otherwise it is said to be *inhomogeneous*.

Remarks.

(i) The principle of superposition applies to linear ODEs as to all linear equations.

(ii) Although the solution may be of interest only for real x, it is often informative to analyse the solution in the complex domain.

7.2 Homogeneous Second-Order Linear ODEs

7.2.1 Linearly independent solutions

Recall from § 2.2.1 that if $y_1(x)$ and $y_2(x)$ are two solutions of the homogeneous equation

$$y'' + p(x)y' + q(x)y = 0\,, \tag{7.4a}$$

they are *linearly independent* if

$$\alpha y_1(x) + \beta y_2(x) = 0 \quad \text{for all } x \text{ implies} \quad \alpha = \beta = 0\,, \tag{7.4b}$$

i.e. if one is not simply a constant multiple of the other.

If $y_1(x)$ and $y_2(x)$ are linearly independent solutions, then the *general solution* of (7.4a)

$$y(x) = \alpha y_1(x) + \beta y_2(x)\,, \tag{7.4c}$$

where α and β are arbitrary constants, and there are two arbitrary constants because the equation is of second order.

7.2.2 The Wronskian

Recall from (2.17a) that the *Wronskian* $W(x)$ of two solutions $y_1(x)$ and $y_2(x)$ of a second-order ODE is the determinant of the Wronskian matrix:

$$W[y_1, y_2] = \begin{vmatrix} y_1 & y_2 \\ y_1' & y_2' \end{vmatrix} = y_1 y_2' - y_2 y_1'\,. \tag{7.5a}$$

Recall also that if $\alpha y_1(x) + \beta y_2(x) = 0$ in some interval of x then, by differentiation, $\alpha y_1'(x) + \beta y_2'(x) = 0$, and so in matrix form

$$\begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}\,. \tag{7.5b}$$

If this is satisfied for non-trivial α and β, then $W = 0$ in that interval of x. Hence if $W \neq 0$, the solutions y_1 and y_2 must be linearly independent

7.2.3 The Calculation of W

We can derive a differential equation for the Wronskian, since

$$\begin{aligned} W' &= y_1 y_2'' - y_1'' y_2 && \text{from (7.5a) since the } y_1' y_2' \text{ terms cancel} \\ &= -y_1(p y_2' + q y_2) + (p y_1' + q y_1) y_2 && \text{using equation (7.4a)} \\ &= -p(y_1 y_2' - y_1' y_2) && \text{since the } q y_1 y_2 \text{ terms cancel} \\ &= -pW && \text{from definition (7.5a).} \end{aligned} \tag{7.6a}$$

This is a first-order equation for W, viz.

$$W' + p(x)W = 0\,, \tag{7.6b}$$

with solution, cf. (7.1c),

$$W(x) = \kappa \exp\left(-\int^x p(\zeta)\,\mathrm{d}\zeta\right)\,, \tag{7.6c}$$

where κ is a constant (a change in lower limit of integration can be absorbed by a rescaling of κ).

Remarks.

(i) Up to the multiplicative constant κ, the Wronskian W can be shown to be the same for any two linearly independent solutions y_1 and y_2, and hence it is an intrinsic property of the ODE.

(ii) If $W \neq 0$ for one value of x (and p is integrable) then $W \neq 0$ for all x (since $\exp y > 0$ for all y). Hence if y_1 and y_2 are linearly independent for one value of x, they are linearly independent for all values of x; it follows that linear independence need be checked at only one value of x. In the case that y_1 and y_2 are known implicitly, e.g. in terms of series or integrals, this means that we just have to find one value of x where is it relatively easy to evaluate W in order to confirm (or
18/02 otherwise) linear independence.

7.2.4 A Second Solution via the Wronskian

Suppose that we already have one solution, say y_1, to the homogeneous equation. Then we can calculate a second linearly independent solution, y_2, using the Wronskian as follows.

First, the definition of the Wronskian, (7.5a), provides a first-order linear ODE for the unknown y_2:

$$y_1y_2' - y_1'y_2 = W(x)\,. \tag{7.7}$$

To solve, divide by y_1^2 to obtain

$$\left(\frac{y_2}{y_1}\right)' = \frac{y_2'}{y_1} - \frac{y_2y_1'}{y_1^2} = \frac{W}{y_1^2}\,.$$

Now integrate both sides and use (7.6c) to obtain

$$y_2(x) = y_1(x)\int^x \frac{W(\eta)}{y_1^2(\eta)}\,\mathrm{d}\eta \tag{7.8a}$$

$$= y_1(x)\int^x \frac{\kappa}{y_1^2(\eta)}\,\exp\left(-\int^\eta p(\zeta)\,\mathrm{d}\zeta\right)\mathrm{d}\eta\,. \tag{7.8b}$$

In principle this allows us to compute y_2 given y_1.

Remarks.

(i) The indefinite integral involves an arbitrary additive constant, since any amount of y_1 can be added to y_2.

(ii) W involves an arbitrary multiplicative constant, since y_2 can be multiplied by any constant.

(iii) This expression for y_2 therefore provides the general solution of the homogeneous ODE.

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Example. Given that $y = x^n$ is a solution of $x^2y'' - (2n-1)xy' + n^2y = 0$, find the general solution.

Answer. First write the ODE in the standard form (7.3c):

$$y'' - \left(\frac{2n-1}{x}\right)y' + \left(\frac{n^2}{x^2}\right)y = 0 \tag{7.9a}$$

Next calculate the Wronskian (7.6c):

$$W = \kappa\exp\left(-\int^x p(\zeta)\,\mathrm{d}\zeta\right) = \kappa\exp\int^x\left(\frac{2n-1}{\zeta}\right)\mathrm{d}\zeta$$

$$= \kappa\exp\left((2n-1)\ln x + \textsf{constant}\right)$$

$$= \Lambda x^{2n-1}\,, \tag{7.9b}$$

for any non-zero constant Λ Finally, calculate the second solution from (7.8a):

$$y_2 = y_1\int^x \frac{W(\eta)}{y_1^2(\eta)}\,\mathrm{d}\eta = x^n\left(\int^x \frac{\Lambda}{\eta}\,\mathrm{d}\eta\right)$$

$$= \Lambda x^n\ln x + Bx^n\,. \tag{7.9c}$$

Remark. The same result can be obtained by writing $y_2(x) = y_1(x)u(x)$ and obtaining a first-order linear ODE for u'. This method applies to higher-order linear ODEs and is reminiscent of the factorization of polynomial equations.

Example. Given that $y_1(x)$ is a solution of Bessel's equation of zeroth order,

$$y'' + \frac{1}{x}y' + y = 0\,, \tag{7.10a}$$

find another independent solution in terms of y_1 for $x > 0$.

Answer. In this case $p(x) = 1/x$ and hence

$$y_2(x) = y_1(x)\int^x \frac{\kappa}{y_1^2(\eta)}\,\exp\left(-\int^\eta \frac{1}{\zeta}\,\mathrm{d}\zeta\right)\mathrm{d}\eta$$

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$$= \kappa y_1(x)\int^x \frac{1}{\eta\,y_1^2(\eta)}\,\mathrm{d}\eta\,. \tag{7.10b}$$

7.3 Taylor Series Solutions

7.3.1 Ordinary and singular points

It is useful now to generalize to complex functions $y(z)$ of a complex variable z. The homogeneous linear second-order ODE (7.4a) in standard form then becomes

$$y''(z) + p(z)y'(z) + q(z)y(z) = 0\,. \tag{7.11}$$

Definition: ordinary and singular points. If

$$p(z) \text{ and } q(z) \text{ are both analytic at } z = z_0$$

(i.e. they have power series expansions (6.44) about $z = z_0$), then $z = z_0$ is called an *ordinary point* of the ODE. A point at which p and/or q is singular, i.e. a point at which p and/or q or one of its derivatives is infinite, is called a *singular point* of the ODE.

Definition: regular singular points. A singular point $z = z_0$ is *regular* if:

$$(z - z_0)p(z) \text{ and } (z - z_0)^2 q(z) \text{ are both analytic at } z = z_0.$$

Example. Consider Legendre's equation

$$(1 - z^2)y'' - 2zy' + \ell(\ell + 1)y = 0\,, \tag{7.12a}$$

where ℓ is a constant. To identify the singular points and their nature, we divide through by $(1 - z^2)$ to obtain the standard form with

$$p(z) = -\frac{2z}{1 - z^2}, \qquad q(z) = \frac{\ell(\ell + 1)}{1 - z^2}. \tag{7.12b}$$

Both $p(z)$ and $q(z)$ are analytic for all z except $z = \pm 1$, which are the singular points. However, they are both regular since

$$(z - 1)p(z) = \frac{2z}{1 + z}, \qquad \text{and} \qquad (z - 1)^2 q(z) = \ell(\ell + 1)\left(\frac{1 - z}{1 + z}\right) \tag{7.12c}$$

22/22 are both analytic at $z = 1$, and similarly for $z = -1$.

7.3.2 The solution at ordinary points in terms of a power series

If $z = z_0$ is an ordinary point of (7.11), then we claim that $y(z)$ is analytic at $z = z_0$, and consequently the equation has two linearly independent solutions of the form (see (6.44))

$$y = \sum_{n=0}^{\infty} a_n (z - z_0)^n \quad \text{when} \quad |z - z_0| < R\,, \tag{7.13}$$

where R is the radius of convergence. The coefficients a_n can be determined by substituting the series into the equation and comparing powers of $(z - z_0)$. The radius of convergence turns out to be the distance to the nearest singular point of the equation in the complex plane.

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For simplicity we will assume henceforth wlog that $z_0 = 0$ (which corresponds to a shift in the origin of the z-plane, e.g. define $z' = z - z_0$ so that $z' = 0$ is the singular point, and then substitute z for z'). Hence we seek solutions of the form

$$y = \sum_{n=0}^{\infty} a_n z^n \equiv \sum_{m=0}^{\infty} a_m z^m\,, \tag{7.14a}$$

for which

$$y' = \sum_{n=\cancel{0}1}^{\infty} n a_n z^{n-1} = \sum_{m=0}^{\infty} (m + 1) a_{m+1} z^m \qquad \text{substituting } m = n - 1, \tag{7.14b}$$

$$y'' = \sum_{n=\cancel{0}2}^{\infty} n(n - 1) a_n z^{n-2} = \sum_{r=0}^{\infty} (r + 2)(r + 1) a_{r+2} z^r \qquad \text{substituting } r = n - 2. \tag{7.14c}$$

At an ordinary point $p(z)$ and $q(z)$ are analytic so we can write

$$p(z) = \sum_{n=0}^{\infty} p_n z^n \quad \text{and} \quad q(z) = \sum_{n=0}^{\infty} q_n z^n \,. \tag{7.15}$$

On substituting the above series into equation (7.11) we will need a rule for multiplying double sums of the form

$$\sum_{n=0}^{\infty} A_n z^n \sum_{m=0}^{\infty} B_m z^m \tag{7.16a}$$

to only include powers like z^r. Let $r = n + m$ and then note that (cf. a change of variables in a double integral)

$$\sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \bullet(n,m) = \sum_{r=0}^{\infty}\sum_{m=0}^{r} \bullet(r-m,m)\,, \tag{7.16b}$$

since $n = r - m \geqslant 0$. In which case (7.16a) can be rewritten as

$$\sum_{r=0}^{\infty}\left(\sum_{m=0}^{r} A_{r-m}B_m\right) z^r\,. \tag{7.16c}$$

Hence from series (7.14a), (7.14b) and (7.15)

$$p(z)y'(z) = \sum_{n=0}^{\infty} p_n z^n \sum_{m=0}^{\infty}(m+1)a_{m+1}z^m = \sum_{r=0}^{\infty}\left(\sum_{m=0}^{r} p_{r-m}(m+1)a_{m+1}\right) z^r\,, \tag{7.17a}$$

$$q(z)y(z) = \sum_{n=0}^{\infty} q_n z^n \sum_{m=0}^{\infty} a_m z^m = \sum_{r=0}^{\infty}\left(\sum_{m=0}^{r} q_{r-m}a_m\right) z^r\,. \tag{7.17b}$$

Now substitute series (7.14c), (7.17a) and (7.17b) into equation (7.11), and group powers of z^r, to obtain

$$\sum_{r=0}^{\infty}\left((r+2)(r+1)a_{r+2} + \sum_{m=0}^{r}\Big((m+1)a_{m+1}p_{r-m} + a_m q_{r-m}\Big)\right) z^r = 0\,. \tag{7.18}$$

Since this expression is true for all $|z| < R$, each coefficient of z^r $(r = 0, 1, \dots)$ must be zero. Thus we deduce the *recurrence relation*

$$a_{r+2} = -\frac{1}{(r+2)(r+1)}\sum_{m=0}^{r}\Big((m+1)a_{m+1}p_{r-m} + a_m q_{r-m}\Big) \quad \text{for} \quad r \geqslant 0\,. \tag{7.19}$$

This is a *recurrence relation* that determines a_{r+2} (for $r \geqslant 0$) in terms of the preceding coefficients $a_0, a_1, \dots, a_{r+1}$. This means that if a_0 and a_1 are known then so are all the a_r. The first two coefficients a_0 and a_1 play the rôle of the *two integration constants* in the general solution.

Remarks.

(i) The above procedure is rarely followed to the letter. For instance, if p and q are *rational functions* (i.e. ratios of polynomials) it is a much better idea to multiply the equation through by a suitable factor to clear denominators *before* substituting in the power series for y, y' and y''.

(ii) Proof that the radius of convergence of the series (7.14a) is non-zero is more difficult, and we will not attempt such a task in general. However we shall discuss the issue for examples.

7.3.3 Example (possibly unlectured)

Consider

$$y'' - \frac{2}{(1-z)^2}y = 0\,. \tag{7.20}$$

$z = 0$ is an ordinary point so try

$$y = \sum_{n=0}^{\infty} a_n z^n\,. \tag{7.21}$$

We note that

$$p = 0\,, \quad q = -\frac{2}{(1-z)^2} = -2\sum_{m=0}^{\infty}(m+1)z^m\,, \tag{7.22a}$$

and hence in the terminology of the previous subsection $p_m = 0$ and $q_m = -2(m+1)$. Substituting into (7.19) we obtain the recurrence relation

$$a_{r+2} = \frac{2}{(r+2)(r+1)}\sum_{n=0}^{r} a_n(r-n+1) \quad \text{for} \quad r \geqslant 0\,. \tag{7.22b}$$

However, with a small amount of forethought we can obtain a simpler, if equivalent, recurrence relation. First multiply (7.20) by $(1-z)^2$ to obtain

$$(1-z)^2y'' - 2y = 0\,,$$

and then substitute (7.21) into this equation. We find, on expanding $(1-z)^2 = 1 - 2z + z^2$, that

$$\sum_{n=\cancel{0}2}^{\infty} n(n-1)a_nz^{n-2} - 2\sum_{n=\cancel{0}1}^{\infty} n(n-1)a_nz^{n-1} + \sum_{n=0}^{\infty}(n^2-n-2)a_nz^n = 0\,.$$

After the substitutions $r = n-2$, $r = n-1$ and $r = n$ in the first, second and third terms respectively, we obtain

$$\sum_{r=0}^{\infty}(r+1)\big((r+2)a_{r+2} - 2ra_{r+1} + (r-2)a_r\big)z^r = 0\,,$$

which leads to the recurrence relation

$$a_{r+2} = \frac{1}{r+2}(2ra_{r+1} - (r-2)a_r) \quad \text{for} \quad r \geqslant 0\,. \tag{7.23}$$

This two-term recurrence relation again determines a_r for $r \geqslant 2$ in terms of a_0 and a_1, but is simpler than (7.22b).

Exercise for those with time. Show that the recurrence relations (7.22b) and (7.23) are equivalent.

Two solutions. For $r = 0$ the recurrence relation (7.23) yields $a_2 = a_0$, while for $r = 1$ and $r = 2$ we obtain

$$a_3 = \tfrac{1}{3}(2a_2 + a_1) \quad \text{and} \quad a_4 = a_3\,. \tag{7.24a}$$

First we note that if $2a_2 + a_1 = 0$, then $a_3 = a_4 = 0$, and hence $a_r = 0$ for $r \geqslant 3$. We thus have as our first solution (with $a_0 = \alpha \neq 0$)

$$y_1 = \alpha(1-z)^2\,. \tag{7.24b}$$

Next we note that $a_r = a_0$ for all r is a solution of (7.23). In this case we can sum the series to obtain (with $a_0 = \beta \neq 0$)

$$y_2 = \beta\sum_{n=0}^{\infty} z^n = \frac{\beta}{1-z}\,. \tag{7.24c}$$

Linear independence. The linear independence of (7.24b) and (7.24c) is clear, as confirmed by the calculation of the Wronskian:

$$W = y_1y_2' - y_1'y_2 = \alpha(1-z)^2\frac{\beta}{(1-z)^2} + 2\alpha(1-z)\frac{\beta}{(1-z)} = 3\alpha\beta \neq 0\,. \tag{7.25}$$

Hence the general solution is

$$y(z) = \alpha(1-z)^2 + \frac{\beta}{1-z}\,, \tag{7.26}$$

for constants α and β.

Radius of convergence. From (6.58b) the radius of convergence of (7.24c) is $R = 1$, which is consistent with the general solution being singular at $z = 1$, and the equation having a singular point at $z = 1$ since $q(z) = -2(1-z)^{-2}$.

7.3.4 Example: Legendre's Equation

Legendre's equation is

$$(1-z^2)y'' - 2zy' + \ell(\ell+1)\,y = 0\,, \tag{7.27}$$

where $\ell \in \mathbb{R}$, and for the sequel it is more convenient not to write it in standard form. The points $z = \pm 1$ are singular points but $z = 0$ is an ordinary point, so for smallish z seek a power series solution

$$y = \sum_{n=0}^{\infty} a_n z^n\,, \quad y' = \sum_{n=0}^{\infty} n a_n z^{n-1}\,, \quad y'' = \sum_{n=0}^{\infty} n(n-1) a_n z^{n-2}\,. \tag{7.28}$$

On substituting this into (7.27) we obtain

$$\sum_{n=\cancel{0}2}^{\infty} n(n-1)a_n z^{n-2} - \sum_{n=0}^{\infty} n(n-1)a_n z^n - 2\sum_{n=0}^{\infty} n a_n z^n + \sum_{n=0}^{\infty} \ell(\ell+1) a_n z^n = 0\,.$$

From substituting $r = n-2$ in the first sum and $r = n$ in the next three sums, and from grouping powers of z^r, we obtain

$$\sum_{r=0}^{\infty} \big((r+2)(r+1)a_{r+2} - (r(r+1) - \ell(\ell+1))\,a_r\big) z^r = 0\,.$$

The recurrence relation is therefore

$$a_{r+2} = \frac{r(r+1) - \ell(\ell+1)}{(r+1)(r+2)}\, a_r = \frac{(r-\ell)(r+\ell+1)}{(r+1)(r+2)}\, a_r \quad \text{for} \quad r = 0, 1, 2, \ldots. \tag{7.29}$$

a_0 and a_1 are arbitrary constants, with the other coefficients following from the recurrence relation. For instance:

(i) if $a_0 = 1$ and $a_1 = 0$, then $\qquad y_1 = 1 - \dfrac{\ell(\ell+1)}{2} z^2 + O(z^4) \qquad$ is an even solution; (7.30a)

(ii) if $a_0 = 0$ and $a_1 = 1$, then $\qquad y_2 = z + \dfrac{2 - \ell(\ell+1)}{6} z^3 + O(z^5) \qquad$ is an odd solution. (7.30b)

The Wronskian at the ordinary point $z = 0$ is thus given by

$$W = y_1 y_2' - y_1' y_2 = 1 \cdot 1 - 0 \cdot 0 = 1\,. \tag{7.31}$$

Since $W \neq 0$, y_1 and y_2 are linearly independent (although it should have been obvious already ☺).

Radius of convergence. The series (7.30a) and (7.30b) are effectively power series in z^2 rather than z. Hence to find the radius of convergence we either need to re-express our series (e.g. $z^2 \to y$ and $a_{2n} \to b_n$), or use a slightly modified D'Alembert's ratio test. We adopt the latter approach and observe from (7.29) that

$$\lim_{n\to\infty} \left| \frac{a_{n+2} z^{n+2}}{a_n z^n} \right| = \lim_{n\to\infty} \left| \frac{n(n+1) - \ell(\ell+1)}{(n+1)(n+2)} \right| |z|^2 = |z|^2\,. \tag{7.32}$$

It then follows from a straightforward extension of D'Alembert's ratio test (6.20b) that the series converges for $|z| < 1$. Moreover, the series diverges for $|z| > 1$ (since $a_n z^n \not\to 0$), and so the radius of convergence $R = 1$. On the radius of convergence, determination of whether the series converges is more difficult.

Remark. The radius of convergence is the distance to nearest singularity of the ODE. This is a general feature.

Legendre polynomials. In the generic situations both series (7.30a) and (7.30b) have an infinite number of terms. However, for $\ell = 0, 1, 2, \ldots$ it follows from (7.29)

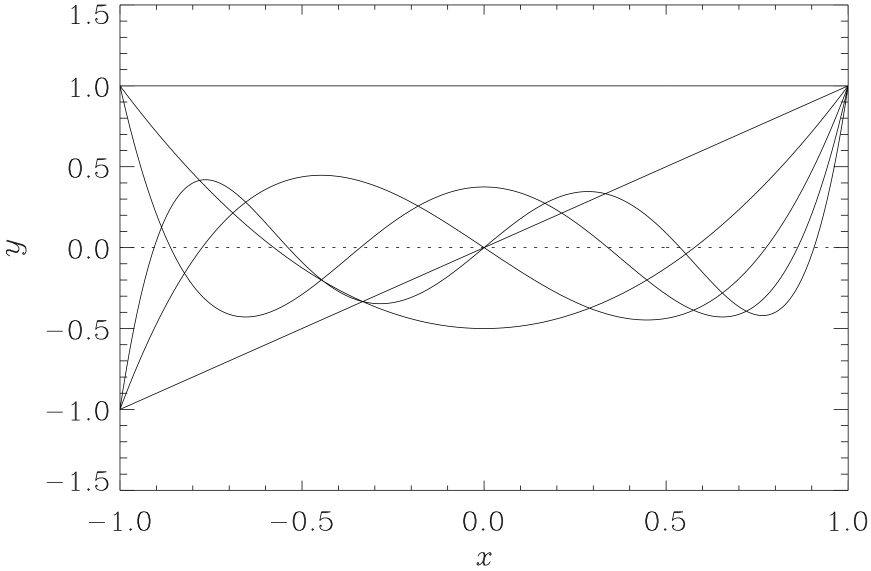
$$a_{\ell+2} = \frac{\ell(\ell+1) - \ell(\ell+1)}{(\ell+1)\,(\ell+2)} a_\ell = 0\,, \tag{7.33}$$

and so the series *terminates*. For instance,

$$\begin{aligned} \ell = 0: &\quad y = a_0\,, \\ \ell = 1: &\quad y = a_1 z\,, \\ \ell = 2: &\quad y = a_0(1 - 3z^2)\,. \end{aligned}$$

These functions are proportional to the *Legendre polynomials*, $P_\ell(z)$, which are conventionally normalized (by suitable choice of a_0 or a_1) so that $P_\ell(1) = 1$. Thus

$$P_0(z) = 1\,, \quad P_1(z) = z\,, \quad P_2(z) = \tfrac{1}{2}(3z^2 - 1)\,, \quad \text{etc.} \tag{7.34}$$



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7.4 Regular Singular Points

Let $z = z_0$ be a regular singular point of equation (7.11) where, as before, wlog we can take $z_0 = 0$. If we write

$$p(z) = \frac{1}{z}s(z) \quad \text{and} \quad q(z) = \frac{1}{z^2}t(z)\,, \tag{7.35a}$$

then the homogeneous equation (7.11) becomes, after multiplying by z^2,

$$z^2y'' + zs(z)y' + t(z)y = 0\,, \tag{7.35b}$$

where, from the definition of a regular singular point, $s(z)$ and $t(z)$ are both analytic at $z = 0$. It follows
19/03 that $s_0 \equiv s(0)$ and $t_0 \equiv t(0)$ are finite.

7.4.1 The Indicial Equation

If $z = 0$ is a regular singular point, *Fuchs's theorem* guarantees that there is always *at least one* solution to (7.35b) of the form

$$y = z^\sigma \sum_{n=0}^{\infty} a_n z^n \quad \text{with} \quad a_0 \neq 0 \quad \text{and} \quad \sigma \in \mathbb{C}\,, \tag{7.36}$$

i.e. a Taylor series multiplied by a power z^σ, where the index σ is to be determined.
Remarks.

(i) This is a Taylor series only if σ is a non-negative integer.

(ii) There may be one or two solutions of this form (see below).

(iii) The condition $a_0 \neq 0$ is required to define σ uniquely.

To understand why the solutions behave in this way, substitute (7.36) into (7.35b) to obtain, after division by z^σ,

$$\sum_{n=0}^{\infty} \big((\sigma+n)(\sigma+n-1) + (\sigma+n)s(z) + t(z)\big)a_n z^n = 0\,. \tag{7.37a}$$

We now evaluate this sum at $z = 0$, recalling that $z^n = 0$ except for $n = 0$, to obtain

$$(\sigma(\sigma-1) + \sigma s_0 + t_0)a_0 = 0\,. \tag{7.37b}$$

Since by definition $a_0 \neq 0$ (see (7.36)) we obtain the *indicial equation* for σ:

$$\sigma^2 + \sigma(s_0 - 1) + t_0 = 0\,. \tag{7.38}$$

19/01 The roots σ_1, σ_2 of this equation are called the *indices* of the regular singular point.

7.4.2 Series Solutions

For each choice of σ from σ_1 and σ_2 we can find a *recurrence relation* for a_n by comparing powers of z in (7.37a), i.e. after expanding s and t in power series.

$\sigma_1 - \sigma_2 \notin \mathbb{Z}$. If $\sigma_1 - \sigma_2 \notin \mathbb{Z}$ we can find *both* linearly independent solutions this way.

$\sigma_1 - \sigma_2 \in \mathbb{Z}$. If $\sigma_1 = \sigma_2$ we note that we can find only one solution by the ansatz (7.36). However, as we shall see, it's worse than this. The ansatz (7.36) also fails (in general) to give both solutions when σ_1 and σ_2 differ by an integer (although there are exceptions).

Frobenius's method is used to find the series solutions about a regular singular point. This is best demonstrated by example.

7.4.3 Example: Bessel's Equation of Order ν

Bessel's equation of order ν is

$$y'' + \frac{1}{z}y' + \left(1 - \frac{\nu^2}{z^2}\right) y = 0\,, \tag{7.39}$$

where $\nu \geqslant 0$ wlog. The origin $z = 0$ is a regular singular point with

$$s(z) = 1 \quad \text{and} \quad t(z) = z^2 - \nu^2\,. \tag{7.40}$$

A power series solution of the form (7.36) solves (7.39) if, from (7.37a),

$$\sum_{n=0}^{\infty} \big((\sigma+n)(\sigma+n-1) + (\sigma+n) - \nu^2\big)a_n z^n + \sum_{n=0}^{\infty} a_n z^{n+2} = 0\,, \tag{7.41a}$$

i.e. after the transformation $n \to n-2$ in the second sum, if

$$\sum_{n=0}^{\infty} \big((\sigma+n)^2 - \nu^2\big)a_n z^n + \sum_{n=2}^{\infty} a_{n-2} z^n = 0\,. \tag{7.41b}$$

Now compare powers of z to obtain

$$n = 0: \quad \sigma^2 - \nu^2 = 0 \qquad\qquad \text{since } a_0 \neq 0 \tag{7.42a}$$

$$n = 1: \quad \big((\sigma+1)^2 - \nu^2\big)a_1 = 0 \tag{7.42b}$$

$$n \geqslant 2: \quad \big((\sigma+n)^2 - \nu^2\big)a_n + a_{n-2} = 0\,. \tag{7.42c}$$

(7.42a) is the indicial equation and implies that

$$\sigma = \pm\nu\,. \tag{7.43}$$

Substituting this result into (7.42b) and (7.42c) yields

$$(1 \pm 2\nu)\, a_1 = 0 \tag{7.44a}$$

$$n(n \pm 2\nu)\, a_n = -a_{n-2} \quad \text{for} \quad n \geqslant 2\,. \tag{7.44b}$$

Radius of convergence. The radius of convergence of the solution is infinite since from (7.44b)

$$\lim_{n\to\infty} \left| \frac{a_n}{a_{n-2}} \right| = \lim_{n\to\infty} \left| \frac{1}{n(n \pm 2\nu)} \right| = 0\,.$$

This is consistent with p and q having no singularities other than at $z = 0$.

Remark. We note that there is no difficulty in solving for a_n from a_{n-2} using (7.44b) if $\sigma = +\nu$. However, if $\sigma = -\nu$ the recursion will fail with a_n predicted to be infinite if at any point $n = 2\nu$. There are hence potential problems if $\sigma_1 - \sigma_2 = 2\nu \in \mathbb{Z}$, i.e. if the indices σ_1 and σ_2 differ by an integer.

$2\nu \notin \mathbb{Z}$. First suppose that $2\nu \notin \mathbb{Z}$ so that σ_1 and σ_2 do *not* differ by an integer. In this case (7.44a) and (7.44b) imply

$$a_n = \begin{cases} 0 & n = 1, 3, 5, \dots\,, \\ -\dfrac{a_{n-2}}{n(n \pm 2\nu)} & n = 2, 4, 6, \dots\,, \end{cases} \tag{7.45a}$$

and so we get *two* linearly independent solutions

$$y_1 = a_0 z^{+\nu} \left(1 - \frac{z^2}{4(1+\nu)} + \frac{z^4}{32(1+\nu)(2+\nu)} + \cdots \right), \tag{7.45b}$$

$$y_2 = a_0 z^{-\nu} \left(1 - \frac{z^2}{4(1-\nu)} + \frac{z^4}{32(1-\nu)(2-\nu)} + \cdots \right). \tag{7.45c}$$

$2\nu = 2m+1$, $m \in \mathbb{N}$. It so happens in this case that even though σ_1 and σ_2 differ by an *odd* integer there is no problem; the solutions are still given by (7.45a), (7.45b) and (7.45c). This is because for Bessel's equation the power series proceed in even powers of z, and hence the problem recursion when $n = 2\nu = 2m+1$ is never encountered. We conclude that the condition for the recursion relation (7.44b) to fail is that ν is an integer.

Remark. If $\nu = \frac{1}{2}$, then (7.44a) does *not* force the choice $a_1 = 0$. However, if $a_1 \neq 0$ the effect is to add a multiple of y_1 to y_2; hence, wlog, one can choose $a_1 = 0$.

$2\nu = 0$. If $\nu = 0$ then $\sigma_1 = \sigma_2$ and we can only find *one* power series solution of the form (7.36), viz.

$$y = a_0 \left(1 - \tfrac{1}{4} z^2 + \dots \right). \tag{7.46}$$

$2\nu = 2m$, $m \in \mathbb{N}$. If ν is a positive integer, m, then we can find one solution by choosing $\sigma = \nu$. However if we take $\sigma = -\nu$ then a_{2m} is predicted to be infinite, i.e. a second series solution of the form (7.36) fails.

Remark. The existence of two power series solutions for $2\nu = 2m+1$, $m \in \mathbb{N}$ is a 'lucky' accident. In general there exists only one solution of the form (7.36) whenever the indices σ_1 and σ_2 differ by an integer.

7.4.4 The Second Solution when $\sigma_1 - \sigma_2 \in \mathbb{Z}$

A Preliminary: Bessel's equation with $\nu = 0$. In order to obtain an idea how to proceed when $\sigma_1 - \sigma_2 \in \mathbb{Z}$, first consider the example of Bessel's equation of zeroth order, i.e. $\nu = 0$. Let y_1 denote the solution (7.46). Then, from (7.10b) (after the transformations $x \to z$)

$$y_2(z) = \kappa y_1(z) \int^z \frac{1}{\eta\, y_1^2(\eta)}\, \mathrm{d}\eta\,. \tag{7.47a}$$

For small (positive) z we can deduce using (7.46) that

$$\begin{aligned} y_2(z) &= \kappa a_0 \left(1 + O(z^2)\right) \int^z \frac{1}{\eta\, a_0^2} \left(1 + O(\eta^2)\right) \mathrm{d}\eta \\ &= \frac{\kappa}{a_0} \log z + \dots\,. \end{aligned} \tag{7.47b}$$

We conclude that the second solution contains a logarithm.

The claim. Let σ_1, σ_2 be the two (possibly complex) solutions to the indicial equation for a regular singular point at $z = 0$. Order them so that

$$\operatorname{Re}(\sigma_1) \geqslant \operatorname{Re}(\sigma_2)\,. \tag{7.48a}$$

Then we can always find *one* solution of the form

$$y_1(z) = z^{\sigma_1} \sum_{n=0}^{\infty} a_n z^n \quad \text{with, say, the normalisation } a_0 = 1\,. \tag{7.48b}$$

If $\sigma_1 - \sigma_2 \in \mathbb{Z}$ we claim that the second-order solution takes the form

$$y_2(z) = z^{\sigma_2} \sum_{n=0}^{\infty} b_n z^n + k\, y_1(z) \log z\,, \tag{7.48c}$$

for some number k. The coefficients b_n can be found by substitution into the ODE. In some very special cases k may vanish but $k \neq 0$ in general.

Example: Bessel's equation of integer order.[25] Suppose that y_1 is the series solution with $\sigma = +m$ to

$$z^2 y'' + z y' + \left(z^2 - m^2\right) y = 0\,, \tag{7.49}$$

where, compared with (7.39), we have written m for ν. Hence from (7.36) and (7.45a)

$$y_1 = z^m \sum_{\ell=0}^{\infty} a_{2\ell} z^{2\ell}\,, \tag{7.50}$$

since $a_{2\ell+1} = 0$ for integer ℓ. Let

$$y = k y_1 \log z + w\,, \tag{7.51}$$

then

$$y' = k y_1' \log z + \frac{k y_1}{z} + w' \quad \text{and} \quad y'' = k y_1'' \log z + \frac{2k y_1'}{z} - \frac{k y_1}{z^2} + w''\,.$$

On substituting into (7.49), and using the fact that y_1 is a solution of (7.49), we find that

$$z^2 w'' + z w' + (z^2 - m^2) w = -2kz y_1'\,. \tag{7.52}$$

Based on (7.43), (7.48a) and (7.48c) we now seek a series solution of the form

$$w = k\, z^{-m} \sum_{n=0}^{\infty} b_n z^n\,. \tag{7.53}$$

On substitution into (7.52) we have that

$$k \sum_{n=\cancel{0}1}^{\infty} n(n-2m) b_n z^{n-m} + k \sum_{n=0}^{\infty} b_n z^{n-m+2} = -2k \sum_{\ell=0}^{\infty} (2\ell+m) a_{2\ell} z^{2\ell+m}\,.$$

After multiplying by z^m and making the transformations $n \to n-2$ and $2\ell \to n-2m$ in the second and third sums respectively, it follows that

$$\sum_{n=1}^{\infty} n(n-2m) b_n z^n + \sum_{n=2}^{\infty} b_{n-2} z^n = -2 \sum_{\substack{n=2m \\ n \text{ even}}}^{\infty} (n-m) a_{n-2m} z^n\,.$$

We now demand that the combined coefficient of z^n is zero. Consider the even and odd powers of z^n in turn.

$n = 1, 3, 5, \ldots$. From equating powers of z^1 it follows that $b_1 = 0$. Next, from writing $n = 2\ell + 1$ ($\ell = 1, 2, \ldots$) and equating powers of $z^{2\ell+1}$, we obtain the following recurrence relation for the $b_{2\ell+1}$:

$$(2\ell+1)(2\ell+1-2m) b_{2\ell+1} = -b_{2\ell-1}\,.$$

Since $b_1 = 0$, we conclude that $b_{2\ell+1} = 0$ ($\ell = 1, 2, \ldots$).

$n = 2, 4, \ldots, 2m, \ldots$. Let $n = 2\ell$ ($\ell = 1, 2, \ldots$), then from equating powers of $z^{2\ell}$ we obtain

$$b_{2\ell-2} = -4\ell(\ell-m) b_{2\ell} \qquad \text{for } 1 \leqslant \ell \leqslant m-1\,, \tag{7.54a}$$

$$b_{2m-2} = -2m a_0 \qquad \text{for } \ell = m\,, \tag{7.54b}$$

$$b_{2\ell} = -\frac{1}{4\ell(\ell-m)}\, b_{2\ell-2} - \frac{(2\ell-m)}{2\ell(\ell-m)}\, a_{2\ell-2m} \qquad \text{for } \ell \geqslant m+1\,. \tag{7.54c}$$

To determine the even coefficients, $b_{2\ell}$,

[25] The schedules specifically state "without full discussion of logarithmic singularities", hence you may assume that the details in this example are not examinable.

- first, after noting that $2m-2 \geqslant 0$, solve for b_{2m-2} in terms of a_0 from (7.54b);
- next, if $m \geqslant 2$, solve for the $b_{2\ell}$ ($\ell = m-2, m-3, \dots, 0$) recurrently, in terms of the known $b_{2m-2} = -2ma_0$, using (7.54a);
- then, having noted that a non-zero value of b_{2m} simply generates a solution proportional to y_1, choose a value for b_{2m}, e.g., wlog, $b_{2m} = 0$;
- finally, having fixed b_{2m}, solve for the $b_{2\ell}$ ($\ell = m+1, m+2 \dots$) recurrently, in terms of b_{2m} and the a_{2k} ($k = 1, 2, \dots$), using (7.54c);

For example, we find for $\nu = 0$

$$y_1 = 1 - \frac{z^2}{4} + \frac{z^4}{64} + \cdots\,, \tag{7.55a}$$

$$y_2 = y_1 \ln z + \frac{z^2}{4} - \frac{3z^4}{128} + \cdots\,, \tag{7.55b}$$

and for $\nu = 1$

$$y_1 = z - \frac{z^3}{8} + \frac{z^5}{192} + \cdots\,, \tag{7.55c}$$

$$y_2 = y_1 \ln z - \frac{2}{z} + \frac{3z^3}{32} + \cdots\,. \tag{7.55d}$$

Remark. These examples illustrate a feature that is commonly encountered in scientific applications: one solution is regular (i.e. analytic) and the other is singular. Often only the regular solution is an
20/02 acceptable solution of the scientific problem.

7.4.5 Irregular singular points

If either $(z-z_0)p(z)$ or $(z-z_0)^2 q(z)$ is not analytic at the point $z = z_0$, it is an *irregular* singular point of the equation (7.11). The solutions can have worse kinds of singular behaviour there.

Example: the equation $z^4 y'' + 2z^2 y' - y = 0$ has an irregular singular point at $z = 0$. Its solutions are $\exp(\pm z^{-1})$, both of which have an essential singularity at $z = 0$.

20/01 In fact this example is just the familiar equation $\mathrm{d}^2 y/\mathrm{d}x^2 = y$ with the substitution $z = 1/x$. Even this
20/03 simple ODE has an irregular singular point at $x = \infty$.

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7.5 The Method of Variation of Parameters (Unlectured and Not in Schedule)

The question that remains is how to find the particular solution. To that end first suppose that we have solved the homogeneous equation and found two linearly-independent solutions y_1 and y_2. Then in order to find a particular solution consider

$$y_0(x) = u(x)y_1(x) + v(x)y_2(x)\,. \tag{7.56}$$

If u and v were constants ('parameters') y_0 would solve the homogeneous equation. However, we allow the 'parameters' to vary, i.e. to be functions of x, in such a way that y_0 solves the inhomogeneous problem.

Remark. We have gone from one unknown function, i.e. y_0 and one equation (i.e. (2.15a)), to two unknown functions, i.e. u and v and one equation. We will need to find, or in fact choose, another equation.

We now differentiate (7.56) to find that

$$y_0' = (uy_1' + vy_2') + (u'y_1 + v'y_2) \tag{7.57a}$$

$$y_0'' = (uy_1'' + vy_2'' + u'y_1' + v'y_2') + (u''y_1 + v''y_2 + u'y_1' + v'y_2')\,. \tag{7.57b}$$

If we substitute the above into the inhomogeneous equation (2.15a) we will have not apparently made much progress because we will still have a second-order equation involving terms like u'' and v''. However, suppose that we eliminate the u' and v' terms from (7.57a) by demanding that u and v satisfy the extra equation

$$u'y_1 + v'y_2 = 0\,. \tag{7.58}$$

Then (7.57a) and (7.57b) become

$$y_0' = uy_1' + vy_2' \tag{7.59a}$$
$$y_0'' = uy_1'' + vy_2'' + u'y_1' + v'y_2' . \tag{7.59b}$$

It follows from (7.56), (7.59a) and (7.59b) that

$$\begin{aligned} y_0'' + py_0' + qy_0 &= u(y_1'' + py_1' + qy_1) + v(y_2'' + py_2' + qy_2) + u'y_1' + v'y_2' \\ &= u'y_1' + v'y_2' , \end{aligned}$$

since y_1 and y_2 solve the homogeneous equation (7.11). Hence y_0 solves the inhomogeneous equation (2.15a) if

$$u'y_1' + v'y_2' = f . \tag{7.60}$$

We now have two simultaneous equations for u', v', i.e. (7.58) and (7.60), with solution

$$u' = -\frac{fy_2}{W} \quad \text{and} \quad v' = \frac{fy_1}{W} , \tag{7.61}$$

where W is the Wronskian,

$$W = y_1y_2' - y_2y_1' . \tag{7.62}$$

W is non-zero because y_1 and y_2 were chosen to be linearly independent. Integrating we obtain

$$u = -\int_a^x \frac{y_2(\zeta)f(\zeta)}{W(\zeta)}\,\mathrm{d}\zeta \quad \text{and} \quad v = \int_a^x \frac{y_1(\zeta)f(\zeta)}{W(\zeta)}\,\mathrm{d}\zeta , \tag{7.63}$$

where a is arbitrary. We could have chosen different lower limits for the two integrals, but we do not need to find the general solution, only a particular one. Substituting this result back into (7.56) we obtain as our particular solution

$$y_0(x) = \int_a^x \frac{f(\zeta)}{W(\zeta)} \big(y_1(\zeta)y_2(x) - y_1(x)y_2(\zeta) \big)\,\mathrm{d}\zeta . \tag{7.64}$$

Remark. We observe that, since the integrand is zero when $\zeta = x$,

$$y_0'(x) = \int_a^x \frac{f(\zeta)}{W(\zeta)} \big(y_1(\zeta)y_2'(x) - y_1'(x)y_2(\zeta) \big)\,\mathrm{d}\zeta . \tag{7.65}$$

Hence the particular solution (7.64) satisfies the *initial value homogeneous boundary conditions*

$$y(a) = y'(a) = 0 . \tag{7.66}$$

More general initial value boundary conditions would be inhomogeneous, e.g.

$$y(a) = k_1 , \quad y'(a) = k_2 , \tag{7.67}$$

where k_1 and k_2 are constants which are not simultaneously zero. Such inhomogeneous boundary conditions can be satisfied by adding suitable multiples of the linearly-independent solutions of the homogeneous equation, i.e. y_1 and y_2.

Example. Find the general solution to the equation

$$y'' + y = \sec x . \tag{7.68}$$

Answer. Two linearly independent solutions of the homogeneous equation are

$$y_1 = \cos x \quad \text{and} \quad y_2 = \sin x , \tag{7.69a}$$

with a Wronskian

$$W = y_1y_2' - y_2y_1' = \cos x(\cos x) - \sin x(-\sin x) = 1 . \tag{7.69b}$$

Hence from (7.64) a particular solution is given by

$$\begin{aligned} y_0(x) &= \int^x \sec\zeta \big(\cos\zeta \sin x - \cos x \sin\zeta \big)\,\mathrm{d}\zeta \\ &= \sin x \int^x \mathrm{d}\zeta - \cos x \int^x \tan\zeta\,\mathrm{d}\zeta \\ &= x\sin x + \cos x \log|\cos x| . \end{aligned} \tag{7.70}$$

The general solution is thus

$$y(x) = (\alpha + \log|\cos x|)\cos x + (\beta + x)\sin x . \tag{7.71}$$