Natural Sciences Tripos: IB Mathematical Methods I

Contents

0   Introduction

0.1   Schedule

This is a copy from the booklet of schedules.[1] Schedules are minimal for lecturing and maximal for examining; that is to say, all the material in the schedules will be lectured and only material in the schedules will be examined. The numbers in square brackets at the end of paragraphs of the schedules indicate roughly the number of lectures that will be devoted to the material in the paragraph.

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

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]

Vector calculus
Reminder of grad, div, curl, ∇^2. Divergence theorem and Stokes' theorem. Vector differential operators in orthogonal curvilinear coordinates, e.g. cylindrical and spherical polar coordinates.   [**4**]

Partial differential equations
Linear second-order partial differential equations; physical examples of occurrence, the method of separation of variables (Cartesian coordinates only).   [**3**]

Fourier transform
Fourier transforms; relation to Fourier series, simple properties and examples, delta function, convolution theorem and Parseval's theorem treated heuristically, application to diffusion equation.   [**3**]

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

Elementary Analysis
Idea of convergence and limits. Convergence of series; comparison and ratio tests. Power series of a complex variable; circle of convergence. O notation. The integral as a sum. Differentiation of an integral with respect to its limits. Schwarz's inequality.   [**2**]

Ordinary differential equations
Homogeneous equations; solution by series (without full discussion of logarithmic singularities), exemplified by Legendre's equation. Inhomogeneous equations; solution by variation of parameters, introduction to Green's function.

Sturm-Liouville theory; self-adjoint operators, eigenfunctions and eigenvalues, reality of eigenvalues and orthogonality of eigenfunctions. Eigenfunction expansions and determination of coefficients. Legendre polynomials; orthogonality.   [**7**]

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[1] See `http://www.maths.cam.ac.uk/undergrad/NST/sched/`.

[2] However, if you took course A rather than B, then you might like to recall the following extract from the schedules: *Students are ... 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.*

[3] Time is always short.

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.

† G Arfken & H Weber *Mathematical Methods for Physicists, 5th edition.* Elsevier/Academic Press, 2001 (£46.95 hardback).

† J W Dettman *Mathematical Methods in Physics and Engineering.* Dover, 1988 (£13.60 paperback).

H F Jones *Groups, Representation and Physics, 2nd edition.* Institute of Physics Publishing, 1998 (£24.99 paperback)

E Kreyszig *Advanced Engineering Mathematics, 8th edition.* Wiley, 1999 (£30.95 paperback, £92.50 hardback)

J W Leech & D J Newman *How to Use Groups.* Chapman & Hall, 1993 (out of print)

† J Mathews & R L Walker *Mathematical Methods of Physics, 2nd edition.* Pearson/Benjamin Cummings, 1970 (£68.99 hardback).

† K F Riley, M P Hobson & S J Bence *Mathematical Methods for Physics and Engineering.* 2nd ed., Cambridge University Press, 2002 (£29.95 paperback, £75.00 hardback).

R N Snieder *A guided tour of mathematical methods for the physical sciences.* Cambridge University Press, 2001 (£21.95 paperback)

There is likely to be an uncanny resemblance between my notes and Riley, Hobson & Bence. This is because we both used the same source, i.e. previous Cambridge lecture notes, and not because I have just copied out their textbook (although it is true that I have tried to align my notation with theirs)![4] Having said that, it really is a good book. A must buy.

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 15 years ago to aeronautics students at Imperial), my notes bore an uncanny resemblance to Kreyszig . . . and that was not because we were using a common source!

0.3 Lectures

- Lectures will start at 11:05 promptly with a summary of the last lecture. Please be on time since it is distracting to have people walking in late.

- I will endeavour to have a 2 minute break in the middle of the lecture for a rest and/or jokes and/or politics and/or paper aeroplanes[5]; students seem to find that the break makes it easier to concentrate throughout the lecture.[6]

- I will aim to finish by 11:55, but am not going to stop dead in the middle of a long proof/explanation.

- I will stay around for a few minutes at the front after lectures in order to answer questions.

- By all means chat to each other *quietly* if I am unclear, but please do not discuss, say, last night's football results, or who did (or did not) get drunk and/or laid. Such chatting is a distraction.

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[4] In a previous year a student hoped that Riley *et al.* were getting royalties from my lecture notes; my view is that I hope that my lecturers from 30 years ago are getting royalties from Riley *et al.*!

[5] If you throw paper aeroplanes please pick them up. I will pick up the first one to stay in the air for 5 seconds.

[6] Having said that, research suggests that within the first 20 minutes I will, at some point, have lost the attention of all of you.

- 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.

- I welcome *constructive* heckling. If I am inaudible, illegible, unclear or just plain wrong then please shout out.

- I aim to avoid the words *trivial*, *easy*, *obvious* and *yes*[7]. Let me know if I fail. I will occasionally use *straightforward* or *similarly to last time*; if it is not, email me (S.J.Cowley@damtp.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. Hence you will not get pure mathematical levels of rigour; having said that all the outline/sketch 'proofs' could in principle be tightened up given sufficient time.

- In Part IA all NST students were required to study mathematics. Consequently the lecturers adapted their presentation to account for the presence of students who might like to have been somewhere else, e.g. there were lots of how to do it 'recipes' and not much theory. This is an optional course, and as a result there will more theory than last year (although less than in the comparable mathematics courses). If you are really to use a method, or extend it as might be necessary in research, you need to understand *why* a method works, as well as *how* to apply it. FWIW the NST mathematics schedules are decided by scientists in conjunction with mathematicians.

- If anyone is colour blind please come and tell me which colour pens you cannot read.

0.4 Printed Notes

- Printed notes will be handed out for the course . . . so that you can listen to me rather than having to scribble things down. If it is not in the printed notes or on the example sheets it should not be in the exam.

- Any notes will only be available in lectures and only *once* for each set of notes.

- I do not keep back-copies (otherwise my office would be an even worse mess) . . . from which you may conclude that I will not have copies of last time's notes (so do not ask).

- There will only be approximately as many copies of the notes as there were students at the previous lecture. We are going to fell a forest as it is, and I have no desire to be even more environmentally unsound.

- Please do not take copies for your absent friends unless they are *ill*.

- The notes are deliberately *not* available on the WWW; they are an adjunct to lectures and are not meant to be used independently.

- If you do not want to attend lectures then use one of the excellent textbooks, e.g. Riley, Hobson & Bence.

- 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.

- 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 me corrections to the notes and example sheets (S.J.Cowley@damtp.cam.ac.uk).

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

0.5 Example Sheets

- There will be five example sheets. They will be available on the WWW at about the same time as I hand them out (see `http://damtp.cam.ac.uk/user/examples/`).

- You should be able to do 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 do example sheets 1/2/3/4 after lectures 6/12/18/24 respectively. Please bear this in mind when arranging supervisions.

0.6 Acknowledgements.

The following notes were adapted from those of Paul Townsend, Stuart Dalziel, Mike Proctor and Paul Metcalfe.

0.7 Revision.

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), phi (i.e. φ), and rho (i.e. ϱ).

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

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

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

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

The Gaussian. The function

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

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.

$$\frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{2\sigma^2}\right) \mathrm{d}x = 1 \,. \tag{0.4}$$
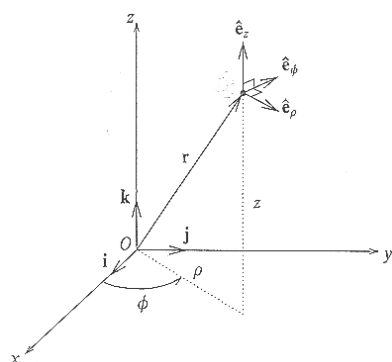
Cylindrical polar co-ordinates (ρ, ϕ, z).

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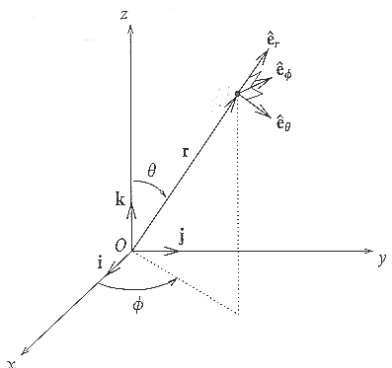
In spherical polar co-ordinates the position vector $\mathbf{r}$ is given in terms of a radial distance r from the origin, a 'latitude' angle θ, and a 'longitude' angle ϕ:

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

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

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

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

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

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 $j = 1, \ldots, m$

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

An identity. If δ_{ij} is the Kronecker delta, then for a_j $(j = 1, 2, 3)$,

$$\sum_{j=1}^{3} a_j \delta_{1j} = a_1\delta_{11} + a_2\delta_{12} + a_3\delta_{13} = a_1 , \tag{0.11a}$$

and more generally

$$\sum_{j=1}^{3} a_j \delta_{ij} = a_1\delta_{i1} + a_2\delta_{i2} + a_3\delta_{i3} = a_i . \tag{0.11b}$$

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

$$\int_{\mathcal{C}} \mathrm{d}\mathbf{r} = -\int_{-\mathcal{C}} \mathrm{d}\mathbf{r} . \tag{0.12}$$

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

$$\mathsf{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} . \tag{0.13a}$$

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

$$\mathsf{A}^{\mathrm{T}} = \begin{pmatrix} A_{11} & A_{21} & A_{31} \\ A_{12} & A_{22} & A_{32} \\ A_{13} & A_{23} & A_{33} \end{pmatrix} . \tag{0.13b}$$

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

$$f(x) = \tfrac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi nx}{\mathcal{L}}\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{2\pi nx}{\mathcal{L}}\right) , \tag{0.14a}$$

where

$$a_n = \frac{2}{\mathcal{L}} \int_{x_0}^{x_0+\mathcal{L}} f(x) \cos\left(\frac{2\pi nx}{\mathcal{L}}\right) \mathrm{d}x , \tag{0.14b}$$

$$b_n = \frac{2}{\mathcal{L}} \int_{x_0}^{x_0+\mathcal{L}} f(x) \sin\left(\frac{2\pi nx}{\mathcal{L}}\right) \mathrm{d}x , \tag{0.14c}$$

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

$$\int_0^{\mathcal{L}} \sin \frac{2\pi n x}{\mathcal{L}} \sin \frac{2\pi m x}{\mathcal{L}} \, \mathrm{d}x = \frac{\mathcal{L}}{2} \delta_{nm} , \tag{0.15a}$$

$$\int_0^{\mathcal{L}} \cos \frac{2\pi n x}{\mathcal{L}} \cos \frac{2\pi m x}{\mathcal{L}} \, \mathrm{d}x = \frac{\mathcal{L}}{2} \delta_{nm} , \tag{0.15b}$$

$$\int_0^{\mathcal{L}} \sin \frac{2\pi n x}{\mathcal{L}} \cos \frac{2\pi m x}{\mathcal{L}} \, \mathrm{d}x = 0 . \tag{0.15c}$$

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

$$g_\mathrm{e}(x) = \tfrac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi x}{L}\right) , \tag{0.16a}$$

where

$$a_n = \frac{2}{L} \int_0^L g_\mathrm{e}(x) \cos\left(\frac{n\pi x}{L}\right) \mathrm{d}x . \tag{0.16b}$$

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

$$g_\mathrm{o}(x) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right) , \tag{0.17a}$$

where

$$b_n = \frac{2}{L} \int_0^L g_\mathrm{o}(x) \sin\left(\frac{n\pi x}{L}\right) \mathrm{d}x . \tag{0.17b}$$

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

$$\int_0^L \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L} \, \mathrm{d}x = \frac{L}{2} \delta_{nm} , \tag{0.18a}$$

$$\int_0^L \cos \frac{n\pi x}{L} \cos \frac{m\pi x}{L} \, \mathrm{d}x = \frac{L}{2} \delta_{nm} , \tag{0.18b}$$

but

$$\int_0^L \sin \frac{n\pi x}{L} \cos \frac{m\pi x}{L} \, \mathrm{d}x = \begin{cases} 0 & \text{if } n+m \text{ is even,} \\[2mm] \dfrac{2nL}{\pi(n^2 - m^2)} & \text{if } n+m \text{ is odd.} \end{cases} \tag{0.18c}$$

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 §3.3.2 and §3.3.1.
6. Swap §4.2 and §4.3.
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?

Many scientific quantities just have a magnitude, e.g. time, temperature, density, concentration. 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.

1.1 Vectors and Bases

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.

Vectors exist independently of any coordinate system. However, it is often very useful to describe them in term of a *basis*. 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 in terms of scalar multiples of the basis vectors:

$$\mathbf{a} = a_1\mathbf{e}_1 + a_2\mathbf{e}_2 + a_3\mathbf{e}_3. \tag{1.1}$$

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

Note that 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*, i.e. if the basis vectors

- have unit magnitude — $|\mathbf{e}_i| = 1$ $(i = 1, 2, 3)$;

- are mutually orthogonal — $\mathbf{e}_i \cdot \mathbf{e}_j = 0$ if $i \neq j$.

These conditions can be expressed more concisely as

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \quad (i, j = 1, 2, 3), \tag{1.2}$$

where δ_{ij} is the *Kronecker delta*:

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}. \tag{1.3}$$

The orthonormal basis is *right-handed* if

$$\mathbf{e}_1 \times \mathbf{e}_2 = \mathbf{e}_3, \tag{1.4}$$

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

$$[\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3] = \mathbf{e}_1 \times \mathbf{e}_2 \cdot \mathbf{e}_3 = 1. \tag{1.5}$$

Exercise. Show using (1.2) and (1.4) that

$$\mathbf{e}_2 \times \mathbf{e}_3 = \mathbf{e}_1 \quad \text{and that} \quad \mathbf{e}_3 \times \mathbf{e}_1 = \mathbf{e}_2 \, . \tag{1.6}$$

1.1.1   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

$$\begin{aligned} \mathbf{r} &= x\,\mathbf{e}_1 + y\,\mathbf{e}_2 + z\,\mathbf{e}_3 && \text{(1.7a)} \\ &= (x, y, z)\, . && \text{(1.7b)} \end{aligned}$$

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

$$\mathbf{e}_1 = \mathbf{e}_x = \mathbf{i}\, , \quad \mathbf{e}_2 = \mathbf{e}_y = \mathbf{j} \quad \text{and} \quad \mathbf{e}_3 = \mathbf{e}_z = \mathbf{k}\, , \tag{1.8}$$

for the unit vectors in the x, y and z directions respectively. Hence from (1.2) and (1.6)

$$\mathbf{i}.\mathbf{i} = \mathbf{j}.\mathbf{j} = \mathbf{k}.\mathbf{k} = 1\, , \quad \mathbf{i}.\mathbf{j} = \mathbf{j}.\mathbf{k} = \mathbf{k}.\mathbf{i} = 0\, , \tag{1.9a}$$

$$\mathbf{i} \times \mathbf{j} = \mathbf{k}\, , \quad \mathbf{j} \times \mathbf{k} = \mathbf{i}\, , \quad \mathbf{k} \times \mathbf{i} = \mathbf{j}\, . \tag{1.9b}$$

1.2   Vector Calculus in Cartesian Coordinates.

1.2.1   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:

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

In the limit when $\delta\bullet$ becomes infinitesimal we write $\mathrm{d}\bullet$ for $\delta\bullet$.[8] Thus we have that

$$\mathrm{d}\psi = \boldsymbol{\nabla}\psi \cdot \mathrm{d}\mathbf{r}\, , \tag{1.10}$$

---

[8] 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.

where the *gradient* of ψ is defined by

$$\text{grad}\,\psi \equiv \boldsymbol{\nabla}\psi = \frac{\partial \psi}{\partial x}\mathbf{e}_x + \frac{\partial \psi}{\partial y}\mathbf{e}_y + \frac{\partial \psi}{\partial z}\mathbf{e}_z = \sum_{j=1}^{3} \frac{\partial \psi}{\partial x_j}\mathbf{e}_j \tag{1.11}$$

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

$$\boldsymbol{\nabla} \equiv \mathbf{e}_x \frac{\partial}{\partial x} + \mathbf{e}_y \frac{\partial}{\partial y} + \mathbf{e}_z \frac{\partial}{\partial z} = \sum_{j} \mathbf{e}_j \frac{\partial}{\partial x_j}\,, \tag{1.12}$$

Key Result

where $\displaystyle\sum_{j}$ will henceforth be used as a shorthand for $\displaystyle\sum_{j=1}^{3}$.

1.2.2 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

$$2r\frac{\partial r}{\partial x} = 2x\,, \quad \text{i.e.} \quad \frac{\partial r}{\partial x} = \frac{x}{r}\,. \tag{1.13a}$$

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

$$\frac{\partial r}{\partial y} = \frac{y}{r}\,, \quad \frac{\partial r}{\partial z} = \frac{z}{r}\,. \tag{1.13b}$$

Hence, from the definition of gradient (1.11),

$$\boldsymbol{\nabla}r = \left(\frac{\partial r}{\partial x}\,,\ \frac{\partial r}{\partial y}\,,\ \frac{\partial r}{\partial z}\right) = \left(\frac{x}{r}\,,\ \frac{y}{r}\,,\ \frac{z}{r}\right) = \frac{\mathbf{r}}{r}\,. \tag{1.14}$$

Key Result

Similarly, from the definition of gradient (1.11) (and from standard results for the derivative of a function of a function),

$$\begin{aligned}
\boldsymbol{\nabla}f(r) &= \left(\frac{\partial f(r)}{\partial x}\,,\ \frac{\partial f(r)}{\partial y}\,,\ \frac{\partial f(r)}{\partial z}\right) \\
&= \left(\frac{\mathrm{d}f}{\mathrm{d}r}\frac{\partial r}{\partial x}\,,\ \frac{\mathrm{d}f}{\mathrm{d}r}\frac{\partial r}{\partial y}\,,\ \frac{\mathrm{d}f}{\mathrm{d}r}\frac{\partial r}{\partial z}\right) \\
&= f'(r)\boldsymbol{\nabla}r \tag{1.15a} \\
&= f'(r)\frac{\mathbf{r}}{r}\,. \tag{1.15b}
\end{aligned}$$

1.2.3 The Geometrical Significance of Gradient

The normal to a surface. Suppose that a surface in 3D space is defined by the condition that $\psi(\mathbf{r}) = $ constant. Also suppose that for an infinitesimal, but non-zero, displacement vector $\mathrm{d}\mathbf{r}$

$$\mathrm{d}\psi \equiv \psi(\mathbf{r} + \mathrm{d}\mathbf{r}) - \psi(\mathbf{r}) = 0\,. \tag{1.16}$$

Then $\mathrm{d}\mathbf{r}$ is a tangent to the surface.

Further suppose that $\boldsymbol{\nabla}\psi \neq 0$, then from (1.10) it follows that $\boldsymbol{\nabla}\psi$ is orthogonal to $\mathrm{d}\mathbf{r}$. Moreover, since we can choose $\mathrm{d}\mathbf{r}$ to be in the direction of any tangent, we conclude that $\boldsymbol{\nabla}\psi$ is orthogonal to all tangents.

Hence $\boldsymbol{\nabla}\psi$ must be *orthogonal/normal to surfaces of constant* ψ, and so if $\widehat{\mathbf{n}}$ is the unit normal to a surface of constant ψ, then (upto a sign)

$$\widehat{\mathbf{n}} = \frac{\boldsymbol{\nabla}\psi}{|\boldsymbol{\nabla}\psi|}\,. \tag{1.17}$$

We also note from (1.10) that $\mathrm{d}\psi$ is a maximum when $\mathrm{d}\mathbf{r}$ is parallel to $\boldsymbol{\nabla}\psi$, i.e. the *direction of* $\boldsymbol{\nabla}\psi$ is *the direction in which ψ is changing most rapidly.*

The directional derivative. More generally consider the rate of change of ψ in the direction given by the unit vector $\mathbf{l}$. To this end consider $\psi(\mathbf{r} + s\mathbf{l})$. If we regard this as a function of the single variable s then we may use a Taylor series to deduce that

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

or in the limit of δs becoming infinitesimal,

$$\mathrm{d}\psi = \mathrm{d}s\,\left.\frac{\mathrm{d}}{\mathrm{d}s}\psi(\mathbf{r} + s\mathbf{l})\right|_{s=0}\,. \tag{1.18}$$

Next we note that if we substitute

$$\mathrm{d}\mathbf{r} = \mathrm{d}s\,\mathbf{l} \tag{1.19}$$

into (1.10), then we obtain

$$\mathrm{d}\psi = \mathrm{d}s\,(\mathbf{l}\cdot\boldsymbol{\nabla}\psi)\,. \tag{1.20}$$

Equating (1.18) and (1.20) yields

$$\mathbf{l}\cdot\boldsymbol{\nabla}\psi = \left.\frac{\mathrm{d}}{\mathrm{d}s}\psi(\mathbf{r} + s\mathbf{l})\right|_{s=0}\,. \tag{1.21}$$

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.*

1.2.4   Applications

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

$$\psi(\mathbf{r}) \equiv xy + yz + zx = -c\,, \tag{1.22}$$

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

$$\boldsymbol{\nabla}\psi = (y + z, x + z, y + x)\,. \tag{1.23}$$

Then from (1.17) the unit normal is given by

$$\widehat{\mathbf{n}} = \frac{\boldsymbol{\nabla}\psi}{|\boldsymbol{\nabla}\psi|} = \frac{(y + z, x + z, y + x)}{\sqrt{2(x^2 + y^2 + z^2 + xy + xz + yz)}}\,. \tag{1.24}$$

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

$$y = -z \quad \text{and} \quad x = -z\,. \tag{1.25}$$

Hence from the equation for the surface, i.e. (1.22), the points where the tangents to the surface are parallel to the (x, y) plane satisfy

$$z^2 = c. \tag{1.26}$$

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:

$$\mathbf{r}(s) = (x(s), y(s), h(x(s), y(s))). \tag{1.27}$$

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

$$\begin{aligned} \text{slope} &= \frac{\frac{\mathrm{d}h}{\mathrm{d}s}}{\sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}s}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}s}\right)^2}} \\ &= \frac{\frac{\partial h}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}s} + \frac{\partial h}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}s}}{\sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}s}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}s}\right)^2}} \qquad \text{from (0.10a)} \\ &= \mathbf{l} \cdot \boldsymbol{\nabla} h, \tag{1.28} \end{aligned}$$

where

$$\mathbf{l} = \frac{1}{\sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}s}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}s}\right)^2}} \left(\frac{\mathrm{d}x}{\mathrm{d}s}, \frac{\mathrm{d}y}{\mathrm{d}s}, 0\right). \tag{1.29}$$

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

$$\text{slope} = \frac{-4x^3 \frac{\mathrm{d}x}{\mathrm{d}s}}{\left|\frac{\mathrm{d}x}{\mathrm{d}s}\right|} = -4x^3 \operatorname{sign}\left(\frac{\mathrm{d}x}{\mathrm{d}s}\right). \tag{1.30}$$

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 $\max|\text{slope}| = 4$.

1.3 The Divergence and Curl

1.3.1 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 $\mathbf{F}(\mathbf{r})$,

$$\mathbf{F}(\mathbf{r}) = F_x(\mathbf{r})\mathbf{e}_x + F_y(\mathbf{r})\mathbf{e}_y + F_z(\mathbf{r})\mathbf{e}_z = \sum_j F_j(\mathbf{r})\mathbf{e}_j, \tag{1.31}$$

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.

1.3.2 The Divergence and Curl of a Vector Field

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

$$
\begin{aligned}
\mathrm{div}\,\mathbf{F} \;\equiv\; \boldsymbol{\nabla}\cdot\mathbf{F} \;&=\; \left(\mathbf{e}_x\frac{\partial}{\partial x}+\mathbf{e}_y\frac{\partial}{\partial y}+\mathbf{e}_z\frac{\partial}{\partial z}\right)\cdot(F_x\mathbf{e}_x+F_y\mathbf{e}_y+F_z\mathbf{e}_z)\\[1mm]
&=\; \frac{\partial F_x}{\partial x}+\frac{\partial F_y}{\partial y}+\frac{\partial F_z}{\partial z} \qquad\qquad\qquad\qquad (1.32)\\[1mm]
&=\; \sum_j \frac{\partial F_j}{\partial x_j}\,, \qquad\qquad\qquad\qquad\qquad\qquad\quad (1.33)
\end{aligned}
$$

<div align="right">Key Result</div>

from using (1.2) and remembering that in a Cartesian coordinate system the basis vectors do not depend on position.

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

$$
\begin{aligned}
\mathrm{curl}\,\mathbf{F} \;\equiv\; \boldsymbol{\nabla}\times\mathbf{F} \;&=\; \left(\mathbf{e}_x\frac{\partial}{\partial x}+\mathbf{e}_y\frac{\partial}{\partial y}+\mathbf{e}_z\frac{\partial}{\partial z}\right)\times(F_x\mathbf{e}_x+F_y\mathbf{e}_y+F_z\mathbf{e}_z)\\[1mm]
&=\; \left(\frac{\partial F_z}{\partial y}-\frac{\partial F_y}{\partial z}\right)\mathbf{e}_x+\left(\frac{\partial F_x}{\partial z}-\frac{\partial F_z}{\partial x}\right)\mathbf{e}_y+\left(\frac{\partial F_y}{\partial x}-\frac{\partial F_x}{\partial y}\right)\mathbf{e}_z \; (1.34a)\\[1mm]
&=\; \begin{vmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ \partial_x & \partial_y & \partial_z \\ F_x & F_y & F_z \end{vmatrix} \qquad\qquad\qquad\qquad (1.34b)\\[1mm]
&=\; \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ \partial_{x_1} & \partial_{x_2} & \partial_{x_3} \\ F_1 & F_2 & F_3 \end{vmatrix}\,, \qquad\qquad\qquad\quad (1.34c)
\end{aligned}
$$

<div align="right">Key Result</div>

from using (1.8) and (1.9b), and remembering that in a Cartesian coordinate system the basis vectors do not depend on position. Here $\partial_x = \frac{\partial}{\partial x}$, etc..

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1.3.3 Examples

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

   Answer.
   $$
   \boldsymbol{\nabla}\cdot\mathbf{F} = \frac{\partial(x^2 y)}{\partial x}+\frac{\partial(y^2 z)}{\partial y}+\frac{\partial(z^2 x)}{\partial z} = 2xy+2yz+2zx\,. \qquad (1.35)
   $$

   $$
   \begin{aligned}
   \boldsymbol{\nabla}\times\mathbf{F} \;&=\; \begin{vmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ \partial_x & \partial_y & \partial_z \\ x^2 y & y^2 z & z^2 x \end{vmatrix}\\[1mm]
   &=\; -y^2\mathbf{e}_x - z^2\mathbf{e}_y - x^2\mathbf{e}_z\\[1mm]
   &=\; -(y^2, z^2, x^2)\,. \qquad\qquad\qquad\qquad\qquad (1.36)
   \end{aligned}
   $$

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

   Answer. From the definition of divergence (1.32), and recalling that $\mathbf{r}=(x,y,z)$, it follows that

   $$
   \boldsymbol{\nabla}\cdot\mathbf{r} = \frac{\partial x}{\partial x}+\frac{\partial y}{\partial y}+\frac{\partial z}{\partial z} = 3\,. \qquad\qquad (1.37)
   $$

   Next, from the definition of curl (1.34a) it follows that

   $$
   \boldsymbol{\nabla}\times\mathbf{r} = \left(\frac{\partial z}{\partial y}-\frac{\partial y}{\partial z},\; \frac{\partial x}{\partial z}-\frac{\partial z}{\partial x},\; \frac{\partial y}{\partial x}-\frac{\partial x}{\partial y}\right) = 0. \qquad (1.38)
   $$

1.3.4 $\mathbf{F} \cdot \boldsymbol{\nabla}$.

In (1.32) 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

$$(\mathbf{F} \cdot \boldsymbol{\nabla}) \equiv F_x \frac{\partial}{\partial x} + F_y \frac{\partial}{\partial y} + F_z \frac{\partial}{\partial z} = \sum_j F_j \frac{\partial}{\partial x_j} \,. \qquad (1.39)$$

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

$$\mathbf{F} \cdot (\boldsymbol{\nabla} \psi) = \sum_j F_j \left(\frac{\partial \psi}{\partial x_j} \right) = \sum_j \left(F_j \frac{\partial}{\partial x_j} \right) \psi = (\mathbf{F} \cdot \boldsymbol{\nabla}) \psi \,.$$

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

$$((\mathbf{F} \cdot \boldsymbol{\nabla}) \mathbf{G})_i = \sum_j F_j \frac{\partial G_i}{\partial x_j} \,, \qquad (1.40)$$

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

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

1.4 Vector Differential Identities

Calculations involving $\boldsymbol{\nabla}$ can be much speeded 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.

$$\boldsymbol{\nabla} \cdot (\psi \, \mathbf{F}) = \psi \, \boldsymbol{\nabla} \cdot \mathbf{F} + (\mathbf{F} \cdot \boldsymbol{\nabla}) \psi \,, \qquad (1.41a)$$

$$\boldsymbol{\nabla} \times (\psi \mathbf{F}) = \psi \, (\boldsymbol{\nabla} \times \mathbf{F}) + (\boldsymbol{\nabla} \psi) \times \mathbf{F} \,, \qquad (1.41b)$$

$$\boldsymbol{\nabla} \cdot (\mathbf{F} \times \mathbf{G}) = \mathbf{G} \cdot (\boldsymbol{\nabla} \times \mathbf{F}) - \mathbf{F} \cdot (\boldsymbol{\nabla} \times \mathbf{G}) \,, \qquad (1.41c)$$

$$\boldsymbol{\nabla} \times (\mathbf{F} \times \mathbf{G}) = \mathbf{F} \, (\boldsymbol{\nabla} \cdot \mathbf{G}) - \mathbf{G} \, (\boldsymbol{\nabla} \cdot \mathbf{F}) + (\mathbf{G} \cdot \boldsymbol{\nabla}) \mathbf{F} - (\mathbf{F} \cdot \boldsymbol{\nabla}) \mathbf{G} \,, \qquad (1.41d)$$

$$\boldsymbol{\nabla} (\mathbf{F} \cdot \mathbf{G}) = (\mathbf{F} \cdot \boldsymbol{\nabla}) \mathbf{G} + (\mathbf{G} \cdot \boldsymbol{\nabla}) \mathbf{F} + \mathbf{F} \times (\boldsymbol{\nabla} \times \mathbf{G}) + \mathbf{G} \times (\boldsymbol{\nabla} \times \mathbf{F}) \,. \qquad (1.41e)$$

Example Verifications.

(1.41a):

$$
\begin{aligned}
\boldsymbol{\nabla} \cdot (\psi \, \mathbf{F}) &= \frac{\partial (\psi \, F_x)}{\partial x} + \frac{\partial (\psi \, F_y)}{\partial y} + \frac{\partial (\psi \, F_z)}{\partial z} \\
&= \psi \frac{\partial F_x}{\partial x} + F_x \frac{\partial \psi}{\partial x} + \psi \frac{\partial F_y}{\partial y} + F_y \frac{\partial \psi}{\partial y} + \psi \frac{\partial F_z}{\partial z} + F_z \frac{\partial \psi}{\partial z} \\
&= \psi \frac{\partial F_x}{\partial x} + \psi \frac{\partial F_y}{\partial y} + \psi \frac{\partial F_z}{\partial z} + F_x \frac{\partial \psi}{\partial x} + F_y \frac{\partial \psi}{\partial y} + F_z \frac{\partial \psi}{\partial z} \\
&= \psi \, \boldsymbol{\nabla} \cdot \mathbf{F} + (\mathbf{F} \cdot \boldsymbol{\nabla}) \psi \,.
\end{aligned}
$$

Unlectured. (1.41c):

$$\boldsymbol{\nabla}\cdot(\mathbf{F}\times\mathbf{G}) \;=\; \frac{\partial}{\partial x}(F_yG_z-F_zG_y)+\frac{\partial}{\partial y}(F_zG_x-F_xG_z)+\frac{\partial}{\partial z}(F_xG_y-F_yG_x)$$

$$=\; G_z\frac{\partial F_y}{\partial x}+F_y\frac{\partial G_z}{\partial x}-F_z\frac{\partial G_y}{\partial x}-G_y\frac{\partial F_z}{\partial x}+G_x\frac{\partial F_z}{\partial y}+F_z\frac{\partial G_x}{\partial y}$$

$$-F_x\frac{\partial G_z}{\partial y}-G_z\frac{\partial F_x}{\partial y}+G_y\frac{\partial F_x}{\partial z}+F_x\frac{\partial G_y}{\partial z}-F_y\frac{\partial G_x}{\partial z}-G_x\frac{\partial F_y}{\partial z}$$

$$=\; G_x\left(\frac{\partial F_z}{\partial y}-\frac{\partial F_y}{\partial z}\right)+G_y\left(\frac{\partial F_x}{\partial z}-\frac{\partial F_z}{\partial x}\right)+G_z\left(\frac{\partial F_y}{\partial x}-\frac{\partial F_x}{\partial y}\right)$$

$$+F_x\left(\frac{\partial G_y}{\partial z}-\frac{\partial G_z}{\partial y}\right)+F_y\left(\frac{\partial G_z}{\partial x}-\frac{\partial G_x}{\partial z}\right)+F_z\left(\frac{\partial G_x}{\partial y}-\frac{\partial G_y}{\partial x}\right)$$

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

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

$$\mathbf{F}\cdot(\boldsymbol{\nabla}\times\mathbf{G}) \;=\; F_x\left(\frac{\partial G_z}{\partial y}-\frac{\partial G_y}{\partial z}\right)+F_y\left(\frac{\partial G_x}{\partial z}-\frac{\partial G_z}{\partial x}\right)+F_z\left(\frac{\partial G_y}{\partial x}-\frac{\partial G_x}{\partial y}\right)\,,$$

while

$$\boldsymbol{\nabla}\cdot(\mathbf{G}\times\mathbf{F}) \;=\; F_x\left(\frac{\partial G_z}{\partial y}-\frac{\partial G_y}{\partial z}\right)+F_y\left(\frac{\partial G_x}{\partial z}-\frac{\partial G_z}{\partial x}\right)+F_z\left(\frac{\partial G_y}{\partial x}-\frac{\partial G_x}{\partial y}\right)$$

$$+G_x\left(\frac{\partial F_y}{\partial z}-\frac{\partial F_z}{\partial y}\right)+G_y\left(\frac{\partial F_z}{\partial x}-\frac{\partial F_x}{\partial z}\right)+G_z\left(\frac{\partial F_x}{\partial y}-\frac{\partial F_y}{\partial x}\right)\,.$$

1.5 Second Order Vector Differential Operators

1.5.1 $\operatorname{div}\operatorname{curl}$ **and** $\operatorname{curl}\operatorname{grad}$

Using the definitions grad, div and curl, i.e. (1.11), (1.32) and (1.34a), and assuming the equality of mixed derivatives, we have that

$$\operatorname{curl}(\operatorname{grad}\psi) \;=\; \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\psi) \;=\; \left(\frac{\partial}{\partial y}\frac{\partial\psi}{\partial z}-\frac{\partial}{\partial z}\frac{\partial\psi}{\partial y},\frac{\partial}{\partial z}\frac{\partial\psi}{\partial x}-\frac{\partial}{\partial x}\frac{\partial\psi}{\partial z},\frac{\partial}{\partial x}\frac{\partial\psi}{\partial y}-\frac{\partial}{\partial y}\frac{\partial\psi}{\partial x}\right)$$

$$=\; 0\,. \tag{1.42}$$

and

$$\operatorname{div}(\operatorname{curl}\mathbf{F}) \;=\; \boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\times\mathbf{F}) \;=\; \frac{\partial}{\partial x}\left(\frac{\partial F_z}{\partial y}-\frac{\partial F_y}{\partial z}\right)+\frac{\partial}{\partial y}\left(\frac{\partial F_x}{\partial z}-\frac{\partial F_z}{\partial x}\right)+\frac{\partial}{\partial z}\left(\frac{\partial F_y}{\partial x}-\frac{\partial F_x}{\partial y}\right)$$

$$=\; 0\,, \tag{1.43}$$

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

$$\boldsymbol{\nabla} \times \boldsymbol{\nabla} \equiv 0\,. \qquad (1.44)$$

2. There are important converses to (1.42) and (1.43). 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

   $$\mathbf{F} = \boldsymbol{\nabla}\varphi\,. \qquad (1.45)$$

   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

   $$\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}\,. \qquad (1.46)$$

   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 (1.41c). Then it follows from using (1.44) that

$$\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}p \times \boldsymbol{\nabla}q) = \boldsymbol{\nabla}q \cdot (\boldsymbol{\nabla} \times \boldsymbol{\nabla}p) - \boldsymbol{\nabla}p \cdot (\boldsymbol{\nabla} \times \boldsymbol{\nabla}q) = 0\,. \qquad (1.47)$$

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1.5.2 The Laplacian Operator ∇^2

From the definitions of div and grad

$$\mathrm{div}(\mathrm{grad}\,\psi) = \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}\psi) = \frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\partial\psi}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{\partial\psi}{\partial z}\right) = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi\,. \qquad (1.48)$$

We conclude that the *Laplacian operator*, $\nabla^2 = \boldsymbol{\nabla} \cdot \boldsymbol{\nabla}$, is given in *Cartesian coordinates* by

$$\nabla^2 = \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\,. \qquad (1.49)$$

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 $\varphi(\mathbf{r})$:

   $$\nabla^2\varphi = \rho\,, \qquad (1.50a)$$

   where (with a suitable normalisation)
      i. $\rho(\mathbf{r})$ is charge density in electromagnetism (when (1.50a) relates charge and electric potential);
      ii. $\rho(\mathbf{r})$ is mass density in gravitation (when (1.50a) relates mass and gravitational potential).

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

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{r})\psi = i\hbar\frac{\partial\psi}{\partial t}\,,\qquad(1.50\text{b})$$

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

(c) Helmholtz's equation

$$\nabla^2 f + \omega^2 f = 0\,,\qquad(1.50\text{c})$$

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

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

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

$$\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{F}) = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{F}) - \nabla^2\mathbf{F}\,.\qquad(1.51\text{a})$$

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

$$\nabla^2\mathbf{F} = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{F}) - \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{F})\,.\qquad(1.51\text{b})$$

1.5.3   Examples

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

   Answer. Put $f(r) = r^n$ in (1.15b) to obtain

$$\boldsymbol{\nabla}r^n \;=\; nr^{n-1}\frac{\mathbf{r}}{r} \;=\; nr^{n-2}\,(x,y,z)\,.\qquad(1.52)$$

So from the definition of divergence (1.32):

$$
\begin{aligned}
\nabla^2 r^n = \boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}r^n) &= \frac{\partial(nr^{n-2}x)}{\partial x} + \frac{\partial(nr^{n-2}y)}{\partial y} + \frac{\partial(nr^{n-2}z)}{\partial z}\\
&= nr^{n-2} + n(n-2)r^{n-3}\frac{x}{r}x + \ldots && \text{using (1.13a)}\\
&= 3nr^{n-2} + n(n-2)r^{n-4}(x^2+y^2+z^2)\\
&= n(n+1)r^{n-2}\,. && (1.53)
\end{aligned}
$$

From the definition of curl (1.34a):

$$
\begin{aligned}
\boldsymbol{\nabla}\times(\boldsymbol{\nabla}r^n) &= \left(\frac{\partial(nr^{n-2}z)}{\partial y} - \frac{\partial(nr^{n-2}y)}{\partial z}, \ldots, \ldots\right)\\
&= \left(n(n-2)r^{n-3}\frac{y}{r}z - n(n-2)r^{n-3}\frac{z}{r}y, \ldots, \ldots\right) && \text{using (1.13a)}\\
&= 0\,. && (1.54)
\end{aligned}
$$

Check. Note that from setting $n=2$ in (1.52) we have that $\boldsymbol{\nabla}r^2 = 2\mathbf{r}$. It follows that (1.53) and (1.54) with $n=2$ reproduce (1.37) and (1.38) respectively. (1.54) also follows from (1.42).

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 (1.15a), i.e. $\boldsymbol{\nabla}f(r) = f'(r)\boldsymbol{\nabla}r$, that

$$\boldsymbol{\nabla}\left(\frac{\sin r}{r}\right) = \left(\frac{\cos r}{r} - \frac{\sin r}{r^2}\right)\boldsymbol{\nabla}r\,.\qquad(1.55\text{a})$$

Further, we recall from (1.14) that

$$\boldsymbol{\nabla} r = \frac{\mathbf{r}}{r}\,,\tag{1.55b}$$

and also from (1.53) with $n = 1$ that

$$\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla} r) = \frac{2}{r}\,.\tag{1.55c}$$

Hence

$$
\begin{aligned}
\nabla^2\left(\frac{\sin r}{r}\right) &= \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\left(\frac{\sin r}{r}\right) \\
&= \boldsymbol{\nabla}\cdot\left(\left(\frac{\cos r}{r} - \frac{\sin r}{r^2}\right)\boldsymbol{\nabla} r\right) && \text{from (1.55a)} \\
&= \left(\frac{\cos r}{r} - \frac{\sin r}{r^2}\right)\boldsymbol{\nabla}\cdot\boldsymbol{\nabla} r + \boldsymbol{\nabla} r\cdot\boldsymbol{\nabla}\left(\frac{\cos r}{r} - \frac{\sin r}{r^2}\right) && \text{from identity (1.41a)} \\
&= 2\left(\frac{\cos r}{r^2} - \frac{\sin r}{r^3}\right) + \frac{\mathbf{r}}{r}\cdot\boldsymbol{\nabla}\left(\frac{\cos r}{r} - \frac{\sin r}{r^2}\right) && \text{from (1.55b) \& (1.55c)} \\
&= 2\left(\frac{\cos r}{r^2} - \frac{\sin r}{r^3}\right) + \frac{\mathbf{r}}{r}\cdot\left(-\frac{\sin r}{r} - \frac{2\cos r}{r^2} + \frac{2\sin r}{r^3}\right)\boldsymbol{\nabla} r && \text{using (1.15a) again} \\
&= -\frac{\sin r}{r}\,. && (1.56)
\end{aligned}
$$

Remark. It follows that $f = \frac{\sin r}{r}$ satisfies Helmholtz's equation (1.50c) for $\omega = 1$.

1.6   The Divergence Theorem and Stokes' Theorem

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

1.6.1   The Divergence Theorem (Gauss' Theorem)

Divergence Theorem. Let $\mathcal{S}$ be a 'nice' surface[9] 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.[10] Then

$$\iiint\limits_{\mathcal{V}} \boldsymbol{\nabla}\cdot\mathbf{u}\,\mathrm{d}V = \iint\limits_{\mathcal{S}(\mathcal{V})} \mathbf{u}\cdot\mathrm{d}\mathbf{S}\,,\tag{1.57}$$

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*

$$\mathrm{d}V = \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,,\tag{1.58a}$$

and

$$\mathrm{d}\mathbf{S} = \sigma_x\mathrm{d}y\,\mathrm{d}z\,\mathbf{e}_x + \sigma_y\mathrm{d}z\,\mathrm{d}x\,\mathbf{e}_y + \sigma_z\mathrm{d}x\,\mathrm{d}y\,\mathbf{e}_z\,,\tag{1.58b}$$

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.

---

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

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

$$\int_{h_1}^{h_2} \frac{\mathrm{d}f}{\mathrm{d}z} \, \mathrm{d}z = f(h_2) - f(h_1) \,, \tag{1.59}$$

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

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

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

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

Then using the second fundamental theorem of calculus (1.59)

$$\begin{aligned} \iiint_{\mathcal{V}} \frac{\partial u_z}{\partial z} \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z &= \iint_{\mathcal{A}} \left[\int_{z=h_1}^{h_2} \frac{\partial u_z}{\partial z} \mathrm{d}z \right] \mathrm{d}x \, \mathrm{d}y \\ &= \iint_{\mathcal{A}} \left(u_z(x, y, h_2(x,y)) - u_z(x, y, h_1(x,y)) \right) \mathrm{d}x \, \mathrm{d}y \,. \end{aligned} \tag{1.60}$$

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 $\mathcal{S}_2$

$$\mathrm{d}x \, \mathrm{d}y = \mathbf{e_z} \cdot \widehat{\mathbf{n}} \, \mathrm{d}S = \mathbf{e_z} \cdot \mathrm{d}\mathbf{S} \,. \tag{1.61a}$$

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

$$\mathrm{d}x \, \mathrm{d}y = -\mathbf{e_z} \cdot \mathrm{d}\mathbf{S} \,. \tag{1.61b}$$

We note that (1.61a) and (1.61b) are consistent with (1.58b) once the tricky issue of signs is sorted out. Using (1.58a), (1.61a) and (1.61b), equation (1.60) can be rewritten as

$$\iiint_{\mathcal{V}} \frac{\partial u_z}{\partial z} \, \mathrm{d}V = \iint_{\mathcal{S}_2} u_z \, \mathbf{e}_z \cdot \mathrm{d}\mathbf{S} \; + \; \iint_{\mathcal{S}_1} u_z \, \mathbf{e}_z \cdot \mathrm{d}\mathbf{S} = \iint_{\mathcal{S}} u_z \, \mathbf{e}_z \cdot \mathrm{d}\mathbf{S} \,, \tag{1.62a}$$

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

$$\iiint_{\mathcal{V}} \frac{\partial u_y}{\partial y} \, \mathrm{d}V = \iint_{\mathcal{S}} u_y \, \mathbf{e}_y \cdot \mathrm{d}\mathbf{S} \,, \qquad \iiint_{\mathcal{V}} \frac{\partial u_x}{\partial x} \, \mathrm{d}V = \iint_{\mathcal{S}} u_x \, \mathbf{e}_x \cdot \mathrm{d}\mathbf{S} \,. \tag{1.62b}$$

Adding the above results we obtain the divergence theorem (1.57):

$$\iiint_{\mathcal{V}} \boldsymbol{\nabla} \cdot \mathbf{u} \, \mathrm{d}V = \iint_{\mathcal{S}} \mathbf{u} \cdot \mathrm{d}\mathbf{S} \,.$$

1.6.2 Stokes' Theorem

Let $\mathcal{S}$ be a 'nice' open surface bounded by a 'nice' closed curve $\mathcal{C}$.[11] Let $\mathbf{u}(\mathbf{r})$ be a 'nice' vector field.[12] Then

$$\iint_{\mathcal{S}} \boldsymbol{\nabla} \times \mathbf{u} \cdot \mathrm{d}\mathbf{S} = \oint_{\mathcal{C}} \mathbf{u} \cdot \mathrm{d}\mathbf{r} \,, \tag{1.63}$$

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

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 $\mathcal{C}$.

Outline Proof. Given an extra half lecture I might just be able to get somewhere without losing too many of you. If you are really interested then my *IA Mathematical Tripos* notes on *Vector Calculus* are available on the WWW at

`http://damtp.cam.ac.uk/user/cowley/teaching/`.

1.6.3 Examples and Applications

1. 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

$$\mathbf{F} = -\iint_{\mathcal{S}} p \, \mathrm{d}\mathbf{S} \,. \tag{1.64}$$

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

$$\mathbf{e}_z \cdot \mathbf{F} = -\iint_{\mathcal{S}} p \, \mathbf{e}_z \cdot \mathrm{d}\mathbf{S} = -\iiint_{\mathcal{V}} \boldsymbol{\nabla} \cdot (p \, \mathbf{e}_z) \, \mathrm{d}V = -\iiint_{\mathcal{V}} \frac{\partial(-\rho g z)}{\partial z} \, \mathrm{d}V = g \iiint_{\mathcal{V}} \rho \, \mathrm{d}V = Mg \,, \tag{1.65a}$$

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

$$\mathbf{e}_x \cdot \mathbf{F} = -\iiint_{\mathcal{V}} \boldsymbol{\nabla} \cdot (p \, \mathbf{e}_x) \, \mathrm{d}V = -\iiint_{\mathcal{V}} \frac{\partial(-\rho g z)}{\partial x} \, \mathrm{d}V = 0 \,, \tag{1.65b}$$

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

$$\mathbf{F} = Mg \, \mathbf{e}_z \,. \tag{1.65c}$$

2. Show that provided there are no singularities, the integral

$$\int_{\mathcal{C}} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r} \,, \tag{1.66}$$

---

[11] 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 $\mathcal{C}$.

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

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 (1.42) that a curl of a gradient is zero, we have that

$$
\begin{aligned}
\int_{\mathcal{C}_1} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r} - \int_{\mathcal{C}_2} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r} \;&=\; \oint_{\widehat{\mathcal{C}}} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r} \\
&=\; \iint_{\widehat{\mathcal{S}}} \boldsymbol{\nabla} \times (\boldsymbol{\nabla}\varphi) \cdot \mathrm{d}\mathbf{S} \\
&=\; 0 \,.
\end{aligned}
$$

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

$$
\int_{\mathcal{C}_1} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r} = \int_{\mathcal{C}_2} \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\mathbf{r} \,. \qquad (1.67)
$$

Application. If 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.

3/02

1.6.4 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 (1.57)

$$
\boldsymbol{\nabla} \cdot \mathbf{u} = \lim_{|\mathcal{V}| \to 0} \frac{1}{|\mathcal{V}|} \iint_{\mathcal{S}} \mathbf{u} \cdot \mathrm{d}\mathbf{S} \,, \qquad (1.68)
$$

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

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

1.6.5 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 (1.63)

$$\widehat{\mathbf{n}} \cdot (\boldsymbol{\nabla} \times \mathbf{u}) = \lim_{\mathcal{S} \to 0} \; \frac{1}{|\mathcal{S}|} \oint_C \mathbf{u} \cdot \mathrm{d}\mathbf{r} \,, \tag{1.69}$$

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 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 $\mathbf{0}$. Then the velocity at a point $\mathbf{r}$ in the body is given by

$$\mathbf{v} = \boldsymbol{\omega} \times \mathbf{r} \,. \tag{1.70}$$

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

$$\oint_C \mathbf{v} \cdot \mathrm{d}\mathbf{r} = \int_0^{2\pi} (\omega a) \, a \, \mathrm{d}\phi = 2\pi a^2 \omega \,. \tag{1.71}$$

Hence from (1.69)

$$\widehat{\boldsymbol{\omega}} \cdot (\boldsymbol{\nabla} \times \mathbf{v}) = \lim_{a \to 0} \; \frac{1}{\pi a^2} \oint_C \mathbf{v} \cdot \mathrm{d}\mathbf{r} = 2\omega \,. \tag{1.72}$$

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

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

1.7 Orthogonal Curvilinear Coordinates

1.7.1 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 not generally much use unless the orthonormality condition (1.2), i.e. $\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$, holds; in which case they are called *orthogonal curvilinear coordinates*. The most 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

Key
Point

to a spherical shell changes direction with position on the shell. It is sometimes helpful to display this dependence on position explicitly:

$$\mathbf{e}_i \equiv \mathbf{e}_i(\mathbf{r}) \,. \tag{1.73}$$

1.7.2 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.

$$q_i \equiv q_i(x, y, z) \quad (i = 1, 2, 3) \,. \tag{1.74}$$

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 (1.74) 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

$$x = x(q_1, q_2, q_3) \,, \quad y = y(q_1, q_2, q_3) \,, \quad z = z(q_1, q_2, q_3) \,. \tag{1.75}$$

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	$r \cos \theta$

3/01

1.7.3 Incremental Change in Position or Length.

Consider an infinitesimal change in position. Then, by the chain rule, the change dx in $x(q_1, q_2, q_3)$ due to changes dq_j in q_j $(i = 1, 2, 3)$ is

$$\mathrm{d}x = \frac{\partial x}{\partial q_1}\mathrm{d}q_1 + \frac{\partial x}{\partial q_2}\mathrm{d}q_2 + \frac{\partial x}{\partial q_3}\mathrm{d}q_3 = \sum_j \frac{\partial x}{\partial q_j}\,\mathrm{d}q_j \,. \tag{1.76}$$

Using similar results for $\mathrm{d}y$ and $\mathrm{d}z$, the vector displacement $\mathrm{d}\mathbf{r}$ is

$$
\begin{aligned}
\mathrm{d}\mathbf{r} &= \mathrm{d}x\,\mathbf{e}_x + \mathrm{d}y\,\mathbf{e}_y + \mathrm{d}z\,\mathbf{e}_z \\[2mm]
&= \left(\sum_j \frac{\partial x}{\partial q_j}\,\mathrm{d}q_j \right) \mathbf{e}_x + \left(\sum_j \frac{\partial y}{\partial q_j}\,\mathrm{d}q_j \right) \mathbf{e}_y + \left(\sum_j \frac{\partial z}{\partial q_j}\,\mathrm{d}q_j \right) \mathbf{e}_z \\[2mm]
&= \sum_j \left(\frac{\partial x}{\partial q_j}\,\mathbf{e}_x + \frac{\partial y}{\partial q_j}\,\mathbf{e}_y + \frac{\partial z}{\partial q_j}\,\mathbf{e}_z \right) \mathrm{d}q_j \\[2mm]
&= \sum_j \mathbf{h}_j\,\mathrm{d}q_j\,, \quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad (1.77a)
\end{aligned}
$$

where

$$
\mathbf{h}_j = \frac{\partial x}{\partial q_j}\,\mathbf{e}_x + \frac{\partial y}{\partial q_j}\,\mathbf{e}_y + \frac{\partial z}{\partial q_j}\,\mathbf{e}_z = \frac{\partial \mathbf{r}(\mathbf{q})}{\partial q_j} \quad (j = 1, 2, 3)\,. \quad (1.77b)
$$

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 $\mathbf{r}$.

Remark. Note that the $\mathbf{h}_j$ are in general functions of $\mathbf{r}$, and hence the directions of the q-axes vary in space. Consequently the q-axes are *curves* rather than straight lines; the coordinate system is said to be a *curvilinear* one.

The vectors $\mathbf{h}_j$ are not necessarily unit vectors, so it is convenient to write

$$
\mathbf{h}_j = h_j\,\mathbf{e}_j \quad (j = 1, 2, 3)\,, \quad\quad\quad\quad\quad\quad\quad (1.78)
$$

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

$$
h_j = \left| \frac{\partial \mathbf{r}}{\partial q_j} \right| \quad \text{and} \quad \mathbf{e}_j = \frac{1}{h_j} \frac{\partial \mathbf{r}}{\partial q_j} \quad (j = 1, 2, 3)\,. \quad\quad (1.79)
$$

Again we emphasise that the *directions* of the $\mathbf{e}_j(\mathbf{r})$ will, in general, *depend on position*.

1.7.4 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

$$
\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}\,. \quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad (1.80)
$$

An identity. Recall from (0.11b) that

$$
\sum_{j=1}^{3} a_j \delta_{ij} = a_i\,. \quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad (1.81)
$$

Incremental Distance. In an orthogonal curvilinear coordinate system the expression for the incremental distance, $|d\mathbf{r}|^2$ simplifies. We find that

$$|d\mathbf{r}|^2 = d\mathbf{r} \cdot d\mathbf{r} = \left(\sum_i h_i dq_i \, \mathbf{e}_i \right) \cdot \left(\sum_j h_j dq_j \, \mathbf{e}_j \right) \qquad \text{from (1.77a) and (1.78)}$$

$$= \sum_{i,j} (h_i dq_i)(h_j dq_j) \, \mathbf{e}_i \cdot \mathbf{e}_j$$

$$= \sum_{i,j} (h_i dq_i)(h_j dq_j) \, \delta_{ij} \qquad \text{from (1.80)}$$

$$= \sum_i h_i^2 (dq_i)^2 \, . \qquad \text{from (1.81) with } a_j = h_j dq_j \qquad (1.82)$$

Key Result

Remarks.

1. All information about orthogonal curvilinear coordinate systems is encoded in the three functions h_j ($j = 1, 2, 3$).

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

1.7.5   Spherical Polar Coordinates

In this case $q_1 = r$, $q_2 = \theta$, $q_3 = \phi$ and

$$\mathbf{r} = r \sin\theta \cos\phi \, \mathbf{e}_x + r \sin\theta \sin\phi \, \mathbf{e}_y + r \cos\theta \, \mathbf{e}_z$$

$$= (r \sin\theta \cos\phi, \ r \sin\theta \sin\phi, \ r \cos\theta) \, . \qquad (1.83)$$

Hence

$$\frac{\partial \mathbf{r}}{\partial q_1} = \frac{\partial \mathbf{r}}{\partial r} = (\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta) \, ,$$

$$\frac{\partial \mathbf{r}}{\partial q_2} = \frac{\partial \mathbf{r}}{\partial \theta} = (r \cos\theta \cos\phi, r \cos\theta \sin\phi, -r \sin\theta) \, ,$$

$$\frac{\partial \mathbf{r}}{\partial q_3} = \frac{\partial \mathbf{r}}{\partial \phi} = (-r \sin\theta \sin\phi, r \sin\theta \cos\phi, 0) \, .$$

It follows from (1.79) that

$$h_1 = \left| \frac{\partial \mathbf{r}}{\partial q_1} \right| = 1 \, , \qquad \mathbf{e}_1 = \mathbf{e}_r = (\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta) \, , \qquad (1.84a)$$

$$h_2 = \left| \frac{\partial \mathbf{r}}{\partial q_2} \right| = r \, , \qquad \mathbf{e}_2 = \mathbf{e}_\theta = (\cos\theta \cos\phi, \cos\theta \sin\phi, -\sin\theta) \, , \qquad (1.84b)$$

$$h_3 = \left| \frac{\partial \mathbf{r}}{\partial q_3} \right| = r \sin\theta \, , \qquad \mathbf{e}_3 = \mathbf{e}_\phi = (-\sin\phi, \cos\phi, 0) \, . \qquad (1.84c)$$

Remarks.

- $\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$ 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.

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

- Recalling from (1.77a) and (1.78) that the h_j give the components of the displacement vector $d\mathbf{r}$ along the r, θ, and ϕ axes, we have that

$$d\mathbf{r} = \sum_j h_j \, dq_j \, \mathbf{e}_j = dr \, \mathbf{e}_r + r \, d\theta \, \mathbf{e}_\theta + r \sin\theta \, d\phi \, \mathbf{e}_\phi \, . \qquad (1.85)$$

1.7.6 Cylindrical Polar Coordinates

In this case $q_1 = \rho$, $q_2 = \phi$, $q_3 = z$ and

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

Exercise. Show that

$$
\frac{\partial \mathbf{r}}{\partial q_1} = \frac{\partial \mathbf{r}}{\partial \rho} = (\cos\phi, \sin\phi, \ 0) \,,
$$

$$
\frac{\partial \mathbf{r}}{\partial q_2} = \frac{\partial \mathbf{r}}{\partial \phi} = (-\rho \sin\phi, \ \rho \cos\phi, \ 0) \,,
$$

$$
\frac{\partial \mathbf{r}}{\partial q_3} = \frac{\partial \mathbf{r}}{\partial z} = (0, 0, 1) \,.
$$

and hence that

$$
h_1 = \left| \frac{\partial \mathbf{r}}{\partial q_1} \right| = 1 \,, \qquad \mathbf{e}_1 = \mathbf{e}_\rho = (\cos\phi, \sin\phi, 0) \,, \tag{1.86a}
$$

$$
h_2 = \left| \frac{\partial \mathbf{r}}{\partial q_2} \right| = \rho \,, \qquad \mathbf{e}_2 = \mathbf{e}_\phi = (-\sin\phi, \cos\phi, 0) \,, \tag{1.86b}
$$

$$
h_3 = \left| \frac{\partial \mathbf{r}}{\partial q_3} \right| = 1 \,, \qquad \mathbf{e}_3 = \mathbf{e}_z = (0, 0, 1) \,. \tag{1.86c}
$$

Remarks.

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

- $\mathbf{e}_\rho$ and $\mathbf{e}_\phi$ are functions of position.

1.7.7 Volume and Surface Elements in Orthogonal Curvilinear Coordinates

Consider the volume element defined by the three displacement vectors $\mathrm{d}\mathbf{r}_i \equiv h_i \, \mathbf{e}_i \mathrm{d}q_i$ along each of the three q-axes. For *orthogonal* curvilinear coordinate systems this is

$$
\begin{aligned}
\mathrm{d}V &= \mathrm{d}\mathbf{r}_1 \times \mathrm{d}\mathbf{r}_2 \cdot \mathrm{d}\mathbf{r}_3 \\
&= h_1 h_2 h_3 \, \mathrm{d}q_1 \mathrm{d}q_2 \mathrm{d}q_3 \, \mathbf{e}_1 \times \mathbf{e}_2 \cdot \mathbf{e}_3 \\
&= h_1 h_2 h_3 \, \mathrm{d}q_1 \mathrm{d}q_2 \mathrm{d}q_3 \,. \tag{1.87}
\end{aligned}
$$

Example: Spherical Polar Coordinates. For spherical polar coordinates we have from (1.84a), (1.84b), (1.84c) and (1.87) that

$$
\mathrm{d}V = r^2 \sin\theta \, \mathrm{d}r \mathrm{d}\theta \mathrm{d}\phi \,. \tag{1.88}
$$

The volume of the sphere of radius a is therefore

$$
\iiint_{\mathcal{V}} \mathrm{d}V = \int_0^a \mathrm{d}r \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \ r^2 \sin\theta = \frac{4}{3}\pi a^3 \,. \tag{1.89}
$$

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

$$
\begin{aligned}
\mathrm{d}\mathbf{S} &= (h_1 \mathrm{d}q_1 \mathbf{e}_1) \times (h_2 \mathrm{d}q_2 \mathbf{e}_2) \\
&= h_1 h_2 \, \mathrm{d}q_1 \mathrm{d}q_2 \, \mathbf{e}_3 \,.
\end{aligned} \tag{1.90}
$$

In general

$$
\mathrm{d}\mathbf{S} = \mathrm{sign}(\widehat{\mathbf{n}} \cdot \mathbf{e}_1) h_2 h_3 \, \mathrm{d}q_2 \mathrm{d}q_3 \, \mathbf{e}_1 + \mathrm{sign}(\widehat{\mathbf{n}} \cdot \mathbf{e}_2) h_3 h_1 \, \mathrm{d}q_3 \mathrm{d}q_1 \, \mathbf{e}_2 + \mathrm{sign}(\widehat{\mathbf{n}} \cdot \mathbf{e}_3) h_1 h_2 \, \mathrm{d}q_1 \mathrm{d}q_2 \, \mathbf{e}_3 \,. \tag{1.91}
$$

1.7.8 Gradient in Orthogonal Curvilinear Coordinates

First we recall from (1.10) 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 $\mathrm{d}\mathbf{r}$

$$
\mathrm{d}\psi = \boldsymbol{\nabla}\psi \cdot \mathrm{d}\mathbf{r} \,. \tag{1.92}
$$

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

$$
\boldsymbol{\nabla}\psi = \sum_i \mathbf{e}_i \alpha_i \,, \tag{1.93}
$$

then from (1.77a), (1.78), (1.80), (1.81) and (1.92)

$$
\mathrm{d}\psi = \sum_i \mathbf{e}_i \alpha_i \cdot \sum_j h_j \mathbf{e}_j \mathrm{d}q_j = \sum_{i,j} \alpha_i \, (h_j \mathrm{d}q_j) \mathbf{e}_i \cdot \mathbf{e}_j = \sum_i \alpha_i \, (h_i \mathrm{d}q_i) \,. \tag{1.94}
$$

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

$$
\begin{aligned}
\mathrm{d}\psi &= \sum_i \frac{\partial \psi}{\partial q_i} \mathrm{d}q_i \\
&= \sum_i \left(\frac{1}{h_i} \frac{\partial \psi}{\partial q_i} \right) (h_i \mathrm{d}q_i) \,.
\end{aligned} \tag{1.95}
$$

Hence, since (1.94) and (1.95) must hold for all $\mathrm{d}q_i$,

$$
\alpha_i = \frac{1}{h_i} \frac{\partial \psi}{\partial q_i} \,, \tag{1.96}
$$

and from (1.93)

$$
\boldsymbol{\nabla}\psi = \sum_i \frac{\mathbf{e}_i}{h_i} \frac{\partial \psi}{\partial q_i} = \left(\frac{1}{h_1} \frac{\partial \psi}{\partial q_1}, \frac{1}{h_2} \frac{\partial \psi}{\partial q_2}, \frac{1}{h_3} \frac{\partial \psi}{\partial q_3} \right) \,. \tag{1.97}
$$

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

$$
\boldsymbol{\nabla} = \sum_i \mathbf{e}_i \frac{1}{h_i} \frac{\partial}{\partial q_i} \,. \tag{1.98}
$$

Key
Result

1.7.9 Examples of Gradients

Cylindrical Polar Coordinates. In cylindrical polar coordinates, the gradient is given from (1.86a), (1.86b) and (1.86c) to be

$$\boldsymbol{\nabla} = \mathbf{e}_\rho \, \frac{\partial}{\partial \rho} \; + \; \mathbf{e}_\phi \, \frac{1}{\rho} \frac{\partial}{\partial \phi} \; + \; \mathbf{e}_z \, \frac{\partial}{\partial z} \,. \tag{1.99a}$$

Spherical Polar Coordinates. In spherical polar coordinates the gradient is given from (1.84a), (1.84b) and (1.84c) to be

$$\boldsymbol{\nabla} = \mathbf{e}_r \, \frac{\partial}{\partial r} \; + \; \mathbf{e}_\theta \, \frac{1}{r} \frac{\partial}{\partial \theta} \; + \; \mathbf{e}_\phi \, \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \,. \tag{1.99b}$$

1.7.10 Divergence and Curl

We can now use (1.98) 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 (1.79). Using (1.98), and the fact that (see (0.8b))

$$\frac{\partial q_i}{\partial q_j} = \delta_{ij} \,, \quad \text{i.e. that} \quad \left(\frac{\partial q_1}{\partial q_1} \right)_{q_2, q_3} = 1 \,, \quad \left(\frac{\partial q_1}{\partial q_2} \right)_{q_1, q_3} = 0 \,, \quad \text{etc.,} \tag{1.100a}$$

we can show that

$$\boldsymbol{\nabla} q_i = \sum_j \mathbf{e}_j \, \frac{1}{h_j} \frac{\partial q_i}{\partial q_j} = \sum_j \frac{\mathbf{e}_j}{h_j} \, \delta_{ij} = \frac{\mathbf{e}_i}{h_i} \,, \quad \text{i.e. that} \quad \mathbf{e}_i = h_i \boldsymbol{\nabla} q_i \,. \tag{1.100b}$$

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 (1.100b)

$$\mathbf{e}_1 = h_2 \boldsymbol{\nabla} q_2 \times h_3 \boldsymbol{\nabla} q_3 \,, \quad \text{and cyclic permutations.} \tag{1.100c}$$

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

$$\boldsymbol{\nabla} \cdot \mathbf{F} = \boldsymbol{\nabla} \cdot \left(\sum_i F_i \mathbf{e}_i \right)$$

$$= \boldsymbol{\nabla} \cdot \left((h_2 h_3 F_1) \left(\frac{\mathbf{e}_1}{h_2 h_3} \right) \right) + \text{cyclic permutations}$$

$$= \frac{\mathbf{e}_1}{h_2 h_3} \cdot \boldsymbol{\nabla} (h_2 h_3 F_1) + h_2 h_3 F_1 \boldsymbol{\nabla} \cdot \left(\frac{\mathbf{e}_1}{h_2 h_3} \right) + \text{cyclic permutations} \qquad \text{using (1.41a)}$$

$$= \frac{\mathbf{e}_1}{h_2 h_3} \cdot \sum_j \mathbf{e}_j \left(\frac{1}{h_j} \frac{\partial}{\partial q_j} (h_2 h_3 F_1) \right) + h_2 h_3 F_1 \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} q_2 \times \boldsymbol{\nabla} q_3)$$

$$+ \text{cyclic permutations} \,. \qquad \text{using (1.98) \& (1.100c)}$$

Recall from (1.80) that $\mathbf{e}_1 \cdot \mathbf{e}_j = \delta_{1j}$, and from example (1.47), 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

$$\boldsymbol{\nabla} \cdot \mathbf{F} = \frac{1}{h_1 h_2 h_3} \left(\frac{\partial}{\partial q_1} (h_2 h_3 F_1) + \frac{\partial}{\partial q_2} (h_3 h_1 F_2) + \frac{\partial}{\partial q_3} (h_1 h_2 F_3) \right) \,. \tag{1.101}$$

Key Result

Cylindrical Polar Coordinates. From (1.86a), (1.86b), (1.86c) and (1.101)

$$\operatorname{div} \mathbf{F} = \frac{1}{\rho} \frac{\partial}{\partial \rho} (\rho F_\rho) + \frac{1}{\rho} \frac{\partial F_\phi}{\partial \phi} + \frac{\partial F_z}{\partial z} \,. \tag{1.102a}$$

Spherical Polar Coordinates. From (1.84a), (1.84b), (1.84c) and (1.101)

$$\operatorname{div} \mathbf{F} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 F_r \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \; F_\theta) + \frac{1}{r \sin \theta} \frac{\partial F_\phi}{\partial \phi} \,. \tag{1.102b}$$

Curl. With a little bit of inspired rearrangement we have that

$$
\begin{aligned}
\boldsymbol{\nabla} \times \mathbf{F} = \boldsymbol{\nabla} \times \left(\sum_i F_i \mathbf{e}_i \right) \\
= \sum_i \boldsymbol{\nabla} \times \left((h_i F_i) \left(\frac{\mathbf{e}_i}{h_i} \right) \right) \\
= \sum_i \boldsymbol{\nabla}(h_i F_i) \times \frac{\mathbf{e}_i}{h_i} + \sum_i h_i F_i \left(\boldsymbol{\nabla} \times \boldsymbol{\nabla} q_i \right) \qquad \text{using (1.41b) \& (1.100b)} \\
= \sum_i \sum_j \left(\frac{1}{h_i h_j} \frac{\partial (h_i F_i)}{\partial q_j} \right) \mathbf{e}_j \times \mathbf{e}_i \,. \qquad \text{using (1.42) \& (1.98)}
\end{aligned}
$$

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

$$
\begin{aligned}
\boldsymbol{\nabla} \times \mathbf{F} = & \frac{\mathbf{e}_1}{h_2 h_3} \left(\frac{\partial (h_3 F_3)}{\partial q_2} - \frac{\partial (h_2 F_2)}{\partial q_3} \right) + \frac{\mathbf{e}_2}{h_3 h_1} \left(\frac{\partial (h_1 F_1)}{\partial q_3} - \frac{\partial (h_3 F_3)}{\partial q_1} \right) \\
& + \frac{\mathbf{e}_3}{h_1 h_2} \left(\frac{\partial (h_2 F_2)}{\partial q_1} - \frac{\partial (h_1 F_1)}{\partial q_2} \right) \,.
\end{aligned} \tag{1.103a}
$$

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

$$\boldsymbol{\nabla} \times \mathbf{F} = \frac{1}{h_1 h_2 h_3} \begin{vmatrix} h_1 \mathbf{e}_1 & h_2 \mathbf{e}_2 & h_3 \mathbf{e}_3 \\ \frac{\partial}{\partial q_1} & \frac{\partial}{\partial q_2} & \frac{\partial}{\partial q_3} \\ h_1 F_1 & h_2 F_2 & h_3 F_3 \end{vmatrix} \,. \tag{1.103b}$$

Key
Result

Cylindrical Polar Coordinates. From (1.86a), (1.86b), (1.86c) and (1.103b)

$$\operatorname{curl} \mathbf{F} = \frac{1}{\rho} \begin{vmatrix} \mathbf{e}_\rho & \rho \, \mathbf{e}_\phi & \mathbf{e}_z \\ \partial_\rho & \partial_\phi & \partial_z \\ F_\rho & \rho \, F_\phi & F_z \end{vmatrix} \tag{1.104a}$$

$$= \left(\frac{1}{\rho} \frac{\partial F_z}{\partial \phi} - \frac{\partial F_\phi}{\partial z}, \frac{\partial F_\rho}{\partial z} - \frac{\partial F_z}{\partial \rho}, \frac{1}{\rho} \frac{\partial (\rho F_\phi)}{\partial \rho} - \frac{1}{\rho} \frac{\partial F_\rho}{\partial \phi} \right) \,. \tag{1.104b}$$

Spherical Polar Coordinates. From (1.84a), (1.84b), (1.84c) and (1.103b)

$$\operatorname{curl} \mathbf{F} = \frac{1}{r^2 \sin \theta} \begin{vmatrix} \mathbf{e}_r & r \mathbf{e}_\theta & r \sin \theta \mathbf{e}_\phi \\ \partial_r & \partial_\theta & \partial_\phi \\ F_r & r F_\theta & r \sin \theta F_\phi \end{vmatrix} \tag{1.105a}$$

$$= \left(\frac{1}{r \sin \theta} \left(\frac{\partial (\sin \theta \; F_\phi)}{\partial \theta} - \frac{\partial F_\theta}{\partial \phi} \right), \frac{1}{r \sin \theta} \frac{\partial F_r}{\partial \phi} - \frac{1}{r} \frac{\partial (r F_\phi)}{\partial r}, \frac{1}{r} \frac{\partial (r F_\theta)}{\partial r} - \frac{1}{r} \frac{\partial F_r}{\partial \theta} \right). \tag{1.105b}$$

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.

1.7.11 Laplacian in Orthogonal Curvilinear Coordinates

Suppose we substitute $\mathbf{F} = \boldsymbol{\nabla}\psi$ into formula (1.101) for the divergence. Then since from (1.97)

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

we have that

$$\nabla^2\psi \equiv \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\psi = \frac{1}{h_1 h_2 h_3}\left(\frac{\partial}{\partial q_1}\left(\frac{h_2 h_3}{h_1}\frac{\partial \psi}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(\frac{h_3 h_1}{h_2}\frac{\partial \psi}{\partial q_2}\right) + \frac{\partial}{\partial q_3}\left(\frac{h_1 h_2}{h_3}\frac{\partial \psi}{\partial q_3}\right)\right). \tag{1.106}$$

We thereby deduce that in a general orthogonal curvilinear coordinate system

$$\nabla^2 = \frac{1}{h_1 h_2 h_3}\left(\frac{\partial}{\partial q_1}\left(\frac{h_2 h_3}{h_1}\frac{\partial}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(\frac{h_3 h_1}{h_2}\frac{\partial}{\partial q_2}\right) + \frac{\partial}{\partial q_3}\left(\frac{h_1 h_2}{h_3}\frac{\partial}{\partial q_3}\right)\right). \tag{1.107}$$

Cylindrical Polar Coordinates. From (1.86a), (1.86b), (1.86c) and (1.107)

$$\nabla^2\psi = \frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho\frac{\partial \psi}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 \psi}{\partial \phi^2} + \frac{\partial^2 \psi}{\partial z^2}\,. \tag{1.108a}$$

Spherical Polar Coordinates. From (1.84a), (1.84b), (1.84c) and (1.107)

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial \psi}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 \psi}{\partial \phi^2}\,, \tag{1.108b}$$

$$= \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial \psi}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 \psi}{\partial \phi^2}\,. \tag{1.108c}$$

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

$$\nabla^2\mathbf{F} = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{F}) - \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{F})\,. \tag{1.109}$$

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).

1.7.12 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 (1.102b)

$$\boldsymbol{\nabla}\cdot\mathbf{r} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\cdot r) = 3\,, \quad \text{as in (1.37).}$$

From (1.105b)

$$\boldsymbol{\nabla}\times\mathbf{r} = \left(0\,, \frac{1}{r\sin\theta}\frac{\partial r}{\partial \phi}\,, -\frac{1}{r}\frac{\partial r}{\partial \theta}\right) = (0,0,0)\,, \quad \text{as in (1.38).}$$

From (1.108c) for $r \neq 0$

$$\nabla^2\left(\frac{1}{r}\right) = \frac{1}{r}\frac{\partial^2}{\partial r^2}\left(r\left(\frac{1}{r}\right)\right) = 0\,, \quad \text{as in (1.53) with } n = -1. \tag{1.110}$$

1.7.13 Aide Memoire

Orthogonal Curvilinear Coordinates.

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

$$\operatorname{div} \mathbf{F} = \frac{1}{h_1 h_2 h_3} \left(\frac{\partial}{\partial q_1} (h_2 h_3 F_1) + \frac{\partial}{\partial q_2} (h_3 h_1 F_2) + \frac{\partial}{\partial q_3} (h_1 h_2 F_3) \right) \,.$$

$$\operatorname{curl} \mathbf{F} = \frac{1}{h_1 h_2 h_3} \begin{vmatrix} h_1 \mathbf{e}_1 & h_2 \mathbf{e}_2 & h_3 \mathbf{e}_3 \\ \frac{\partial}{\partial q_1} & \frac{\partial}{\partial q_2} & \frac{\partial}{\partial q_3} \\ h_1 F_1 & h_2 F_2 & h_3 F_3 \end{vmatrix} \,.$$

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

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

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

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

$$\operatorname{curl} \mathbf{F} = \frac{1}{\rho} \begin{vmatrix} \mathbf{e}_\rho & \rho \mathbf{e}_\phi & \mathbf{e}_z \\ \partial_\rho & \partial_\phi & \partial_z \\ F_\rho & \rho F_\phi & F_z \end{vmatrix}$$

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

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

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

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

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

$$\operatorname{curl} \mathbf{F} = \frac{1}{r^2 \sin \theta} \begin{vmatrix} \mathbf{e}_r & r \mathbf{e}_\theta & r \sin \theta \mathbf{e}_\phi \\ \partial_r & \partial_\theta & \partial_\phi \\ F_r & r F_\theta & r \sin \theta F_\phi \end{vmatrix}$$

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

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

2 Partial Differential Equations

2.0 Why Study This?

Many (most?, all?) scientific phenomena can be described by mathematical equations. An important sub-class of these equations is that of *partial differential equations*. If we can solve and/or understand such equations (and note that this is not always possible for a given equation), then this should help us understand the science.

2.1 Nomenclature

Ordinary differential equations (ODEs) are equations relating one or more unknown functions of a variable with one or more of the functions' derivatives, e.g. the second-order equation for the motion of a particle of mass m acted on by a force $\mathbf{F}$

$$m\frac{\mathrm{d}^2\mathbf{r}(t)}{\mathrm{d}t^2} = \mathbf{F}\,, \tag{2.1a}$$

or equivalently the two first-order equations

$$\dot{\mathbf{r}}(t) = \mathbf{v}(t) \quad \text{and} \quad m\dot{\mathbf{v}}(t) = \mathbf{F}(t)\,. \tag{2.1b}$$

The unknown functions are referred to as the *dependent* variables, and the quantity that they depend on is known as the *independent* variable.

Partial differential equations (PDEs) are equations relating one or more unknown functions of two or more variables with one or more of the functions' partial derivatives with respect to those variables, e.g. Schrödinger's equation (1.50b) for the quantum mechanical wave function $\psi(x, y, z, t)$ of a non-relativistic particle:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi + V(\mathbf{r})\psi = \mathrm{i}\hbar\frac{\partial\psi}{\partial t}\,. \tag{2.2}$$

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Linearity. If the system of differential equations is of the first degree in the dependent variables, then the system is said to be *linear*. Hence the above examples are linear equations. However Euler's equation for an inviscid fluid,

$$\rho\left(\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{u}\right) = -\boldsymbol{\nabla}p\,, \tag{2.3}$$

where $\mathbf{u}$ is the velocity, ρ is the density and p is the pressure, is *nonlinear* in $\mathbf{u}$.

Order. The power of the highest derivative determines the *order* of the differential equation. Hence (2.1a) and (2.2) are second-order equations, while each equation in (2.1b) is a first-order equation.

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2.1.1 Linear Second-Order Partial Differential Equations

The most general linear second-order partial differential equation in two independent variables is

$$a(x,y)\frac{\partial^2\psi}{\partial x^2} + b(x,y)\frac{\partial^2\psi}{\partial x\partial y} + c(x,y)\frac{\partial^2\psi}{\partial y^2} + d(x,y)\frac{\partial\psi}{\partial x} + e(x,y)\frac{\partial\psi}{\partial y} + f(x,y)\psi = g(x,y)\,. \tag{2.4}$$

We will concentrate on examples where the coefficients, $a(x, y)$, etc. are constants, and where there are other simplifying assumptions. However, we will not necessarily restrict ourselves to two independent variables (e.g. Schrödinger's equation (2.2) has four independent variables).

2.2 Physical Examples and Applications

2.2.1 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

$$T_2 \cos\theta_2 = T_1 \cos\theta_1 \,, \tag{2.5a}$$

$$(\rho\,\mathrm{d}x)\frac{\partial^2 y}{\partial t^2} = T_2 \sin\theta_2 - T_1 \sin\theta_1$$
$$= T_2 \cos\theta_2 \left(\tan\theta_2 - \tan\theta_1\right). \tag{2.5b}$$

In the light of (2.5a) let

$$T = T_j \cos\theta_j \quad (j = 1, 2)\,, \tag{2.6a}$$

and observe that

$$\tan\theta = \frac{\partial y}{\partial x}\,. \tag{2.6b}$$

Then from (2.5b) it follows after use of Taylor's theorem that

$$\rho\,\mathrm{d}x\,\frac{\partial^2 y}{\partial t^2} = T\left(\tan\theta_2 - \tan\theta_1\right)$$
$$= T\left(\frac{\partial}{\partial x}y(x+\mathrm{d}x, t) - \frac{\partial}{\partial x}y(x, t)\right)$$
$$= T\frac{\partial^2 y}{\partial x^2}\mathrm{d}x + \dots\,, \tag{2.7}$$

and hence, in the infinitesimal limit, that

$$\frac{\partial^2 y}{\partial t^2} = \frac{T}{\rho}\frac{\partial^2 y}{\partial x^2}\,. \tag{2.8}$$

This is the *wave equation* with wavespeed $c = \sqrt{\frac{T}{\rho}}$. In general the *one-dimensional wave equation* is

$$\frac{\partial^2 y}{\partial t^2} = c^2 \frac{\partial^2 y}{\partial x^2}\,. \tag{2.9}$$

2.2.2 Electromagnetic Waves

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 $\mathbf{J}$:

$$\boldsymbol{\nabla} \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}\,, \tag{2.10a}$$

$$\boldsymbol{\nabla} \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}\,, \tag{2.10b}$$

$$\boldsymbol{\nabla} \times \mathbf{B} = \mu_0 \mathbf{J} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}\,, \tag{2.10c}$$

$$\boldsymbol{\nabla} \cdot \mathbf{B} = 0\,, \tag{2.10d}$$

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. If there is no charge or current (i.e. $\rho = 0$ and $\mathbf{J} = 0$), then from (2.10a), (2.10b), (2.10c) and the vector identity (1.51a):

$$\frac{1}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} = \boldsymbol{\nabla} \times \frac{\partial \mathbf{B}}{\partial t} \qquad\qquad \text{using (2.10c) with } \mathbf{J} = 0$$
$$= -\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \mathbf{E}) \qquad\qquad \text{using (2.10b)}$$
$$= \nabla^2 \mathbf{E} - \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \mathbf{E}) \qquad\qquad \text{using identity (1.51a)}$$
$$= \nabla^2 \mathbf{E}\,. \qquad\qquad \text{using (2.10a) with } \rho = 0 \tag{2.11}$$

We have therefore recovered the *three-dimensional wave equation* (cf. (2.9))

$$\frac{\partial^2 \mathbf{E}}{\partial t^2} = c^2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \mathbf{E} \,. \tag{2.12}$$

Remark. The pressure perturbation of a sound waves satisfies the scalar equivalent of this equation (but with c equal to the speed of sound rather than that of light).

2.2.3 Electrostatic Fields

Suppose instead a steady electric field is generated by a known charge density ρ. Then from (2.10b)

$$\boldsymbol{\nabla} \times \mathbf{E} = 0 \,,$$

which implies from (1.45) that there exists an electric potential φ such that

$$\mathbf{E} = -\boldsymbol{\nabla}\varphi \,. \tag{2.13}$$

It then follows from the first of Maxwell's equations, (2.10a), that φ satisfies *Poisson's equation*

$$\nabla^2 \varphi = -\frac{\rho}{\epsilon_0} \,, \tag{2.14a}$$

i.e.

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \varphi = -\frac{\rho}{\epsilon_0} \,. \tag{2.14b}$$

2.2.4 Gravitational Fields

A Newtonian *gravitational field* $\mathbf{g}$ satisfies

$$\boldsymbol{\nabla} \cdot \mathbf{g} = -4\pi G \rho \,, \tag{2.15a}$$

and

$$\boldsymbol{\nabla} \times \mathbf{g} = 0 \,, \tag{2.15b}$$

where G is the gravitational constant and ρ is mass density. From the latter equation and (1.45) it follows that there exists a gravitational potential φ such that

$$\mathbf{g} = -\boldsymbol{\nabla}\varphi \,. \tag{2.16}$$

Thence from (2.15a) we deduce that the gravitational potential satisfies *Poisson's equation*

$$\nabla^2 \varphi = 4\pi G \rho \,. \tag{2.17}$$

Remark. Electrostatic and gravitational fields are similar! 5/01

2.2.5 Diffusion of a Passive Tracer

Suppose we want describe how an inert chemical diffuses through a solid or stationary fluid.[13]

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 $d\mathbf{S}$ in time δt is

$$\text{local flux} = (\mathbf{q} \cdot d\mathbf{S})\, \delta t \,.$$

---

[13] Reacting chemicals and moving fluids are slightly more tricky.

Hence the flux of chemical out of a closed surface $\mathcal{S}$ enclosing a volume $\mathcal{V}$ in time δt is

$$\text{surface flux} = \left(\iint_{\mathcal{S}} \mathbf{q} \cdot d\mathbf{S} \right) \delta t \,. \tag{2.18}$$

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

$$\left(\iint_{\mathcal{S}} \mathbf{q} \cdot d\mathbf{S} \right) \delta t = - \left(\frac{d}{dt} \iiint_{\mathcal{V}} C \, dV \right) \delta t + \left(\iiint_{\mathcal{V}} Q \, dV \right) \delta t \,. \tag{2.19a}$$

Hence using the divergence theorem (1.57), and exchanging the order of differentiation and integration,

$$\iiint_{\mathcal{V}} \left(\boldsymbol{\nabla} \cdot \mathbf{q} + \frac{\partial C}{\partial t} - Q \right) dV = 0 \,. \tag{2.19b}$$

But this is true for any volume, and so

$$\frac{\partial C}{\partial t} = -\boldsymbol{\nabla} \cdot \mathbf{q} + Q \,. \tag{2.20}$$

The simplest empirical law relating concentration flux to concentration gradient is *Fick's law*

$$\mathbf{q} = -D\boldsymbol{\nabla} C \,, \tag{2.21}$$

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

$$\frac{\partial C}{\partial t} = D\nabla^2 C + Q \,. \tag{2.22}$$

Special Cases.

Diffusion Equation. If there is no chemical source then $Q = 0$, and the governing equation becomes the *diffusion equation*

$$\frac{\partial C}{\partial t} = D\nabla^2 C \,. \tag{2.23}$$

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*

$$\nabla^2 C = -f \,. \tag{2.24}$$

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*

$$\nabla^2 C = 0 \,. \tag{2.25}$$

2.2.6 Heat Flow

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 (2.18). 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. (2.19a))

$$\left(\iint_{\mathcal{S}} \mathbf{q} \cdot \mathrm{d}\mathbf{S} \right) \delta t = -\left(\frac{\mathrm{d}}{\mathrm{d}t} \iiint_{\mathcal{V}} \rho E \, \mathrm{d}V \right) \delta t + \left(\iiint_{\mathcal{V}} Q \, \mathrm{d}V \right) \delta t \,.$$

For 'slow' changes at constant pressure (1st and 2nd law of thermodynamics)

$$E(\mathbf{r}, t) = c_p \theta(\mathbf{r}, t) \,, \tag{2.26}$$

where θ is the *temperature* and c_p is the *specific heat* (assumed constant here). Hence using the divergence theorem (1.57), and exchanging the order of differentiation and integration (cf. (2.19b)),

$$\iiint_{\mathcal{V}} \left(\boldsymbol{\nabla} \cdot \mathbf{q} + \rho c_p \frac{\partial \theta}{\partial t} - Q \right) \mathrm{d}V = 0 \,.$$

But this is true for any volume, hence

$$\rho c_p \frac{\partial \theta}{\partial t} = -\boldsymbol{\nabla} \cdot \mathbf{q} + Q \,. \tag{2.27}$$

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 (2.21))

$$\mathbf{q} = -k \boldsymbol{\nabla} \theta \,, \tag{2.28}$$

where k is the *heat conductivity*. If k is constant then the partial differential equation governing the temperature is (cf. (2.22))

$$\frac{\partial \theta}{\partial t} = \nu \nabla^2 \theta + \frac{Q}{\rho c_p} \tag{2.29}$$

where $\nu = k/(\rho c_p)$ is the *diffusivity* (or coefficient of diffusion).

2.2.7 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

$$\frac{\partial w}{\partial t} = rw - rx \frac{\partial w}{\partial x} - \tfrac{1}{2} v^2 x^2 \frac{\partial^2 w}{\partial x^2} \,, \tag{2.30}$$

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![14]

Also, despite the impression given above where all the equations except (2.3) are linear, many of the most interesting scientific (and non-scientific) equations are *nonlinear*. For instance the nonlinear Schrödinger equation

$$\mathrm{i} \frac{\partial A}{\partial t} + \frac{\partial^2 A}{\partial x^2} = A|A|^2 \,,$$

where i is the square root of -1, admits *soliton* solutions (which is one of the reasons that optical fibres work).

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[14] It's by no means clear to me what these terms mean, but `http://www.physics.uci.edu/~silverma/bseqn/bs/bs.html` is one place to start!

2.3 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

$$\underbrace{X(x)\mathrm{d}x}_{\text{function of }x} = \underbrace{Y(y)\mathrm{d}y}_{\text{function of }y} = \text{constant}.$$

Sometimes functions can we written in separable form. For instance,

$$f(x,y) = \cos x \exp y = X(x)Y(y), \quad \text{where} \quad X = \cos x \text{ and } Y = \exp y,$$

is separable in Cartesian coordinates, while

$$g(x,y,z) = \frac{1}{(x^2 + y^2 + z^2)^{\frac{1}{2}}}$$

is not separable in Cartesian coordinates, but is separable in spherical polar coordinates since

$$g = R(r)\Theta(\theta)\Phi(\phi) \quad \text{where} \quad R = \tfrac{1}{r}, \ \Theta = 1 \text{ and } \Phi = 1.$$

Solutions to partial differential equations can *sometimes* be found by seeking solutions that can be written in separable form, e.g.

$$\begin{aligned} \text{Time \& 1D Cartesians:} \quad y(x,t) &= X(x)T(t), & \text{(2.31a)}\\ \text{2D Cartesians:} \quad \psi(x,y) &= X(x)Y(y), & \text{(2.31b)}\\ \text{3D Cartesians:} \quad \psi(x,y,z) &= X(x)Y(y)Z(z), & \text{(2.31c)}\\ \text{Cylindrical Polars:} \quad \psi(\rho,\phi,z) &= R(\rho)\Phi(\phi)Z(z), & \text{(2.31d)}\\ \text{Spherical Polars:} \quad \psi(r,\theta,\phi) &= R(r)\Theta(\theta)\Phi(\phi). & \text{(2.31e)} \end{aligned}$$

However, we emphasise that *not* all solutions of partial differential equations can be written in this form.

2.4 The One Dimensional Wave Equation

2.4.1 Separable Solutions

Seek solutions $y(x,t)$ to the one dimensional wave equation (2.9), i.e.

$$\frac{\partial^2 y}{\partial t^2} = c^2 \frac{\partial^2 y}{\partial x^2}, \tag{2.32a}$$

of the form

$$y(x,t) = X(x)T(t). \tag{2.32b}$$

On substituting (2.32b) into (2.32a) we obtain

$$X\ddot{T} = c^2 T X'',$$

where a $\dot{}$ and a $'$ denote differentiation by t and x respectively. After rearrangement we have that

$$\underbrace{\frac{1}{c^2}\frac{\ddot{T}(t)}{T(t)}}_{\text{function of }t} = \underbrace{\frac{X''(x)}{X(x)}}_{\text{function of }x} = \lambda, \tag{2.33a}$$

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:

$$\ddot{T} - c^2\lambda T = 0 \quad \text{and} \quad X'' - \lambda X = 0. \tag{2.33b}$$

There are three cases to consider.

$\lambda = 0$. In this case

$$\ddot{T}(t) = X''(x) = 0 \quad \Rightarrow \quad T = A_0 + B_0 t \quad \text{and} \quad X = C_0 + D_0 x \,,$$

where A_0, B_0, C_0 and D_0 are constants, i.e.

$$y = (A_0 + B_0 t)(C_0 + D_0 x) \,. \tag{2.34a}$$

$\lambda = \sigma^2 > 0$. In this case

$$\ddot{T} - \sigma^2 c^2 T = 0 \quad \text{and} \quad X'' - \sigma^2 X = 0 \,.$$

Hence

$$T = A_\sigma e^{\sigma ct} + B_\sigma e^{-\sigma ct} \quad \text{and} \quad X = C_\sigma \cosh \sigma x + D_\sigma \sinh \sigma x \,,$$

where A_σ, B_σ, C_σ and D_σ are constants, i.e.

$$y = \left(A_\sigma e^{\sigma ct} + B_\sigma e^{-\sigma ct} \right) \left(C_\sigma \cosh \sigma x + D_\sigma \sinh \sigma x \right) \,. \tag{2.34b}$$

Alternatively we could express this as

$$y = \left(\tilde{A}_\sigma \cosh \sigma ct + \tilde{B}_\sigma \sinh \sigma ct \right) \left(\tilde{C}_\sigma e^{\sigma x} + \tilde{D}_\sigma e^{-\sigma x} \right) \,, \quad \text{or as} \ldots$$

where $\tilde{A}_\sigma$, $\tilde{B}_\sigma$, $\tilde{C}_\sigma$ and $\tilde{D}_\sigma$ are constants.

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$\lambda = -k^2 < 0$. In this case

$$\ddot{T} + k^2 c^2 T = 0 \quad \text{and} \quad X'' + k^2 X = 0 \,.$$

Hence

$$T = A_k \cos kct + B_k \sin kct \quad \text{and} \quad X = C_k \cos kx + D_k \sin kx \,,$$

where A_k, B_k, C_k and D_k are constants, i.e.

$$y = (A_k \cos kct + B_k \sin kct) (C_k \cos kx + D_k \sin kx) \,. \tag{2.34c}$$

Remark. Without loss of generality we could also impose a normalisation condition, say, $C_j^2 + D_j^2 = 1$.

2.4.2 Boundary and Initial Conditions

Solutions (2.34a), (2.34b) and (2.34c) represent three families of solutions.[15] 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 §2.2.1 has ends at $x = 0$ and $x = L$ that are fixed; appropriate *boundary conditions* are then

$$y(0, t) = 0 \quad \text{and} \quad y(L, t) = 0 \,. \tag{2.35}$$

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
>
> $$y(x, 0) = d(x) \quad \text{and} \quad \frac{\partial y}{\partial t}(x, 0) = v(x) \,. \tag{2.36}$$
>
> 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.

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[15] Or arguably one family if you wish to nit pick in the complex plane.

2.4.3 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 (2.35) are to be satisfied for all time, then in (2.34a) we must have that $C_0 = D_0 = 0$.

$\lambda > 0$. Again if the boundary conditions (2.35) are to be satisfied for all time, then in (2.34b) we must have that $C_\sigma = D_\sigma = 0$.

$\lambda < 0$. Applying the boundary conditions (2.35) to (2.34c) yields

$$C_k = 0 \quad \text{and} \quad D_k \sin kL = 0. \tag{2.37}$$

If $D_k = 0$ then the entire solution is trivial (i.e. zero), so the only useful solution has

$$\sin kL = 0 \quad \Rightarrow \quad k = \frac{n\pi}{L}, \tag{2.38}$$

where n is a non-zero integer. These special values of k are *eigenvalues* and the corresponding *eigenfunctions*, or *normal modes*, are

$$X_n = D_{\frac{n\pi}{L}} \sin \frac{n\pi x}{L}. \tag{2.39}$$

Hence, from (2.34c), solutions to (2.9) that satisfy the boundary condition (2.35) are

$$y_n(x,t) = \left(\mathcal{A}_n \cos \frac{n\pi ct}{L} + \mathcal{B}_n \sin \frac{n\pi ct}{L} \right) \sin \frac{n\pi x}{L}, \tag{2.40}$$

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 (2.9) is linear we can superimpose (i.e. add) solutions to get the general solution

$$y(x,t) = \sum_{n=1}^{\infty} \left(\mathcal{A}_n \cos \frac{n\pi ct}{L} + \mathcal{B}_n \sin \frac{n\pi ct}{L} \right) \sin \frac{n\pi x}{L}, \tag{2.41}$$

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 it has the form of a Fourier series.   6/01

The solution (2.41) satisfies the boundary conditions (2.35) by construction. The only thing left to do is to satisfy the initial conditions (2.36), i.e. we require that

$$y(x,0) = d(x) = \sum_{n=1}^{\infty} \mathcal{A}_n \sin \frac{n\pi x}{L}, \tag{2.42a}$$

$$\frac{\partial y}{\partial t}(x,0) = v(x) = \sum_{n=1}^{\infty} \mathcal{B}_n \frac{n\pi c}{L} \sin \frac{n\pi x}{L}. \tag{2.42b}$$

$\mathcal{A}_n$ and $\mathcal{B}_n$ can now be found using the orthogonality relations for sin (see (0.18a)), i.e.

$$\int_0^L \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L} \, dx = \frac{L}{2} \delta_{nm}. \tag{2.43}$$

Hence for an integer $m > 0$

$$\frac{2}{L} \int_0^L d(x) \sin \frac{m\pi x}{L} dx = \frac{2}{L} \int_0^L \left(\sum_{n=1}^{\infty} \mathcal{A}_n \sin \frac{n\pi x}{L} \right) \sin \frac{m\pi x}{L} dx$$

$$= \sum_{n=1}^{\infty} \frac{2\mathcal{A}_n}{L} \int_0^L \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L} \, dx$$

$$= \sum_{n=1}^{\infty} \frac{2\mathcal{A}_n}{L} \frac{L}{2} \delta_{nm} \qquad\qquad \text{using (2.43)}$$

$$= \mathcal{A}_m, \qquad\qquad\qquad\qquad\qquad \text{using (0.11b)} \quad\text{(2.44a)}$$

or alternatively invoke standard results for the coefficients of Fourier series. Similarly

$$\mathcal{B}_m = \frac{2}{m\pi c} \int_0^L v(x) \sin \frac{m\pi x}{L} \, \mathrm{d}x \,. \tag{2.44b}$$

2.4.4 Unlectured: Oscillation Energy

A vibrating string has both potential energy (because of the stretching of the string) and kinetic energy (because of the motion of the string). For small displacements the potential energy is approximately

$$PE = \int_0^L \tfrac{1}{2} T y'^2 \, \mathrm{d}x = \int_0^L \tfrac{1}{2} \rho \left(c y' \right)^2 \, \mathrm{d}x \,, \tag{2.45a}$$

since $c^2 = T\rho^{-1}$, and the kinetic energy is approximately

$$KE = \int_0^L \tfrac{1}{2} \rho \dot{y}^2 \, \mathrm{d}x \,. \tag{2.45b}$$

Hence from (2.41) and (2.43)

$$
\begin{aligned}
PE \;=\;& \tfrac{1}{2}\rho c^2 \int_0^L \left(\sum_{n=1}^{\infty} \left(\mathcal{A}_n \cos \frac{n\pi ct}{L} + \mathcal{B}_n \sin \frac{n\pi ct}{L} \right) \frac{n\pi}{L} \cos \frac{n\pi x}{L} \right) \times \\
& \left(\sum_{m=1}^{\infty} \left(\mathcal{A}_m \cos \frac{m\pi ct}{L} + \mathcal{B}_m \sin \frac{m\pi ct}{L} \right) \frac{m\pi}{L} \cos \frac{m\pi x}{L} \right) \mathrm{d}x \\
\;=\;& \tfrac{1}{2}\rho c^2 \sum_{m,n} \left(\mathcal{A}_n \cos \frac{n\pi ct}{L} + \mathcal{B}_n \sin \frac{n\pi ct}{L} \right) \left(\mathcal{A}_m \cos \frac{m\pi ct}{L} + \mathcal{B}_m \sin \frac{m\pi ct}{L} \right) \frac{mn\pi^2}{L^2} \frac{L}{2} \delta_{mn} \\
\;=\;& \frac{\rho \pi^2 c^2}{4L} \sum_{n=1}^{\infty} n^2 \left(\mathcal{A}_n \cos \frac{n\pi ct}{L} + \mathcal{B}_n \sin \frac{n\pi ct}{L} \right)^2 \,, \tag{2.46a}
\end{aligned}
$$

$$
\begin{aligned}
KE \;=\;& \tfrac{1}{2}\rho \int_0^L \left(\sum_{n=1}^{\infty} \frac{n\pi c}{L} \left(-\mathcal{A}_n \sin \frac{n\pi ct}{L} + \mathcal{B}_n \cos \frac{n\pi ct}{L} \right) \sin \frac{n\pi x}{L} \right) \times \\
& \left(\sum_{m=1}^{\infty} \frac{n\pi c}{L} \left(-\mathcal{A}_m \sin \frac{m\pi ct}{L} + \mathcal{B}_m \cos \frac{m\pi ct}{L} \right) \sin \frac{m\pi x}{L} \right) \mathrm{d}x \\
\;=\;& \frac{\rho \pi^2 c^2}{4L} \sum_{n=1}^{\infty} n^2 \left(-\mathcal{A}_n \sin \frac{n\pi ct}{L} + \mathcal{B}_n \cos \frac{n\pi ct}{L} \right)^2 \,. \tag{2.46b}
\end{aligned}
$$

It follows that the total energy is given by

$$E = PE + KE = \sum_{n=1}^{\infty} \frac{\rho \pi^2 c^2 n^2}{4L} \left(\mathcal{A}_n^2 + \mathcal{B}_n^2 \right) = \sum_{\text{normal modes}} (\text{energy in mode}) \,. \tag{2.46c}$$

Remark. The energy is conserved in time (since there is no dissipation). Moreover there is no transfer of energy between modes.

Exercise. Show, by averaging the PE and KE over an oscillation period, that there is equi-partition of energy over an oscillation cycle.

2.5 Poisson's Equation

Suppose we are interested in obtaining solutions to Poisson's equation

$$\nabla^2 \theta = -f \,, \tag{2.47a}$$

where, say, θ is a *steady* temperature distribution and $f = Q/(\rho c_p \nu^2)$ is a scaled heat source (see (2.29)). For simplicity let the world be two-dimensional, then (2.47a) becomes

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \theta = -f \,. \tag{2.47b}$$

Suppose we seek a separable solution as before, i.e. $\theta(x,y) = X(x)Y(y)$. Then on substituting into (2.47b) we obtain

$$\frac{X''}{X} = -\frac{Y''}{Y} - \frac{f}{XY} \,. \tag{2.48}$$

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 (2.47b) (cf. finding a particular solution when solving constant coefficient ODEs last year). The function $\Theta = \theta - \theta_s$ then satisfies Laplace's equation

$$\nabla^2 \Theta = 0 \,. \tag{2.49}$$

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).

2.5.1 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 (2.47b) then reduces to

$$\frac{\mathrm{d}^2 \theta_s}{\mathrm{d}y^2} = -1 \,, \tag{2.50a}$$

which has solution

$$\theta_s = a_0 + b_0 y - \tfrac{1}{2} y^2 \,, \tag{2.50b}$$

where a_0 and b_0 are constants.

2.5.2 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.

$$\theta = g(\mathbf{r}) \,, \tag{2.51a}$$

  where $g(\mathbf{r})$ is a known function;

- the scaled heat flux (a *Neumann* condition), i.e.

$$\frac{\partial \theta}{\partial n} \equiv \widehat{\mathbf{n}} \cdot \boldsymbol{\nabla} \theta = h(\mathbf{r}) \,, \tag{2.51b}$$

  where $h(\mathbf{r})$ is a known function;

- a mixed condition, i.e.

$$\alpha(\mathbf{r})\frac{\partial \theta}{\partial n} + \beta(\mathbf{r})\theta = d(\mathbf{r}) \,, \tag{2.51c}$$

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

$$\theta = 0 \text{ on } x = 0 \ (0 \leqslant y \leqslant 1), \ y = 0 \ (0 \leqslant x < \infty) \text{ and } y = 1 \ (0 \leqslant x < \infty), \text{ and } \frac{\partial \theta}{\partial x} \to 0 \text{ as } x \to \infty \,. \tag{2.52}$$

For these conditions it is appropriate to take $a_0 = 0$ and $b_0 = \frac{1}{2}$ in (2.50b) so that

$$\theta_s = \tfrac{1}{2}y(1 - y) \geqslant 0 \,. \tag{2.53}$$

Let $\Theta = \theta - \theta_s$, then Θ satisfies Laplace's equation (2.49) and, from (2.52) and (2.53), the boundary conditions

$$\Theta = -\tfrac{1}{2}y(1 - y) \text{ on } x = 0 \,, \ \Theta = 0 \text{ on } y = 0 \text{ and } y = 1 \,, \text{ and } \frac{\partial \Theta}{\partial x} \to 0 \text{ as } x \to \infty \,. \tag{2.54}$$

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2.5.3 Separable Solutions

On writing $\Theta(x, y) = X(x)Y(y)$ and substituting into Laplace's equation (2.49) it follows that (cf. (2.48))

$$\underbrace{\frac{X''(x)}{X(x)}}_{\text{function of } x} = \underbrace{-\frac{Y''(y)}{Y(y)}}_{\text{function of } y} = \lambda \,, \tag{2.55a}$$

so that

$$X'' - \lambda X = 0 \quad \text{and} \quad Y'' + \lambda Y = 0 \,. \tag{2.55b}$$

We can now consider each of the possibilities $\lambda = 0$, $\lambda > 0$ and $\lambda < 0$ in turn to obtain, cf. (2.34a), (2.34b) and (2.34c),

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$\lambda = 0$.

$$\Theta = (A_0 + B_0 x)(C_0 + D_0 y) \,. \tag{2.56a}$$

$\lambda = \sigma^2 > 0$.

$$\Theta = \left(A_\sigma e^{\sigma x} + B_\sigma e^{-\sigma x} \right) \left(C_\sigma \cos \sigma y + D_\sigma \sin \sigma y \right) \,. \tag{2.56b}$$

$\lambda = -k^2 < 0$.

$$\Theta = \left(A_k \cos kx + B_k \sin kx \right) \left(C_k e^{ky} + D_k e^{-ky} \right) \,. \tag{2.56c}$$

The boundary conditions at $y = 0$ and $y = 1$ in (2.54) state that $\Theta(x, 0) = 0$ and $\Theta(x, 1) = 0$. 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

$$\Theta_n = \left(\mathcal{A}_n e^{n\pi x} + \mathcal{B}_n e^{-n\pi x} \right) \sin(n\pi y) \,, \tag{2.57}$$

where $\mathcal{A}_n$ and $\mathcal{B}_n$ are constants. However, if the boundary condition in (2.54) as $x \to \infty$ is to be satisfied then $\mathcal{A}_n = 0$. Hence the solution has the form

$$\Theta = \sum_{n=1}^{\infty} \mathcal{B}_n e^{-n\pi x} \sin(n\pi y) \,. \tag{2.58}$$

The $\mathcal{B}_n$ are fixed by the first boundary condition in (2.54), i.e. we require that

$$-\tfrac{1}{2}y(1 - y) = \sum_{n=1}^{\infty} \mathcal{B}_n \sin(n\pi y) \,. \tag{2.59a}$$

Using the orthogonality relations (2.43) it follows that

$$\mathcal{B}_m = 2\frac{(-1)^m - 1}{m^3\pi^3}\,. \tag{2.59b}$$

and hence that

$$\theta \;=\; \tfrac{1}{2}y(1-y) - \sum_{\ell=0}^{\infty}\frac{4}{\pi^3(2\ell+1)^3}\,\sin((2\ell+1)\pi y)\,\mathrm{e}^{-(2\ell+1)\pi x}\,, \tag{2.60a}$$

or equivalently

$$\theta \;=\; \sum_{\ell=0}^{\infty}\frac{4}{\pi^3(2\ell+1)^3}\,\sin((2\ell+1)\pi y)\left(1-\mathrm{e}^{-(2\ell+1)\pi x}\right)\,. \tag{2.60b}$$

2.6 The Diffusion Equation

2.6.1 Separable Solutions

Seek solutions $C(x,t)$ to the one dimensional diffusion equation of the form

$$C(x,t) = X(x)T(t)\,. \tag{2.61}$$

On substituting into the one dimensional version of (2.22),

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}\,,$$

we obtain

$$X\,\dot{T} = D\,T\,X''\,.$$

After rearrangement we have that

$$\underbrace{\frac{1}{D}\frac{\dot{T}(t)}{T(t)}}_{\text{function of }t} \;=\; \underbrace{\frac{X''(x)}{X(x)}}_{\text{function of }x} \;=\; \lambda\,, \tag{2.62a}$$

where λ is again a constant. We have therefore split the PDE into two ODEs:

$$\dot{T} - D\lambda T = 0 \quad\text{and}\quad X'' - \lambda X = 0\,. \tag{2.62b}$$

There are again three cases to consider.

$\lambda = 0$. In this case
$$\dot{T}(t) = X''(x) = 0 \quad\Rightarrow\quad T = \alpha_0 \quad\text{and}\quad X = \beta_0 + \gamma_0 x\,,$$

where α_0, β_0 and γ_0 are constants. Combining these results we obtain

$$C \;=\; \alpha_0(\beta_0 + \gamma_0 x)\,,$$

or

$$C \;=\; \beta_0 + \gamma_0 x\,, \tag{2.63a}$$

since, without loss of generality (wlog), we can take $\alpha_0 = 1$.

$\lambda = \sigma^2 > 0$. In this case
$$\dot{T} - D\sigma^2 T = 0 \quad\text{and}\quad X'' - \sigma^2 X = 0\,.$$

Hence
$$T = \alpha_\sigma \exp(D\sigma^2 t) \quad\text{and}\quad X = \beta_\sigma \cosh\sigma x + \gamma_\sigma \sinh\sigma x\,,$$

where α_σ, β_σ and γ_σ are constants. On taking $\alpha_\sigma = 1$ wlog,

$$C = \exp(D\sigma^2 t)\,(\beta_\sigma \cosh\sigma x + \gamma_\sigma \sinh\sigma x)\,. \tag{2.63b}$$

$\lambda = -k^2 < 0$. In this case

$$\dot{T} + Dk^2 T = 0 \quad \text{and} \quad X'' + k^2 X = 0 \,.$$

Hence

$$T = \alpha_k \exp(-Dk^2 t) \quad \text{and} \quad X = \beta_k \cos kx + \gamma_k \sin kx \,,$$

where α_k, β_k and γ_k are constants. On taking $\alpha_k = 1$ wlog,

$$C = \exp(-Dk^2 t)\left(\beta_k \cos kx + \gamma_k \sin kx\right) \,. \tag{2.63c}$$

2.6.2 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

$$C(x,0) = 0 \,. \tag{2.64a}$$

Note that here we specify *one* initial condition based on the observation that the highest derivative in t in (2.22) 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.

$$C(0,t) = C_0 \quad \text{and} \quad C(L,t) = 0 \quad \text{for} \quad t > 0 \,. \tag{2.64b}$$

Again it is no coincidence that there two boundary conditions and the highest derivative in x is *second* order.

Remark. Equation (2.22) and conditions (2.64a) and (2.64b) 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.

2.6.3 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 (2.63b) and (2.63c) depend on time, while (2.63a) does not.

It therefore seems sensible to try and satisfy the the boundary conditions (2.64b) using the solution (2.63a). 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 (2.63a),

$$C_\infty(x) = C_0 \left(1 - \frac{x}{L}\right) \,, \tag{2.65}$$

which is just a linear variation in C from C_0 at $x = 0$ to 0 at $x = L$. Write

$$C(x,t) = C_\infty(x) + \widetilde{C}(x,t) \,, \tag{2.66}$$

where $\widetilde{C}$ is a sum of the separable time-dependent solutions (2.63b) and (2.63c). Then from the initial condition (2.64a), the boundary conditions (2.64b), and the steady solution (2.65), it follows that

$$\widetilde{C}(x,0) = -C_0 \left(1 - \frac{x}{L}\right) \,, \tag{2.67a}$$

and

$$\widetilde{C}(0,t) = 0 \quad \text{and} \quad \widetilde{C}(L,t) = 0 \quad \text{for} \quad t > 0 \,. \tag{2.67b}$$

If the homogeneous boundary conditions (2.67b) 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

$$\beta_k = 0 \quad \text{and} \quad \gamma_k \sin kL = 0 \,. \tag{2.68a}$$

It follows that if the solution is to be non trivial then

$$k = \frac{n\pi}{L} \,. \tag{2.68b}$$

The eigenfunctions corresponding to (2.68b) are

$$X_n = \Gamma_n \sin \frac{n\pi x}{L} \,, \tag{2.68c}$$

where $\Gamma_n = \gamma_{\frac{n\pi}{L}}$. Again, because (2.22) is a linear equation, we can add individual solutions to get the general solution

$$\widetilde{C}(x,t) = \sum_{n=1}^{\infty} \Gamma_n \exp\left(-\frac{n^2\pi^2 Dt}{L^2}\right) \sin \frac{n\pi x}{L} \,. \tag{2.69}$$

The Γ_n are fixed by the initial condition (2.67b):

$$-C_0\left(1 - \frac{x}{L}\right) = \sum_{n=1}^{\infty} \Gamma_n \sin \frac{n\pi x}{L} \,. \tag{2.70a}$$

Hence

$$\Gamma_m = -\frac{2C_0}{L} \int_0^L \left(1 - \frac{x}{L}\right) \sin \frac{m\pi x}{L} \mathrm{d}x = -\frac{2C_0}{m\pi} \,. \tag{2.70b}$$

The solution is thus given by

$$C \;=\; C_0\left(1 - \frac{x}{L}\right) - \sum_{n=1}^{\infty} \frac{2C_0}{n\pi} \exp\left(-\frac{n^2\pi^2 D t}{L^2}\right) \sin \frac{n\pi x}{L} \,. \tag{2.71a}$$

or from using (2.70a)

$$C \;=\; \sum_{n=1}^{\infty} \frac{2C_0}{n\pi} \left(1 - \exp\left(-\frac{n^2\pi^2 D t}{L^2}\right)\right) \sin \frac{n\pi x}{L} \,. \tag{2.71b}$$
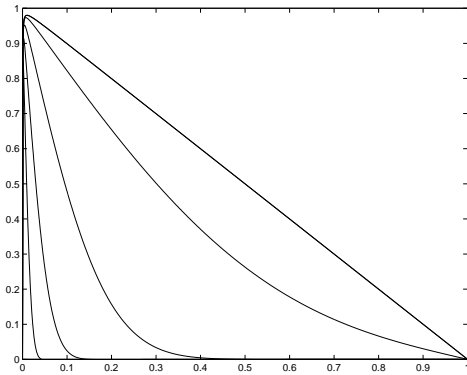
The solution (2.71b) with $C_0 = 1$ and $L = 1$, plotted at times $t = 0.0001$, $t = 0.001$, $t = 0.01$, $t = 0.1$ and $t = 1$ (curves from left to right respectively).

Paradox. $\sin \frac{n\pi x}{L}$ is not a separable solution of the diffusion equation.

Remark. As $t \to \infty$ in (2.71a)

$$C \to C_0\left(1 - \frac{x}{L}\right) = C_\infty(x)\,. \tag{2.72}$$

Remark. Solution (2.71b) 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.

3   Fourier Transforms

3.0   Why Study This?

Fourier transforms, like Fourier series, tell you about the *spectral* (or harmonic) properties of functions. As such they are useful diagnostic tools for experiments. Here we will primarily use Fourier transforms to solve differential equations that model important aspects of science.

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

3.1.1   The Delta Function as the Limit of a Sequence

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

$$\delta_\varepsilon(x) = \begin{cases} 0 & x < -\varepsilon \\ \frac{1}{2\varepsilon} & -\varepsilon \leqslant x \leqslant \varepsilon \\ 0 & \varepsilon < x \end{cases} . \qquad (3.1a)$$

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

$$\int_{-\infty}^{\infty} \delta_\varepsilon(x)\,\mathrm{d}x = 1 . \qquad (3.1b)$$

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 $g'(x) = f(x)$

$$\begin{aligned} \lim_{\varepsilon \to 0+} \int_{-\infty}^{\infty} \delta_\varepsilon(x-\xi)f(x)\,\mathrm{d}x &= \lim_{\varepsilon \to 0+} \frac{1}{2\varepsilon}\Big(\ g(\xi) + \varepsilon g'(\xi) + \tfrac{1}{2}\varepsilon^2 g''(\xi) + \ldots \\ &\qquad\qquad -g(\xi) + \varepsilon g'(\xi) - \tfrac{1}{2}\varepsilon^2 g''(\xi) + \ldots\Big) \\ &= f(\xi). \end{aligned} \qquad (3.1c)$$

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

$$\delta(x) = \lim_{\varepsilon \to 0+} \delta_\varepsilon(x) . \qquad (3.2)$$

Applications. Delta functions are the mathematical way of modelling point objects/properties, e.g. point charges, point forces, point sinks/sources.

3.1.2   Some Properties of the Delta Function

Taking (3.2) as our 'definition' of a delta function, we infer the following.

1. From (3.1a) we see that the delta function has an *infinitely sharp peak of zero width*, i.e.

$$\delta(x) = \begin{cases} \infty & x = 0 \\ 0 & x \neq 0 \end{cases} . \qquad (3.3a)$$

2. From (3.1b) it follows that the delta function has *unit area*, i.e.

$$\int_{-\alpha}^{\beta} \delta(x)\,\mathrm{d}x = 1 \quad \text{for any } \alpha > 0,\ \beta > 0\,. \tag{3.3b}$$

3. From (3.1c), 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.

$$\int_{-\infty}^{\infty} \delta(x - \xi) f(x)\,\mathrm{d}x = f(\xi)\,. \tag{3.3c}$$

3.1.3 An Alternative (And Better) View

- The delta function $\delta(x)$ is *not* a function, but a *distribution* or *generalised function*.

- (3.3c) 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 'good' functions $f(x)$[16]

$$\int_{-\infty}^{\infty} \delta(x - \xi) f(x)\,\mathrm{d}x = f(\xi)\,. \tag{3.4}$$

- Given that $\delta(x)$ is defined within an integrand as a linear operator, it should always be employed in an integrand as a linear operator.[17]

3.1.4 The Delta Function as the Limit of Other Sequences

The sequence represented by (3.1a) is not unique in tending to the delta function in an appropriate limit; there are many such sequences of well-defined functions.

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

$$\delta_\varepsilon(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{\imath kx - \varepsilon|k|}\,\mathrm{d}k \tag{3.5a}$$

$$= \frac{1}{2\pi} \left(\int_{-\infty}^{0} e^{\imath kx + \varepsilon k}\,\mathrm{d}k + \int_{0}^{\infty} e^{\imath kx - \varepsilon k}\,\mathrm{d}k \right)$$

$$= \frac{1}{2\pi} \left(\frac{1}{\imath x + \varepsilon} - \frac{1}{\imath x - \varepsilon} \right)$$

$$= \frac{\varepsilon}{\pi(x^2 + \varepsilon^2)}\,. \tag{3.5b}$$

We note by substituting $x = \varepsilon y$ that (cf. (3.1b))

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

Also, by means of the substitution $x = (\xi + \varepsilon z)$ followed by an application of Taylor's theorem, the analogous result to (3.1c) follows, namely 8/03

$$\lim_{\varepsilon \to 0+} \int_{-\infty}^{\infty} \delta_\varepsilon(x - \xi) f(x)\,\mathrm{d}x = \lim_{\varepsilon \to 0+} \int_{-\infty}^{\infty} \delta_\varepsilon(\varepsilon z) f(\xi + \epsilon z)\,\varepsilon\mathrm{d}z$$

$$= \lim_{\varepsilon \to 0+} \int_{-\infty}^{\infty} \frac{1}{\pi(z^2 + 1)} \left(f(\xi) + \varepsilon z f'(\xi) + \dots \right)\mathrm{d}z$$

$$= f(\xi)\,.$$

---

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

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

[17] However we will not always be holier than thou: see (3.6).

Hence, if we are willing to break the injunction that $\delta(x)$ should always be employed in an integrand as a linear operator, we can infer from (3.5a) that

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{\imath kx} \, dk \,. \tag{3.6}$$

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

$$\delta_\varepsilon(x) = \frac{1}{\sqrt{2\pi\varepsilon^2}} \exp\left(-\frac{x^2}{2\varepsilon^2}\right) \,. \tag{3.7a}$$

The analogous result to (3.1b) follows by means of the substitution $x = \sqrt{2}\,\varepsilon y$:

$$\int_{-\infty}^{\infty} \delta_\varepsilon(x) \, dx = \frac{1}{\sqrt{2\pi\varepsilon^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{2\varepsilon^2}\right) \, dx = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp\left(-y^2\right) \, dy = 1 \,. \tag{3.7b}$$

The equivalent result to (3.1c) can also be recovered, as above, by the substitution $x = (\xi + \sqrt{2}\,\varepsilon z)$ followed by an application of Taylor's theorem.

3.1.5 Further Properties of the Delta Function

The following properties hold for all the definitions of $\delta_\varepsilon(x)$ above (i.e. (3.1a), (3.5a) and (3.7a)), and thence for δ by the limiting process. Alternatively they can be deduced from (3.6).

1. $\delta(x)$ is symmetric. From (3.6) it follows using the substitution $k = -\ell$ that

$$\delta(-x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-\imath kx} \, dk = -\frac{1}{2\pi} \int_{\infty}^{-\infty} e^{\imath \ell x} \, d\ell = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{\imath \ell x} \, d\ell = \delta(x) \,. \tag{3.8a}$$

2. $\delta(x)$ is real. From (3.6) and (3.8a), with * denoting a complex conjugate, it follows that

$$\delta^*(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-\imath kx} \, dk = \delta(-x) = \delta(x) \,. \tag{3.8b}$$

3.1.6 The Heaviside Step Function

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

$$H(x) = \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases} \,. \tag{3.9}$$

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 (3.3a) and (3.3b)

$$H(x) = \int_{-\infty}^{x} \delta(\xi) \, d\xi. \tag{3.10a}$$

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

$$H'(x) = \delta(x) \,. \tag{3.10b}$$

Unlectured Remark. As a check on (3.10b) we see from integrating by parts that

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

Hence from the definition the delta function (3.4) we may identify $H'(x)$ with $\delta(x)$.   8/01

3.1.7   The Derivative of the Delta Function

We can define the derivative of $\delta(x)$ by using (3.3a), (3.3c) and a formal integration by parts:

$$
\int_{-\infty}^{\infty} \delta'(x-\xi)f(x)\,\mathrm{d}x = \left[\delta(x-\xi)f(x) \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \delta(x-\xi)f'(x)\,\mathrm{d}x = -f'(\xi). \tag{3.11}
$$

3.2   The Fourier Transform

3.2.1   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

$$
\widetilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath k x} f(x)\,\mathrm{d}x\,. \tag{3.12}
$$

Notation. Sometimes it will be clearer to denote the Fourier transform of a function f by $\mathcal{F}[f]$ rather than $\widetilde{f}$, i.e.

$$
\mathcal{F}[\bullet] \equiv \widetilde{\bullet}\,. \tag{3.13}
$$

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 $-\imath k x$ is replaced by $+\imath k x$.

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*:

$$
\begin{aligned}
\widetilde{f}^*(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\imath k x} f^*(x)\,\mathrm{d}x && \text{from c.c. of (3.12)} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\imath k x} f(-x)\,\mathrm{d}x && \text{since } f^*(x) = f(-x) \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath k y} f(y)\,\mathrm{d}y && \text{let } x = -y \\
&= \widetilde{f}(k)\,. && \text{from (3.12)} \qquad (3.14)
\end{aligned}
$$

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.

3.2.2 Examples of Fourier Transforms

The Fourier Transform (FT) of $\mathrm{e}^{-b|x|}$ $(b > 0)$**.** First, from (3.5a) and (3.5b) 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

$$\int_{-\infty}^{\infty} \mathrm{e}^{\imath \ell x - b|x|} \, \mathrm{d}x = \frac{2b}{\ell^2 + b^2} \, . \tag{3.15}$$

We deduce from the definition of a Fourier transform, (3.12), and (3.15) with $\ell = -k$, that

$$\mathcal{F}[\mathrm{e}^{-b|x|}] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx - b|x|} \, \mathrm{d}x$$

$$= \frac{1}{\sqrt{2\pi}} \frac{2b}{k^2 + b^2} \, . \tag{3.16}$$

The FTs of $\cos(ax)\,\mathrm{e}^{-b|x|}$ **and** $\sin(ax)\,\mathrm{e}^{-b|x|}$ $(b > 0)$**.** *Unlectured.* From (3.12), the definition of cosine, and (3.15) first with $\ell = a - k$ and then with $\ell = a + k$, it follows that

$$\mathcal{F}[\cos(ax)\,\mathrm{e}^{-b|x|}] = \frac{1}{2\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\mathrm{e}^{\imath ax} + \mathrm{e}^{-\imath ax}\right) \mathrm{e}^{-\imath kx - b|x|} \, \mathrm{d}x$$

$$= \frac{b}{\sqrt{2\pi}} \left(\frac{1}{(a-k)^2 + b^2} + \frac{1}{(a+k)^2 + b^2} \right) \, . \tag{3.17a}$$

This is real, as it has to be since $\cos(ax)\,\mathrm{e}^{-b|x|}$ is even.

Similarly, from (3.12), the definition of sine, and (3.15) first with $\ell = a - k$ and then with $\ell = a + k$, it follows that

$$\mathcal{F}[\sin(ax)\,\mathrm{e}^{-b|x|}] = \frac{1}{2\imath\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\mathrm{e}^{\imath ax} - \mathrm{e}^{-\imath ax}\right) \mathrm{e}^{-\imath kx - b|x|} \, \mathrm{d}x$$

$$= \frac{-\imath b}{\sqrt{2\pi}} \left(\frac{1}{(a-k)^2 + b^2} - \frac{1}{(a+k)^2 + b^2} \right) \, . \tag{3.17b}$$

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 (3.12), the completion of a square, and the substitution $x = (\varepsilon y - \imath \varepsilon^2 k)$,[18] it follows that

$$\mathcal{F}\left[\frac{1}{\sqrt{2\pi\varepsilon^2}} \exp\left(-\frac{x^2}{2\varepsilon^2} \right) \right] = \frac{1}{2\pi\varepsilon} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{2\varepsilon^2} - \imath kx \right) \, \mathrm{d}x$$

$$= \frac{1}{2\pi\varepsilon} \int_{-\infty}^{\infty} \exp\left(-\tfrac{1}{2}\left(\frac{x}{\varepsilon} + \imath\varepsilon k \right)^2 - \tfrac{1}{2}\varepsilon^2 k^2 \right) \, \mathrm{d}x$$

$$= \frac{1}{2\pi} \exp\left(-\tfrac{1}{2}\varepsilon^2 k^2 \right) \int_{-\infty}^{\infty} \exp\left(-\tfrac{1}{2}y^2 \right) \, \mathrm{d}y$$

$$= \frac{1}{\sqrt{2\pi}} \exp\left(-\tfrac{1}{2}\varepsilon^2 k^2 \right) \, . \tag{3.18}$$

Hence the FT of a Gaussian is a Gaussian.

The FT of the delta function. From definitions (3.4) and (3.12) it follows that

$$\mathcal{F}[\delta(x-a)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x-a)\mathrm{e}^{-\imath kx} \, \mathrm{d}x$$

$$= \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-\imath ka} \, . \tag{3.19a}$$

---

[18] 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.

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 (3.7a), we note that this result with $a = 0$ is consistent with (3.18) in the limit $\varepsilon \to 0+$.

The FT of the step function. From (3.9) and (3.12) it follows that

$$
\begin{aligned}
\mathcal{F}[H(x - a)] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} H(x - a) \mathrm{e}^{-\imath kx} \, \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi}} \int_{a}^{\infty} \mathrm{e}^{-\imath kx} \, \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi}} \left[\frac{\mathrm{e}^{-\imath kx}}{-\imath k} \right]_{a}^{\infty}
\end{aligned}
$$

We now have 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 §3.1.4) to find $\mathcal{F}[H(x - a)\mathrm{e}^{-\varepsilon(x-a)}]$ for $\varepsilon > 0$, and then let $\varepsilon \to 0+$. So

$$
\begin{aligned}
\mathcal{F}[H(x - a)\mathrm{e}^{-\varepsilon(x-a)}] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} H(x - a)\mathrm{e}^{-\varepsilon(x-a)-\imath kx} \, \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi}} \left[\frac{\mathrm{e}^{-\varepsilon(x-a)-\imath kx}}{-\varepsilon - \imath k} \right]_{a}^{\infty} \\
&= \frac{1}{\sqrt{2\pi}} \frac{\mathrm{e}^{-\imath ka}}{\varepsilon + \imath k} .
\end{aligned}
\tag{3.19b}
$$

On taking the limit $\varepsilon \to 0$ we have that

$$
\mathcal{F}[H(x - a)] = \frac{\mathrm{e}^{-\imath ka}}{\sqrt{2\pi}\, \imath k} .
\tag{3.19c}
$$

Remark. For future reference we observe from a comparison of (3.19a) and (3.19c) that

$$
\imath k \mathcal{F}[H(x - a)] = \mathcal{F}[\delta(x - a)] .
\tag{3.19d}
$$

9/02
9/04

3.2.3 The Fourier Inversion Theorem

Given a function f we can compute its Fourier transform $\widetilde{f}$ from (3.12). 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)

$$
\begin{aligned}
\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\imath kx} \widetilde{f}(k) \, \mathrm{d}k &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\imath kx} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath k\bullet} f(\bullet) \, \mathrm{d}\bullet \right) \mathrm{d}k && \text{from definition (3.12)} \\
&= \int_{-\infty}^{\infty} \mathrm{d}\bullet \, f(\bullet) \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k \, \mathrm{e}^{\imath k(x-\bullet)} \right) && \text{swap integration order} \\
&= \int_{-\infty}^{\infty} \mathrm{d}\bullet \, f(\bullet) \, \delta(x - \bullet) && \text{from definition (3.6)} \\
&= f(x) . && \text{from definition (3.4)}
\end{aligned}
$$

We thus have the result that if the Fourier transform of $f(x)$ is defined by

$$
\widetilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} f(x) \, \mathrm{d}x \equiv \mathcal{F}[f] ,
\tag{3.20a}
$$

then the *inverse transform* (note the change of sign in the exponent) acting on $\widetilde{f}(k)$ recovers $f(x)$, i.e.

$$
f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\imath kx} \widetilde{f}(k) \, \mathrm{d}k \equiv \mathcal{I}[\widetilde{f}] .
\tag{3.20b}
$$

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Note that

$$\mathcal{I}\left[\mathcal{F}\left[f\right]\right] = f\,, \quad \text{and} \quad \mathcal{F}\left[\mathcal{I}\left[\widetilde{f}\right]\right] = \widetilde{f}\,. \tag{3.20c}$$

Example. Find the Fourier transform of $(x^2 + b^2)^{-1}$.

Answer. From (3.16)

$$\mathcal{F}\left[\mathrm{e}^{-b|x|}\right](k) = \frac{1}{\sqrt{2\pi}}\,\frac{2b}{k^2 + b^2}\,.$$

Hence from (3.20c)

$$\sqrt{\frac{\pi}{2b^2}}\,\mathrm{e}^{-b|x|} = \mathcal{I}\left[\frac{1}{k^2 + b^2}\right](x)\,,$$

or, after applying the transformation $x \leftrightarrow k$,

$$\mathcal{I}\left[\frac{1}{x^2 + b^2}\right](k) = \sqrt{\frac{\pi}{2b^2}}\,\mathrm{e}^{-b|k|}\,. \tag{3.21a}$$

But, from the transformation $x \leftrightarrow k$ in (3.20b) and comparison with (3.20a), we see that

$$\mathcal{F}[f(x)](k) = \mathcal{I}[f(x)](-k)\,. \tag{3.21b}$$

Hence, making the transformation $k \to -k$ in (3.21a), we find that

$$\mathcal{F}\left[\frac{1}{x^2 + b^2}\right](k) = \sqrt{\frac{\pi}{2b^2}}\,\mathrm{e}^{-b|k|}\,. \tag{3.21c}$$

3.2.4 Properties of Fourier Transforms

A couple of useful properties of Fourier transforms follow from (3.20a) and (3.20b). In particular we shall see that an important property of the Fourier transform is that it allows a simple representation of derivatives of $f(x)$. This has important consequences when we come to solve differential equations. However, before we derive these properties we need to get Course A students upto speed.

Lemma. Suppose $g(x,k)$ is a function of two variables, then for constants a and b

$$\frac{\mathrm{d}}{\mathrm{d}x}\int_a^b g(x,k)\,\mathrm{d}k = \int_a^b \frac{\partial g(x,k)}{\partial x}\,\mathrm{d}k\,. \tag{3.22}$$

Proof. Work from first principles, then

$$\frac{\mathrm{d}}{\mathrm{d}x}\int_a^b g(x,k)\,\mathrm{d}k = \lim_{\varepsilon \to 0}\frac{1}{\varepsilon}\left(\int_a^b g(x+\varepsilon,k)\,\mathrm{d}k - \int_a^b g(x,k)\,\mathrm{d}k\right)$$

$$= \int_a^b \lim_{\varepsilon \to 0}\left(\frac{g(x+\varepsilon,k) - g(x,k)}{\varepsilon}\right)\mathrm{d}k$$

$$= \int_a^b \frac{\partial g(x,k)}{\partial x}\,\mathrm{d}k\,.$$

Differentiation. If we differentiate the inverse Fourier transform (3.20b) with respect to x we obtain

$$\frac{\mathrm{d}f}{\mathrm{d}x}(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{e}^{\imath k x}\left(\imath k \widetilde{f}(k)\right)\mathrm{d}k = \mathcal{I}\left[\imath k \widetilde{f}\right]\,. \tag{3.23}$$

Now Fourier transform this equation to conclude from using (3.20c) that

$$\mathcal{F}\left[\frac{\mathrm{d}f}{\mathrm{d}x}\right] = \mathcal{F}\left[\mathcal{I}\left[\imath k \widetilde{f}\right]\right] = \imath k \widetilde{f}\,. \tag{3.24a}$$

In other words, each time we differentiate a function we multiply its Fourier transform by $\imath k$. Hence

$$\mathcal{F}\left[\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right] = -k^2 \widetilde{f} \quad \text{and} \quad \mathcal{F}\left[\frac{\mathrm{d}^n f}{\mathrm{d}x^n}\right] = (\imath k)^n \widetilde{f}\,. \tag{3.24b}$$

Multiplication by x. This time we differentiate (3.20a) with respect to k to obtain

$$\frac{\mathrm{d}\widetilde{f}}{\mathrm{d}k}(k) \;=\; \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx}\left(-\imath x f(x)\right)\mathrm{d}x\,.$$

Hence, after multiplying by $\imath$, we deduce from (3.12) that (cf. (3.24a))

$$\imath\,\frac{\mathrm{d}\widetilde{f}}{\mathrm{d}k} \;=\; \mathcal{F}\left[xf(x)\right]\,. \tag{3.25}$$

Translation. The Fourier transform of $f(x-a)$ is given by

$$
\begin{aligned}
\mathcal{F}[f(x-a)] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} f(x-a)\,\mathrm{d}x && \text{from (3.12)}\\[2mm]
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath k(y+a)} f(y)\,\mathrm{d}y && x = y+a\\[2mm]
&= \mathrm{e}^{-\imath ka}\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath ky} f(y)\,\mathrm{d}y && \text{rearrange}\\[2mm]
&= \mathrm{e}^{-\imath ka}\mathcal{F}[f(x)] && \text{from (3.12).} \tag{3.26}
\end{aligned}
$$

See (3.19a) and (3.19c) for a couple of examples that we have already done.

3.2.5 Parseval's Theorem

Parseval's theorem states that if $f(x)$ is a complex function of x with Fourier transform $\widetilde{f}(k)$, then

$$\int_{-\infty}^{\infty} \left|f(x)\right|^2\mathrm{d}x = \int_{-\infty}^{\infty} \left|\widetilde{f}(k)\right|^2\mathrm{d}k\,. \tag{3.27}$$

'Proof'.

$$
\begin{aligned}
\int_{-\infty}^{\infty}\left|f(x)\right|^2\mathrm{d}x &= \int_{-\infty}^{\infty}\mathrm{d}x\,f(x)f^*(x)\\[2mm]
&= \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x\left[\int_{-\infty}^{\infty}\mathrm{d}k\,\mathrm{e}^{\imath kx}\widetilde{f}(k)\right]\left[\int_{-\infty}^{\infty}\mathrm{d}\ell\,\mathrm{e}^{-\imath \ell x}\widetilde{f}^*(\ell)\right] && \text{from (3.20b) \& (3.20b)}^*\\[2mm]
&= \int_{-\infty}^{\infty}\mathrm{d}k\,\widetilde{f}(k)\int_{-\infty}^{\infty}\mathrm{d}\ell\,\widetilde{f}^*(\ell)\left(\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x\,\mathrm{e}^{\imath(k-\ell)x}\right) && \text{swap integration order}\\[2mm]
&= \int_{-\infty}^{\infty}\mathrm{d}k\,\widetilde{f}(k)\int_{-\infty}^{\infty}\mathrm{d}\ell\,\widetilde{f}^*(\ell)\,\delta(k-\ell) && \text{from (3.6)}\\[2mm]
&= \int_{-\infty}^{\infty}\mathrm{d}k\,\widetilde{f}(k)\widetilde{f}^*(k) && \text{from (3.4) \& (3.8a)}\\[2mm]
&= \int_{-\infty}^{\infty}\left|\widetilde{f}(k)\right|^2\mathrm{d}k\,.
\end{aligned}
$$

Unlectured Example. Find the Fourier transform of $x\mathrm{e}^{-|x|}$ and use Parseval's theorem to evaluate the integral

$$\int_{-\infty}^{\infty}\frac{k^2}{(1+k^2)^4}\,\mathrm{d}k\,.$$

Answer. From (3.16) with $b=1$

$$\mathcal{F}\left[\mathrm{e}^{-|x|}\right] = \frac{1}{\sqrt{2\pi}}\frac{2}{1+k^2}\,. \tag{3.28a}$$

Next employ (3.25) to obtain

$$\mathcal{F}\left[x\mathrm{e}^{-|x|}\right] = \imath\,\frac{\partial}{\partial k}\mathcal{F}\left[\mathrm{e}^{-|x|}\right] = -\imath\,\sqrt{\frac{2}{\pi}}\frac{2k}{(1+k^2)^2}\,. \tag{3.28b}$$

Then from Parseval's theorem (3.27) and a couple of integrations by parts

$$\int_{-\infty}^{\infty} \frac{k^2}{(1+k^2)^4}\,\mathrm{d}k = \frac{\pi}{8}\int_{-\infty}^{\infty} x^2 \mathrm{e}^{-2|x|}\,\mathrm{d}x = \frac{\pi}{4}\int_{0}^{\infty} x^2 \mathrm{e}^{-2x}\,\mathrm{d}x = \frac{\pi}{16}\,. \tag{3.28c}$$

An Application: Heisenberg's Uncertainty Principle. Suppose that

$$\psi(x) = \frac{1}{(2\pi\Delta_x^2)^{\frac{1}{4}}}\,\exp\left(-\frac{x^2}{4\Delta_x^2}\right) \tag{3.29}$$

is the [real] wave-function of a particle in quantum mechanics. Then, according to quantum mechanics,

$$|\psi^2(x)| = \frac{1}{\sqrt{2\pi\Delta_x^2}}\,\exp\left(-\frac{x^2}{2\Delta_x^2}\right)\,, \tag{3.30}$$

is the probability of finding the particle at position x, and Δ_x is the root mean square deviation in position. Note that since $|\psi^2|$ is the Gaussian of width Δ_x,

$$\int_{-\infty}^{\infty} |\psi^2(x)|\,\mathrm{d}x = \frac{1}{\sqrt{2\pi\Delta_x^2}}\int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{2\Delta_x^2}\right)\,\mathrm{d}x = 1\,. \tag{3.31}$$

Hence there is unit probability of finding the particle somewhere! The Fourier transform of $\psi(x)$ follows from (3.18) after the substitution $\varepsilon = \sqrt{2}\,\Delta_x$ and a multiplicative normalisation:

$$\widetilde{\psi}(k) = \left(\frac{2\Delta_x^2}{\pi}\right)^{\frac{1}{4}}\exp\left(-\Delta_x^2 k^2\right)$$

$$= \frac{1}{(2\pi\Delta_k^2)^{\frac{1}{4}}}\,\exp\left(-\frac{k^2}{4\Delta_k^2}\right) \quad \text{where} \quad \Delta_k = \frac{1}{2\Delta_x}\,. \tag{3.32}$$

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

$$\int_{-\infty}^{\infty} |\widetilde{\psi}(k)^2|\,\mathrm{d}k = 1\,. \tag{3.33}$$

We note that for the Gaussian $\Delta_k \Delta_x = \frac{1}{2}$. More generally, one can show that for *any* (possibly complex) wave-function $\psi(x)$,

$$\Delta_k \Delta_x \geqslant \tfrac{1}{2} \tag{3.34}$$

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 (3.34), 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 (3.34), namely

$$\Delta p\,\Delta x \geqslant \tfrac{1}{2}\hbar\,. \tag{3.35}$$

A general property of Fourier transforms that follows from (3.34) 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 obtain an approximately monochromatic signal.

3.2.6 The Convolution Theorem

The *convolution*, $f * g$, of a function $f(x)$ with a function $g(x)$ is defined by

$$(f * g)(x) = \int_{-\infty}^{\infty} dy \, f(y) \, g(x - y). \tag{3.36}$$

Property: $*$ is commutative. $f * g = g * f$ since

$$
\begin{aligned}
(f * g)(x) &= \int_{-\infty}^{\infty} dy \, f(y) \, g(x - y) && \text{from (3.36)} \\
&= \int_{\infty}^{-\infty} (-\, dz) \, f(x - z) \, g(z) && z = x - y \\
&= \int_{-\infty}^{\infty} dy \, f(x - y) \, g(y) && z \to y \\
&= (g * f)(x) && \text{from (3.36).}
\end{aligned}
$$

The Fourier transform $\mathcal{F}[f * g]$. If the functions f and g have Fourier transforms $\mathcal{F}[f]$ and $\mathcal{F}[g]$ respectively, then

$$\mathcal{F}[f * g] = \sqrt{2\pi}\, \mathcal{F}[f]\mathcal{F}[g], \tag{3.37}$$

since

$$
\begin{aligned}
\mathcal{F}[f * g] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, e^{-\imath kx} \left(\int_{-\infty}^{\infty} dy \, f(y) \, g(x - y) \right) && \text{from (3.12) \& (3.36)} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy \, f(y) \int_{-\infty}^{\infty} dx \, e^{-\imath kx} g(x - y) && \text{swap integration order} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy \, f(y) \int_{-\infty}^{\infty} dz \, e^{-\imath k(z + y)} g(z) && x = z + y \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy \, f(y) \, e^{-\imath ky} \int_{-\infty}^{\infty} dz \, e^{-\imath kz} g(z) && \text{rearrange} \\
&= \sqrt{2\pi}\, \mathcal{F}[f]\mathcal{F}[g] && \text{from (3.12).}
\end{aligned}
$$

The Fourier transform $\mathcal{F}[fg]$. 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.

$$\mathcal{F}[fg] = \frac{1}{\sqrt{2\pi}}\, \mathcal{F}[f] * \mathcal{F}[g], \tag{3.38}$$

since

$$
\begin{aligned}
\mathcal{F}[fg](k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, e^{-\imath kx} f(x)g(x) && \text{from (3.12)} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, e^{-\imath kx} \, g(x) \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\ell \, e^{\imath \ell x} \widetilde{f}(\ell) \right) && \text{from (3.20b) with } k \to \ell \\
&= \frac{1}{\sqrt{2\pi}} \int_{\infty}^{\infty} d\ell \, \widetilde{f}(\ell) \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, e^{-i(k-\ell)x} \, g(x) \right) && \text{swap integration order} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\ell \, \widetilde{f}(\ell) \, \widetilde{g}(k - \ell) && \text{from (3.12)} \\
&= \frac{1}{\sqrt{2\pi}} (\widetilde{f} * \widetilde{g})(k) \equiv \frac{1}{\sqrt{2\pi}} \left(\mathcal{F}[f] * \mathcal{F}[g] \right)(k) && \text{from (3.36).}
\end{aligned}
$$

Application. 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 $R(\omega)\exp{(\imath\omega t)} = G(\omega)F(\omega)\exp{(\imath\omega t)}$.

Moreover, since the 'black box' is *linear* we can superpose input/output, and hence an input

$$f(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(\omega)\,\mathrm{e}^{\imath\omega t}\,\mathrm{d}\omega\,, \tag{3.39}$$

will produce an output

$$\begin{aligned}
r(t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} G(\omega)F(\omega)\,\mathrm{e}^{\imath\omega t}\,\mathrm{d}\omega \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left(\frac{1}{\sqrt{2\pi}}\mathcal{F}[f*g]\right)\mathrm{e}^{\imath\omega t}\mathrm{d}\omega && \text{from (3.37)} \\
&= \frac{1}{\sqrt{2\pi}}\,(f*g)(t)\,, && \text{from (3.20b)} \tag{3.40}
\end{aligned}$$

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.

Remark. If the know the output of a linear black box for all possible harmonic inputs, then we know everything about the black box.

10/02
10/0

Unlectured Example. A linear electronic device is such that an input $f(t) = H(t)\mathrm{e}^{-\alpha t}$ yields an output

$$r(t) = \frac{H(t)(\mathrm{e}^{-\alpha t} - \mathrm{e}^{-\beta t})}{\beta - \alpha}\,.$$

What is the output for an input $h(t)$?

Answer. Let $F(\omega)$ and $R(\omega)$ be the Fourier transforms of $f(t)$ and $r(t)$ respectively. Then, since the device is linear, the principle of superposition means that an input $F(\omega)\exp{(\imath\omega t)}$ produces an output $R(\omega)\exp{(\imath\omega t)}$, and that an input $\exp{(\imath\omega t)}$ produces an output $G(\omega)\exp{(\imath\omega t)}$ where $G = R/F$.

Next we note from (3.19b) with $\varepsilon = \alpha$, $a = 0$ and $k = \omega$, that the Fourier transform of the input is

$$F(\omega) \equiv \mathcal{F}[H(t)\mathrm{e}^{-\alpha t}] = \frac{1}{\sqrt{2\pi}}\frac{1}{\alpha + \imath\omega}\,. \tag{3.41a}$$

Similarly, the Fourier transform of the output is

$$R(\omega) \equiv \mathcal{F}\left[\frac{H(t)(\mathrm{e}^{-\alpha t} - \mathrm{e}^{-\beta t})}{\beta - \alpha}\right] = \frac{1}{\sqrt{2\pi}\,(\beta - \alpha)}\left(\frac{1}{\alpha + \imath\omega} - \frac{1}{\beta + \imath\omega}\right)\,. \tag{3.41b}$$

Hence

$$G(\omega) = \frac{R(\omega)}{F(\omega)} = \frac{1}{\beta - \alpha}\left(1 - \frac{\alpha + \imath\omega}{\beta + \imath\omega}\right) = \frac{1}{\beta + \imath\omega}\,. \tag{3.42a}$$

It then follows from (3.41a) that the inverse transform of $G(\omega)$ is given by

$$g(t) = \sqrt{2\pi}H(t)\mathrm{e}^{-\beta t}\,. \tag{3.42b}$$

We can now use the result from the previous example to deduce from (3.40) (with the change of notation $f \to h$) that the output $\mathcal{H}(t)$ to an input $h(t)$ is given by

$$\begin{aligned}
\mathcal{H}(t) &= \frac{1}{\sqrt{2\pi}}\,(h*g)(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}y\,h(y)\,g(t-y) && \text{from definition (3.36)} \\
&= \int_{-\infty}^{\infty}\mathrm{d}y\,h(y)H(t-y)\,\mathrm{e}^{-\beta(t-y)} && \text{from (3.42b)} \\
&= \int_{-\infty}^{t}\mathrm{d}y\,h(y)\,\mathrm{e}^{\beta(y-t)} && H(t-y) = 0 \quad\text{for}\quad y > t \\
&= \int_{0}^{\infty}\mathrm{d}\sigma\,h(t-\sigma)\,\mathrm{e}^{-\beta\sigma}\,. && y = t - \sigma \tag{3.43}
\end{aligned}$$

3.2.7 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

$$f(x) = \sum_{n=-\infty}^{\infty} a_n \exp\left(\frac{2\pi \imath n x}{L}\right), \tag{3.44a}$$

where

$$a_n = \frac{1}{L} \int_{-\frac{1}{2}L}^{\frac{1}{2}L} f(x) \exp\left(-\frac{2\pi \imath n x}{L}\right) \mathrm{d}x. \tag{3.44b}$$

Expression (3.44a) can be viewed as a superposition of an infinite number of waves with wavenumbers $k_n = 2\pi n/L$ $(n = -\infty, \ldots, \infty)$. 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.

$$\int_{-\infty}^{\infty} g(k)\,\mathrm{d}k = \lim_{\Delta k \to 0} \sum_{n=-\infty}^{\infty} g(k_n)\Delta k \quad \text{where} \quad k_n = n\Delta k. \tag{3.45}$$

Rewrite (3.44a) and (3.44b) as

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \widetilde{f}(k_n) \exp\left(\imath x k_n\right) \Delta k,$$

and

$$\widetilde{f}(k_n) = \frac{1}{\sqrt{2\pi}} \int_{-\frac{1}{2}L}^{\frac{1}{2}L} f(x) \exp\left(-\imath x k_n\right) \mathrm{d}x,$$

where

$$\widetilde{f}(k_n) = \frac{L a_n}{\sqrt{2\pi}}.$$

We then see that in the limit $\Delta k \to 0$, i.e. $L \to \infty$,

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{f}(k) \exp\left(\imath x k\right) \mathrm{d}k, \tag{3.46a}$$

and

$$\widetilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp\left(-\imath x k\right) \mathrm{d}x. \tag{3.46b}$$

These are just our earlier definitions of the inverse Fourier transform (3.20b) and Fourier transform (3.12) respectively.

3.3 Application: Solution of Differential Equations

Fourier transforms can be used as a method for solving differential equations. We consider two examples.

3.3.1 An Ordinary Differential Equation.

Suppose that $\psi(x)$ satisfies

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - a^2\psi = -f(x), \tag{3.47}$$

where a is a constant and f is a known function. Suppose also that ψ satisfies the [two] boundary conditions $|\psi| \to 0$ as $|x| \to \infty$.

Suppose that we multiply the left-hand side (3.47) by $\frac{1}{\sqrt{2\pi}}\exp\left(-\imath kx\right)$ and integrate over x. Then

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} \left(\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - a^2\psi\right) \mathrm{d}x = \mathcal{F}\left(\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}\right) - a^2\mathcal{F}\left(\psi\right) \qquad \text{from (3.12)}$$

$$= -k^2\mathcal{F}\left(\psi\right) - a^2\mathcal{F}\left(\psi\right) \qquad \text{from (3.24b)}. \qquad (3.48\mathrm{a})$$

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

$$-k^2\mathcal{F}\left(\psi\right) - a^2\mathcal{F}\left(\psi\right) = -\mathcal{F}\left(f\right). \qquad (3.48\mathrm{b})$$

Rearranging this equation we have that

$$\mathcal{F}\left(\psi\right) = \frac{\mathcal{F}\left(f\right)}{k^2 + a^2}, \qquad (3.48\mathrm{c})$$

and so from the inverse transform (3.20b) we have the solution

$$\psi = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{\imath kx} \frac{\mathcal{F}\left(f\right)}{k^2 + a^2} \, \mathrm{d}k. \qquad (3.48\mathrm{d})$$

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?

3.3.2 The Diffusion Equation

Consider the diffusion equation (see (2.23) or (2.29)) governing the evolution of, say, temperature, $\theta(x,t)$:

$$\frac{\partial\theta}{\partial t} = \nu\frac{\partial^2\theta}{\partial x^2}. \qquad (3.49)$$

In § 2.6 we have seen how separable solutions and Fourier series can be used to solve (3.49) over finite x-intervals. Fourier transforms can be used to solve (3.49) when the range of x is infinite.[19]

We will assume boundary conditions such as

$$\theta \to \text{constant} \quad \text{and} \quad \frac{\partial\theta}{\partial x} \to 0 \quad \text{as} \quad |x| \to \infty, \qquad (3.50)$$

so that the Fourier transform of θ exists (at least in a generalised sense):

$$\widetilde{\theta}(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} \, \theta \, \mathrm{d}x. \qquad (3.51)$$

If we then multiply the left hand side of (3.49) by $\frac{1}{\sqrt{2\pi}}\exp\left(-\imath kx\right)$ and integrate over x we obtain the time derivative of $\widetilde{\theta}$:

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} \frac{\partial\theta}{\partial t} \, \mathrm{d}x = \frac{\partial}{\partial t}\left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} \, \theta \, \mathrm{d}x\right) \qquad \text{swap differentiation and integration}$$

$$= \frac{\partial\widetilde{\theta}}{\partial t} \qquad \text{from (3.51)}.$$

A similar manipulation of the right hand side of (3.49) yields

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\imath kx} \left(\nu\frac{\partial^2\theta}{\partial x^2}\right) \mathrm{d}x = -\nu k^2\widetilde{\theta} \qquad \text{from (3.24b)}.$$

---

[19] Semi-infinite ranges can also be tackled by means of suitable 'tricks': see the example sheet.

Putting the left hand side and the right hand side together it follows that $\widetilde{\theta}(k,t)$ satisfies

$$\frac{\partial \widetilde{\theta}}{\partial t} + \nu k^2 \widetilde{\theta} = 0\,. \tag{3.52a}$$

This equation has solution

$$\widetilde{\theta}(k,t) = \gamma(k)\exp(-\nu k^2 t)\,, \tag{3.52b}$$

where $\gamma(k)$ is an unknown function of k (cf. the Γ_n in (2.69)).

Suppose that the temperature distribution is known at a specific time, wlog $t = 0$. Then from evaluating (3.52b) at $t = 0$ we have that

$$\gamma(k) = \widetilde{\theta}(k,0) \quad \text{and so} \quad \widetilde{\theta}(k,t) = \widetilde{\theta}(k,0)\exp(-\nu k^2 t)\,. \tag{3.53}$$

But from definition (3.12)

$$\widetilde{\theta}(k,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\imath k y} \theta(y,0)\,\mathrm{d}y\,, \tag{3.54a}$$

and so

$$\widetilde{\theta}(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(-\imath k y - \nu k^2 t)\,\theta(y,0)\,\mathrm{d}y\,. \tag{3.54b}$$

We can now use the Fourier inversion formula to find $\theta(x,t)$:

$$\theta(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k\, e^{\imath k x}\widetilde{\theta}(k,t) \qquad\qquad \text{from (3.20b)}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k\, e^{\imath k x} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(-\imath k y - \nu k^2 t)\,\theta(y,0)\,\mathrm{d}y \right) \qquad \text{from (3.54b)}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}y\, \theta(y,0) \int_{-\infty}^{\infty} \mathrm{d}k\, \exp(\imath k(x-y) - \nu k^2 t) \qquad\qquad \text{swap integration order.}$$

From completing the square, or alternatively from our earlier calculation of the Fourier transform of a Gaussian (see (3.18) and apply the transformations $\varepsilon \to (2\nu t)^{-\frac{1}{2}}$, $k \to (y-x)$ and $x \to k$), we have that

$$\int_{-\infty}^{\infty} \mathrm{d}k\, \exp\left(\imath k(x-y) - \nu k^2 t\right) = \sqrt{\frac{\pi}{\nu t}} \exp\left(-\frac{(x-y)^2}{4\nu t}\right)\,. \tag{3.55}$$

Substituting into the above expression for $\theta(x,t)$ we obtain a solution to the diffusion equation in terms of the initial condition at $t = 0$:

$$\theta(x,t) = \frac{1}{\sqrt{4\pi\nu t}} \int_{-\infty}^{\infty} \mathrm{d}y\, \theta(y,0) \exp\left(-\frac{(x-y)^2}{4\nu t}\right)\,. \tag{3.56a}$$

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

$$\theta(x,t) = \frac{\theta_0}{\sqrt{4\pi\nu t}}\ \exp\left(-\frac{x^2}{4\nu t}\right)\,. \tag{3.56b}$$

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 $t^{\frac{1}{2}}$.

4 Matrices

4.0 Why Study This?

A very good question (since this material is as dry as the Sahara). A general answer is that matrices are essential mathematical tools: you have to know how to manipulate them. A more specific answer is that we will study Hermitian matrices, and observables in quantum mechanics are Hermitian operators. We will also study eigenvalues, and you should have come across these sufficiently often in your science courses to know that they are an important mathematical concept.

4.1 Vector Spaces

The concept of a vector in three-dimensional Euclidean space can be generalised to n dimensions.

4.1.1 Some Notation

First some notation.

Notation	Meaning
$\in$	in
$\exists$	there exists
$\forall$	for all

4.1.2 Definition

A set of elements, or 'vectors', are said to form a *complex linear vector space* V if

1. there exists a *binary operation*, say *addition*, under which the set V is *closed* so that

$$\text{if} \quad \mathbf{u}, \mathbf{v} \in V, \quad \text{then} \quad \mathbf{u} + \mathbf{v} \in V; \tag{4.1a}$$

2. addition is *commutative and associative*, i.e. for all $\mathbf{u}, \mathbf{v}, \mathbf{w} \in V$

$$\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u}, \tag{4.1b}$$
$$(\mathbf{u} + \mathbf{v}) + \mathbf{w} = \mathbf{u} + (\mathbf{v} + \mathbf{w}); \tag{4.1c}$$

3. there exists *closure under multiplication by a complex scalar*, i.e.

$$\text{if} \quad a \in \mathbb{C} \quad \text{and} \quad \mathbf{v} \in V \quad \text{then} \quad a\mathbf{v} \in V; \tag{4.1d}$$

4. multiplication by a scalar is *distributive and associative*, i.e. for all $a, b \in \mathbb{C}$ and $\mathbf{u}, \mathbf{v} \in V$

$$a(\mathbf{u} + \mathbf{v}) = a\mathbf{u} + a\mathbf{v}, \tag{4.1e}$$
$$(a + b)\mathbf{u} = a\mathbf{u} + b\mathbf{u}, \tag{4.1f}$$
$$a(b\mathbf{u}) = (ab)\mathbf{u}; \tag{4.1g}$$

5. there exists a *null, or zero, vector* $\mathbf{0} \in V$ such that for all $\mathbf{v} \in V$

$$\mathbf{v} + \mathbf{0} = \mathbf{v}; \tag{4.1h}$$

6. for all $\mathbf{v} \in V$ there exists a *negative, or inverse, vector* $(-\mathbf{v}) \in V$ such that

$$\mathbf{v} + (-\mathbf{v}) = \mathbf{0}. \tag{4.1i}$$

Remarks.

- The existence of a negative/inverse vector (see (4.1i)) allows us to *subtract* as well as add vectors, by defining

$$\mathbf{u} - \mathbf{v} \equiv \mathbf{u} + (-\mathbf{v}) \,. \tag{4.2}$$

- If we restrict all scalars to be real, we have a *real linear vector space*, or a *linear vector space over reals*.

- We will often refer to V as a *vector space*, rather than the more correct *linear vector space*.

4.1.3 Linear Independence

A set of m non-zero vectors $\{\mathbf{u}_1, \mathbf{u}_2, \dots \ \mathbf{u}_m\}$ is *linearly independent* if

$$\sum_{i=1}^{m} a_i \mathbf{u}_i = \mathbf{0} \quad \Rightarrow \quad a_i = 0 \quad \text{for} \quad i = 1, 2, \dots, m \,. \tag{4.3}$$

Otherwise, the vectors are *linearly dependent*, i.e. there exist scalars a_i, at least one of which is *non-zero*, such that

$$\sum_{i=1}^{m} a_i \mathbf{u}_i = \mathbf{0} \,.$$

Definition: Dimension of a Vector Space. If a vector space V contains a set of n linearly independent vectors but all sets of $n+1$ vectors are linearly dependent, then V is said to be of *dimension n*.   11/04

Examples.

1. $(1,0,0)$, $(0,1,0)$ and $(0,0,1)$ are linearly independent since

$$a(1,0,0) + b(0,1,0) + c(0,0,1) = (a,b,c) = \mathbf{0} \quad \Rightarrow \quad a = 0, \ b = 0, \ c = 0 \,.$$

2. $(1,0,0)$, $(0,1,0)$ and $(1,1,0) = (1,0,0) + (0,1,0)$ are linearly dependent.

3. Since

$$(a,b,c) = a(1,0,0) + b(0,1,0) + c(0,0,1) \,, \tag{4.4}$$

   the vectors $(1,0,0)$, $(0,1,0)$ and $(0,0,1)$ *span* a linear vector space of dimension 3.

4.1.4 Basis Vectors

If V is an n-dimensional vector space then *any* set of n linearly independent vectors $\{\mathbf{u}_1, \dots, \mathbf{u}_n\}$ is a *basis* for V. The are a couple of *key properties* of a basis.   11/02
11/03

1. We claim that for all vectors $\mathbf{v} \in V$, there exist scalars v_i such that

$$\mathbf{v} = \sum_{i=1}^{n} v_i \mathbf{u}_i \ . \tag{4.5}$$

   The v_i are said to be the components of $\mathbf{v}$ with respect to the basis $\{\mathbf{u}_1, \dots, \mathbf{u}_n\}$.

Proof. 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

$$\sum_{i=1}^{n} a_i \mathbf{u}_i + b\mathbf{v} = \mathbf{0}. \tag{4.6}$$

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

$$\mathbf{v} = -\sum_{i=1}^{n} \left(b^{-1} a_i\right) \mathbf{u}_i$$

$$= \sum_{i=1}^{n} v_i \mathbf{u}_i, \tag{4.7}$$

where $v_i = -b^{-1} a_i$ $(i = 1, \ldots, n)$. □

2. The scalars $v_1, \ldots, v_n$ are *unique*.

Proof. Suppose that

$$\mathbf{v} = \sum_{i=1}^{n} v_i \mathbf{u}_i \quad \text{and that} \quad \mathbf{v} = \sum_{i=1}^{n} w_i \mathbf{u}_i. \tag{4.8}$$

Then, because $\mathbf{v} - \mathbf{v} = \mathbf{0}$,

$$\mathbf{0} = \sum_{i=1}^{n} (v_i - w_i)\mathbf{u}_i. \tag{4.9}$$

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 (4.8) are identical. □

Remark. Let $\{\mathbf{u}_1, \ldots, \mathbf{u}_m\}$ be a set of vectors in an n-dimensional vector space.

- 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.
- If $m < n$ then there exists a vector that cannot be expressed as a linear combination of the $\mathbf{u}_i$.

Examples.

1. *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. (4.4))

$$\mathbf{v} = v_x \mathbf{e}_x + v_y \mathbf{e}_y + v_z \mathbf{e}_z \tag{4.10a}$$

$$= v_1 \mathbf{u}_1 + v_2 \mathbf{u}_2 + v_3 \mathbf{u}_3, \tag{4.10b}$$

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.

2. *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

$$z = \alpha \cdot 1 \quad \text{where} \quad \alpha \in \mathbb{C}, \tag{4.11a}$$

and moreover

$$\alpha \cdot 1 = 0 \quad \Rightarrow \quad \alpha = 0 \quad \text{for} \quad \alpha \in \mathbb{C}. \tag{4.11b}$$

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

$$z = a \cdot 1 + b \cdot \imath \quad \text{where} \quad a, b \in \mathbb{R}, \tag{4.12a}$$

and

$$a \cdot 1 + b \cdot \imath = 0 \quad \Rightarrow \quad a = b = 0 \quad \text{if} \quad a, b, \in \mathbb{R}. \tag{4.12b}$$

Thus we have that

$$\dim_{\mathbb{C}} \mathbb{C} = 1 \quad \text{but} \quad \dim_{\mathbb{R}} \mathbb{C} = 2, \tag{4.13}$$

where the subscript indicates whether the vector space $\mathbb{C}$ is considered over $\mathbb{C}$ or $\mathbb{R}$.

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.

1. We note that addition is closed since $\mathsf{A} + \mathsf{B}$ is a real symmetric matrix.

2. Addition is commutative and associative since for all [real symmetric] matrices, $\mathsf{A} + \mathsf{B} = \mathsf{B} + \mathsf{A}$ and $(\mathsf{A} + \mathsf{B}) + \mathsf{C} = \mathsf{A} + (\mathsf{B} + \mathsf{C})$.

3. Multiplication by a scalar is closed since if $p \in \mathbb{R}$, then $p\mathsf{A}$ is a real symmetric matrix.

4. 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 $p(q\mathsf{A}) = (pq)\mathsf{A}$.

5. The zero matrix,

$$\mathsf{0} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix},$$

   is real and symmetric (and hence in V), and such that for all [real symmetric] matrices $\mathsf{A} + \mathsf{0} = \mathsf{A}$.

6. 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

$$\mathsf{U}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathsf{U}_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \text{and} \quad \mathsf{U}_3 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{4.15}$$

are independent, since for $p, q, r \in \mathbb{R}$

$$p\mathsf{U}_1 + q\mathsf{U}_2 + r\mathsf{U}_3 = \begin{pmatrix} p & q \\ q & r \end{pmatrix} = \mathsf{0} \quad \Rightarrow \quad p = q = r = 0.$$

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 under addition, and that the 'vectors' U_i defined in (4.15) form a basis. 11/01

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.

4.2 Change of Basis: the Rôle of Matrices

4.2.1 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

$$\mathbf{u}'_j = \sum_{i=1}^{n} \mathbf{u}_i \, A_{ij} \quad (j = 1, \ldots, n) \, , \tag{4.16}$$

for some numbers A_{ij}. From (4.5) we see that A_{ij} is the ith component of the vector $\mathbf{u}'_j$ in the basis $\{\mathbf{u}_i : i = 1, \ldots, n\}$. The numbers A_{ij} can be represented by a square $n \times n$ *transformation matrix* A

$$\mathsf{A} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{pmatrix} . \tag{4.17}$$

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

$$\mathbf{u}_i = \sum_{k=1}^{n} \mathbf{u}'_k B_{ki} \quad (i = 1, 2, \ldots, n) \, , \tag{4.18}$$

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

$$\mathsf{B} = \begin{pmatrix} B_{11} & B_{12} & \cdots & B_{1n} \\ B_{21} & B_{22} & \cdots & B_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ B_{n1} & B_{n2} & \cdots & B_{nn} \end{pmatrix} . \tag{4.19}$$

4.2.2 Properties of Transformation Matrices

From substituting (4.18) into (4.16) we have that

$$\mathbf{u}'_j = \sum_{i=1}^{n} \left[\sum_{k=1}^{n} \mathbf{u}'_k B_{ki} \right] A_{ij} = \sum_{k=1}^{n} \mathbf{u}'_k \left[\sum_{i=1}^{n} B_{ki} A_{ij} \right] . \tag{4.20}$$

However, because of the uniqueness of a basis representation and the fact that

$$\mathbf{u}'_j = \mathbf{u}'_j \cdot 1 = \sum_{k=1}^{n} \mathbf{u}'_k \, \delta_{kj} \, ,$$

it follows that

$$\sum_{i=1}^{n} B_{ki} A_{ij} = \delta_{kj} \, . \tag{4.21}$$

Hence in matrix notation, $\mathsf{BA} = \mathsf{I}$, where I is the identity matrix. Conversely, substituting (4.16) into (4.18) leads to the conclusion that $\mathsf{AB} = \mathsf{I}$ (alternatively argue by a relabeling symmetry). Thus

$$\mathsf{B} = \mathsf{A}^{-1} \, , \tag{4.22a}$$

and

$$\det \mathsf{A} \neq 0 \quad \text{and} \quad \det \mathsf{B} \neq 0 \, . \tag{4.22b}$$

4.2.3   Transformation Law for Vector Components

Consider a vector $\mathbf{v}$, then in the $\{\mathbf{u}_i : i = 1, \ldots, n\}$ basis we have from (4.5)

$$\mathbf{v} = \sum_{i=1}^{n} v_i \mathbf{u}_i \,.$$

Similarly, in the $\{\mathbf{u}'_i : i = 1, \ldots, n\}$ basis we can write

$$\mathbf{v} = \sum_{j=1}^{n} v'_j \mathbf{u}'_j \tag{4.23}$$

$$= \sum_{j=1}^{n} v'_j \sum_{i=1}^{n} \mathbf{u}_i A_{ij} \qquad\qquad \text{from (4.16)}$$

$$= \sum_{i=1}^{n} \mathbf{u}_i \sum_{j=1}^{n} (A_{ij} v'_j) \qquad\qquad \text{swap summation order.}$$

Since a basis representation is unique it follows from (4.5) that

$$v_i = \sum_{j=1}^{n} A_{ij} v'_j \,, \tag{4.24}$$

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

$$\mathsf{v} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} \quad \text{and} \quad \mathsf{v}' = \begin{pmatrix} v'_1 \\ v'_2 \\ \vdots \\ v'_n \end{pmatrix} \quad \text{respectively.} \tag{4.25}$$

Note that we now have **bold** $\mathbf{v}$ denoting a vector, *italic* v_i denoting a component of a vector, and sans serif v denoting a column matrix of components. Then (4.24) can be expressed as

$$\mathsf{v} = \mathsf{A}\mathsf{v}' \,. \tag{4.26a}$$

By applying A^{-1} to either side of (4.26a) it follows that

$$\mathsf{v}' = \mathsf{A}^{-1}\mathsf{v} \,. \tag{4.26b}$$

Unlectured Remark. Observe by comparison between (4.16) and (4.26b) 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:

$$\mathbf{v} = \sum_{j=1}^{n} v'_j \mathbf{u}'_j \qquad\qquad \text{from (4.23)}$$

$$= \sum_{j=1}^{n} \left(\sum_{k=1}^{n} (\mathsf{A}^{-1})_{jk} v_k \right) \left(\sum_{i=1}^{n} \mathbf{u}_i A_{ij} \right) \qquad\qquad \text{from (4.26b) and (4.16)}$$

$$= \sum_{i=1}^{n} \mathbf{u}_i \left(\sum_{k=1}^{n} v_k \left(\sum_{j=1}^{n} A_{ij} (\mathsf{A}^{-1})_{jk} \right) \right) \qquad\qquad \text{swap summation order}$$

$$= \sum_{i=1}^{n} \mathbf{u}_i \left(\sum_{k=1}^{n} v_k \delta_{ik} \right) \qquad\qquad \mathsf{A}\mathsf{A}^{-1} = \mathsf{I}$$

$$= \sum_{i=1}^{n} v_i \mathbf{u}_i \,. \qquad\qquad \text{contract using (0.11b)}$$

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 that

$$\mathbf{u}'_1 = (1,1) = (1,0) + (0,1) = \mathbf{u}_1 + \mathbf{u}_2,$$
$$\mathbf{u}'_2 = (-1,1) = -1 \cdot (1,0) + (0,1) = -\mathbf{u}_1 + \mathbf{u}_2.$$

Hence from comparison with (4.16)

$$A_{11} = 1, \quad A_{21} = 1, \quad A_{12} = -1 \quad \text{and} \quad A_{22} = 1,$$

i.e.

$$\mathsf{A} = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \quad \text{with inverse} \quad \mathsf{A}^{-1} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}.$$

First Check. Note that A^{-1} is consistent with the observation that

$$\mathbf{u}_1 = (1,0) = \tfrac{1}{2}(\,(1,1) - (-1,1)\,) = \tfrac{1}{2}(\mathbf{u}'_1 - \mathbf{u}'_2),$$
$$\mathbf{u}_2 = (0,1) = \tfrac{1}{2}(\,(1,1) + (-1,1)\,) = \tfrac{1}{2}(\mathbf{u}'_1 + \mathbf{u}'_2).$$

Second Check. Consider an arbitrary vector $\mathbf{v}$, then

$$\begin{aligned}
\mathbf{v} &= v_1 \mathbf{u}_1 + v_2 \mathbf{u}_2 \\
&= \tfrac{1}{2} v_1 (\mathbf{u}'_1 - \mathbf{u}'_2) + \tfrac{1}{2} v_2 (\mathbf{u}'_1 + \mathbf{u}'_2) \\
&= \tfrac{1}{2}(v_1 + v_2)\mathbf{u}'_1 - \tfrac{1}{2}(v_1 - v_2)\mathbf{u}'_2.
\end{aligned}$$

Thus

$$v'_1 = \tfrac{1}{2}(v_1 + v_2) \quad \text{and} \quad v'_2 = -\tfrac{1}{2}(v_1 - v_2).$$

From (4.26b), i.e. $\mathbf{v}' = \mathsf{A}^{-1}\mathbf{v}$, we obtain as above that

$$\mathsf{A}^{-1} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

4.3 Scalar Product (Inner Product)

4.3.1 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.

1. If we [again] denote a complex conjugate with * then we require that

$$\mathbf{u} \cdot \mathbf{v} = (\mathbf{v} \cdot \mathbf{u})^*. \tag{4.27a}$$

   Note that 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

$$\mathbf{v} \cdot \mathbf{v} = (\mathbf{v} \cdot \mathbf{v})^*, \tag{4.27b}$$

   i.e. $\mathbf{v} \cdot \mathbf{v}$ is *real*.

2. The scalar product should be *linear in its second argument*, i.e. for $a, b \in \mathbb{C}$

$$\mathbf{u} \cdot (a\mathbf{v}_1 + b\mathbf{v}_2) = a\,\mathbf{u} \cdot \mathbf{v}_1 + b\,\mathbf{u} \cdot \mathbf{v}_2. \tag{4.27c}$$

3. The scalar product of a vector with itself should be positive, i.e.

$$\mathbf{v} \cdot \mathbf{v} \geqslant 0. \tag{4.27d}$$

   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 $\mathbf{v}$.

4. We shall also require that the only vector of zero norm should be the zero vector, i.e.

$$|\mathbf{v}| = 0 \quad \Rightarrow \quad \mathbf{v} = \mathbf{0}\,. \tag{4.27e}$$

Remark. Properties (4.27a) and (4.27c) imply that for $a, b \in \mathbb{C}$

$$
\begin{aligned}
(a\mathbf{u}_1 + b\mathbf{u}_2) \cdot \mathbf{v} &= (\mathbf{v} \cdot (a\mathbf{u}_1 + b\mathbf{u}_2))^* \\
&= (a\mathbf{v} \cdot \mathbf{u}_1 + b\mathbf{v} \cdot \mathbf{u}_2)^* \\
&= a^* (\mathbf{v} \cdot \mathbf{u}_1)^* + b^* (\mathbf{v} \cdot \mathbf{u}_2)^* \\
&= a^* (\mathbf{u}_1 \cdot \mathbf{v}) + b^* (\mathbf{u}_2 \cdot \mathbf{v})\,,
\end{aligned} \tag{4.28}
$$

i.e. the scalar product is 'anti-linear' in the first argument.

<div align="center">Failure to remember this is a common cause of error.</div>

However, if $a, b \in \mathbb{R}$ then (4.28) reduces to linearity in *both* arguments.

Alternative notation. An alternative notation for the scalar product and associated norm is

$$\langle\, \mathbf{u} \mid \mathbf{v} \,\rangle \equiv \mathbf{u} \cdot \mathbf{v}\,, \tag{4.29a}$$

$$\|\mathbf{v}\| \equiv |\mathbf{v}| = (\mathbf{v} \cdot \mathbf{v})^{\frac{1}{2}}\,. \tag{4.29b}$$

4.3.2 Worked Exercise

Question. Find a definition of 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 (4.43a), i.e. that the scalar product of a vector with itself is zero only if the vector is zero. Hence for real symmetric 2×2 matrices A and B consider the inner product defined by

$$\langle\, \mathsf{A} \mid \mathsf{B} \,\rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij}^* B_{ij} \tag{4.30a}$$

$$= A_{11}^* B_{11} + A_{12}^* B_{12} + A_{21}^* B_{21} + A_{22}^* B_{22}\,, \tag{4.30b}$$

where we are using the alternative notation (4.29a) for the inner product. For this definition of inner product we have for real symmetric 2×2 matrices A, B and C, and $a, b \in \mathbb{C}$:

- as in (4.27a)

$$\langle\, \mathsf{B} \mid \mathsf{A} \,\rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} B_{ij}^* A_{ij} = \langle\, \mathsf{A} \mid \mathsf{B} \,\rangle^*\,;$$

- as in (4.27c)

$$
\begin{aligned}
\langle\, \mathsf{A} \mid (\beta\mathsf{B} + \gamma\mathsf{C}) \,\rangle &= \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij}^* (\beta B_{ij} + \gamma C_{ij}) \\
&= \beta \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij}^* B_{ij} + \gamma \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij}^* C_{ij} \\
&= \beta \langle\, \mathsf{A} \mid \mathsf{B} \,\rangle + \gamma \langle\, \mathsf{A} \mid \mathsf{C} \,\rangle\,;
\end{aligned}
$$

- as in (4.27d)

$$\langle\, \mathsf{A} \mid \mathsf{A} \,\rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij}^* A_{ij} = \sum_{i=1}^{n} \sum_{j=1}^{n} |A_{ij}|^2 \geqslant 0\,;$$

- as in (4.27e)

$$\langle\, \mathsf{A} \mid \mathsf{A} \,\rangle = 0 \quad \Rightarrow \quad \mathsf{A} = 0\,.$$

Hence we have a well defined inner product.

4.3.3 Some Inequalities

Schwarz's Inequality. This states that

$$|\langle\, \mathbf{u}\mid\mathbf{v}\,\rangle| \leqslant \|\mathbf{u}\|\,\|\mathbf{v}\|\,, \tag{4.31}$$

with equality only when $\mathbf{u}$ is a scalar multiple of $\mathbf{v}$.

Proof. Write $\langle\,\mathbf{u}\mid\mathbf{v}\,\rangle = |\langle\,\mathbf{u}\mid\mathbf{v}\,\rangle|e^{\imath\alpha}$, and for $\lambda \in \mathbb{C}$ consider

$$
\begin{aligned}
\|\mathbf{u}+\lambda\mathbf{v}\|^2 &= \langle\,\mathbf{u}+\lambda\mathbf{v}\mid\mathbf{u}+\lambda\mathbf{v}\,\rangle && \text{from (4.29b)}\\
&= \langle\,\mathbf{u}\mid\mathbf{u}\,\rangle + \lambda\langle\,\mathbf{u}\mid\mathbf{v}\,\rangle + \lambda^*\langle\,\mathbf{v}\mid\mathbf{u}\,\rangle + |\lambda|^2\langle\,\mathbf{v}\mid\mathbf{v}\,\rangle && \text{from (4.27c) and (4.28)}\\
&= \langle\,\mathbf{u}\mid\mathbf{u}\,\rangle + (\lambda e^{\imath\alpha} + \lambda^* e^{-\imath\alpha})|\langle\,\mathbf{u}\mid\mathbf{v}\,\rangle| + |\lambda|^2\langle\,\mathbf{v}\mid\mathbf{v}\,\rangle && \text{from (4.27a).}
\end{aligned}
$$

First, suppose that $\mathbf{v} = \mathbf{0}$. 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

$$\langle\,\mathbf{u}\mid\mathbf{v}\,\rangle = 0 \quad \text{if} \quad \mathbf{v} = \mathbf{0}\,,$$

in which case (4.31) is satisfied as an equality. Next suppose that $\mathbf{v} \neq \mathbf{0}$ and choose $\lambda = r e^{-\imath\alpha}$ so that from (4.27d)

$$0 \leqslant \|\mathbf{u}+\lambda\mathbf{v}\|^2 = \|\mathbf{u}\|^2 + 2r|\langle\,\mathbf{u}\mid\mathbf{v}\,\rangle| + r^2\|\mathbf{v}\|^2\,.$$

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 $\mathbf{u} = -\lambda\mathbf{v}$. $\square$

The Triangle Inequality. This states that

$$\|\mathbf{u}+\mathbf{v}\| \leqslant \|\mathbf{u}\| + \|\mathbf{v}\|\,. \tag{4.32}$$

Proof. This follows from taking square roots of the following inequality:

$$
\begin{aligned}
\|\mathbf{u}+\mathbf{v}\|^2 &= \langle\,\mathbf{u}\mid\mathbf{u}\,\rangle + \langle\,\mathbf{u}\mid\mathbf{v}\,\rangle + \langle\,\mathbf{u}\mid\mathbf{v}\,\rangle^* + \langle\,\mathbf{v}\mid\mathbf{v}\,\rangle && \text{from above with } \lambda = 1\\
&= \|\mathbf{u}\|^2 + 2\,\mathrm{Re}\,\langle\,\mathbf{u}\mid\mathbf{v}\,\rangle + \|\mathbf{v}\|^2 && \text{from (4.27a)}\\
&\leqslant \|\mathbf{u}\|^2 + 2|\langle\,\mathbf{u}\mid\mathbf{v}\,\rangle| + \|\mathbf{v}\|^2 \\
&\leqslant \|\mathbf{u}\|^2 + 2\|\mathbf{u}\|\,\|\mathbf{v}\| + \|\mathbf{v}\|^2 && \text{from (4.31)}\\
&\leqslant (\|\mathbf{u}\| + \|\mathbf{v}\|)^2\,.
\end{aligned}
$$

4.3.4 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

$$G_{ij} = \mathbf{u}_i \cdot \mathbf{u}_j \quad (i,j = 1,\ldots,n)\,. \tag{4.33}$$

Then, for *any* two vectors

$$\mathbf{v} = \sum_{i=1}^{n} v_i \mathbf{u}_i \quad \text{and} \quad \mathbf{w} = \sum_{j=1}^{n} w_j \mathbf{u}_j\,, \tag{4.34}$$

we have that

$$
\begin{aligned}
\mathbf{v}\cdot\mathbf{w} &= \Big(\sum_{i=1}^{n} v_i \mathbf{u}_i\Big) \cdot \Big(\sum_{j=1}^{n} w_j \mathbf{u}_j\Big) \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} v_i^* w_j\,\mathbf{u}_i \cdot \mathbf{u}_j && \text{from (4.27c) and (4.28)}\\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} v_i^* G_{ij} w_j\,. && \tag{4.35}
\end{aligned}
$$

We can simplify this expression (which determines the scalar product in terms of the G_{ij}), but first it helps to have a definition.

Definition. The *Hermitian conjugate* of a matrix A is defined to be

$$\mathsf{A}^\dagger = (\mathsf{A}^\mathrm{T})^* = (\mathsf{A}^*)^\mathrm{T}, \tag{4.36}$$

where $^\mathrm{T}$ denotes a transpose.

Example.

$$\text{If} \quad \mathsf{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \quad \text{then} \quad \mathsf{A}^\dagger = \begin{pmatrix} A_{11}^* & A_{21}^* \\ A_{12}^* & A_{22}^* \end{pmatrix}.$$

Properties. 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

$$(\mathsf{AB})^\dagger = \mathsf{B}^\dagger \mathsf{A}^\dagger. \tag{4.37a}$$

Also, from (4.36),

$$\mathsf{A}^{\dagger\dagger} = \left(\mathsf{A}^{*\mathrm{T}}\right)^{\mathrm{T}*} = \mathsf{A}. \tag{4.37b}$$

Let w be the column matrix

$$\mathsf{w} = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix}, \tag{4.38a}$$

and let $\mathsf{v}^\dagger$ be the Hermitian conjugate of the column matrix v, i.e. $\mathsf{v}^\dagger$ is the row matrix

$$\mathsf{v}^\dagger \equiv (\mathsf{v}^*)^\mathrm{T} = \begin{pmatrix} v_1^* & v_2^* & \cdots & v_n^* \end{pmatrix}. \tag{4.38b}$$

Then the scalar product (4.35) can be written as

$$\mathbf{v} \cdot \mathbf{w} = \mathsf{v}^\dagger \mathsf{G}\, \mathsf{w}, \tag{4.39}$$

where G is the matrix, or *metric*, with entries G_{ij} (metrics are a key ingredient of General Relativity).

4.3.5 Properties of the Metric

First two definitions for a $n \times n$ matrix A.

Definition. The matrix A is said to be a *Hermitian* if it is equal to its own Hermitian conjugate, i.e. if

$$\mathsf{A}^\dagger = \mathsf{A}. \tag{4.40}$$

Definition. The matrix A is said to be *positive definite* if for all column matrices v of length n,

$$\mathsf{v}^\dagger \mathsf{A} \mathsf{v} \geqslant 0, \quad \text{with equality iff } \mathsf{v} = \mathbf{0}. \tag{4.41}$$

Remark. If equality to zero were possible in (4.41) for non-zero v, then A would said to be *positive* rather than *positive definite*.

Property: a metric is Hermitian. The elements of the Hermitian conjugate of the metric G are the complex numbers

$$
\begin{aligned}
(\mathsf{G}^\dagger)_{ij} \equiv G_{ij}^\dagger = (G_{ji})^* && \text{from (4.36)} && \text{(4.42a)} \\
= (\mathbf{u}_j \cdot \mathbf{u}_i)^* && \text{from (4.33)} && \\
= \mathbf{u}_i \cdot \mathbf{u}_j && \text{from (4.27a)} && \\
= G_{ij}. && \text{from (4.33)} && \text{(4.42b)}
\end{aligned}
$$

Hence G is Hermitian, i.e.

$$\mathsf{G}^\dagger = \mathsf{G}. \tag{4.42c}$$

Remark. That G is Hermitian is consistent with the requirement (4.27b) that $|\mathbf{v}|^2 = \mathbf{v} \cdot \mathbf{v}$ is real, since

$$
\begin{aligned}
(\mathbf{v} \cdot \mathbf{v})^* &= ((\mathbf{v} \cdot \mathbf{v})^*)^{\mathrm{T}} && \text{since a scalar is its own transpose} \\
&= (\mathbf{v} \cdot \mathbf{v})^\dagger && \text{from definition (4.36)} \\
&= (\mathsf{v}^\dagger \mathsf{G} \mathsf{v})^\dagger && \text{from (4.39)} \\
&= \mathsf{v}^\dagger \mathsf{G}^\dagger \mathsf{v} && \text{from (4.37a) and (4.37b)} \\
&= \mathsf{v}^\dagger \mathsf{G} \mathsf{v} && \text{from (4.42c)} \\
&= \mathbf{v} \cdot \mathbf{v}\,. && \text{from (4.39)}
\end{aligned}
$$

Property: a metric is positive definite. From (4.27d) and (4.27e) we have from the properties of a scalar product that for any $\mathbf{v}$

$$|\mathbf{v}|^2 \geqslant 0 \quad \text{with equality iff} \quad \mathbf{v} = \mathbf{0}\,, \tag{4.43a}$$

where 'iff' means if and only if. Hence, from (4.39), for any $\mathbf{v}$

$$\mathsf{v}^\dagger \mathsf{G} \mathsf{v} \geqslant 0 \quad \text{with equality iff} \quad \mathsf{v} = \mathbf{0}\,. \tag{4.43b}$$

It follows that G is *positive definite*.

4.4 Change of Basis: Diagonalization

4.4.1 Transformation Law for Metrics

In §4.2 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 §4.3 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 (4.26a) 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

$$\mathsf{v}^\dagger = \mathsf{v}'^\dagger \mathsf{A}^\dagger\,. \tag{4.44}$$

Hence for arbitrary vectors $\mathbf{v}$ and $\mathbf{w}$

$$
\begin{aligned}
\mathbf{v} \cdot \mathbf{w} &= \mathsf{v}^\dagger \mathsf{G} \mathsf{w} && \text{from (4.39)} \\
&= \mathsf{v}'^\dagger \mathsf{A}^\dagger \mathsf{G} \mathsf{A} \mathsf{w}' && \text{from (4.26a) and (4.44).}
\end{aligned}
$$

But from (4.39) we must also have that in terms of the new basis

$$\mathbf{v} \cdot \mathbf{w} = \mathsf{v}'^\dagger \mathsf{G}' \mathsf{w}'\,, \tag{4.45}$$

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

$$\mathsf{G}' = \mathsf{A}^\dagger \mathsf{G} \mathsf{A}\,. \tag{4.46}$$

Unlectured Alternative Derivation. (4.46) can also be derived from the definition of the metric since

$$
\begin{aligned}
(\mathsf{G}')_{ij} \equiv G'_{ij} &= \mathbf{u}'_i \cdot \mathbf{u}'_j && \text{from (4.33)} \\
&= \left(\sum_{k=1}^{n} \mathbf{u}_k A_{ki} \right) \cdot \left(\sum_{\ell=1}^{n} \mathbf{u}_\ell A_{\ell j} \right) && \text{from (4.16)} \\
&= \sum_{k=1}^{n} \sum_{\ell=1}^{n} A^*_{ki} (\mathbf{u}_k \cdot \mathbf{u}_\ell) A_{\ell j} && \text{from (4.27c) and (4.28)} \\
&= \sum_{k=1}^{n} \sum_{\ell=1}^{n} A^\dagger_{ik} G_{k\ell} A_{\ell j} && \text{from (4.33) and (4.42a)} \\
&= (\mathsf{A}^\dagger \mathsf{G} \mathsf{A})_{ij}\,. && \tag{4.47}
\end{aligned}
$$

Remark. As a check we observe that

$$(\mathsf{G}')^\dagger = (\mathsf{A}^\dagger \mathsf{G} \mathsf{A})^\dagger = \mathsf{A}^\dagger \mathsf{G}^\dagger (\mathsf{A}^\dagger)^\dagger = \mathsf{A}^\dagger \mathsf{G} \mathsf{A} = \mathsf{G}' \,. \tag{4.48}$$

Thus G' is confirmed to be Hermitian.

4.4.2 Diagonalization of the Metric

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} \,.$$

Let us *suppose* that there exists an invertible matrix A such that

$$\mathsf{G}' = \mathsf{A}^\dagger \mathsf{G} \mathsf{A} = \Lambda \,, \tag{4.49a}$$

where Λ is a *diagonal matrix*, i.e. a matrix such that

$$\Lambda_{ij} = \lambda_i \delta_{ij} \,. \tag{4.49b}$$

The matrix A is said to *diagonalize* G. Subsequently we shall (almost) show that for any Hermitian matrix G a matrix A can be found to diagonalize G.

Properties of the λ_i.

1. Because $\mathsf{G}' = \Lambda$ is Hermitian,

$$\lambda_i^* = \Lambda_{ii}^* = \Lambda_{ii} = \lambda_i \qquad (i = 1, \dots, n), \tag{4.50}$$

   and hence the diagonal entries λ_i are *real*.

2. From (4.45), (4.49a) and (4.49b) we have that

$$0 \leqslant |\mathbf{v}|^2 = \mathsf{v}'^\dagger \mathsf{G}' \mathsf{v}'$$

$$= \sum_{i=1}^n \sum_{j=1}^n v_i'^* \lambda_i \delta_{ij} v_j'$$

$$= \sum_{i=1}^n \lambda_i |v_i'|^2 \,, \tag{4.51}$$

   with equality only if $\mathbf{v} = 0$ (see (4.27e)). This can only be true for all vectors $\mathbf{v}$ if

$$\lambda_i > 0 \quad \text{for} \quad i = 1, \dots, n \,, \tag{4.52}$$

   i.e. if the diagonal entries λ_i are *strictly positive*.

4.4.3 Orthonormal Bases

From (4.33), (4.49a) and (4.49b) we see that

$$\mathbf{u}_i' \cdot \mathbf{u}_j' = G_{ij}' = \Lambda_{ij} = \lambda_i \delta_{ij} \,. \tag{4.53}$$

Hence $\mathbf{u}_i' \cdot \mathbf{u}_j' = 0$ when $i \neq j$, i.e. the new basis vectors are orthogonal. Further, because the λ_i are strictly positive we can normalise the basis, viz.

$$\mathbf{e}_i = \frac{1}{\sqrt{\lambda_i}} \mathbf{u}_i' \,, \tag{4.54a}$$

so that

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \,. \tag{4.54b}$$

The $\{\mathbf{e}_i : i = 1, \dots, n\}$ are thus an *orthonormal basis*. We conclude, subject to showing that G can be diagonalized (because it is an Hermitian matrix), that:

Any vector space with a scalar product has an orthonormal basis.

It also follows, since from (4.33) the elements of the metric are just $\mathbf{e}_i \cdot \mathbf{e}_j$, that 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 (4.39)

$$\mathbf{v} \cdot \mathbf{w} = \mathsf{v}^\dagger \mathsf{I} \, \mathsf{w} = \mathsf{v}^\dagger \, \mathsf{w} \,. \tag{4.55}$$

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

$$\mathsf{v}^\dagger \mathsf{w} = 0 \,. \tag{4.56}$$

4.5 Unitary and Orthogonal Matrices

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

$$\mathbf{e}'_i = \sum_{k=1}^{n} \mathbf{e}_k \, U_{ki} \,, \tag{4.57}$$

where U is the transformation matrix (cf. (4.16)). Then from (4.46) the metric for the new basis is given by

$$\mathsf{G}' = \mathsf{U}^\dagger \mathsf{I} \, \mathsf{U} = \mathsf{U}^\dagger \mathsf{U} \,. \tag{4.58a}$$

For the new basis to be orthonormal we require that the new metric to be the identity matrix, i.e. we require that

$$\mathsf{U}^\dagger \mathsf{U} = \mathsf{I} \,. \tag{4.58b}$$

Since $\det \mathsf{U} \neq 0$, the inverse U^{-1} exists and hence

$$\mathsf{U}^\dagger = \mathsf{U}^{-1} \,. \tag{4.59}$$

Definition. A matrix for which the Hermitian conjugate is equal to the inverse is said to be *unitary*.

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

$$\mathsf{R}^{\mathrm{T}} = \mathsf{R}^{-1} \,. \tag{4.60}$$

Definition. A real matrix with this property is said to be *orthogonal*.

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).

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4.6 Diagonalization of Matrices: Eigenvectors and Eigenvalues

Suppose that M is a square $n \times n$ matrix. Then a *non-zero* column vector x such that

$$\mathsf{M}\mathsf{x} = \lambda\mathsf{x}\,, \tag{4.61a}$$

where $\lambda \in \mathbb{C}$, is said to be an eigenvector of the matrix M with eigenvalue λ. If we rewrite this equation as

$$(\mathsf{M} - \lambda\mathsf{I})\mathsf{x} = 0\,, \tag{4.61b}$$

then since x is non-zero it must be that

$$\det(\mathsf{M} - \lambda\mathsf{I}) = 0\,. \tag{4.62}$$

This is called the *characteristic equation* of the matrix M. The left-hand-side of (4.62) is an nth order polynomial in λ called the *characteristic polynomial* of M. The roots of the characteristic polynomial are the eigenvalues of M.

Example. Find the eigenvalues of

$$\mathsf{M} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{4.63a}$$

Answer. From (4.62)

$$0 = \det(\mathsf{M} - \lambda\mathsf{I}) = \left\| \begin{matrix} -\lambda & 1 \\ -1 & -\lambda \end{matrix} \right\| = \lambda^2 + 1 = (\lambda - \imath)(\lambda + \imath)\,, \tag{4.63b}$$

and so the eigenvalues of M are $\pm\imath$.

Since an nth order polynomial has exactly n, possibly complex, roots (counting multiplicities in the case of repeated roots), there are always n eigenvalues $\lambda_i, i = 1, \ldots, n$. Let x^i be the respective eigenvectors, i.e.

$$\mathsf{M}\mathsf{x}^i = \lambda_i \mathsf{x}^i \tag{4.64a}$$

or in component notation

$$\sum_{k=1}^{n} M_{jk} x_k^i = \lambda_i x_j^i\,. \tag{4.64b}$$

Let X be the $n \times n$ matrix defined by

$$(\mathsf{X})_{ij} \equiv X_{ij} = x_i^j\,, \tag{4.65a}$$

i.e.

$$\mathsf{X} = \begin{pmatrix} x_1^1 & x_1^2 & \cdots & x_1^n \\ x_2^1 & x_2^2 & \cdots & x_2^n \\ \vdots & \vdots & \ddots & \vdots \\ x_n^1 & x_n^2 & \cdots & x_n^n \end{pmatrix}. \tag{4.65b}$$

Then (4.64b) can be rewritten as

$$\sum_{k=1}^{n} M_{jk} X_{ki} = \lambda_i X_{ji} = \sum_{k=1}^{n} X_{jk}\, \delta_{ki}\lambda_i \tag{4.66a}$$

or, in matrix notation,

$$\mathsf{M}\mathsf{X} = \mathsf{X}\Lambda\,, \tag{4.66b}$$

where Λ is the diagonal matrix

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}. \tag{4.66c}$$

If X has an inverse, X^{-1}, then

$$\mathsf{X}^{-1}\mathsf{M}\mathsf{X} = \Lambda, \tag{4.67}$$

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.

4.7 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.

4.7.1 The Eigenvalues of an Hermitian Matrix are Real

Let H be an Hermitian matrix, and suppose that e is a non-zero eigenvector with eigenvalue λ. Then

$$\mathsf{H}\mathsf{e} = \lambda\mathsf{e}, \tag{4.68a}$$

and hence

$$\mathsf{e}^{\dagger}\mathsf{H}\mathsf{e} = \lambda\mathsf{e}^{\dagger}\mathsf{e}. \tag{4.68b}$$

Take the Hermitian conjugate of both sides; first the left hand side

$$\begin{aligned} \left(\mathsf{e}^{\dagger}\mathsf{H}\mathsf{e}\right)^{\dagger} &= \mathsf{e}^{\dagger}\mathsf{H}^{\dagger}\mathsf{e} && \text{since } (\mathsf{A}\mathsf{B})^{\dagger} = \mathsf{B}^{\dagger}\mathsf{A}^{\dagger} \text{ and } (\mathsf{A}^{\dagger})^{\dagger} = \mathsf{A} \\ &= \mathsf{e}^{\dagger}\mathsf{H}\mathsf{e} && \text{since } \mathsf{H} \text{ is Hermitian,} \end{aligned} \tag{4.69a}$$

and then the right

$$(\lambda\mathsf{e}^{\dagger}\mathsf{e})^{\dagger} = \lambda^{*}\mathsf{e}^{\dagger}\mathsf{e}. \tag{4.69b}$$

On equating the above two results we have that

$$\mathsf{e}^{\dagger}\mathsf{H}\mathsf{e} = \lambda^{*}\mathsf{e}^{\dagger}\mathsf{e}. \tag{4.70}$$

It then follows from (4.68b) and (4.70) that

$$(\lambda - \lambda^{*})\,\mathsf{e}^{\dagger}\mathsf{e} = 0. \tag{4.71}$$

However we have assumed that e is a *non-zero* eigenvector, so

$$\mathsf{e}^{\dagger}\mathsf{e} = \sum_{i=1}^{n} e_i^* e_i = \sum_{i=1}^{n} |e_i|^2 > 0, \tag{4.72}$$

and hence it follows from (4.71) that $\lambda = \lambda^*$, i.e. that λ is real.

4.7.2 An n-Dimensional Hermitian Matrix has n Orthogonal Eigenvectors

$\lambda_i \neq \lambda_j$. Let e^i and e^j be two eigenvectors of an Hermitian matrix H. First of all suppose that their respective eigenvalues λ_i and λ_j are different, i.e. $\lambda_i \neq \lambda_j$. From pre-multiplying (4.68a), with $\mathsf{e} \rightarrow \mathsf{e}^i$, by $(\mathsf{e}^j)^\dagger$ we have that

$$\mathsf{e}^{j\dagger}\,\mathsf{H}\,\mathsf{e}^i = \lambda_i\,\mathsf{e}^{j\dagger}\,\mathsf{e}^i \,. \tag{4.73a}$$

Similarly

$$\mathsf{e}^{i\dagger}\,\mathsf{H}\,\mathsf{e}^j = \lambda_j\,\mathsf{e}^{i\dagger}\,\mathsf{e}^j \,. \tag{4.73b}$$

On taking the Hermitian conjugate of (4.73b) it follows that

$$\mathsf{e}^{j\dagger}\,\mathsf{H}^\dagger\,\mathsf{e}^i = \lambda_j^*\,\mathsf{e}^{j\dagger}\,\mathsf{e}^i \,.$$

However, H is Hermitian, i.e. $\mathsf{H}^\dagger = \mathsf{H}$, and we have seen above that the eigenvalue λ_j is real, hence

$$\mathsf{e}^{j\dagger}\mathsf{H}\,\mathsf{e}^i = \lambda_j\,\mathsf{e}^{j\dagger}\,\mathsf{e}^i \,. \tag{4.74}$$

On subtracting (4.74) from (4.73a) we obtain

$$0 = (\lambda_i - \lambda_j)\,\mathsf{e}^{j\dagger}\,\mathsf{e}^i \,. \tag{4.75}$$

Hence if $\lambda_i \neq \lambda_j$ it follows that

$$\mathsf{e}^{j\dagger}\,\mathsf{e}^i = 0 \,. \tag{4.76}$$

Now if the column vectors e^i and e^j are interpreted as the components of two vectors *in an orthonormal basis*, then from (4.56) we see that the two vectors $\mathbf{e}^i$ and $\mathbf{e}^j = 0$ are orthogonal in the scalar product sense.

$\lambda_i = \lambda_j$. 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 (3.19b) 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 $\varepsilon \rightarrow 0$. For all non-zero values of ε (both positive and negative) there will be n orthogonal eigenvectors. On appealing to a continuity argument there will be n orthogonal eigenvectors for the specific case $\varepsilon = 0$.

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Lemma. Orthogonal eigenvectors e^i and e^j are linearly independent.

> *Proof.* Suppose there exist a_i and a_j such that

$$a_i\mathsf{e}^i + a_j\mathsf{e}^j = 0 \,. \tag{4.77}$$

Then from pre-multiplying (4.77) by $\mathsf{e}^{j\dagger}$ and using (4.76) it follows that

$$0 = a_j \mathsf{e}^{j\dagger}\mathsf{e}^j = a_j \sum_{k=1}^{n}(\mathsf{e}^j)_k^*(\mathsf{e}^j)_k = a_j \sum_{k=1}^{n}\left|(\mathsf{e}^j)_k\right|^2 . \tag{4.78}$$

Since e^j is non-zero it follows that $a_j = 0$. By the relabeling symmetry, or by using the Hermitian conjugate of (4.76), it similarly follows that $a_i = 0$. $\qquad\square$

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.

Remark. We can tighten this is result a little further by noting that, for any $\mu \in \mathbb{C}$,

$$\text{if}\quad \mathsf{H}\mathsf{e}^i = \lambda_i \mathsf{e}^i, \quad \text{then}\quad \mathsf{H}(\mu\mathsf{e}^i) = \lambda_i(\mu\mathsf{e}^i) . \tag{4.79a}$$

This allows us to normalise the eigenvectors so that

$$\mathsf{e}^{i\dagger}\,\mathsf{e}^i = 1 . \tag{4.79b}$$

Hence for Hermitian matrices it is always possible to find n *orthonormal* eigenvectors that are linearly independent.

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4.7.3 Diagonalization of Hermitian Matrices

It follows from the above result, §4.6, and specifically (4.65b), that an Hermitian matrix H can be 'diagonalized' to the matrix Λ by means of the transformation $\mathsf{X}^{-1}\mathsf{H}\mathsf{X}$ if

$$\mathsf{X} = \begin{pmatrix} e_1^1 & e_1^2 & \cdots & e_1^n \\ e_2^1 & e_2^2 & \cdots & e_2^n \\ \vdots & \vdots & \ddots & \vdots \\ e_n^1 & e_n^2 & \cdots & e_n^n \end{pmatrix} . \tag{4.80}$$

Remark. If the e^i are orthonormal eigenvectors of H then X is a *unitary* matrix. To see this note that

$$\begin{aligned} (\mathsf{X}^\dagger \mathsf{X})_{ij} &= \sum_{k=1}^{n}(\mathsf{X}^\dagger)_{ik}(\mathsf{X})_{kj} \\ &= \sum_{k=1}^{n}(e_k^i)^* e_k^j \\ &= \mathsf{e}^{i\dagger}\,\mathsf{e}^j \\ &= \delta_{ij} \qquad\qquad\qquad\text{by orthonormality,} \end{aligned} \tag{4.81a}$$

or, in matrix notation,

$$\mathsf{X}^\dagger \mathsf{X} = \mathsf{I}. \tag{4.81b}$$

Hence $\mathsf{X}^\dagger = \mathsf{X}^{-1}$, and we conclude X is a unitary matrix.

We deduce that every Hermitian matrix, H, is diagonalizable by a transformation $\mathsf{X}^\dagger\mathsf{H}\mathsf{X}$, where X is a unitary matrix. Hence, if in (4.49a) we identify H and X with G and A respectively, we see that

   a metric can always be diagonalized by a suitable choice of basis,

namely the basis made up of the eigenvectors of G. Similarly, if we restrict ourselves to real matrices, then every real symmetric matrix, S, is diagonalizable by a transformation $\mathsf{R}^\mathsf{T}\mathsf{S}\mathsf{R}$, where R is an orthogonal matrix.

Example. Find the orthogonal matrix that diagonalizes the real symmetric matrix

$$\mathsf{S} = \begin{pmatrix} 1 & \beta \\ \beta & 1 \end{pmatrix} \quad \text{where} \quad \beta \geqslant 0 \quad \text{is real.} \tag{4.82}$$

Answer. The characteristic equation is

$$0 = \left\| \begin{matrix} 1 - \lambda & \beta \\ \beta & 1 - \lambda \end{matrix} \right\| = (1 - \lambda)^2 - \beta^2. \tag{4.83}$$

The solutions to (4.83) are

$$\lambda = \begin{cases} \lambda_+ = 1 + \beta \\ \lambda_- = 1 - \beta \end{cases}. \tag{4.84}$$

The corresponding eigenvectors $\mathsf{e}^\pm$ are found from

$$\begin{pmatrix} 1 - \lambda_\pm & \beta \\ \beta & 1 - \lambda_\pm \end{pmatrix} \begin{pmatrix} e_1^\pm \\ e_2^\pm \end{pmatrix} = 0, \tag{4.85a}$$

or

$$\beta \begin{pmatrix} \mp 1 & 1 \\ 1 & \mp 1 \end{pmatrix} \begin{pmatrix} e_1^\pm \\ e_2^\pm \end{pmatrix} = 0. \tag{4.85b}$$

$\beta \neq 0.$ If $\beta \neq 0$ (in which case $\lambda_+ \neq \lambda_-$) we have that

$$e_2^\pm = \pm e_1^\pm. \tag{4.86a}$$

On normalising $\mathsf{e}^\pm$ so that $\mathsf{e}^{\pm\dagger} \mathsf{e}^\pm = 1$, it follows that

$$\mathsf{e}^+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \mathsf{e}^- = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{4.86b}$$

Note that $\mathsf{e}^{+\dagger} \mathsf{e}^- = 0$, 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. e^+ and e^- 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 (4.80):

$$\mathsf{R} \equiv \mathsf{X} = \begin{pmatrix} e_1^+ & e_1^- \\ e_2^+ & e_2^- \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{4.87}$$

As a check we note that

$$\mathsf{R}^\mathrm{T}\mathsf{R} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{4.88}$$

and

$$\begin{aligned} \mathsf{R}^\mathrm{T}\mathsf{S}\,\mathsf{R} &= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & \beta \\ \beta & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 + \beta & 1 - \beta \\ 1 + \beta & -1 + \beta \end{pmatrix} \\ &= \begin{pmatrix} 1 + \beta & 0 \\ 0 & 1 - \beta \end{pmatrix} \\ &= \Lambda. \end{aligned} \tag{4.89}$$

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4.7.4 Diagonalization of Matrices

For a general $n \times n$ matrix M with n *distinct* eigenvalues λ_i, $(i = 1, \ldots, n)$, it is possible to show (but not here) that there are n linearly independent eigenvectors e^i. It then follows from our earlier results in §4.6 that M is diagonalized by the matrix

$$\mathsf{X} = \begin{pmatrix} e_1^1 & e_1^2 & \cdots & e_1^n \\ e_2^1 & e_2^2 & \cdots & e_2^n \\ \vdots & \vdots & \ddots & \vdots \\ e_n^1 & e_n^2 & \cdots & e_n^n \end{pmatrix}. \tag{4.90}$$

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 consider the matrix

$$\mathsf{M} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \tag{4.91}$$

with the characteristic equation $\lambda^2 = 0$; hence $\lambda_1 = \lambda_2 = 0$. Moreover, M has only one linearly independent eigenvector, namely

$$\mathsf{e} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{4.92}$$

and so M is *not* diagonalizable.

Normal Matrices. However, *normal matrices*, i.e. matrices such that $\mathsf{M}^\dagger \mathsf{M} = \mathsf{M} \mathsf{M}^\dagger$, always have n linearly independent eigenvectors and can always be diagonalized. Hence, as well as Hermitian matrices, skew-symmetric Hermitian matrices ($\mathsf{H}^\dagger = -\mathsf{H}$) and unitary matrices (and their real restrictions) can always be diagonalized.

4.8 Hermitian and Quadratic Forms

Definition. Let H be an Hermitian matrix. The expression

$$\mathsf{x}^\dagger \mathsf{H} \mathsf{x} = \sum_{i=1}^n \sum_{j=1}^n x_i^* H_{ij} x_j \,, \tag{4.93a}$$

is called an *Hermitian form*; it is a function of the complex numbers $(x_1, x_2, \ldots, x_n)$. Moreover, we note that

$$\begin{aligned} (\mathsf{x}^\dagger \mathsf{H} \mathsf{x})^* = (\mathsf{x}^\dagger \mathsf{H} \mathsf{x})^\dagger && \text{since a scalar is its own transpose} \\ = \mathsf{x}^\dagger \mathsf{H}^\dagger \mathsf{x} && \text{since } (\mathsf{A}\mathsf{B})^\dagger = \mathsf{B}^\dagger \mathsf{A}^\dagger \\ = \mathsf{x}^\dagger \mathsf{H} \mathsf{x} \,. && \text{since } \mathsf{H} \text{ is Hermitian} \end{aligned}$$

Hence an Hermitian form is real.

The Real Case. 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

$$\mathsf{x}^{\mathrm{T}} \mathsf{S} \mathsf{x} = \sum_{i=1}^n \sum_{j=1}^n x_i S_{ij} x_j \,. \tag{4.93b}$$

When considered as a function of the real variables $x_1, x_2, \ldots, x_n$, this expression called a *quadratic form*.

Remark. In the same way that an Hermitian matrix can be viewed as a generalisation to complex matrices of a real symmetric matrix, an Hermitian form can be viewed a generalisation to vector spaces over $\mathbb{C}$ of a quadratic form for a vector space over $\mathbb{R}$.

4.8.1 Eigenvectors and Principal Axes

Let us consider the equation
$$x^{\mathrm{T}}Sx = \text{constant}\,, \tag{4.94}$$

where S is a real symmetric matrix.

Conic Sections. First suppose that $n = 2$, then with
$$x = \left(\begin{array}{c} x \\ y \end{array} \right) \quad \text{and} \quad S = \left(\begin{array}{cc} \alpha & \beta \\ \beta & \gamma \end{array} \right)\,, \tag{4.95}$$

(4.94) becomes
$$\alpha x^2 + 2\beta xy + \gamma y^2 = \text{constant}\,. \tag{4.96}$$

This is the equation of a *conic section*. Now suppose that $x = Rx'$, where $x' = (x', y')^{\mathrm{T}}$ and R is a real orthogonal matrix. The equation of the conic section then becomes
$$x'^{\mathrm{T}}S'x' = \text{constant}, \quad \text{where} \quad S' = R^{\mathrm{T}}SR\,. \tag{4.97}$$

Now choose R to diagonalize S so that
$$S' = \left(\begin{array}{cc} \lambda_1 & 0 \\ 0 & \lambda_2 \end{array} \right)\,, \tag{4.98}$$

where λ_1 and λ_2 are the eigenvalues of S; from our earlier results in § 4.7.3 we know that such a matrix can always be found (and wlog $\det R = 1$). The conic section then takes the simple form
$$\lambda_1 x'^2 + \lambda_2 y'^2 = \text{constant}\,. \tag{4.99}$$

The 'prime' axes are identical to the eigenvectors of S', and hence in terms of the 'prime' axes the normalised eigenvectors of S' are
$$e'^{\,1} = \left(\begin{array}{c} 1 \\ 0 \end{array} \right) \quad \text{and} \quad e'^{\,2} = \left(\begin{array}{c} 0 \\ 1 \end{array} \right)\,, \tag{4.100}$$

with eigenvalues λ_1 and λ_2 respectively. Axes that coincide with the eigenvectors are known as *principal axes*. In the terms of the original axes, the principal axes are given by $e^i = Re'^{\,i}$ $(i = 1, 2)$.

Interpretation. If $\lambda_1\lambda_2 > 0$ then (4.99) is the equation for an ellipse with principal axes coinciding with the x' and y' axes.

    Scale. The *scale* of the ellipse is determined by the constant on the right-hand-side of (4.94) (or (4.99)).

    Orientation. The *orientation* of the ellipse is determined by the eigenvectors of S.

    Shape. The *shape* of the ellipse is determined by the eigenvalues of S.

    In the *degenerate case*, $\lambda_1 = \lambda_2$, the ellipse becomes a circle with no preferred principal axes. Any two linearly independent vectors may be chosen as the principal axes, which are no longer necessarily orthogonal but can be be chosen to be so.

    If $\lambda_1\lambda_2 < 0$ then (4.99) is the equation for a hyperbola with principal axes coinciding with the x' and y' axes. Similar results to above hold for the scale, orientation and shape.

Quadric Surfaces. For a real 3×3 symmetric matrix S, the equation
$$x^{\mathrm{T}}Sx = k\,, \tag{4.101}$$

where k is a constant, is called a *quadric surface*. After a rotation of axes such that $S \rightarrow S' = \Lambda$, a diagonal matrix, its equation takes the form
$$\lambda_1 x'^2 + \lambda_2 y'^2 + \lambda_3 z'^2 = k\,. \tag{4.102}$$

The axes in the new 'prime' coordinate system are again known as principal axes, and the eigenvectors of S' (or S) are again aligned with the principal axes. We note that when $\lambda_i k > 0$,

$$\text{the distance to surface along the } i\text{th principal axes} = \sqrt{\frac{k}{\lambda_i}}. \qquad (4.103)$$

Special Cases.

- In the case of metric matrices we know that S is positive definite, and hence that λ_1, λ_2 and λ_3 are all positive. The quadric surface is then an *ellipsoid*
- If $\lambda_1 = \lambda_2$ then we have a *surface of revolution* about the z' axis.
- If $\lambda_1 = \lambda_2 = \lambda_3$ we have a *sphere*.
- If $\lambda_3 \to 0$ then we have a *cylinder*.
- If $\lambda_2, \lambda_3 \to 0$, then we recover the *planes* $x' = \pm\sqrt{\frac{k}{\lambda_1}}$.

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4.8.2 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 (4.55) 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.

$$(\text{relative distance to surface})^2 = \frac{\mathsf{x}^{\mathrm{T}}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}}. \qquad (4.104)$$

Let us consider the directions for which this relative distance, or equivalently its inverse

$$\lambda(\mathsf{x}) = \frac{\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}, \qquad (4.105)$$

is *stationary*. We can find the so-called *first variation* in $\lambda(\mathsf{x})$ by letting

$$\mathsf{x} \to \mathsf{x} + \delta\mathsf{x} \quad \text{and} \quad \mathsf{x}^{\mathrm{T}} \to \mathsf{x}^{\mathrm{T}} + \delta\mathsf{x}^{\mathrm{T}}, \qquad (4.106)$$

by performing a Taylor expansion, and by ignoring terms quadratic or higher in $|\delta\mathsf{x}|$. First note that

$$\begin{aligned}
(\mathsf{x}^{\mathrm{T}} + \delta\mathsf{x}^{\mathrm{T}})(\mathsf{x} + \delta\mathsf{x}) &= \mathsf{x}^{\mathrm{T}}\mathsf{x} + \mathsf{x}^{\mathrm{T}}\delta\mathsf{x} + \delta\mathsf{x}^{\mathrm{T}}\mathsf{x} + \ldots \\
&= \mathsf{x}^{\mathrm{T}}\mathsf{x} + 2\delta\mathsf{x}^{\mathrm{T}}\mathsf{x} + \ldots . \qquad \text{since the transpose of a scalar is itself}
\end{aligned}$$

Hence

$$\begin{aligned}
\frac{1}{(\mathsf{x}^{\mathrm{T}} + \delta\mathsf{x}^{\mathrm{T}})(\mathsf{x} + \delta\mathsf{x})} &= \frac{1}{\mathsf{x}^{\mathrm{T}}\mathsf{x} + 2\delta\mathsf{x}^{\mathrm{T}}\mathsf{x} + \ldots} \\
&= \frac{1}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\left(1 + \frac{2\delta\mathsf{x}^{\mathrm{T}}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} + \ldots\right)^{-1} \\
&= \frac{1}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\left(1 - \frac{2\delta\mathsf{x}^{\mathrm{T}}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} + \ldots\right).
\end{aligned}$$

Similarly

$$\begin{aligned}
(\mathsf{x}^{\mathrm{T}} + \delta\mathsf{x}^{\mathrm{T}})\mathsf{S}(\mathsf{x} + \delta\mathsf{x}) &= \mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + \mathsf{x}^{\mathrm{T}}\mathsf{S}\delta\mathsf{x} + \delta\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + \ldots \\
&= \mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + 2\delta\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + \ldots . \qquad \text{since } \mathsf{S}^{\mathrm{T}} = \mathsf{S}
\end{aligned}$$

Putting the above results together we have that

$$
\begin{aligned}
\delta\lambda(\mathsf{x}) &= \frac{(\mathsf{x}^{\mathrm{T}} + \delta\mathsf{x}^{\mathrm{T}})\mathsf{S}(\mathsf{x} + \delta\mathsf{x})}{(\mathsf{x}^{\mathrm{T}} + \delta\mathsf{x}^{\mathrm{T}})(\mathsf{x} + \delta\mathsf{x})} - \frac{\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} \\
&= \frac{\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + 2\delta\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} + \ldots}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\left(1 - \frac{2\delta\mathsf{x}^{\mathrm{T}}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} + \ldots\right) - \frac{\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} \\
&= \frac{2\delta\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} - \frac{\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\frac{2\delta\mathsf{x}^{\mathrm{T}}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} + \ldots \\
&= \frac{2}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\left(\delta\mathsf{x}^{\mathrm{T}}\mathsf{S}\mathsf{x} - \lambda(\mathsf{x})\delta\mathsf{x}^{\mathrm{T}}\mathsf{x}\right) \\
&= \frac{2}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\delta\mathsf{x}^{\mathrm{T}}\left(\mathsf{S}\mathsf{x} - \lambda(\mathsf{x})\mathsf{x}\right).
\end{aligned}
\tag{4.107}
$$

Hence the first variation is zero for all possible $\delta\mathsf{x}$ when

$$
\mathsf{S}\mathsf{x} = \lambda(\mathsf{x})\mathsf{x}, \tag{4.108}
$$

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 (4.104) stationary, and the eigenvalues are the values of (4.105) 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

$$
\lambda(\mathsf{x}) = \frac{\mathsf{x}^{\dagger}\mathsf{H}\mathsf{x}}{\mathsf{x}^{\dagger}\mathsf{x}} \tag{4.109}
$$

at its stationary points.

4.9 Mechanical Oscillations (Unlectured: See Easter Term Course)

4.9.0 Why Have We Studied Hermitian Matrices, etc.?

The above discussion of quadratic forms, etc. may have appeared rather dry. There is a nice application concerning *normal modes* and *normal coordinates* for mechanical oscillators (e.g. molecules). If you are interested read on, if not wait until the first few lectures of the Easter term course where the following material appears in the schedules.

4.9.1 Governing Equations

Suppose we have a mechanical system described by coordinates $q_1, \ldots, q_n$, where the q_i may be distances, angles, etc. Suppose that the system is in equilibrium when $\mathsf{q} = \mathsf{0}$, and consider *small* oscillations about the equilibrium. The velocities in the system will depend on the $\dot{q}_i$, and for *small* oscillations the velocities will be *linear* in the $\dot{q}_i$, and total kinetic energy T will be quadratic in the $\dot{q}_i$. The most general quadratic expression for T is

$$
T = \sum_i \sum_j a_{ij}\dot{q}_i\dot{q}_j = \dot{\mathsf{q}}^{\mathrm{T}}\mathsf{A}\dot{\mathsf{q}}. \tag{4.110}
$$

Since kinetic energies are positive, A should be positive definite. We will also assume that, by a suitable choice of coordinates, A can be chosen to be symmetric.

Consider next the potential energy, V. This will depend on the coordinates, but not on the velocities, i.e. $V \equiv V(\mathsf{q})$. For small oscillations we can expand V about the equilibrium position:

$$
V(\mathsf{q}) = V(\mathsf{0}) + \sum_i q_i \frac{\partial V}{\partial q_i}(\mathsf{0}) + \tfrac{1}{2}\sum_i\sum_j q_i q_j \frac{\partial^2 V}{\partial q_i \partial q_j}(\mathsf{0}) + \ldots. \tag{4.111}
$$

Normalise the potential so that $V(0) = 0$. Also, since the system is in equilibrium when $\mathsf{q} = 0$, we require that there is no force when $\mathsf{q} = 0$. Hence

$$\frac{\partial V}{\partial q_i}(0) = 0\,. \tag{4.112}$$

Hence for small oscillations we may approximate (4.111) by

$$V = \sum_i \sum_j b_{ij} q_i q_j = \mathsf{q}^{\mathrm{T}} \mathsf{B} \mathsf{q}\,. \tag{4.113}$$

We note that if the mixed derivatives of V are equal, then B is symmetric. Assume next that there are no dissipative forces so that there is conservation of energy. Then we have that

$$\frac{\mathrm{d}}{\mathrm{d}t}(T + V) = 0\,. \tag{4.114}$$

In matrix form this equation becomes, after using the symmetry of A and B,

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}(T + V) = \ddot{\mathsf{q}}^{\mathrm{T}} \mathsf{A} \dot{\mathsf{q}} + \dot{\mathsf{q}}^{\mathrm{T}} \mathsf{A} \ddot{\mathsf{q}} + \dot{\mathsf{q}}^{\mathrm{T}} \mathsf{B} \mathsf{q} + \mathsf{q}^{\mathrm{T}} \mathsf{B} \dot{\mathsf{q}}$$

$$= 2\dot{\mathsf{q}}^{\mathrm{T}} \left(\mathsf{A} \ddot{\mathsf{q}} + \mathsf{B} \mathsf{q} \right)\,. \tag{4.115}$$

We will assume that the solution of this matrix equation that we need is the one in which the coefficient of each $\dot{q}_i$ is zero, i.e. we will require

$$\mathsf{A} \ddot{\mathsf{q}} + \mathsf{B} \mathsf{q} = 0\,. \tag{4.116}$$

4.9.2 Normal Modes

We will seek solutions to (4.116) that all oscillate with the same frequency, i.e. we seek solutions

$$\mathsf{q} = \mathsf{x} \cos(\omega t + \phi)\,, \tag{4.117}$$

where ϕ is a constant. Substituting into (4.116) we find that

$$(\mathsf{B} - \omega^2 \mathsf{A})\mathsf{q} = 0\,, \tag{4.118}$$

or, on the assumption that A is invertible,

$$(\mathsf{A}^{-1} \mathsf{B} - \omega^2 \mathsf{I})\mathsf{q} = 0\,. \tag{4.119}$$

Thus the solutions ω^2 are the eigenvalues of $\mathsf{A}^{-1}\mathsf{B}$, and are referred to as *eigenfrequencies* or *normal frequencies*. The eigenvectors are referred to as normal modes, and in general there will be n of them.

4.9.3 Normal Coordinates

We have seen how, for a quadratic form, we can change coordinates so that the matrix for a particular form is diagonalized. We assert, but do not prove, that a transformation can be found that simultaneously diagonalizes A and B, say to M and N. The new coordinates, say u, are referred to as normal coordinates. In terms of them the kinetic and potential energies become

$$T = \sum_i \mu_i \dot{u}_i^2 = \dot{\mathsf{u}}^{\mathrm{T}} \mathsf{M} \dot{\mathsf{u}} \quad \text{and} \quad V = \sum_i \nu_i u_i^2 = \mathsf{u}^{\mathrm{T}} \mathsf{N} \mathsf{u} \tag{4.120}$$

respectively, where

$$\mathsf{M} = \begin{pmatrix} \mu_1 & 0 & \cdots & 0 \\ 0 & \mu_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mu_n \end{pmatrix} \quad \text{and} \quad \mathsf{N} = \begin{pmatrix} \nu_1 & 0 & \cdots & 0 \\ 0 & \nu_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \nu_n \end{pmatrix}\,. \tag{4.121}$$

The equations of motion are then the *uncoupled* equations

$$\mu_i \ddot{u}_i + \nu_i u_i = 0 \quad (i = 1, \ldots, n)\,. \tag{4.122}$$

4.9.4 Example

Consider a system in which three particles of mass m, μm and m are connected in a straight line by light springs with a force constant k (cf. an idealised model of CO_2).[20]

The kinetic energy of the system is then

$$T = \tfrac{1}{2}(m\dot{x}_1^2 + \mu m\dot{x}_2^2 + m\dot{x}_3^2)\,, \qquad (4.123\text{a})$$

while the potential energy stored in the springs is

$$V = \tfrac{1}{2}k((x_2 - x_1)^2 + (x_3 - x_2)^2)\,. \qquad (4.123\text{b})$$

The kinetic and potential energy matrices are thus

$$\mathsf{A} = \tfrac{1}{2}m\begin{pmatrix} 1 & 0 & 0 \\ 0 & \mu & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \mathsf{B} = \tfrac{1}{2}k\begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}\,, \qquad (4.124)$$

respectively. In order to find the normal frequencies we therefore need to find the roots to $\|\mathsf{B} - \omega^2\mathsf{A}\| = 0$ (see (4.118)), i.e. we need the roots to

$$\left\| \begin{matrix} 1-\lambda & -1 & 0 \\ -1 & 2-\mu\lambda & -1 \\ 0 & -1 & 1-\lambda \end{matrix} \right\| = \lambda(1-\lambda)(\mu\lambda - (\mu+2)) = 0\,, \qquad (4.125)$$

where $\lambda = m\omega^2/k$. The eigenfrequencies are thus

$$\omega_1 = 0\,, \quad \omega_2 = \left(\frac{k}{m}\right)^{\frac{1}{2}}\,, \quad \omega_3 = \left(\frac{k}{m}\right)^{\frac{1}{2}}\left(1+\frac{2}{\mu}\right)^{\frac{1}{2}}\,, \qquad (4.126)$$

with corresponding (non-normalised) eigenvectors

$$\mathsf{x}^1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}\,, \quad \mathsf{x}^2 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}\,, \quad \mathsf{x}^3 = \begin{pmatrix} 1 \\ -2/\mu \\ 1 \end{pmatrix}\,. \qquad (4.127)$$

Remark.   Note that the centre of mass of the system is at rest in the case of x^2 and x^3.

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[20] See Riley, Hobson & Bence (1997).

5 Elementary Analysis

5.0 Why Study This?

Analysis is one of the foundations upon which mathematics is built. At some point you ought to at least inspect the foundations! Also, you need to have an idea of when, and when not, you can sum a series, e.g. a Fourier series.

5.1 Sequences and Limits

5.1.1 Sequences

A *sequence* is a set of numbers 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

$$1, \tfrac{1}{2}, \tfrac{1}{3}, \tfrac{1}{4}, \ldots . \tag{5.1}$$

5.1.2 Sequences Tending to a Limit, or Not.

Sequences tending to a 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

$$|s_n - s| < \varepsilon \quad \text{for all} \quad n > N . \tag{5.2a}$$

We then write

$$\lim_{n \to \infty} s_n = s . \tag{5.2b}$$

Example. 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,

$$N > \frac{\log 1/\varepsilon}{\log 1/|x|} . \tag{5.3}$$

Then, if $n > N$,

$$|s_n - 0| = |x|^n < |x|^N < \varepsilon . \tag{5.4a}$$

Hence

$$\lim_{n \to \infty} x^n = 0 . \tag{5.4b}$$

Property. An increasing sequence tends either to a limit or to $+\infty$. Hence a bounded increasing sequence tends to a limit, i.e. if

$$s_{n+1} > s_n , \quad \text{and} \quad s_n < \mathcal{K} \in \mathbb{R} \quad \text{for all } n, \text{ then} \quad s = \lim_{n \to \infty} s_n \quad \text{exists.} \tag{5.5}$$

Remark. You really ought to have a proof of this property, but I do not have time.[21]

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

$$s_n > A \quad \text{for all} \quad n > N . \tag{5.6a}$$

We then write

$$s_n \to \infty \quad \text{as} \quad n \to \infty . \tag{5.6b}$$

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

$$s_n < -A \quad \text{for all} \quad n > N . \tag{5.6c}$$

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*.

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[21] Alternatively you can view this property as an axiom that specifies the real numbers $\mathbb{R}$ essentially uniquely.

5.2   Convergence of Infinite Series

5.2.1   Convergent Series

Given an infinite sequence of numbers $u_1, u_2, \ldots$, define the *partial sum* s_n by

$$s_n = \sum_{r=1}^{n} u_r \,. \tag{5.7}$$

If as $n \to \infty$, s_n tends to a finite limit, s, then we say that the infinite series

$$\sum_{r=1}^{\infty} u_r \,, \tag{5.8}$$

converges (or is convergent), and that s is its sum.

Example: the convergence of a geometric series. The series

$$\sum_{r=0}^{\infty} x^r = 1 + x + x^2 + x^3 + \ldots \,, \tag{5.9}$$

converges to $(1 - x)^{-1}$ provided that $|x| < 1$.

Answer. Consider the partial sum

$$s_n = 1 + x + \cdots + x^{n-1} = \frac{1 - x^n}{1 - x} \,. \tag{5.10}$$

If $|x| < 1$, then from (5.4b) we have that $x^n \to 0$ as $n \to \infty$, and hence

$$s = \lim_{n \to \infty} s_n = \frac{1}{1 - x} \quad \text{for } |x| < 1. \tag{5.11}$$

However if $|x| \geqslant 1$ the series diverges.

5.2.2   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

$$\lim_{r \to \infty} u_r = \lim_{r \to \infty} (s_r - s_{r-1}) = \lim_{r \to \infty} s_r - \lim_{r \to \infty} s_{r-1} = s - s = 0 \,. \tag{5.12}$$

However, as we are about to see with the example $u_r = \frac{1}{r}$ (see (5.13) and (5.14)), $u_r \to 0$ as $r \to \infty$ is *not* a sufficient condition for convergence.

5.2.3   Divergent Series

An infinite series which is not convergent is called *divergent*.

Example. Suppose that

$$u_r = \frac{1}{r} \quad \text{so that} \quad s_n = \sum_{r=1}^{n} \frac{1}{r} = 1 + \tfrac{1}{2} + \tfrac{1}{3} \cdots + \tfrac{1}{n} \,. \tag{5.13}$$

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)

$$s_{2^m} > 1 + \tfrac{m}{2} \,, \tag{5.14}$$

and hence the series is divergent.

5.2.4 Absolutely Convergent Series

A series $\sum u_r$ is said to *converge absolutely* if

$$\sum_{r=1}^{\infty} |u_r| \tag{5.15}$$

converges, otherwise any convergence of the series is said to be *conditional*.

Example. Suppose that

$$u_r = (-1)^{r-1}\frac{1}{r} \quad \text{so that} \quad s_n = \sum_{r=1}^{n}(-1)^{r-1}\frac{1}{r} = 1 - \tfrac{1}{2} + \tfrac{1}{3}\cdots + (-1)^{n-1}\tfrac{1}{n} \,. \tag{5.16}$$

Then, from the Taylor expansion

$$\log(1+x) = -\sum_{r=1}^{\infty}\frac{(-x)^r}{r} \,, \tag{5.17}$$

we spot that $s = \lim_{n\to\infty} s_n = \log 2$; hence $\sum_{r=1}^{\infty} u_r$ converges. However, from (5.13) and (5.14) we already know that $\sum_{r=1}^{\infty} |u_r|$ diverges. Hence $\sum_{r=1}^{\infty} u_r$ is conditionally convergent.

Property. If $\sum |u_r|$ converges then so does $\sum u_r$ (see the Example Sheet for a proof).

5.3 Tests of Convergence

5.3.1 The Comparison Test

If we are given that $v_r > 0$ and

$$S = \sum_{r=1}^{\infty} v_r \tag{5.18}$$

is convergent, the infinite series $\sum_{r=1}^{\infty} u_r$ is also convergent if $0 < u_r < \mathcal{K}v_r$ for some $\mathcal{K}$ independent of r.

Proof. Since $u_r > 0$, $s_n = \sum_{r=1}^{n} u_r$ is an increasing sequence. Further

$$s_n = \sum_{r=1}^{n} u_r < \mathcal{K}\sum_{r=1}^{n} v_r \,, \tag{5.19}$$

and thus

$$\lim_{n\to\infty} s_n < \mathcal{K}\sum_{r=1}^{\infty} v_r = \mathcal{K}\,S \,, \tag{5.20}$$

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i.e. s_n is an increasing bounded sequence. Thence from (5.5) $\sum_{r=1}^{\infty} u_r$ is convergent.

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.

5.3.2 D'Alembert's Ratio Test

Suppose that $u_r > 0$ and that

$$\lim_{r \to \infty} \left(\frac{u_{r+1}}{u_r} \right) = \rho. \tag{5.21}$$

Then $\sum u_r$ converges if $\rho < 1$, while $\sum u_r$ diverges if $\rho > 1$.

Proof. First suppose that $\rho < 1$. Choose σ with $\rho < \sigma < 1$. Then there exists $N \equiv N(\sigma)$ such that

$$\frac{u_{r+1}}{u_r} < \sigma \quad \text{for all} \quad r > N. \tag{5.22}$$

So

$$\sum_{r=1}^{\infty} u_r = \sum_{r=1}^{N} u_r + u_{N+1} \left\{ 1 + \frac{u_{N+2}}{u_{N+1}} + \frac{u_{N+2}}{u_{N+1}} \frac{u_{N+3}}{u_{N+2}} + \dots \right\}$$

$$< \sum_{r=1}^{N} u_r + u_{N+1}(1 + \sigma + \sigma^2 + \dots) \qquad \text{by hypothesis}$$

$$< \sum_{r=1}^{N} u_r + \frac{u_{N+1}}{1 - \sigma} \qquad \text{by (5.11) since } \sigma < 1. \tag{5.23}$$

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 (5.5) that $\sum u_r$ converges.

Next suppose that $\rho > 1$. Choose τ with $1 < \tau < \rho$. Then there exists $M \equiv M(\tau)$ such that

$$\frac{u_{r+1}}{u_r} > \tau > 1 \quad \text{for all} \quad r > M, \tag{5.24a}$$

and hence

$$\frac{u_r}{u_M} > \tau^{r-M} > 1 \quad \text{for all} \quad r > M. \tag{5.24b}$$

Thus, since $u_r \not\to 0$ as $r \to \infty$, we conclude that $\sum u_r$ diverges.

5.3.3 Cauchy's Test

Suppose that $u_r > 0$ and that

$$\lim_{r \to \infty} u_r^{1/r} = \rho. \tag{5.25}$$

Then $\sum u_r$ converges if $\rho < 1$, while $\sum u_r$ diverges if $\rho > 1$.

Proof. First suppose that $\rho < 1$. Choose σ with $\rho < \sigma < 1$. Then there exists $N \equiv N(\sigma)$ such that

$$u_r^{1/r} < \sigma, \quad \text{i.e.} \quad u_r < \sigma^r \quad \text{for all} \quad r > N. \tag{5.26}$$

It follows that

$$\sum_{r=1}^{\infty} u_r < \sum_{r=1}^{N} u_r + \sum_{r=N+1}^{\infty} \sigma^r. \tag{5.27}$$

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 (5.5) we also conclude that $\sum u_r$ converges.

Next suppose that $\rho > 1$. Choose τ with $1 < \tau < \rho$. Then there exists $M \equiv M(\tau)$ such that

$$u_r^{1/r} > \tau > 1, \quad \text{i.e.} \quad u_r > \tau^r > 1, \quad \text{for all} \quad r > M. \tag{5.28}$$

Thus, since $u_r \not\to 0$ as $r \to \infty$, $\sum u_r$ must diverge.

5.4   Power Series of a Complex Variable

A power series of a complex variable, z, has the form

$$f(z) = \sum_{r=0}^{\infty} a_r z^r \quad \text{where} \quad a_r \in \mathbb{C}. \tag{5.29}$$

Remark. Many of the above results for real series can be generalised for complex series. For instance, 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 $\sum |a_r z^r|$ converges, so does $\sum a_r z^r$.

5.4.1   Convergence of Power Series

If the sum $\sum_{r=0}^{\infty} a_r z^r$ converges for $z = z_1$, then it converges absolutely for all z such that $|z| < |z_1|$.

Proof. First we note that

$$|a_r z^r| = |a_r z_1^r| \left| \frac{z}{z_1} \right|^r . \tag{5.30}$$

Also, since $\sum a_r z_1^r$ converges, then from § 5.2.2, $a_r z_1^r \to 0$ as $r \to \infty$. Hence for a given ε there exists $N \equiv N(\varepsilon)$ such that if $r > N$ then $|a_r z_1^r| < \varepsilon$ and

$$|a_r z^r| < \varepsilon \left| \frac{z}{z_1} \right|^r \quad \text{if } |z| < |z_1|. \tag{5.31}$$

Thus $\sum a_r z^r$ converges for $|z| < |z_1|$ by comparison with a geometric series.

Corollary. If the sum diverges for $z = z_1$ then it diverges for all z such that $|z| > |z_1|$. For suppose that it were to converge for some such $z = z_2$ with $|z_2| > |z_1|$, then it would converge for $z = z_1$ by the above result; this is in contradiction to the hypothesis.

5.4.2   Radius of Convergence

The results of § 5.4.1 imply that there exists some circle in the complex z-plane of radius ϱ (possibly 0 or ∞) such that:

$$\left. \begin{array}{l} \sum a_r z^r \text{ converges for } |z| < \varrho \\ \sum a_r z^r \text{ diverges for } |z| > \varrho \end{array} \right\} \quad |z| = \varrho \quad \text{is the } \textit{circle of convergence.} \tag{5.32}$$

The real number ϱ is called the *radius of convergence*. On $|z| = \varrho$ the sum may or may not converge.

5.4.3   Determination of the Radius of Convergence

Let

$$f(z) = \sum_{r=0}^{\infty} u_r \quad \text{where} \quad u_r = a_r z^r . \tag{5.33}$$

Use D'Alembert's ratio test. If the limit exists, then

$$\lim_{r \to \infty} \left| \frac{a_{r+1}}{a_r} \right| = \frac{1}{\varrho} . \tag{5.34}$$

Proof. We have that

$$\lim_{r \to \infty} \left| \frac{u_{r+1}}{u_r} \right| = \lim_{r \to \infty} \left| \frac{a_{r+1}}{a_r} \right| |z| = \frac{|z|}{\varrho} \quad \text{by hypothesis.}$$

Hence the series converges absolutely by D'Alembert's ratio test if $|z| < \varrho$. On the other hand if $|z| > \varrho$, then

$$\lim_{r \to \infty} \left| \frac{u_{r+1}}{u_r} \right| = \frac{|z|}{\varrho} > 1 \,. \tag{5.35}$$

Hence $u_r \nrightarrow 0$ as $r \to \infty$, and so the series does not converge. It follows that ϱ is the radius of convergence.

Remark. The limit (5.34) may not exist, e.g. if $a_r = 0$ for r odd then $\left| \frac{a_{r+1}}{a_r} \right|$ is alternately 0 or ∞.

Use Cauchy's test. If the limit exists, then

$$\lim_{r \to \infty} |a_r|^{1/r} = \frac{1}{\varrho} \,. \tag{5.36}$$

Proof. We have that

$$\lim_{r \to \infty} |u_r|^{1/r} = \lim_{r \to \infty} |a_r|^{1/r} |z| = \frac{|z|}{\varrho} \quad \text{by hypothesis.} \tag{5.37}$$

Hence the series converges absolutely by Cauchy's test if $|z| < \varrho$.

On the other hand if $|z| > \varrho$, choose τ with $1 < \tau < |z|/\varrho$. Then there exists $M \equiv M(\tau)$ such that

$$|u_r|^{1/r} > \tau > 1 \,, \quad \text{i.e.} \quad |u_r| > \tau^r > 1 \,, \quad \text{for all} \quad r > M \,.$$

Thus, since $u_r \nrightarrow 0$ as $r \to \infty$, $\sum u_r$ must diverge. It follows that ϱ is the radius of convergence.

5.4.4 Examples

1. Suppose that $f(z)$ is the geometric series

$$f(z) = \sum_{r=0}^{\infty} z^r \,.$$

Then $a_r = 1$ for all r, and hence

$$\left| \frac{a_{r+1}}{a_r} \right| = 1 \quad \text{and} \quad |a_r|^{1/r} = 1 \quad \text{for all } r. \tag{5.38}$$

Hence $\varrho = 1$ by either D'Alembert's ratio test or Cauchy's test, and the series converges for $|z| < 1$. In fact

$$f(z) = \frac{1}{1-z} \,.$$

Note the *singularity* at $z = 1$ which determines the radius of convergence.

2. Suppose that $f(z) = -\sum_{r=1}^{\infty} \frac{(-z)^r}{r}$. Then $a_r = \frac{(-1)^{r-1}}{r}$, and hence

$$\left| \frac{a_{r+1}}{a_r} \right| = \frac{r}{r+1} \to 1 \quad \text{as} \quad r \to \infty \,. \tag{5.39}$$

Hence $\varrho = 1$ by D'Alembert's ratio test. As a check we observe that

$$|a_r|^{1/r} = \left(\frac{1}{r} \right)^{1/r} , \quad \text{and} \quad \log |a_r|^{1/r} = \frac{1}{r} \log \frac{1}{r} \to 0 \text{ as } r \to \infty \,.$$

Thus

$$|a_r|^{1/r} \to 1 \quad \text{as} \quad r \to \infty \,, \tag{5.40}$$

and we confirm by Cauchy's test that $\varrho = 1$. In fact the series converges to $\log(1 + z)$ for $|z| < 1$; the singularity at $z = -1$ fixes the radius of convergence.

3. Next suppose $f(z) = \sum_{r=0}^{\infty} \dfrac{z^r}{r!}$. Then $a_r = \frac{1}{r!}$ and

$$\frac{a_{r+1}}{a_r} = \frac{1}{r+1} \to 0 \quad \text{as} \quad r \to \infty. \tag{5.41}$$

Hence $\varrho = \infty$ by D'Alembert's ratio test. As a check we observe that

$$|a_r|^{1/r} = \left(\frac{1}{r!}\right)^{1/r}, \quad \text{and} \quad \log |a_r|^{1/r} = -\frac{1}{r} \log r!.$$

But Stirling's formula gives that

$$\log r! \sim r \log r + \tfrac{1}{2} \log r - r + \ldots \quad \text{as} \quad r \to \infty,$$

and so

$$\log |a_r|^{1/r} \to -\log r \to -\infty \quad \text{as} \quad r \to \infty.$$

Thus

$$|a_r|^{\frac{1}{r}} \to 0 \quad \text{as} \quad r \to \infty, \tag{5.42}$$

and we confirm by Cauchy's test that $\varrho = \infty$. In fact the series converges to e^z for all finite z.

4. Finally suppose $f(z) = \sum_{r=0}^{\infty} r! z^r$. Then $a_r = r!$ and

$$\frac{a_{r+1}}{a_r} = r + 1 \to \infty \quad \text{as} \quad r \to \infty. \tag{5.43}$$

Hence $\varrho = 0$ by D'Alembert's ratio test. As a check we observe, using Stirling's formula, that

$$|a_r|^{1/r} = (r!)^{1/r}, \quad \text{and} \quad \log |a_r|^{1/r} = \frac{1}{r} \log r! \sim \log r \to \infty \quad \text{as} \quad r \to \infty,$$

and so

$$|a_r|^{1/r} \to \infty \quad \text{as} \quad r \to \infty. \tag{5.44}$$

Thus we confirm by Cauchy's test this series has *zero radius of convergence*; it fails to define the function $f(z)$ for any non-zero z.

5.4.5 Analytic Functions

A function $f(z)$ is said to be analytic at $z = z_0$ if it has Taylor series expansion about $z = z_0$ with a *non-zero radius of convergence*, i.e. $f(z)$ is analytic at $z = z_0$ if for some $\varrho > 0$

$$f(z) = \sum_{r=0}^{\infty} a_r (z - z_0)^r \quad \text{for } |z - z_0| < \varrho. \tag{5.45a}$$

The coefficients of the Taylor series can be evaluated by differentiating (5.45a) n times and then evaluating the result at $z = z_0$, whence

$$a_n = \frac{1}{n!} \frac{\mathrm{d}^n f}{\mathrm{d}z^n}(z_0). \tag{5.45b}$$

5.4.6 The O Notation

Suppose that $f(z)$ and $g(z)$ are functions of z. Then

$$\text{if} \quad f(z)/g(z) \text{ is bounded} \quad \text{as } z \to 0 \text{ we say that } f(z) = O(g(z));$$

$$\text{if} \quad f(z)/g(z) \to 0 \quad \text{as } z \to 0 \text{ we say that } f(z) = o(g(z)).$$

Example. As $x \to 0$ we have that

$$\sin x = O(1) \qquad\qquad \text{since } \sin x/1 \text{ is bounded as } x \to 0;$$
$$\sin x = o(1) \qquad\qquad \text{since } \sin x/1 \to 0 \text{ as } x \to 0;$$
$$\sin x = O(x) \qquad\qquad \text{since } \sin x/x \text{ is bounded as } x \to 0.$$

Remark. The O notation is often used in conjunction with truncated Taylor series, e.g. for small $(z - z_0)$

$$f(z) = f(z_0) + (z - z_0)f'(z_0) + \tfrac{1}{2}(z - z_0)^2 f''(z_0) + O((z - z_0)^3). \qquad (5.46)$$

5.5   Integration

You have already encountered integration as both

- the inverse of differentiation, and

- some form of of summation.

The aim of this part of the course is to emphasize that these two definitions are equivalent for continuous functions.

5.5.1   Why Do We Have To Do This Again?

You already know the 'definition'

$$\int_a^b f(t)\mathrm{d}t = \lim_{N\to\infty} \sum_{j=1}^N f(a + jh)\,h \quad \text{where} \quad h = (b-a)/N, \qquad (5.47)$$

so why are mathematicians not really content with it?

One answer is that while (5.47) is OK for OK functions, consider Dirichlet's function

$$f = \begin{cases} 0 & \text{on irrationals,} \\ 1 & \text{on rationals.} \end{cases} \qquad (5.48)$$

If

- $a = 0$ and $b = \pi$, then (5.47) evaluates to 0,

- $a = 0$ and $b = p/q$, where p/q is a rational approximation to π (e.g. 22/7 or better), then (5.47) evaluates to p/q.

Since we can choose p/q to be arbitrarily close to π we would appear to have a problem.[22] We conclude that we need a better definition of an integral. In particular

- we need a better way of dividing up $[a, b]$;

- we need to be more precise about the limit as the subdivisions tend to zero.

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[22] In fact Dirichlet's function is not Riemann integrable, so this example is a bit of a cheat.

5.5.2 The Riemann Integral

Dissection. A *dissection*, *partition* or *subdivision* D of the interval $[a, b]$ is a finite set of points $t_0, \ldots, t_N$ such that

$$a = t_0 < t_1 < \ldots < t_N = b \,.$$

Modulus. Define the *modulus*, *gauge* or *norm* of a dissection D, written $|D|$, to be the length of the longest subinterval $(t_j - t_{j-1})$ of D, i.e.

$$|D| = \max_{1 \leqslant j \leqslant N} |t_j - t_{j-1}| \,. \tag{5.49a}$$

Riemann Sum. A *Riemann sum*, $\sigma(D, \boldsymbol{\zeta})$, for a bounded function $f(t)$ is any sum

$$\sigma(D, \boldsymbol{\zeta}) = \sum_{j=1}^{N} f(\zeta_j)(t_j - t_{j-1}) \quad \text{where} \quad \zeta_j \in [t_{j-1}, t_j] \,. \tag{5.49b}$$

Note that if the subintervals all have the same length so that $t_j = (a + jh)$ and $t_j - t_{j-1} = h$ where $h = (t_N - t_0)/N$, and if we take $\zeta_j = t_j$, then (cf. (5.47))

$$\sigma(D, \boldsymbol{\zeta}) = \sum_{j=1}^{N} f(a + jh)\, h \,. \tag{5.49c}$$

Integrability. A bounded function $f(t)$ is *integrable* if there exists $I \in \mathbb{R}$ such that

$$\lim_{|D| \to 0} \sigma(D, \boldsymbol{\zeta}) = I \,, \tag{5.49d}$$

where the limit of the Riemann sum must exist *independent of the dissection* (subject to the condition that $|D| \to 0$) and *independent of the choice of $\boldsymbol{\zeta}$ for a given dissection D.*[23]

Definite Integral. For an integrable function f the *Riemann definite integral* of f over the interval $[a, b]$ is defined to be the limiting value of the Riemann sum, i.e.

$$\int_a^b f(t)\, \mathrm{d}t = I \,. \tag{5.49e}$$

Remark. An integral should be thought of as the limiting value of a sum, *not* as the area under a curve. Of course this is not to say that integrals are not a handy way of calculating the areas under curves.

Example. Suppose that $f(t) = c$, where c is a real constant. Then from (5.49b)

$$\sigma(D, \boldsymbol{\zeta}) = \sum_{j=1}^{N} c(t_j - t_{j-1}) = c(b - a) \,, \tag{5.50a}$$

whatever the choice of D and $\boldsymbol{\zeta}$. Hence the required limit in (5.49d) exists. We conclude that $f(t) = c$ is integrable, and that

$$\int_a^b c\, \mathrm{d}t = c(b - a) \,. \tag{5.50b}$$

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[23] More precisely, f is integrable if given $\varepsilon > 0$, there exists $I \in \mathbb{R}$ and $\delta > 0$ such that whatever the choice of $\boldsymbol{\zeta}$ for a given dissection D

$$|\sigma(D, \boldsymbol{\zeta}) - I| < \varepsilon \quad \text{when} \quad |D| < \delta \,.$$

Note that this is far more restrictive than saying that the sum (5.49c) converges as $h \to 0$.

Remark. Proving integrability using (5.49d) is in general non trivial (since there are a rather large number of dissections and sample points $\boldsymbol{\zeta}$ to consider).[24] However *if* we know that a function is integrable then the limit (5.49d) needs only to be evaluated once, i.e. for a limiting dissection and sample points of our choice (usually those that make the calculation easiest).

5.5.3 Properties of the Riemann Integral

Using (5.49d) and (5.49e) it is possible to show for integrable functions f and g, $a < c < b$, and $k \in \mathbb{R}$, that

$$\int_a^b f(t)\,\mathrm{d}t = -\int_b^a f(t)\,\mathrm{d}t\,, \tag{5.51a}$$

$$\int_a^b f(t)\,\mathrm{d}t = \int_a^c f(t)\,\mathrm{d}t + \int_c^b f(t)\,\mathrm{d}t\,, \tag{5.51b}$$

$$\int_a^b kf(t)\,\mathrm{d}t = k\int_a^b f(t)\,\mathrm{d}t\,, \tag{5.51c}$$

$$\int_a^b (f(t) + g(t))\,\mathrm{d}t = \int_a^b f(t)\,\mathrm{d}t + \int_a^b g(t)\,\mathrm{d}t\,, \tag{5.51d}$$

$$\left| \int_a^b f(t)\,\mathrm{d}t \right| \leqslant \int_a^b |f(t)|\,\mathrm{d}t\,. \tag{5.51e}$$

It is also possible to deduce that if f and g are integrable then so if fg.

Schwarz's Inequality. For integrable functions f and g (cf. (4.31))

$$\left(\int_a^b fg\,\mathrm{d}t \right)^2 \leqslant \left(\int_a^b f^2\mathrm{d}t \right) \left(\int_a^b g^2\mathrm{d}t \right)\,. \tag{5.52}$$

Proof. Using the above properties it follows that

$$0 \leqslant \int_a^b (\lambda f + g)^2 \mathrm{d}t = \lambda^2 \int_a^b f^2\mathrm{d}t + 2\lambda \int_a^b fg\,\mathrm{d}t + \int_a^b g^2\mathrm{d}t\,. \tag{5.53}$$

- If $\int_a^b f^2\mathrm{d}t = 0$ then

$$2\lambda \int_a^b fg\,\mathrm{d}t + \int_a^b g^2\mathrm{d}t \geqslant 0\,.$$

This can only be true for all λ if $\int_a^b fg\,\mathrm{d}t = 0$; the [in]equality follows.

- If $\int_a^b f^2\mathrm{d}t \neq 0$ then choose (cf. the proof of (4.31))

$$\lambda = -\frac{\displaystyle\int_a^b fg\,\mathrm{d}t}{\displaystyle\int_a^b f^2\mathrm{d}t}\,, \tag{5.54}$$

and the inequality again follows.

Remark. This will not be the last time that we will find an analogy between scalar/inner products and integrals.

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[24] As you might guess, there is a better way to do it.

5.5.4 The Fundamental Theorems of Calculus

Suppose f is integrable. Define

$$F(x) = \int_a^x f(t)\,\mathrm{d}t\,. \tag{5.55}$$

F is continuous. F is a continuous function of x since

$$|F(x+h) - F(x)| = \left| \int_x^{x+h} f(t)\,\mathrm{d}t \right|$$

$$\leqslant \int_x^{x+h} |f(t)|\,\mathrm{d}t$$

$$\leqslant \left(\max_{x \leqslant t \leqslant x+h} |f(t)| \right) h\,,$$

and hence

$$\lim_{h \to 0} |F(x+h) - F(x)| = 0\,.$$

The First Fundamental Theorem of Calculus. This states that

$$\frac{\mathrm{d}F}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\int_a^x f(t)\,\mathrm{d}t \right) = f(x)\,, \tag{5.56}$$

i.e. *the derivative of the integral of a function is the function.*

Proof. Suppose that

$$m = \min_{x \leqslant t \leqslant x+h} f(t) \quad \text{and} \quad M = \max_{x \leqslant t \leqslant x+h} f(t)\,.$$

We can show from the definition of a Riemann integral that for $h > 0$

$$mh \leqslant \int_x^{x+h} f(t)\,\mathrm{d}t \leqslant Mh\,,$$

so

$$m \leqslant \frac{F(x+h) - F(x)}{h} \leqslant M\,.$$

But if f is continuous, then as $h \to 0$ both m and M tend to $f(x)$. We can similarly 'sandwich' $(F(x+h) - F(x))/h$ if $h < 0$. (5.56) then follows from the definition of a derivative.

The Second Fundamental Theorem of Calculus. This essentially states that *the integral of the derivative of a function is the function*, i.e. if g is differentiable then

$$\int_a^x \frac{\mathrm{d}g}{\mathrm{d}t}\,\mathrm{d}t = g(x) - g(a)\,. \tag{5.57}$$

Proof. Define $f(x)$ by

$$f(x) = \frac{\mathrm{d}g}{\mathrm{d}x}(x)\,,$$

and then define F as in (5.55). Then using (5.56) we have that

$$\frac{\mathrm{d}}{\mathrm{d}x}(F - g) = 0\,.$$

Hence from integrating and using the fact that $F(a) = 0$ from (5.55),

$$F(x) - g(x) = -g(a).$$

Thus using the definition (5.55)

$$\int_a^x \frac{\mathrm{d}g}{\mathrm{d}t}\,\mathrm{d}t = g(x) - g(a). \tag{5.58}$$

The Indefinite Integral. Let f be integrable, and suppose $f = F'(x)$ for some function F. Then, based on the observation that the lower limit a in (5.55), etc. is arbitrary, we define the *indefinite integral* of f by

$$\int^x f(t)\,\mathrm{d}t = F(x) + c \tag{5.59}$$

for any constant c.

6 Ordinary Differential Equations

6.0 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 study a sub-class of ordinary differential equations of 'Sturm-Liouville' type. In addition we will consider eigenvalue problems for 'Sturm-Liouville' operators. In subsequent courses you will learn that such eigenvalues fix, say, the angular momentum of electrons in an atom.

6.1 Second-Order Linear Ordinary Differential Equations

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

$$y'' + p(x)y' + q(x)y = f(x). \tag{6.1}$$

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

6.2 Homogeneous Second-Order Linear ODEs

If $f = 0$ then any two solutions of

$$y'' + py' + qy = 0, \tag{6.2}$$

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

$$y = \alpha y_1 + \beta y_2. \tag{6.3}$$

Further, suppose that y_1 and y_2 are two *linearly independent* solutions, where by linearly independent we mean, as in (4.3), that

$$\alpha y_1(x) + \beta y_2(x) \equiv 0 \quad \Rightarrow \quad \alpha = \beta = 0. \tag{6.4}$$

Then since (6.2) is second order, the *general solution* of (6.2) will be of the form (6.3); 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 (6.3) becomes

$$y = (\alpha + \beta\gamma)y_1, \tag{6.5}$$

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

6.2.1 The Wronskian

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

$$\begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0, \tag{6.6}$$

has a non-zero solution. 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

$$\begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \quad \Rightarrow \quad \alpha = \beta = 0. \tag{6.7}$$

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

$$\left\| \begin{array}{cc} y_1 & y_2 \\ y_1' & y_2' \end{array} \right\| = y_1 y_2' - y_2 y_1' \neq 0 \,. \tag{6.8}$$

The function,

$$W(x) = y_1 y_2' - y_2 y_1' \,, \tag{6.9}$$

is called the *Wronskian* of the two solutions. To recap: if W is non-zero then y_1 and y_2 are linearly independent.

6.2.2 The Calculation of W

We can derive a differential equation for the Wronskian, since

$$
\begin{aligned}
W' &= y_1 y_2'' - y_1'' y_2 && \text{from (6.9) since the } y_1' y_2' \text{ terms cancel} \\
&= -y_1(py_2' + qy_2) + (py_1' + qy_1)y_2 && \text{using equation (6.2)} \\
&= -p(y_1 y_2' - y_1' y_2) && \text{since the } qy_1 y_2 \text{ terms cancel} \\
&= -pW && \text{from definition (6.9).} \tag{6.10}
\end{aligned}
$$

This is a first-order equation for W, viz.

$$W' + p(x)W = 0 \,, \tag{6.11}$$

with solution

$$W(x) = \kappa \, \exp\left(-\int^x p(\zeta) \, \mathrm{d}\zeta \right) \,, \tag{6.12}$$

where κ is a constant (a change in lower limit of integration can be absorbed by a rescaling of κ).

Remark. If for one value of x we have that $W \neq 0$, then W is non-zero for all values of x (since $\exp x > 0$ for all x). Hence if y_1 and y_2 are linearly independent for one value of x, they are linearly independent for all values of x. In the case that y_1 and y_2 are known implicitly, e.g. in terms of series or integrals, this is a welcome result since it means that we just have to find one value of x where is it relatively easy to evaluate W in order to confirm (or otherwise) linear independence.   18/02

6.2.3 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 using the Wronskian as follows.

First, from the definition of the Wronskian (6.9)

$$y_1 y_2' - y_1' y_2 = W(x) \,. \tag{6.13}$$

Hence from dividing by y_1^2

$$\left(\frac{y_2}{y_1} \right)' = \frac{y_2'}{y_1} - \frac{y_2 y_1'}{y_1^2} = \frac{W}{y_1^2} \,.$$

Now integrate both sides and use (6.12) to obtain

$$
\begin{aligned}
y_2(x) &= y_1(x) \int^x \frac{W(\eta)}{y_1^2(\eta)} \, \mathrm{d}\eta \\
&= y_1(x) \int^x \frac{\kappa}{y_1^2(\eta)} \, \exp\left(-\int^\eta p(\zeta) \, \mathrm{d}\zeta \right) \mathrm{d}\eta \,. \tag{6.14}
\end{aligned}
$$

In principle this allows us to compute y_2 given y_1.   18/04

Example. Given that $y_1(x)$ is a solution of Bessel's equation of zeroth order,

$$y'' + \frac{1}{x} y' + y = 0 \,, \qquad (6.15)$$

find another independent solution in terms of y_1 for $x > 0$.

Answer. In this case $p(x) = 1/x$ and hence

$$y_2(x) = y_1(x) \int^x \frac{\kappa}{y_1^2(\eta)} \exp\left(-\int^\eta \frac{1}{\zeta} \, d\zeta\right) d\eta$$

$$= \kappa y_1(x) \int^x \frac{1}{\eta \, y_1^2(\eta)} \, d\eta \,. \qquad (6.16)$$

18/03

6.3 Taylor Series Solutions

It is useful now to generalize to complex functions $y(z)$ of a complex variable z. The homogeneous ODE (6.2) then becomes

$$y'' + p(z)y' + q(z)y = 0 \,. \qquad (6.17)$$

If p and q are analytic at $z = z_0$ (i.e. they have power series expansions (5.45a) 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.

6.3.1 The Solution at Ordinary Points in Terms of a Power Series

If $z = z_0$ is an ordinary point of the ODE for $y(z)$, then we claim that $y(z)$ is analytic at $z = z_0$, i.e. there exists $\varrho > 0$ for which (see (5.45a))

$$y = \sum_{n=0}^{\infty} a_n (z - z_0)^n \quad \text{when} \quad |z - z_0| < \varrho \,. \qquad (6.18a)$$

18/01

For simplicity we will assume henceforth wlog that $z_0 = 0$ (which corresponds to a shift in the origin of the z-plane). Then we seek a solution of the form

$$y = \sum_{n=0}^{\infty} a_n z^n \,. \qquad (6.18b)$$

Next we substitute (6.18b) into the governing equation (6.17) to obtain

$$\sum_{n=\cancel{0}2}^{\infty} n(n-1)a_n z^{n-2} + \sum_{n=\cancel{0}1}^{\infty} n a_n p(z) z^{n-1} + \sum_{n=0}^{\infty} a_n q(z) z^n = 0 \,,$$

or, after the substitution $k = n - 2$ and $\ell = n - 1$ in the first and second terms respectively,

$$\sum_{k=0}^{\infty} (k+2)(k+1)a_{k+2} z^k + \sum_{\ell=0}^{\infty} (\ell+1)a_{\ell+1}p(z) z^\ell + \sum_{n=0}^{\infty} a_n q(z) z^n = 0 \,. \qquad (6.19)$$

At an ordinary point $p(z)$ and $q(z)$ are analytic so we can write

$$p(z) = \sum_{m=0}^{\infty} p_m z^m \quad \text{and} \quad q(z) = \sum_{m=0}^{\infty} q_m z^m \,. \qquad (6.20)$$

Then, after the substitutions $k \to r$ and $\ell \to n$, (6.19) can be written as

$$\sum_{r=0}^{\infty} (r+2)(r+1)a_{r+2} z^r + \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left((n+1)a_{n+1}p_m + a_n q_m\right) z^{n+m} = 0 \,. \qquad (6.21)$$

We now want to rewrite the double sum to include powers like z^r. Hence let $r = n + m$ and then note that (cf. a change of variables in a double integral)

$$\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\bullet(n,m) = \sum_{r=0}^{\infty}\sum_{n=0}^{r}\bullet(n, r-n)\,, \qquad (6.22)$$

since $m = r - n \geqslant 0$. Hence (6.21) can be rewritten as

$$\sum_{r=0}^{\infty}\left((r+2)(r+1)a_{r+2} + \sum_{n=0}^{r}\Big((n+1)a_{n+1}p_{r-n} + a_n q_{r-n}\Big)\right) z^r = 0\,. \qquad (6.23)$$

Since this expression is true for all $|z| < \varrho$, each coefficient of z^r $(r = 0, 1, \dots)$ must be zero. Thus we deduce the *recurrence relation*

$$a_{r+2} = -\frac{1}{(r+2)(r+1)}\sum_{n=0}^{r}\Big((n+1)a_{n+1}p_{r-n} + a_n q_{r-n}\Big) \quad \text{for} \quad r \geqslant 0\,. \qquad (6.24)$$

Therefore a_{r+2} is determined in terms of $a_0, a_1, \dots, a_{r+1}$. This means that if a_0 and a_1 are known then so are all the a_r; a_0 and a_1 play the rôle of the *two integration constants* in the general solution.

Remark. Proof that the radius of convergence of (6.18b) is non-zero is more difficult, and we will not attempt such a task in general. However we shall discuss the issue for examples.

6.3.2 Example

Consider

$$y'' - \frac{2}{(1-z)^2}y = 0\,. \qquad (6.25)$$

$z = 0$ is an ordinary point so try

$$y = \sum_{n=0}^{\infty} a_n z^n\,. \qquad (6.26)$$

We note that

$$p = 0\,, \quad q = -\frac{2}{(1-z)^2} = -2\sum_{m=0}^{\infty}(m+1)z^m\,, \qquad (6.27)$$

and hence in the terminology of the previous subsection $p_m = 0$ and $q_m = -2(m+1)$. Substituting into (6.24) we obtain the recurrence relation

$$a_{r+2} = \frac{2}{(r+2)(r+1)}\sum_{n=0}^{r}a_n(r-n+1) \quad \text{for} \quad r \geqslant 0\,. \qquad (6.28)$$

However, with a small amount of forethought we can obtain a simpler, if equivalent, recurrence relation. First multiply (6.25) by $(1-z)^2$ to obtain

$$(1-z)^2 y'' - 2y = 0\,,$$

and then substitute (6.26) into this equation. We find, on expanding $(1-z)^2 = 1 - 2z + z^2$, that

$$\sum_{n=\emptyset 2}^{\infty} n(n-1)a_n z^{n-2} - 2\sum_{n=\emptyset 1}^{\infty} n(n-1)a_n z^{n-1} + \sum_{n=0}^{\infty}(n^2 - n - 2)a_n z^n = 0\,,$$

after the substitution $k = n - 2$ and $\ell = n - 1$ in the first and second terms respectively,

$$\sum_{k=0}^{\infty}(k+2)(k+1)a_{k+2}z^k - 2\sum_{\ell=0}^{\infty}(\ell+1)\ell a_{\ell+1}z^\ell + \sum_{n=0}^{\infty}(n+1)(n-2)a_n z^n = 0\,.$$

Then after the substitutions $k \to n$ and $\ell \to n$, we group powers of z to obtain

$$\sum_{n=0}^{\infty} (n+1)\left((n+2)a_{n+2} - 2na_{n+1} + (n-2)a_n\right) z^n = 0 \,,$$

which leads to the recurrence relation

$$a_{n+2} = \frac{1}{n+2}(2na_{n+1} - (n-2)a_n) \quad \text{for} \quad n \geqslant 0 \,. \tag{6.29}$$

This two-term recurrence relation again determines a_n for $n \geqslant 2$ in terms of a_0 and a_1, but is simpler than (6.28).

Exercise for those with time! Show that the recurrence relations (6.28) and (6.29) are equivalent.

Two solutions. For $n = 0$ the recurrence relation (6.29) yields $a_2 = a_0$, while for $n = 1$ and $n = 2$ we obtain

$$a_3 = \tfrac{1}{3}(2a_2 + a_1) \quad \text{and} \quad a_4 = a_3 \,. \tag{6.30}$$

First we note that if $2a_2 + a_1 = 0$, then $a_3 = a_4 = 0$, and hence $a_n = 0$ for $n \geqslant 3$. We thus have as our first solution (with $a_0 = \alpha \neq 0$)

$$y_1 = \alpha(1 - z)^2 \,. \tag{6.31a}$$

Next we note that $a_n = a_0$ for all n is a solution of (6.29). In this case we can sum the series to obtain (with $a_0 = \beta \neq 0$)

$$y_2 = \beta \sum_{n=0}^{\infty} z^n = \frac{\beta}{1-z} \,. \tag{6.31b}$$

Linear independence. The linear independence of (6.31a) and (6.31b) is clear. However, to be extra sure we calculate the Wronskian:

$$W = y_1 y_2' - y_1' y_2 = \alpha(1-z)^2 \frac{\beta}{(1-z)^2} + 2\alpha(1-z)\frac{\beta}{(1-z)} = 3\alpha\beta \neq 0 \,. \tag{6.32}$$

Hence the general solution is

$$y(z) = \alpha(1-z)^2 + \frac{\beta}{1-z} \,, \tag{6.33}$$

for constants α and β. Observe that the general solution is singular at $z = 1$, which is also a singular point of the equation since $q(z) = -2(1-z)^{-2}$ is singular there.

6.3.3   Example: Legendre's Equation

Legendre's equation is

$$y'' - \frac{2z}{1-z^2}y' + \frac{\ell(\ell+1)}{1-z^2}\, y = 0 \,, \tag{6.34}$$

where $\ell \in \mathbb{R}$. The points $z = \pm 1$ are singular points but $z = 0$ is an ordinary point, so for smallish z try

$$y = \sum_{n=0}^{\infty} a_n z^n \,. \tag{6.35}$$

On substituting this into $(1 - z^2) * (6.34)$ we obtain

$$\sum_{n=\cancel{0}2}^{\infty} n(n-1)a_n z^{n-2} - \sum_{n=0}^{\infty} n(n-1)a_n z^n - 2\sum_{n=0}^{\infty} na_n z^n + \sum_{n=0}^{\infty} \ell(\ell+1)a_n z^n = 0 \,.$$

Hence with $k = n - 2$ in the first sum

$$\sum_{k=0}^{\infty} (k+2)(k+1)a_{k+2}z^k - \sum_{n=0}^{\infty} \left(n(n+1) - \ell(\ell+1)\right) a_n z^n = 0 \,,$$

and thence after the transformation $k \to n$

$$\sum_{n=0}^{\infty} \left((n+2)(n+1)a_{n+2} - (n(n+1) - \ell(\ell+1)) \, a_n \right) z^n = 0 \, .$$

This implies that

$$a_{n+2} = \frac{n(n+1) - \ell(\ell+1)}{(n+1)(n+2)} \, a_n \quad \text{for} \quad n = 0, 1, 2, \ldots . \tag{6.36}$$

Two solutions can be constructed by choosing

- $a_0 = 1$ and $a_1 = 0$, so that
$$y_1 = 1 - \frac{\ell(\ell+1)}{2} z^2 + O(z^4) \, ; \tag{6.37a}$$

- $a_0 = 0$ and $a_1 = 1$, so that
$$y_2 = z + \frac{2 - \ell(\ell+1)}{6} z^3 + O(z^5) \, . \tag{6.37b}$$

The Wronskian at the ordinary point $z = 0$ is thus given by

$$W = y_1 y_2' - y_1' y_2 = 1 \cdot 1 - 0 \cdot 0 = 1 \, . \tag{6.38}$$

Since $W \neq 0$, y_1 and y_2 are linearly independent.

Radius of convergence. The series (6.37a) and (6.37b) 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 (6.36) that

$$\lim_{n \to \infty} \left| \frac{a_{n+2} z^{n+2}}{a_n z^n} \right| = \lim_{n \to \infty} \left| \frac{n(n+1) - \ell(\ell+1)}{(n+1)(n+2)} \right| |z|^2 = |z|^2 \, . \tag{6.39}$$

It then follows from a straightforward extension of D'Alembert's ratio test (5.21) that the series converges for $|z| < 1$. Moreover, the series diverges for $|z| > 1$ (since $a_n z^n \nrightarrow 0$), and so the radius of convergence $\varrho = 1$. On the radius of convergence, determination of whether the series converges is more difficult.

Remark. The radius of convergence is distance to nearest singularity of the ODE. This is a general feature.

Legendre polynomials. In the generic situations both series (6.37a) and (6.37b) have an infinite number of terms. However, for $\ell = 0, 1, 2, \ldots$ it follows from (6.36)

$$a_{\ell+2} = \frac{\ell(\ell+1) - \ell(\ell+1)}{(\ell+1)(\ell+2)} a_\ell = 0 \, , \tag{6.40}$$

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 so that $P_\ell(1) = 1$. Thus

$$P_0 = 1 \, , \quad P_1 = z \, , \quad P_2 = \tfrac{1}{2}(3z^2 - 1) \, , \quad \text{etc.} \tag{6.41}$$

6.4   Regular Singular Points

Let $z = z_0$ be a singular point of the ODE. As before we can take $z_0 = 0$ wlog (otherwise define $z' = z - z_0$ so that $z' = 0$ is the singular point, and then make the transformation $z' \to z$). The origin is then a *regular singular point* if

$$zp(z) \quad \text{and} \quad z^2 q(z) \quad \text{are non-singular at} \quad z = 0. \tag{6.42}$$

In this case we can write

$$p(z) = \frac{1}{z} s(z) \quad \text{and} \quad q(z) = \frac{1}{z^2} t(z), \tag{6.43}$$

where $s(z)$ and $t(z)$ are analytic at $z = 0$. Then the homogeneous ODE (6.17) becomes after multiplying by z^2

$$z^2 y'' + zs(z)y' + t(z)y = 0. \tag{6.44}$$

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6.4.1   The Indicial Equation

We claim that there is always *at least one* solution to (6.44) of the form

$$y = z^\sigma \sum_{n=0}^\infty a_n z^n \quad \text{with} \quad a_0 \neq 0 \quad \text{and} \quad \sigma \in \mathbb{C}. \tag{6.45}$$

To see this substitute (6.45) into (6.44) to obtain

$$\sum_{n=0}^\infty \big((\sigma + n)(\sigma + n - 1) + (\sigma + n)s(z) + t(z) \big) a_n z^{\sigma + n} = 0,$$

or after division by z^σ,

$$\sum_{n=0}^\infty \big((\sigma + n)(\sigma + n - 1) + (\sigma + n)s(z) + t(z) \big) a_n z^n = 0. \tag{6.46}$$

We now evaluate this sum at $z = 0$ (when $z^n = 0$ except when $n = 0$) to obtain

$$(\sigma(\sigma - 1) + \sigma s_0 + t_0) a_0 = 0, \tag{6.47}$$

where $s_0 = s(0)$ and $t_0 = t(0)$; note that since s and t are analytic at $z = 0$, s_0 and t_0 are finite. Since by definition $a_0 \neq 0$ (see (6.45)) we obtain the *indicial equation* for σ:

$$\sigma^2 + \sigma(s_0 - 1) + t_0 = 0. \tag{6.48}$$

The roots σ_1, σ_2 of this equation are called the *indices* of the regular singular point.

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6.4.2   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 (6.46), 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 (6.45). However, as we shall see, it's worse than this. The ansatz (6.45) also fails (in general) to give both solutions when σ_1 and σ_2 differ by an integer (although there are exceptions).

6.4.3   Example: Bessel's Equation of Order ν

Bessel's equation of order ν is

$$y'' + \frac{1}{z}y' + \left(1 - \frac{\nu^2}{z^2}\right)y = 0\,, \tag{6.49}$$

where $\nu \geqslant 0$ wlog. The origin $z = 0$ is a regular singular point with

$$s(z) = 1 \quad \text{and} \quad t(z) = z^2 - \nu^2\,. \tag{6.50}$$

A power series solution of the form (6.45) solves (6.49) if, from (6.46),

$$\sum_{n=0}^{\infty}\big((\sigma+n)(\sigma+n-1)+(\sigma+n)-\nu^2\big)a_n z^n + \sum_{n=0}^{\infty}a_n z^{n+2} = 0\,, \tag{6.51}$$

i.e. after the transformation $n \to n - 2$ in the second sum, if

$$\sum_{n=0}^{\infty}\big((\sigma+n)^2 - \nu^2\big)a_n z^n + \sum_{n=2}^{\infty}a_{n-2}z^n = 0\,. \tag{6.52}$$

Now compare powers of z to obtain

$$n = 0: \quad \sigma^2 - \nu^2 = 0 \tag{6.53a}$$
$$n = 1: \quad \big((\sigma+1)^2 - \nu^2\big)a_1 = 0 \tag{6.53b}$$
$$n \geqslant 2: \quad \big((\sigma+n)^2 - \nu^2\big)a_n + a_{n-2} = 0\,. \tag{6.53c}$$

(6.53a) is the indicial equation and implies that

$$\sigma = \pm\nu\,. \tag{6.54}$$

Substituting this result into (6.53b) and (6.53c) yields

$$(1 \pm 2\nu)\,a_1 = 0 \tag{6.55a}$$
$$n(n \pm 2\nu)\,a_n = -a_{n-2} \quad \text{for} \quad n \geqslant 2\,. \tag{6.55b}$$

Remark. We note that there is no difficulty in solving for a_n from a_{n-2} using (6.55b) 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 (6.55a) and (6.55b) imply

$$a_n = \begin{cases} 0 & n = 1, 3, 5, \ldots\,, \\[2mm] -\dfrac{a_{n-2}}{n(n \pm 2\nu)} & n = 2, 4, 6, \ldots\,, \end{cases} \tag{6.56}$$

and so we get *two* solutions

$$y_{\pm} = a_0 z^{\pm\nu}\left(1 - \frac{1}{4(1 \pm \nu)}z^2 + \ldots\right)\,. \tag{6.57}$$

$2\nu = 2m + 1$, $m \in \mathbb{N}$. 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 (6.56) and (6.57). 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 (6.55b) to fail is that ν is an integer.

$\nu = 0$. If $\nu = 0$ then $\sigma_1 = \sigma_2$ and we can only find *one* power series solution of the form (6.45), viz.

$$y = a_0\left(1 - \tfrac{1}{4}z^2 + \ldots\right)\,. \tag{6.58}$$

$\nu = m \in \mathbb{N}$. If ν is a positive integer 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 (6.45) fails.

Remarks. 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 (6.45) whenever the indices σ_1 and σ_2 differ by an integer. We also note that the radius of convergence of the power series solution is infinite since from (6.56)

$$\lim_{n \to \infty} \left| \frac{a_n}{a_{n-2}} \right| = \lim_{n \to \infty} \left| \frac{1}{n(n \pm 2\nu)} \right| = 0 \,.$$

6.4.4 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 (6.58). Then, from (6.16) (after the transformations $x \to z$)

$$y_2(z) = \kappa y_1(z) \int^z \frac{1}{\eta\, y_1^2(\eta)} \, \mathrm{d}\eta \,. \tag{6.59}$$

For small (positive) z we can deduce using (6.58) that

$$y_2(z) = \kappa a_0 \left(1 + O(z^2)\right) \int^z \frac{1}{\eta\, a_0^2} \left(1 + O(\eta^2)\right) \mathrm{d}\eta$$

$$= \frac{\kappa}{a_0} \, \log z + \dots . \tag{6.60}$$

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

$$\operatorname{Re}(\sigma_1) \geqslant \operatorname{Re}(\sigma_2) \,. \tag{6.61}$$

Then we can always find *one* solution of the form

$$y_1(z) = z^{\sigma_1} \sum_{n=0}^{\infty} a_n z^n \quad \text{with, say, the normalisation } a_0 = 1 \,. \tag{6.62}$$

If $\sigma_1 - \sigma_2 \in \mathbb{Z}$ we claim that the second-order solution takes the form

$$y_2(z) = z^{\sigma_2} \sum_{n=0}^{\infty} b_n z^n + k\, y_1(z) \log z \,, \tag{6.63}$$

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. Suppose that y_1 is the series solution with $\sigma = +m$ to

$$z^2 y'' + z y' + \left(z^2 - m^2\right) y = 0 \,, \tag{6.64}$$

where, compared with (6.49), we have written m for ν. Hence from (6.45) and (6.56)

$$y_1 = z^m \sum_{\ell=0}^{\infty} a_{2\ell} z^{2\ell} \,, \tag{6.65}$$

since $a_{2\ell+1} = 0$ for integer ℓ. Let

$$y = k y_1 \log z + w \,, \tag{6.66}$$

then
$$y' = ky_1' \log z + \frac{ky_1}{z} + w' \quad \text{and} \quad y'' = ky_1'' \log z + \frac{2ky_1'}{z} - \frac{ky_1}{z^2} + w''.$$

On substituting into (6.64), and using the fact that y_1 is a solution of (6.64), we find that
$$z^2 w'' + zw' + (z^2 - m^2)w = -2kzy_1'. \tag{6.67}$$

Based on (6.54), (6.61) and (6.63) we now seek a series solution of the form
$$w = k\, z^{-m} \sum_{n=0}^{\infty} b_n z^n. \tag{6.68}$$

On substitution into (6.67) we have that
$$k \sum_{n=\emptyset 1}^{\infty} n(n-2m)b_n z^{n-m} + k \sum_{n=0}^{\infty} b_n z^{n-m+2} = -2k \sum_{\ell=0}^{\infty} (2\ell + m)a_{2\ell} z^{2\ell+m}.$$

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.

$n = 1, 3, 5, \dots$. From equating powers of z^1 it follows that $b_1 = 0$, and thence from the recurrence relation for powers of $z^{2\ell+1}$, i.e.
$$(2\ell + 1)(2\ell + 1 - 2m)b_{2\ell+1} = -b_{2\ell-1},$$
that $b_{2\ell+1} = 0$ ($\ell = 1, 2, \dots$).

$n = 2, 4, \dots, 2m, \dots$. From equating even powers of z^n:
$$2 \leqslant n \leqslant 2m-2: \quad b_{n-2} = -n(n-2m)b_n, \tag{6.69a}$$
$$n = 2m \qquad : \quad b_{2m-2} = -2ma_0, \tag{6.69b}$$
$$n \geqslant 2m+2: \quad b_n = -\frac{1}{n(n-2m)}b_{n-2} - \frac{2(n-m)}{n(n-2m)}a_{n-2m}. \tag{6.69c}$$

Hence:
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- if $m \geqslant 1$ solve for b_{2m-2} in terms of a_0 from (6.69b);
- if $m \geqslant 2$ solve for $b_{2m-4}, b_{2m-6}, \dots, b_2, b_0$ in terms of b_{2m-2}, etc. from (6.69a);
- finally, on the assumption that b_{2m} is known (see below), solve for $b_{2m+2}, b_{2m+4}, \dots$ in terms of b_{2m} and the $a_{2\ell}$ ($\ell = 1, 2, \dots$) from (6.69c).

b_{2m} is undetermined since this effectively generates a solution proportional to y_1; wlog $b_{2m} = 0$.

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6.5   Inhomogeneous Second-Order Linear ODEs

We now [re]turn to the real inhomogeneous equation
$$y'' + p(x)y' + q(x)y = f(x). \tag{6.70}$$

The general solution, if one exists, has the form
$$y(x) = y_0(x) + \alpha y_1(x) + \beta y_2(x), \tag{6.71}$$

where $y_1(x)$ and $y_2(x)$ are linearly-independent solutions of the homogeneous equation, and are often referred to as *complementary functions*, and $y_0(x)$ is a *particular solution*, which is sometimes also called a *particular integral*.

Remark. The solution (6.71) solves the equation and involves two arbitrary constants.

6.5.1 The Method of Variation of Parameters

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

$$y_0(x) = u(x)y_1(x) + v(x)y_2(x).\tag{6.72}$$

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. (6.70)), 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 (6.72) to find that

$$y_0' = (uy_1' + vy_2') + (u'y_1 + v'y_2)\tag{6.73a}$$
$$y_0'' = (uy_1'' + vy_2'' + u'y_1' + v'y_2') + (u''y_1 + v''y_2 + u'y_1' + v'y_2').\tag{6.73b}$$

If we substitute the above into the inhomogeneous equation (6.70) 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 (6.73a) by demanding that u and v satisfy the extra equation

$$u'y_1 + v'y_2 = 0.\tag{6.74}$$

Then (6.73a) and (6.73b) become

$$y_0' = uy_1' + vy_2'\tag{6.75a}$$
$$y_0'' = uy_1'' + vy_2'' + u'y_1' + v'y_2'.\tag{6.75b}$$

It follows from (6.72), (6.75a) and (6.75b) that

$$y_0'' + py_0' + qy_0 = u(y_1'' + py_1' + qy_1) + v(y_2'' + py_2' + qy_2) + u'y_1' + v'y_2'$$
$$= u'y_1' + v'y_2',$$

since y_1 and y_2 solve the homogeneous equation (6.17). Hence y_0 solves the inhomogeneous equation (6.70) if

$$u'y_1' + v'y_2' = f.\tag{6.76}$$

We now have two simultaneous equations for u', v', i.e. (6.74) and (6.76), with solution

$$u' = -\frac{fy_2}{W} \quad \text{and} \quad v' = \frac{fy_1}{W},\tag{6.77}$$

where W is the Wronskian,

$$W = y_1y_2' - y_2y_1'.\tag{6.78}$$

W is non-zero because y_1 and y_2 were chosen to be linearly independent. Integrating we obtain

$$u = -\int_a^x \frac{y_2(\zeta)f(\zeta)}{W(\zeta)}\,\mathrm{d}\zeta \quad \text{and} \quad v = \int_a^x \frac{y_1(\zeta)f(\zeta)}{W(\zeta)}\,\mathrm{d}\zeta,\tag{6.79}$$

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 (6.72) we obtain as our particular solution

$$y_0(x) = \int_a^x \frac{f(\zeta)}{W(\zeta)}\left(y_1(\zeta)y_2(x) - y_1(x)y_2(\zeta)\right)\mathrm{d}\zeta.\tag{6.80}$$

Remark. We observe that, since the integrand is zero when $\zeta = x$,

$$y_0'(x) = \int_a^x \frac{f(\zeta)}{W(\zeta)} \left(y_1(\zeta)y_2'(x) - y_1'(x)y_2(\zeta) \right) \, \mathrm{d}\zeta \,. \tag{6.81}$$

Hence the particular solution (6.80) satisfies the *initial value homogeneous boundary conditions*

$$y(a) = y'(a) = 0 \,. \tag{6.82}$$

More general initial value boundary conditions would be inhomogeneous, e.g.

$$y(a) = k_1 \,, \quad y'(a) = k_2 \,, \tag{6.83}$$

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

$$y'' + y = \sec x \,. \tag{6.84}$$

Answer. Two linearly independent solutions of the homogeneous equation are

$$y_1 = \cos x \quad \text{and} \quad y_2 = \sin x \,, \tag{6.85a}$$

with a Wronskian

$$W = y_1 y_2' - y_2 y_1' = \cos x (\cos x) - \sin x (-\sin x) = 1 \,. \tag{6.85b}$$

Hence from (6.80) a particular solution is given by

$$\begin{aligned} y_0(x) &= \int^x \sec \zeta \left(\cos \zeta \sin x - \cos x \sin \zeta \right) \mathrm{d}\zeta \\ &= \sin x \int^x \mathrm{d}\zeta - \cos x \int^x \tan \zeta \, \mathrm{d}\zeta \\ &= x \sin x + \cos x \log |\cos x| \,. \end{aligned} \tag{6.86}$$

The general solution is thus

$$y(x) = (\alpha + \log |\cos x|) \cos x + (\beta + x) \sin x \,. \tag{6.87}$$

6.5.2 Two Point Boundary Value Problems

For many important problems ODEs have to be solved subject to boundary conditions at more than one point. For linear second-order ODEs such boundary conditions have the general form

$$Ay(a) + By'(a) = k_a \,, \tag{6.88a}$$
$$Cy(b) + Dy'(b) = k_b \,, \tag{6.88b}$$

for *two points* $x = a$ and $x = b$ (wlog $b > a$), where A, B, C, D, k_a and k_b are constants. If $k_a = k_b = 0$ these boundary conditions are homogeneous, otherwise they are inhomogeneous.

For simplicity we shall consider the special case of homogeneous boundary conditions given by

$$y(a) = 0 \quad \text{and} \quad y(b) = 0 \,. \tag{6.89}$$

The general solution of the inhomogeneous equation (6.70) satisfying the first boundary condition $y(a) = 0$ is, from (6.71), (6.80) and (6.82),

$$y(x) = \mathcal{K}(y_1(a)y_2(x) - y_1(x)y_2(a)) + \int_a^x \frac{f(\zeta)}{W(\zeta)} \left(y_1(\zeta)y_2(x) - y_1(x)y_2(\zeta) \right) \mathrm{d}\zeta \,, \tag{6.90a}$$

where the first term on the right-hand side is the general solution of the homogeneous equation vanishing at $x = a$ and $\mathcal{K}$ is a constant. If we now impose the condition $y(b) = 0$, then we require that

$$\mathcal{K} \left(y_1(a)y_2(b) - y_1(b)y_2(a) \right) + \int_a^b \frac{f(\zeta)}{W(\zeta)} \left(y_1(\zeta)y_2(b) - y_1(b)y_2(\zeta) \right) \mathrm{d}\zeta = 0 \,. \tag{6.90b}$$

This determines $\mathcal{K}$ provided that $y_1(a)y_2(b) - y_1(b)y_2(a) \neq 0$.

Remark. If per chance $y_1(a)y_2(b) - y_1(b)y_2(a) = 0$ then a solution exists to the homogeneous equation satisfying both boundary conditions. As a general rule a solution to the inhomogeneous problem exists if and only if there is no solution of the homogeneous equation satisfying both boundary conditions.

A particular choice of y_1 and y_2. For linearly independent y_1 and y_2 let

$$y_a(x) = y_1(a)y_2(x) - y_1(x)y_2(a) \quad \text{and} \quad y_b(x) = y_1(b)y_2(x) - y_1(x)y_2(b),\qquad (6.91)$$

so that $y_a(a) = 0$ and $y_b(b) = 0$. The Wronskian of y_a and y_b is given by

$$
\begin{aligned}
y_a y_b' - y_a' y_b &= \left(y_1(a)y_2(b) - y_1(b)y_2(a)\right)\left(y_1 y_2' - y_1' y_2\right) \\
&= \left(y_1(a)y_2(b) - y_1(b)y_2(a)\right) W,
\end{aligned}
$$

where W is the Wronskian of y_1 and y_2. Hence y_a and y_b are linearly independent if

$$y_1(a)y_2(b) - y_1(b)y_2(a) \neq 0,\qquad (6.92)$$

i.e. the same condition that allows us to solve for $\mathcal{K}$. Under such circumstances we can redefine y_1 and y_2 to be y_a and y_b respectively.

In general the amount of algebra can be reduced by a sensible choice of y_1 and y_2 so that they satisfy the homogeneous boundary conditions at $x = a$ and $x = b$ respectively, i.e. in the case of (6.89)

$$y_1(a) = y_2(b) = 0.\qquad (6.93)$$

6.5.3   Green's Functions

Suppose that we wish to solve the equation

$$\mathcal{L}_{(x)}\, y(x) = f(x),\qquad (6.94)$$

where $\mathcal{L}_{(x)}$ is the general second-order linear differential operator in x, i.e.

$$\mathcal{L}_{(x)} = \frac{\mathrm{d}^2}{\mathrm{d}x^2} + p(x)\frac{\mathrm{d}}{\mathrm{d}x} + q(x),\qquad (6.95)$$

where p and q are continuous functions. To fix ideas we will assume that the solution should satisfy *homogeneous* boundary conditions at $x = a$ and $x = b$, i.e. $k_a = k_b = 0$ in (6.88a) and (6.88b).

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

$$\mathcal{L}_{(x)}\, G(x, \zeta) = \delta(x - \zeta),\qquad (6.96)$$

subject to

$$A\,G(a, \zeta) + B\,G_x(a, \zeta) = 0 \quad \text{and} \quad C\,G(b, \zeta) + D\,G_x(b, \zeta) = 0,\qquad (6.97)$$

where $G_x(x, \zeta) = \frac{\partial G}{\partial x}(x, \zeta)$ 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 (6.94) is

$$y(x) = \int_a^b G(x, \zeta) f(\zeta)\,\mathrm{d}\zeta.\qquad (6.98)$$

To see this we first note that (6.98) satisfies the boundary conditions, since $\int 0\,\mathrm{d}\zeta = 0$. Further, it also satisfies the inhomogeneous equation (6.94) (or (6.70)) because

$$
\begin{aligned}
\mathcal{L}_{(x)}\, y(x) &= \int_a^b \mathcal{L}_{(x)}\, G(x, \zeta)\, f(\zeta)\,\mathrm{d}\zeta && \text{differential wrt } x, \text{ integral wrt } \zeta \\
&= \int_a^b \delta(x - \zeta)\, f(\zeta)\,\mathrm{d}\zeta && \text{from (6.96)} \\
&= f(x) && \text{from (3.4)}.
\end{aligned}
\qquad (6.99)
$$

The function $G(x, \zeta)$ is called the *Green's function* of $\mathcal{L}_{(x)}$ for the given homogeneous boundary conditions.

6.5.4 Two Properties Green's Functions

In the next section we will construct a Green's function. However, first we need to derive two properties of $G(x, \zeta)$. Suppose that we integrate equation (6.96) from $\zeta - \varepsilon$ to $\zeta + \varepsilon$ for $\varepsilon > 0$ and consider the limit $\varepsilon \to 0$. From (3.4) the right hand side is equal to 1, and hence

$$
\begin{aligned}
1 &= \lim_{\varepsilon \to 0} \int_{\zeta - \varepsilon}^{\zeta + \varepsilon} \mathcal{L}_{(x)} G \, dx \\
&= \lim_{\varepsilon \to 0} \int_{\zeta - \varepsilon}^{\zeta + \varepsilon} \left(\frac{\partial^2 G}{\partial x^2} + p \frac{\partial G}{\partial x} + q \, G \right) dx && \text{from (6.95)} \\
&= \lim_{\varepsilon \to 0} \int_{\zeta - \varepsilon}^{\zeta + \varepsilon} \frac{\partial}{\partial x} \left(\frac{\partial G}{\partial x} + p \, G \right) dx + \lim_{\varepsilon \to 0} \int_{\zeta - \varepsilon}^{\zeta + \varepsilon} \left(-\frac{dp}{dx} G + q \, G \right) dx && \text{rearrange} \\
&= \lim_{\varepsilon \to 0} \left[\frac{\partial G}{\partial x} + p \, G \right]_{x = \zeta - \varepsilon}^{x = \zeta + \varepsilon} - \lim_{\varepsilon \to 0} \int_{\zeta - \varepsilon}^{\zeta + \varepsilon} \left(\frac{dp}{dx} - q \right) G \, dx \, . && (6.100)
\end{aligned}
$$

How can this equation be satisfied? Let us suppose that $G(x, \zeta)$ is continuous at $x = \zeta$, i.e. that

$$
\lim_{\varepsilon \to 0} \left[G(x, \zeta) \right]_{\zeta - \varepsilon}^{\zeta + \varepsilon} = 0 \, . \tag{6.101a}
$$

Then since p and q are continuous, (6.100) reduces to

$$
\lim_{\varepsilon \to 0} \left[\frac{\partial G}{\partial x} \right]_{x = \zeta - \varepsilon}^{x = \zeta + \varepsilon} = 1 \, , \tag{6.101b}
$$

i.e. that there is a unit jump in the derivative of G at $x = \zeta$ (cf. the unit jump in the Heaviside step function (3.9) at $x = 0$). Note that a function can be continuous and its derivative discontinuous, but not vice versa.

6.5.5 Construction of the Green's Function

$G(x, \zeta)$ can be constructed by the following procedure. First we note that when $x \ne \zeta$, 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

$$
G(x, \zeta) = \begin{cases} \alpha_-(\zeta) y_1(x) + \beta_-(\zeta) y_2(x) & \text{for } a \leqslant x < \zeta, \\ \alpha_+(\zeta) y_1(x) + \beta_+(\zeta) y_2(x) & \text{for } \zeta \leqslant x \leqslant b. \end{cases} \tag{6.102}
$$

By construction this satisfies (6.96) for $x \ne \zeta$. 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 (6.101a) and (6.101b) that

$$
\left[\alpha_+(\zeta) y_1(\zeta) + \beta_+(\zeta) y_2(\zeta) \right] - \left[\alpha_-(\zeta) y_1(\zeta) + \beta_-(\zeta) y_2(\zeta) \right] = 0 \, ,
$$
$$
\left[\alpha_+(\zeta) y_1'(\zeta) + \beta_+(\zeta) y_2'(\zeta) \right] - \left[\alpha_-(\zeta) y_1'(\zeta) + \beta_-(\zeta) y_2'(\zeta) \right] = 1 \, ,
$$

i.e.

$$
y_1(\zeta) \left[\alpha_+(\zeta) - \alpha_-(\zeta) \right] + y_2(\zeta) \left[\beta_+(\zeta) - \beta_-(\zeta) \right] = 0 \, ,
$$
$$
y_1'(\zeta) \left[\alpha_+(\zeta) - \alpha_-(\zeta) \right] + y_2'(\zeta) \left[\beta_+(\zeta) - \beta_-(\zeta) \right] = 1 \, ,
$$

i.e.

$$
\begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix} \begin{pmatrix} \alpha_+ - \alpha_- \\ \beta_+ - \beta_- \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} . \tag{6.103}
$$

A solution exists to this equation if

$$
W \equiv \left\| \begin{matrix} y_1 & y_2 \\ y_1' & y_2' \end{matrix} \right\| \ne 0 \, ,
$$

i.e. if y_1 and y_2 are linearly independent; if so then

$$\alpha_+ - \alpha_- = -\frac{y_2(\zeta)}{W(\zeta)} \quad \text{and} \quad \beta_+ - \beta_- = \frac{y_1(\zeta)}{W(\zeta)}\,. \tag{6.104}$$

Finally we impose the boundary conditions. For instance, suppose that the solution y is required to satisfy (6.89) (i.e. $y(a) = 0$ and $y(b) = 0$), then the appropriate boundary conditions for G are

$$G(a, \zeta) = G(b, \zeta) = 0\,, \tag{6.105}$$

i.e. $A = C = 1$ and $B = D = 0$ in (6.97). It follows from (6.102) that we require

$$\alpha_-(\zeta)y_1(a) + \beta_-(\zeta)y_2(a) = 0\,, \tag{6.106a}$$
$$\alpha_+(\zeta)y_1(b) + \beta_+(\zeta)y_2(b) = 0\,. \tag{6.106b}$$

$\alpha_\pm$, $\beta_\pm$ can now be determined from (6.104), (6.106a) and (6.106b). For simplicity choose y_1 and y_2 as in (6.93) so that $y_1(a) = y_2(b) = 0$; then

$$\alpha_+ = \beta_- = 0\,, \tag{6.107a}$$

and thence from (6.104)

$$\alpha_- = \frac{y_2(\zeta)}{W(\zeta)} \quad \text{and} \quad \beta_+ = \frac{y_1(\zeta)}{W(\zeta)}\,. \tag{6.107b}$$

It follows from (6.102) that

$$G(x, \zeta) = \begin{cases} \dfrac{y_1(x)y_2(\zeta)}{W(\zeta)} & \text{for } a \leqslant x < \zeta, \\[2ex] \dfrac{y_1(\zeta)y_2(x)}{W(\zeta)} & \text{for } \zeta \leqslant x \leqslant b. \end{cases} \tag{6.108}$$

Initial value homogeneous boundary conditions. Suppose that instead of the two-point boundary condition (6.89) we require that $y(a) = y'(a) = 0$, and thence that $G(a, \zeta) = \frac{\partial G}{\partial x}(a, \zeta) = 0$. If we choose $y_1(a) = 0$ and $y_2'(a) = 0$, then in place of (6.107a) we have that $\alpha_- = \beta_- = 0$. The conditions that G be continuous and $\frac{\partial G}{\partial x}$ has a unit discontinuity then give that

$$G(x, \zeta) = \begin{cases} 0 & \text{for } a \leqslant x < \zeta, \\[2ex] \dfrac{y_1(\zeta)y_2(x) - y_1(x)y_2(\zeta)}{W(\zeta)} & \text{for } \zeta \leqslant x \leqslant b. \end{cases} \tag{6.109}$$

6.5.6 *Unlectured* Alternative Derivation of a Green's Function

By means of a little bit of manipulation we can also recover (6.108) from our earlier general solution (6.90a) and (6.90b). That solution was derived for the homogeneous boundary conditions (6.89), i.e.

$$y(a) = 0 \quad \text{and} \quad y(b) = 0\,.$$

As above choose y_1 and y_2 so that they satisfy the boundary conditions at $x = a$ and $x = b$ respectively, i.e. let

$$y_1(a) = y_2(b) = 0\,. \tag{6.110}$$

In this case we have from (6.90b) that

$$\mathcal{K} = -\frac{1}{y_2(a)} \int_a^b \frac{f(\zeta)}{W(\zeta)}\, y_2(\zeta)\, \mathrm{d}\zeta\,. \tag{6.111}$$

It follows from (6.90a) that

$$y(x) = \int_a^b \frac{f(\zeta)}{W(\zeta)}\, y_1(x)y_2(\zeta)\, \mathrm{d}\zeta + \int_a^x \frac{f(\zeta)}{W(\zeta)}\left(y_1(\zeta)y_2(x) - y_1(x)y_2(\zeta)\right) \mathrm{d}\zeta$$

$$= \int_a^x \frac{y_1(\zeta)y_2(x)}{W(\zeta)} f(\zeta)\, \mathrm{d}\zeta + \int_x^b \frac{y_1(x)y_2(\zeta)}{W(\zeta)} f(\zeta)\, \mathrm{d}\zeta$$

$$= \int_a^b G(x,\zeta) f(\zeta)\, \mathrm{d}\zeta \tag{6.112}$$

where, as in (6.108), $G(x,\zeta)$ is defined by

$$G(x,\zeta) = \begin{cases} \dfrac{y_1(\zeta)y_2(x)}{W(\zeta)} & \text{for } \zeta \leqslant x, \text{ i.e. } x \geqslant \zeta, \\[2mm] \dfrac{y_1(x)y_2(\zeta)}{W(\zeta)} & \text{for } \zeta > x, \text{ i.e. } x < \zeta. \end{cases} \tag{6.113}$$

Remark. Note from (6.113) that $G(x,\zeta)$ is continuous at $x = \zeta$, and that

$$\frac{\partial G}{\partial x}(x,\zeta) = \begin{cases} \dfrac{y_1(\zeta)y_2'(x)}{W(\zeta)} & \text{for } x \geqslant \zeta, \\[2mm] \dfrac{y_1'(x)y_2(\zeta)}{W(\zeta)} & \text{for } x < \zeta. \end{cases} \tag{6.114}$$

Hence, from using the definition of the Wronskian (6.9), $\frac{\partial G}{\partial x}$ is discontinuous at $x = \zeta$ with discontinuity

$$\lim_{\varepsilon \to 0}\left[\frac{\partial G}{\partial x}(x,\zeta)\right]_{x=\zeta-\varepsilon}^{x=\zeta+\varepsilon} = \frac{y_1(\zeta)y_2'(\zeta)}{W(\zeta)} - \frac{y_1'(\zeta)y_2(\zeta)}{W(\zeta)} = 1\,. \tag{6.115}$$

6.5.7 Example of a Green's Function

Find the Green's function in $0 < a < b$ for

$$\mathcal{L}_{(x)} = \frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x} - \frac{n^2}{x^2}\,, \tag{6.116a}$$

with homogeneous boundary conditions

$$G(a,\zeta) = 0 \quad \text{and} \quad \frac{\partial G}{\partial x}(b,\zeta) = 0\,, \tag{6.116b}$$

i.e. with $A = D = 1$ and $B = C = 0$ in (6.97).

Answer. Seek solutions to the homogeneous equation $\mathcal{L}_{(x)}\, y = 0$ of the form $y = x^r$. Then we require that

$$r(r-1) + r - n^2 = 0\,, \quad \text{i.e.} \quad r = \pm n\,.$$

Let

$$y_1 = \left(\frac{x}{a}\right)^n - \left(\frac{a}{x}\right)^n \quad \text{and} \quad y_2 = \left(\frac{x}{b}\right)^n + \left(\frac{b}{x}\right)^n, \tag{6.117}$$

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 (6.116b) (cf. the choice of $y_1(a) = 0$ and $y_2(b) = 0$ in §6.5.5 since in that case we required the Green's function to satisfy boundary conditions (6.105)). As in (6.102) let

$$G(x,\zeta) = \begin{cases} \alpha_-(\zeta)y_1(x) + \beta_-(\zeta)y_2(x) & \text{for } a \leqslant x < \zeta, \\ \alpha_+(\zeta)y_1(x) + \beta_+(\zeta)y_2(x) & \text{for } \zeta \leqslant x \leqslant b. \end{cases}$$

Since we require that $G(a, \zeta) = 0$ from (6.116b), and by construction $y_1(a) = 0$, it follows that $\beta_- = 0$. Similarly, since we require that $\frac{\partial G}{\partial x}(b, \zeta) = 0$ from (6.116b), and by construction $y_2'(b) = 0$, it follows that $\alpha_+ = 0$. Hence

$$G(x, \zeta) = \begin{cases} \alpha_-(\zeta)y_1(x) & \text{for } a \leqslant x < \zeta, \\ \beta_+(\zeta)y_2(x) & \text{for } \zeta \leqslant x \leqslant b. \end{cases}$$

We also require that G is continuous and $\frac{\partial G}{\partial x}$ has a unit discontinuity at $x = \zeta$, hence

$$\beta_+(\zeta)y_2(\zeta) = \alpha_-(\zeta)y_1(\zeta) \quad \text{and} \quad \beta_+(\zeta)y_2'(\zeta) - \alpha_-(\zeta)y_1'(\zeta) = 1 \,.$$

Thus

$$\alpha_- = \frac{y_2(\zeta)}{W(\zeta)}, \quad \beta_+ = \frac{y_1(\zeta)}{W(\zeta)} \quad \text{and} \quad G(x, \zeta) = \begin{cases} \dfrac{y_1(x)y_2(\zeta)}{W(\zeta)} & \text{for } a \leqslant x < \zeta, \\[2mm] \dfrac{y_1(\zeta)y_2(x)}{W(\zeta)} & \text{for } \zeta \leqslant x \leqslant b. \end{cases} \tag{6.118}$$

This has the same form as (6.108) because we [carefully] chose y_1 and y_2 in (6.117) to satisfy the boundary conditions at $x = a$ and $x = b$ respectively. Note, however, the boundary condition that the solution is required to satisfy at $x = b$ is different in the two cases, i.e. $y_2(b) = 0$ in (6.108) while $y_2'(b) = 0$ in (6.118).

6.6 Sturm-Liouville Theory

Definition. A second-order linear differential operator $\mathcal{L}$ is said to be of *Sturm-Liouville* type if

$$\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) - q(x) \,, \tag{6.119a}$$

where $p(x)$ and $q(x)$ are real functions defined for $a \leqslant x \leqslant b$, with

$$p(x) > 0 \quad \text{for} \quad a < x < b \,. \tag{6.119b}$$

Notation alert. The use of p and q in (6.119a) is different from their use up to now in this section, e.g. in (6.2), (6.70) and (6.95). Unfortunately both uses are 'conventional'.

6.6.1 Inner Products and Self-Adjoint Operators

Given two, possibly complex, piecewise continuous functions $u(x)$ and $v(x)$, define an inner product $\langle\, u \mid v \,\rangle$ by

$$\langle\, u \mid v \,\rangle = \int_a^b u^*(x)v(x)\,w(x)\,\mathrm{d}x \,, \tag{6.120a}$$

where a and b are constants and $w(x)$ is a real *weight function* such that

$$w(x) > 0 \quad \text{for} \quad a < x < b \,. \tag{6.120b}$$

As required in the definition of an inner product in (4.27a), (4.27c), (4.27d) and (4.27e), we note that for piecewise continuous functions u, v and t and complex constants α and β,

$$\langle\, u \mid v \,\rangle = \langle\, v \mid u \,\rangle^* \,; \tag{6.121a}$$

$$\langle\, u \mid \alpha v + \beta t \,\rangle = \alpha\langle\, u \mid v \,\rangle + \beta\langle\, u \mid t \,\rangle \,; \tag{6.121b}$$

$$\langle\, v \mid v \,\rangle \geqslant 0 \,; \tag{6.121c}$$

$$\langle\, v \mid v \,\rangle = 0 \quad \Rightarrow \quad v = 0 \,. \tag{6.121d}$$

Definition. A general differential operator $\widetilde{\mathcal{L}}$ is said to be *self-adjoint* if

$$\left\langle\, u \,\middle|\, \widetilde{\mathcal{L}}v \,\right\rangle = \left\langle\, \widetilde{\mathcal{L}}u \,\middle|\, v \,\right\rangle. \tag{6.122}$$

Remark. Whether or not an operator $\widetilde{\mathcal{L}}$ is self adjoint with respect to an inner product depends on the choice of weight function in the inner product.

6.6.2   The Sturm-Liouville Operator

Consider the Sturm-Liouville operator (6.119a) together with the identity weight function $w = 1$, then

$$
\begin{aligned}
\langle\, u \mid \mathcal{L}v \,\rangle &= \int_a^b \mathrm{d}x\, u^* \mathcal{L}v && \text{from (6.120a)} \\[2mm]
&= -\int_a^b \mathrm{d}x\, u^* \left(\frac{\mathrm{d}}{\mathrm{d}x}\left(p\frac{\mathrm{d}v}{\mathrm{d}x} \right) + qv \right) && \text{from (6.119a)} \\[2mm]
&= -\left[u^* p \frac{\mathrm{d}v}{\mathrm{d}x} \right]_a^b + \int_a^b \mathrm{d}x\, p\, \frac{\mathrm{d}u^*}{\mathrm{d}x}\frac{\mathrm{d}v}{\mathrm{d}x} - \int_a^b \mathrm{d}x\, qu^* v && \text{integrate by parts} \\[2mm]
&= \left[-u^* p \frac{\mathrm{d}v}{\mathrm{d}x} + p\frac{\mathrm{d}u^*}{\mathrm{d}x} v \right]_a^b - \int_a^b \mathrm{d}x\, v\frac{\mathrm{d}}{\mathrm{d}x}\left(p\frac{\mathrm{d}u^*}{\mathrm{d}x} \right) - \int_a^b \mathrm{d}x\, v\, qu^* && \text{integrate by parts} \\[2mm]
&= \left[p\left(v\frac{\mathrm{d}u^*}{\mathrm{d}x} - u^*\frac{\mathrm{d}v}{\mathrm{d}x} \right) \right]_a^b + \int_a^b \mathrm{d}x\, v\, \mathcal{L}u^* && \text{from (6.119a)} \\[2mm]
&= \left[p\left(v\frac{\mathrm{d}u^*}{\mathrm{d}x} - u^*\frac{\mathrm{d}v}{\mathrm{d}x} \right) \right]_a^b + \int_a^b \mathrm{d}x\, (\mathcal{L}u)^* v && \text{since } \mathcal{L} \text{ real} \\[2mm]
&= \left[p\left(v\frac{\mathrm{d}u^*}{\mathrm{d}x} - u^*\frac{\mathrm{d}v}{\mathrm{d}x} \right) \right]_a^b + \langle\, \mathcal{L}u \mid v \,\rangle && \text{from (6.120a).} \quad (6.123a)
\end{aligned}
$$

Suppose we now insist that u and v be such that

$$\left[p\left(v\frac{\mathrm{d}u^*}{\mathrm{d}x} - u^*\frac{\mathrm{d}v}{\mathrm{d}x} \right) \right]_a^b = 0, \tag{6.123b}$$

then (6.122) is satisfied. We conclude that the differential operator

$$\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x} \right) - q(x)$$

acting on functions, say u or v, which satisfy homogeneous boundary conditions at $x = a$ and $x = b$ (e.g. $u(a) = 0$, $v(a) = 0$ and $u(b) = 0$, $v(b) = 0$), is *self-adjoint* with respect to the inner product with $w = 1$.

Remarks.

- The boundary conditions are part of the conditions for an operator to be self-adjoint.

- Suppose that an inner product for column vectors u and v is defined by (cf. (4.55))

$$\langle\, \mathsf{u} \mid \mathsf{v} \,\rangle = \mathsf{u}^\dagger \mathsf{v}. \tag{6.124}$$

  Then for a Hermitian matrix H we have that

$$
\begin{aligned}
\langle\, \mathsf{u} \mid \mathsf{H}\mathsf{v} \,\rangle &= \mathsf{u}^\dagger \mathsf{H}\mathsf{v} = \mathsf{u}^\dagger \mathsf{H}^\dagger \mathsf{v} && \text{since } \mathsf{H} \text{ is Hermitian} \\[2mm]
&= (\mathsf{H}\mathsf{u})^\dagger \mathsf{v} = \langle\, \mathsf{H}\mathsf{u} \mid \mathsf{v} \,\rangle && \text{since } (\mathsf{A}\mathsf{B})^\dagger = \mathsf{B}^\dagger \mathsf{A}^\dagger. \quad (6.125)
\end{aligned}
$$

  A comparison of (6.122) and (6.125) suggests that self-adjoint operators are to general operators what Hermitian matrices are to general matrices.

6.6.3 The Rôle of the Weight Function

Not all second-order linear differential operators have the Sturm-Liouville form (6.119a). However, suppose that $\widetilde{\mathcal{L}}$ is a second-order linear differential operator *not* of Sturm-Liouville form, then there exists a function $w(x)$ so that

$$\mathcal{L} = w\widetilde{\mathcal{L}} \tag{6.126}$$

is of Sturm-Liouville form.

Proof. The general second-order linear differential operator acting on functions defined for $a \leqslant x \leqslant b$ can be written in the form

$$\widetilde{\mathcal{L}} = -P(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2} - R(x)\frac{\mathrm{d}}{\mathrm{d}x} - Q(x)\,, \tag{6.127a}$$

where P, Q and R are real functions; we shall assume that

$$P(x) > 0 \quad \text{for} \quad a < x < b\,. \tag{6.127b}$$

Hence for $\mathcal{L}$ defined by (6.126)

$$
\begin{aligned}
\mathcal{L} &= -wP\frac{\mathrm{d}^2}{\mathrm{d}x^2} - wR\frac{\mathrm{d}}{\mathrm{d}x} - wQ \\
&= -\frac{\mathrm{d}}{\mathrm{d}x}\left(wP\frac{\mathrm{d}}{\mathrm{d}x}\right) + \left(\frac{\mathrm{d}}{\mathrm{d}x}(wP) - wR\right)\frac{\mathrm{d}}{\mathrm{d}x} - wQ\,.
\end{aligned} \tag{6.128}
$$

The operator $\mathcal{L}$ in (6.128) is of Sturm-Liouville form (6.119a) if we choose our *integrating factor* w so that

$$P\frac{\mathrm{d}w}{\mathrm{d}x} + \left(\frac{\mathrm{d}P}{\mathrm{d}x} - R\right)w = 0\,, \tag{6.129a}$$

and let

$$p = wP \quad \text{and} \quad q = wQ\,. \tag{6.129b}$$

On solving (6.129a), and on choosing the constant of integration so that $w(a) = 1$, we obtain

$$w = \exp\int_a^x \frac{1}{P(\zeta)}\left(R(\zeta) - \frac{\mathrm{d}P}{\mathrm{d}x}(\zeta)\right)\mathrm{d}\zeta\,. \tag{6.130}$$

Remark. It follows from (6.130) that $w > 0$, and hence from (6.127b) and (6.129b) that $p > 0$ for $a < x < b$ (cf. (6.119b)).

Examples. Put the operators

$$\widetilde{\mathcal{L}} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{\mathrm{d}}{\mathrm{d}x} \quad \text{and} \quad \widetilde{\mathcal{L}} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}$$

in Sturm-Liouville form.

Answers. For the first operator $P = R = 1$. Hence from (6.130), $w = \exp x$ (wlog $a = 0$), and thus

$$\mathcal{L} = \mathrm{e}^x\widetilde{\mathcal{L}} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(\mathrm{e}^x\frac{\mathrm{d}}{\mathrm{d}x}\right)\,.$$

For the second operator $P = 1$ and $R = x^{-1}$. Hence from (6.130), $w = x$ (wlog $a = 1$), and thus

$$\mathcal{L} = x\widetilde{\mathcal{L}} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(x\frac{\mathrm{d}}{\mathrm{d}x}\right)\,.$$

Is $\widetilde{\mathcal{L}}$ self adjoint? We have seen that the general second-order linear differential operator $\widetilde{\mathcal{L}}$ can be transformed into Sturm-Liouville form by multiplication by a weight function w. It follows from § 6.6.2 that, subject to the boundary conditions (6.123b) being satisfied, $w\widetilde{\mathcal{L}} = \mathcal{L}$ is self-adjoint with respect to an inner product with the identity weight function, i.e.

$$\int_a^b u^* \left(\mathcal{L}\, v \right) \mathrm{d}x = \int_a^b \left(\mathcal{L}\, u^* \right) v \, \mathrm{d}x \,. \tag{6.131a}$$

However suppose that we slightly rearrange this equation to

$$\int_a^b u^* \left(\widetilde{\mathcal{L}}\, v \right) w \, \mathrm{d}x = \int_a^b \left(\widetilde{\mathcal{L}}\, u^* \right) v \, w \, \mathrm{d}x \,. \tag{6.131b}$$

Then from reference to the definition of an inner product with weight function w, i.e. (6.120a), we see that, subject to appropriate boundary conditions being satisfied, i.e.

$$\left[wP \left(v \frac{\mathrm{d}u^*}{\mathrm{d}x} - u^* \frac{\mathrm{d}v}{\mathrm{d}x} \right) \right]_a^b = 0 \,, \tag{6.132}$$

$\widetilde{\mathcal{L}}$ is self-adjoint with respect to an inner product with the weight function w.

6.6.4 Eigenvalues and Eigenfunctions

The equation $\widetilde{\mathcal{L}} y = f$ is analogous to the matrix equation $\mathsf{M}\mathsf{x} = \mathsf{b}$. This analogy suggests that it might be profitable to consider the *eigenvalue equation*

$$\widetilde{\mathcal{L}} y = \lambda y \,, \tag{6.133}$$

where λ is the, possibly complex, *eigenvalue* associated with the *eigenfunction* $y \neq 0$.

Example. The Schrödinger equation for a one-dimensional quantum harmonic oscillator is

$$\left(-\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} + \tfrac{1}{2} k^2 x^2 \right) \psi = E\psi \,.$$

This is an eigenvalue equation where the eigenvalue E is the energy level of the oscillator.

Remark. If $\widetilde{\mathcal{L}}$ is not in Sturm-Liouville form we can multiply by w to get the equivalent eigenvalue equation,

$$\mathcal{L} y = \lambda w y \,, \tag{6.134}$$

where $\mathcal{L}$ is in Sturm-Liouville form.

The Claim. We claim, but do not prove, that if the functions on which $\widetilde{\mathcal{L}}$ [or equivalently $\mathcal{L}$] acts are such that the boundary conditions (6.132) [or equivalently (6.123b)] are satisfied, then it is generally the case that (6.133) [or equivalently (6.134)] has solutions only for a discrete, but infinite, set of values of λ:

$$\{ \lambda_n, n = 1, 2, 3, \dots \} \tag{6.135}$$

These are the eigenvalues of $\widetilde{\mathcal{L}}$ [or equivalently $\mathcal{L}$]. The corresponding solutions $\{ y_n(x), n = 1, 2, 3, \dots \}$ are the eigenfunctions.

Example. Find the eigenvalues and eigenfunctions for the operator

$$\mathcal{L} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} \,, \tag{6.136}$$

on the assumption that $\mathcal{L}$ acts on functions defined on $0 \leqslant x \leqslant \pi$ that vanish at end-points $x = 0$ and $x = \pi$.

Answer. $\mathcal{L}$ is in Sturm-Liouville form with $p = 1$ and $q = 0$. Further, the boundary conditions ensure that (6.123b) is satisfied. Hence $\mathcal{L}$ is self-adjoint. The eigenvalue equation is

$$y'' + \lambda y = 0\,, \tag{6.137a}$$

with general solution

$$y = \alpha \cos \lambda^{\frac{1}{2}} x + \beta \sin \lambda^{\frac{1}{2}} x\,. \tag{6.137b}$$

Non-zero solutions exist with $y(0) = y(\pi) = 0$ only if

$$\alpha = 0 \quad \text{and} \quad \sin \lambda^{\frac{1}{2}} \pi = 0\,. \tag{6.138}$$

Hence $\lambda = n^2$ for integer n, and the corresponding eigenfunctions are

$$y_n(x) = \beta \sin nx\,. \tag{6.139}$$

Remark. The eigenvalues $\lambda_n = n^2$ are real (cf. the eigenvalues of an Hermitian matrix.).

The norm. We define the norm, $\|y\|$, of a (possibly complex) function $y(x)$ by

$$\|y\|^2 \equiv \langle\, y \mid y\,\rangle_w = \int_a^b |y|^2\, w\, \mathrm{d}x\,, \tag{6.140}$$

where we have introduced the subscript w (a non-standard notation) to indicate the weight function w in the inner product. It is conventional to normalize eigenfunctions to have unit norm. For our example (6.139) this results in

$$y_n = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \sin nx\,. \tag{6.141}$$

6.6.5 The Eigenvalues of a Self-Adjoint Operator are Real

Let $\widetilde{\mathcal{L}}$ be a self-adjoint operator with respect to an inner product with weight w, and suppose that y is a non-zero eigenvector with eigenvalue λ satisfying

$$\widetilde{\mathcal{L}}y = \lambda y\,. \tag{6.142a}$$

Take the complex conjugate of this equation, remembering that $\widetilde{\mathcal{L}}$ and w are real, to obtain

$$\widetilde{\mathcal{L}}y^* = \lambda^* y^*\,. \tag{6.142b}$$

Hence

$$\int_a^b \left(y^* \widetilde{\mathcal{L}}y - y \widetilde{\mathcal{L}}y^* \right) w\, \mathrm{d}x = \int_a^b \left(y^* \lambda y - y \lambda^* y^* \right) w\, \mathrm{d}x \qquad \text{from (6.142a) and (6.142b)}$$

$$= (\lambda - \lambda^*) \int_a^b |y|^2 w\, \mathrm{d}x\,.$$

$$= (\lambda - \lambda^*)\langle\, y \mid y\,\rangle_w\,. \tag{6.143}$$

But $\widetilde{\mathcal{L}}$ is self adjoint with respect to an inner product with weight w, and hence the left hand side of (6.143) is zero (e.g. (6.131b) with $u = v = y$). It follows that

$$(\lambda - \lambda^*)\langle\, y \mid y\,\rangle_w = 0\,, \tag{6.144}$$

But $\langle\, y \mid y\,\rangle_w \neq 0$ from (6.121d) since y has been assumed to be a non-zero eigenvector. Hence

$$\lambda = \lambda^*\,, \quad \text{i.e. } \lambda \text{ is real.} \tag{6.145}$$

Remark. This result can also be obtained, arguably in a more elegant fashion, using inner product notation since

$$\begin{aligned}
\lambda\langle\, y \mid y\,\rangle_w &= \langle\, y \mid \lambda y\,\rangle_w & \text{from (6.121b)} \\
&= \langle\, y \mid \widetilde{\mathcal{L}}y\,\rangle_w & \text{from (6.133)} \\
&= \langle\, \widetilde{\mathcal{L}}y \mid y\,\rangle_w & \text{since } \widetilde{\mathcal{L}} \text{ is self-adjoint} \\
&= \langle\, \lambda y \mid y\,\rangle_w & \text{from (6.133)} \\
&= \lambda^*\langle\, y \mid y\,\rangle_w & \text{from (6.121a) and (6.121b).} \tag{6.146}
\end{aligned}$$

This is essentially (6.144), and hence (6.145) follows as above.

6.6.6 Eigenfunctions with Distinct Eigenvalues are Orthogonal

Definition. Two functions u and v are said to be *orthogonal* with respect to a given inner product, if

$$\langle\, u \mid v \,\rangle_w = 0\,. \tag{6.147}$$

As before let $\widetilde{\mathcal{L}}$ be a general second-order linear differential operator that is self-adjoint with respect to an inner product with weight w. Suppose that y_1 and y_2 are eigenvectors of $\widetilde{\mathcal{L}}$, with *distinct* eigenvalues λ_1 and λ_2 respectively. Then

$$\widetilde{\mathcal{L}}y_1 = \lambda_1 y_1\,, \tag{6.148a}$$

$$\widetilde{\mathcal{L}}y_2 = \lambda_2 y_2\,. \tag{6.148b}$$

From taking the complex conjugate of (6.148a) we also have that

$$\widetilde{\mathcal{L}}y_1^* = \lambda_1 y_1^*\,, \tag{6.148c}$$

since $\widetilde{\mathcal{L}}$ and λ_1 are real. Hence

$$\int_a^b \left(y_1^* \,\widetilde{\mathcal{L}}y_2 - y_2 \,\widetilde{\mathcal{L}}y_1^* \right) w \, \mathrm{d}x = \int_a^b \left(y_1^* \,\lambda_2 y_2 - y_2 \,\lambda_1 y_1^* \right) w \, \mathrm{d}x \qquad \text{from (6.148b) and (6.148c)}$$

$$= (\lambda_2 - \lambda_1) \int_a^b y_1^* y_2 \, w \, \mathrm{d}x$$

$$= (\lambda_2 - \lambda_1) \langle\, y_1 \mid y_2 \,\rangle_w\,. \tag{6.149}$$

But $\widetilde{\mathcal{L}}$ is self adjoint, and hence the left hand side of (6.149) is zero (e.g. (6.131b) with $u = y_1$ and $v = y_2$). It follows that

$$(\lambda_2 - \lambda_1) \langle\, y_1 \mid y_2 \,\rangle_w = 0\,. \tag{6.150}$$

Hence if $\lambda_1 \neq \lambda_2$ then the eigenfunctions are orthogonal since

$$\langle\, y_1 \mid y_2 \,\rangle_w = 0\,. \tag{6.151}$$

Remark. As before the same result can be obtained using inner product notation since (6.150) follows from

$$
\begin{aligned}
\lambda_2 \langle\, y_1 \mid y_2 \,\rangle_w &= \langle\, y_1 \mid \lambda_2 y_2 \,\rangle_w && \text{from (6.121b)} \\
&= \langle\, y_1 \mid \widetilde{\mathcal{L}}y_2 \,\rangle_w && \text{from (6.148b)} \\
&= \langle\, \widetilde{\mathcal{L}}y_1 \mid y_2 \,\rangle_w && \text{since } \widetilde{\mathcal{L}} \text{ is self-adjoint} \\
&= \langle\, \lambda_1 y_1 \mid y_2 \,\rangle_w && \text{from (6.148a)} \\
&= \lambda_1^* \langle\, y_1 \mid y_2 \,\rangle_w && \text{from (6.121a) and (6.121b)} \\
&= \lambda_1 \langle\, y_1 \mid y_2 \,\rangle_w && \text{from (6.145).} \tag{6.152}
\end{aligned}
$$

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Example. Returning to our earlier example, we recall that we showed that the eigenfunctions of the Sturm-Liouville operator

$$\mathcal{L} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,, \tag{6.153}$$

acting on functions that vanish at end-points $x = 0$ and $x = \pi$, are

$$y_n = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \sin nx\,. \tag{6.154}$$

Since

$$\int_0^\pi y_n^* y_m \, \mathrm{d}x = \frac{2}{\pi} \int_0^\pi \sin nx \sin mx \, \mathrm{d}x$$

$$= \frac{1}{\pi} \int_0^\pi \big(\cos(n-m)x - \cos(n+m)x \big) \, \mathrm{d}x$$

$$= 0 \quad \text{if } n \neq m, \tag{6.155}$$

we confirm that the eigenfunctions are indeed orthogonal.

Orthonormal set. We have seen that eigenfunctions with different eigenvalues are mutually orthogonal. We claim, but do not prove, that mutually orthogonal eigenfunctions can be constructed even for repeated eigenvalues (cf. the 'experimental error' argument of § 4.7.2). Further, if we normalize all eigenfunctions to have unit norm then we have an *orthonormal* set of eigenfunctions, i.e.

$$\int_a^b w \, y_n^* y_m \, \mathrm{d}x = \langle \, y_n \mid y_m \, \rangle_w = \delta_{mn} \,. \tag{6.156}$$

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6.6.7 Eigenfunction Expansions

Let $\{y_n, n = 1, 2, \dots \}$ be an orthonormal set of eigenfunctions of a self-adjoint operator. Then we claim that any function $f(x)$ with the same boundary conditions as the eigenfunctions can be expressed as an eigenfunction expansion

$$f(x) = \sum_{n=1}^\infty a_n y_n(x) \,, \tag{6.157a}$$

where the coefficients a_n are given by

$$a_n = \langle \, y_n \mid f \, \rangle_w \,, \tag{6.157b}$$

i.e. we claim that the eigenfunctions form a basis. A set of eigenfunctions that has this property is said to be *complete*.

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We will not prove the *existence* of the expansion (6.157a). However, if we assume such an expansion does exist, then we can confirm that the coefficients must be given by (6.157b) since

$$\langle \, y_n \mid f \, \rangle_w = \langle \, y_n \mid \textstyle\sum_{m=1}^\infty a_m y_m \, \rangle_w \qquad \text{from (6.157a)}$$

$$= \sum_{m=1}^\infty a_m \langle \, y_n \mid y_m \, \rangle_w \qquad \text{from inner product property (4.27c)}$$

$$= \sum_{m=1}^\infty a_m \delta_{nm} \qquad \text{from (6.156)}$$

$$= a_n \qquad \text{from (0.11b), and as required.}$$

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The completeness relation. It follows from (6.157a) and (6.157b) that

$$f(x) = \sum_{n=1}^\infty \langle \, y_n \mid f \, \rangle_w \, y_n(x)$$

$$= \sum_{n=1}^\infty y_n(x) \int_a^b w(\zeta) \, y_n^*(\zeta) f(\zeta) \, \mathrm{d}\zeta \qquad \text{from (6.120a)}$$

$$= \int_a^b f(\zeta) \left(w(\zeta) \sum_{n=1}^\infty y_n(x) y_n^*(\zeta) \right) \mathrm{d}\zeta \qquad \text{interchange sum and integral.} \tag{6.158}$$

This expression holds for all functions f satisfying the appropriate homogeneous boundary conditions. Hence from (3.4)

$$w(\zeta) \sum_{n=1}^\infty y_n(x) y_n^*(\zeta) = \delta(x - \zeta) \,. \tag{6.159a}$$

This is the *completeness relation*.

Remark. Suppose we exchange x and ζ in the complex conjugate of (6.159a), then using the facts that the weight function is real and the delta function is real and symmetric (see (3.8a) and (3.8b)), we also have that

$$w(x) \sum_{n=1}^{\infty} y_n(x) y_n^*(\zeta) = \delta(x - \zeta) \,. \tag{6.159b}$$

Example: Fourier series. Again consider the Sturm-Liouville operator

$$\mathcal{L} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} \,. \tag{6.160}$$

In this case assume that it acts on functions that are 2π-periodic. $\mathcal{L}$ is still self-adjoint with weight function $w = 1$ since the periodicity ensures that the boundary conditions (6.123b) are satisfied if, say, $a = 0$ and $b = 2\pi$. This time we choose to write the general solution of the eigenvalue equation (6.134) as

$$y = \alpha \exp\left(\imath \lambda^{\frac{1}{2}} x\right) + \beta \exp\left(-\imath \lambda^{\frac{1}{2}} x\right) \,. \tag{6.161}$$

This solution is 2π-periodic if $\lambda = n^2$ for integer n (as before). Note that now we have two eigenfunctions for each eigenvalue (except for $n = 0$). Label the eigenfunctions by y_n for $n = \ldots, -1, 0, 1, \ldots$, with corresponding eigenvalues $\lambda_n = n^2$. Although there are repeated eigenvalues an orthonormal set of eigenfunctions exists (as claimed), e.g.

$$y_n = \frac{1}{\sqrt{2\pi}} \exp(\imath n x) \quad \text{for } n \in \mathbb{Z}. \tag{6.162}$$

Hence from (6.157a) a 2π-periodic function f has an eigenfunction expansion

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} a_n \exp(\imath n x) \,, \tag{6.163}$$

where a_n is given by (6.157b). This is just the Fourier series representation of f. In this case the completeness relation (6.159a) reads (cf. (3.6))

$$\frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \exp\bigl(\imath n(x - \zeta)\bigr) = \delta(x - \zeta) \,. \tag{6.164}$$

Example: Legendre polynomials. Legendre's equation (6.34),

$$(1 - x^2)y'' - 2xy' + \ell(\ell + 1)y = 0 \,, \tag{6.165a}$$

can be written as an Sturm-Liouville eigenvalue equation $\mathcal{L}y = \lambda y$ where

$$\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left((1 - x^2)\frac{\mathrm{d}}{\mathrm{d}x}\right) \quad \text{and} \quad \lambda = \ell(\ell + 1) \,. \tag{6.165b}$$

In terms of our standard notation

$$p = 1 - x^2 \quad \text{and} \quad q = 0 \,. \tag{6.165c}$$

Suppose now we require that $\mathcal{L}$ operates on functions y that remain *finite* at $x = -1$ and $x = 1$. Then $py = 0$ at $x = -1$ and $x = 1$, and hence the boundary conditions (6.123b) are satisfied if $a = -1$ and $b = 1$. It follows that $\mathcal{L}$ is self-adjoint.

Further, we saw earlier that Legendre's equation has solutions that are finite at $x = \pm 1$ when $\ell = 0, 1, 2, \ldots$, (see (6.40) and following), and that the solutions are Legendre polynomials $P_\ell(x)$. Identify the eigenvalues and eigenfunctions as

$$\lambda_\ell = \ell(\ell + 1) \quad \text{and} \quad y_\ell(x) = P_\ell(x) \quad \text{for} \quad \ell = 0, 1, 2, \ldots \,. \tag{6.166}$$

It then follows from our general theory that the Legendre polynomials are orthogonal in the sense that

$$\int_{-1}^{1} P_m(x) P_n(x) \, \mathrm{d}x = 0 \quad \text{if } m \neq n. \tag{6.167}$$

Remarks.

- With the conventional normalization, $P_\ell(1) = 1$, the Legendre polynomials are orthogonal, but *not* orthonormal.
- As a check on (6.167) we note that if m is odd and n is even, then $P_m P_n$ is an odd polynomial, and hence a symmetric integral like (6.167) must be zero. As a further check we note from (6.41) that

$$\int_{-1}^{1} P_0(x) P_2(x)\, \mathrm{d}x = \tfrac{1}{2} \int_{-1}^{1} (3x^2 - 1)\, \mathrm{d}x = \tfrac{1}{2} \left[x^3 - x \right]_{-1}^{1} = 0 \,. \tag{6.168}$$

6.6.8 Eigenfunction Expansions of Green's Functions for Self-Adjoint Operators

Let $\{\lambda_n\}$ and $\{y_n\}$ be the eigenvalues and the complete *orthonormal* set of eigenfunctions of a self-adjoint operator $\widetilde{\mathcal{L}}$ acting on functions satisfying (6.123b). Provided none of the λ_n vanish, we claim that the Green's function for $\widetilde{\mathcal{L}}$ can be written as

$$G(x, \zeta) = \sum_{n=1}^{\infty} \frac{w(\zeta) y_n^*(\zeta) y_n(x)}{\lambda_n} \,, \tag{6.169}$$

where $G(x, \zeta)$ satisfies the same boundary conditions as the $y_n(x)$. This result follows from the observation that

$$\widetilde{\mathcal{L}} G(x, \zeta) = \sum_{n=1}^{\infty} \frac{w(\zeta)\, y_n^*(\zeta)}{\lambda_n}\, \widetilde{\mathcal{L}} y_n(x) \qquad \text{from (6.169)}$$

$$= \sum_{n=1}^{\infty} w(\zeta) y_n^*(\zeta)\, y_n(x) \qquad \text{from (6.134)}$$

$$= \delta(x - \zeta) \qquad \text{from (6.159a).} \tag{6.170}$$

Remark. The form of the Green's function (6.169) shows that

$$w(x)\, G(x, \zeta) = w(\zeta)\, G^*(\zeta, x) \,. \tag{6.171}$$

Resonance. If $\lambda_n = 0$ for some n then $G(x, \zeta)$ does not exist. This is consistent with our previous observation that $\widetilde{\mathcal{L}} y = f$ has no solution for general f if $\widetilde{\mathcal{L}} y = 0$ has a solution satisfying appropriate boundary conditions; $y_n(x)$ is precisely such a solution if $\lambda_n = 0$. The vanishing of one of the eigenvalues is related to the phenomenon of *resonance*. If a solution to the problem (including the boundary conditions) exists in the *absence* of the 'forcing' function f (i.e. there is a zero eigenvalue of $\widetilde{\mathcal{L}}$) then any non-zero force elicits an infinite response.

6.6.9 Approximation via Eigenfunction Expansions

It is often useful, e.g. in a numerical method, to approximate a function with Sturm-Liouville boundary conditions by a *finite* linear combination of Sturm-Liouville eigenfunctions, i.e.

$$f(x) \approx \sum_{n=1}^{N} a_n y_n(x) \,. \tag{6.172}$$

Define the error of the approximation to be

$$\Sigma_N(a_1, a_2, \ldots, a_N) = \left\| f(x) - \sum_{n=1}^{N} a_n y_n(x) \right\|^2 \,. \tag{6.173}$$

One definition of the 'best' approximation is that the error (6.173) should be minimized with respect to the coefficients $a_1, a_2, \ldots, a_N$. By expanding (6.173) we have that, assuming that the y_n are an orthonormal set,

$$
\begin{aligned}
\Sigma_N &= \left\langle f(x) - \sum_{n=1}^{N} a_n y_n(x) \,\middle|\, f(x) - \sum_{m=1}^{N} a_m y_m(x) \right\rangle \\
&= \langle\, f \mid f \,\rangle - \sum_{n=1}^{N} a_n^* \langle\, y_n \mid f \,\rangle - \sum_{m=1}^{N} a_m \langle\, f \mid y_m \,\rangle + \sum_{n=1}^{N} \sum_{m=1}^{N} a_n^* a_m \langle\, y_n \mid y_m \,\rangle \\
&= \|f\|^2 - \sum_{n=1}^{N} \left(a_n^* \langle\, y_n \mid f \,\rangle + a_n \langle\, y_n \mid f \,\rangle^* \right) + \sum_{n=1}^{N} a_n a_n^* \,.
\end{aligned}
\tag{6.174}
$$

Hence if we perturb the a_n to $a_n + \delta a_n$ we have that

$$
\delta \Sigma_N = -\sum_{n=1}^{N} \left(\delta a_n^* \left(\langle\, y_n \mid f \,\rangle - a_n \right) + \delta a_n \left(\langle\, y_n \mid f \,\rangle^* - a_n^* \right) \right).
\tag{6.175}
$$

By setting $\delta\Sigma_N = 0$ we see that Σ_N is minimized when

$$
a_n = \langle\, y_n \mid f \,\rangle, \quad \text{or equivalently} \quad a_n^* = \langle\, y_n \mid f \,\rangle^*.
\tag{6.176}
$$

We note that this is an identical value for a_n to (6.157b). The value of Σ_N is then, from (6.174),

$$
\Sigma_N = \|f\|^2 - \sum_{n=1}^{N} |a_n|^2 \,.
\tag{6.177}
$$

Since $\Sigma_N \geqslant 0$ from (6.173), we arrive at *Bessel's inequality*

$$
\|f\|^2 \geqslant \sum_{n=1}^{N} |a_n|^2 \,.
\tag{6.178}
$$

It is possible to show, but not here, that this inequality becomes an equality when $N \to \infty$, and hence

$$
\|f\|^2 = \sum_{n=1}^{\infty} |a_n|^2
\tag{6.179}
$$

which is a generalization of *Parseval's theorem*.

Remark. While it is not strictly true that any function satisfying the Sturm-Liouville boundary conditions can be expressed as an eigenfunction expansion (6.157a) (since there are restrictions such as continuity), it is true that $\Sigma_\infty = 0$ for such functions, i.e.

$$
\left\| f(x) - \sum_{n=1}^{\infty} \langle\, y_n \mid f \,\rangle \, y_n(x) \right\|^2 = 0 \,.
\tag{6.180}
$$