**Natural Sciences Tripos, Part IB**

Michaelmas Term 2008

**Mathematical Methods I**

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## Schedule

**Vector calculus**. Suffix notation. Contractions using $\delta_{ij}$ and $\epsilon_{ijk}$. Reminder of vector products, grad, div, curl, $\nabla^2$ and their representations using suffix notation. Divergence theorem and Stokes's theorem. Vector differential operators in orthogonal curvilinear coordinates, e.g. cylindrical and spherical polar coordinates. Jacobians. [6 lectures]

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

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

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

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

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

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

## Course website

## Assumed knowledge

I will assume familiarity with the following topics at the level of Course A of Part IA Mathematics for Natural Sciences.

- Algebra of complex numbers

- Algebra of vectors (including scalar and vector products)

- Algebra of matrices

- Eigenvalues and eigenvectors of matrices

- Taylor series and the geometric series

- Calculus of functions of several variables

- Line, surface and volume integrals

- The Gaussian integral

- First-order ordinary differential equations

- Second-order linear ODEs with constant coefficients

- Fourier series

## Textbooks

The following textbooks are particularly recommended.

- K. F. Riley, M. P. Hobson and S. J. Bence (2006). *Mathematical Methods for Physics and Engineering*, 3rd edition. Cambridge University Press

- G. Arfken and H. J. Weber (2005). *Mathematical Methods for Physicists*, 6th edition. Academic Press

# 1 Vector calculus

## 1.1 Motivation

Scientific quantities are of different kinds:

- *scalars* have only magnitude (and sign), e.g. mass, electric charge, energy, temperature

- *vectors* have magnitude and direction, e.g. velocity, electric field, temperature gradient

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

- air pressure in this room (scalar field)

- electric field in this room (vector field)

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

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

## 1.2 Suffix notation and Cartesian coordinates

### 1.2.1 Three-dimensional Euclidean space

This is a close approximation to our physical space:

- *points* are the elements of the space

- *vectors* are translatable, directed line segments

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

Points and vectors have a geometrical existence without reference to any coordinate system. For definite calculations, however, we must introduce coordinates.

*Cartesian coordinates*:

- measured with respect to an origin $O$ and a system of orthogonal axes $Oxyz$

- points have coordinates $(x, y, z) = (x_1, x_2, x_3)$

- unit vectors $(\boldsymbol{e}_x, \boldsymbol{e}_y, \boldsymbol{e}_z) = (\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$ in the three coordinate directions, also called $(\hat{\boldsymbol{\imath}}, \hat{\boldsymbol{\jmath}}, \hat{\boldsymbol{k}})$ or $(\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}})$

The *position vector* of a point $P$ is

$$\overrightarrow{OP} = \boldsymbol{r} = \boldsymbol{e}_x x + \boldsymbol{e}_y y + \boldsymbol{e}_z z = \sum_{i=1}^{3} \boldsymbol{e}_i x_i$$

### 1.2.2 Properties of the Cartesian unit vectors

The unit vectors form a *basis* for the space. Any vector $\boldsymbol{a}$ belonging to the space can be written uniquely in the form

$$\boldsymbol{a} = \boldsymbol{e}_x a_x + \boldsymbol{e}_y a_y + \boldsymbol{e}_z a_z = \sum_{i=1}^{3} \boldsymbol{e}_i a_i$$

where $a_i$ are the *Cartesian components* of the vector $\boldsymbol{a}$.

The basis is *orthonormal* (orthogonal and normalized):

$$\boldsymbol{e}_1 \cdot \boldsymbol{e}_1 = \boldsymbol{e}_2 \cdot \boldsymbol{e}_2 = \boldsymbol{e}_3 \cdot \boldsymbol{e}_3 = 1$$
$$\boldsymbol{e}_1 \cdot \boldsymbol{e}_2 = \boldsymbol{e}_1 \cdot \boldsymbol{e}_3 = \boldsymbol{e}_2 \cdot \boldsymbol{e}_3 = 0$$

and *right-handed*:

$$[\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3] \equiv \boldsymbol{e}_1 \cdot \boldsymbol{e}_2 \times \boldsymbol{e}_3 = +1$$

This means that

$$\boldsymbol{e}_1 \times \boldsymbol{e}_2 = \boldsymbol{e}_3 \qquad \boldsymbol{e}_2 \times \boldsymbol{e}_3 = \boldsymbol{e}_1 \qquad \boldsymbol{e}_3 \times \boldsymbol{e}_1 = \boldsymbol{e}_2$$

The choice of basis is not unique. Two different bases, if both orthonormal and right-handed, are simply related by a rotation. The Cartesian components of a vector are different with respect to two different bases.

### 1.2.3  Suffix notation

- $x_i$ for a coordinate, $a_i$ (e.g.) for a vector component, $\boldsymbol{e}_i$ for a unit vector

- in three-dimensional space the symbolic index $i$ can have the values 1, 2 or 3

- quantities (*tensors*) with more than one index, such as $a_{ij}$ or $b_{ijk}$, can also be defined

Scalar and vector products can be evaluated in the following way:

$$\begin{aligned}
\boldsymbol{a} \cdot \boldsymbol{b} &= (\boldsymbol{e}_1 a_1 + \boldsymbol{e}_2 a_2 + \boldsymbol{e}_3 a_3) \cdot (\boldsymbol{e}_1 b_1 + \boldsymbol{e}_2 b_2 + \boldsymbol{e}_3 b_3) \\
&= a_1 b_1 + a_2 b_2 + a_3 b_3
\end{aligned}$$

$$\begin{aligned}
\boldsymbol{a} \times \boldsymbol{b} &= (\boldsymbol{e}_1 a_1 + \boldsymbol{e}_2 a_2 + \boldsymbol{e}_3 a_3) \times (\boldsymbol{e}_1 b_1 + \boldsymbol{e}_2 b_2 + \boldsymbol{e}_3 b_3) \\
&= \boldsymbol{e}_1(a_2 b_3 - a_3 b_2) + \boldsymbol{e}_2(a_3 b_1 - a_1 b_3) + \boldsymbol{e}_3(a_1 b_2 - a_2 b_1) \\
&= \begin{vmatrix} \boldsymbol{e}_1 & \boldsymbol{e}_2 & \boldsymbol{e}_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix}
\end{aligned}$$

### 1.2.4  Delta and epsilon

Suffix notation is made easier by defining two symbols. The *Kronecker delta symbol* is

$$\boxed{\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}}$$

In detail:

$$\delta_{11} = \delta_{22} = \delta_{33} = 1$$
$$\text{all others, e.g. } \delta_{12} = 0$$

$\delta_{ij}$ gives the components of the unit matrix. It is *symmetric*:

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

and has the *substitution property*:

$$\sum_{j=1}^{3} \delta_{ij} a_j = a_i \qquad (\text{in matrix notation, } \mathsf{1a} = \mathsf{a})$$

The *Levi-Civita permutation symbol* is

$$\boxed{\epsilon_{ijk} = \begin{cases} 1 & \text{if } (i, j, k) \text{ is an even permutation of } (1, 2, 3) \\ -1 & \text{if } (i, j, k) \text{ is an odd permutation of } (1, 2, 3) \\ 0 & \text{otherwise} \end{cases}}$$

In detail:

$$\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1$$
$$\epsilon_{132} = \epsilon_{213} = \epsilon_{321} = -1$$
$$\text{all others, e.g. } \epsilon_{112} = 0$$

An *even (odd) permutation* is one consisting of an even (odd) number of transpositions (interchanges of two objects). Therefore $\epsilon_{ijk}$ is *totally antisymmetric*: it changes sign when any two indices are interchanged, e.g. $\epsilon_{jik} = -\epsilon_{ijk}$. It arises in vector products and determinants.

$\epsilon_{ijk}$ has three indices because the space has three dimensions. The even permutations of $(1,2,3)$ are $(1,2,3)$, $(2,3,1)$ and $(3,1,2)$, which also happen to be the cyclic permutations. So $\epsilon_{ijk} = \epsilon_{jki} = \epsilon_{kij}$.

Then we can write

$$\boldsymbol{a} \cdot \boldsymbol{b} = \sum_{i=1}^{3} \sum_{j=1}^{3} \delta_{ij} a_i b_j = \sum_{i=1}^{3} a_i b_i$$

$$\boldsymbol{a} \times \boldsymbol{b} = \sum_{i=1}^{3} \sum_{j=1}^{3} \sum_{k=1}^{3} \epsilon_{ijk} \boldsymbol{e}_i a_j b_k$$

### 1.2.5  Einstein summation convention

The summation sign is conventionally omitted in expressions of this type. It is implicit that *a repeated index is to be summed over*. Thus

$$\boxed{\boldsymbol{a} \cdot \boldsymbol{b} = a_i b_i}$$

$$\boxed{\boldsymbol{a} \times \boldsymbol{b} = \epsilon_{ijk} \boldsymbol{e}_i a_j b_k} \qquad \text{or} \quad (\boldsymbol{a} \times \boldsymbol{b})_i = \epsilon_{ijk} a_j b_k$$

The repeated index should occur exactly twice in any term. Examples of *invalid* notation are:

$\boldsymbol{a} \cdot \boldsymbol{a} = a_i^2$ (should be $a_i a_i$)

$(\boldsymbol{a} \cdot \boldsymbol{b})(\boldsymbol{c} \cdot \boldsymbol{d}) = a_i b_i c_i d_i$ (should be $a_i b_i c_j d_j$)

The repeated index is a *dummy index* and can be relabelled at will. Other indices in an expression are *free indices*. The free indices in each term in an equation must agree.

Examples:

$\boldsymbol{a} = \boldsymbol{b}$      $a_i = b_i$

$\boldsymbol{a} = \boldsymbol{b} \times \boldsymbol{c}$      $a_i = \epsilon_{ijk} b_j c_k$

$|\boldsymbol{a}|^2 = \boldsymbol{b} \cdot \boldsymbol{c}$      $a_i a_i = b_i c_i$

$\boldsymbol{a} = (\boldsymbol{b} \cdot \boldsymbol{c})\boldsymbol{d} + \boldsymbol{e} \times \boldsymbol{f}$      $a_i = b_j c_j d_i + \epsilon_{ijk} e_j f_k$

*Contraction* means to set one free index equal to another, so that it is summed over. The contraction of $a_{ij}$ is $a_{ii}$. Contraction is equivalent to multiplication by a Kronecker delta:

$$a_{ij} \delta_{ij} = a_{11} + a_{22} + a_{33} = a_{ii}$$

The contraction of $\delta_{ij}$ is $\delta_{ii} = 1 + 1 + 1 = 3$ (in three dimensions).

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

### 1.2.6  Matrices and suffix notation

Matrix ($\mathsf{A}$) times vector ($\mathsf{x}$):

$$\mathsf{y} = \mathsf{A}\mathsf{x} \qquad y_i = A_{ij} x_j$$

Matrix times matrix:

$$\mathsf{A} = \mathsf{B}\mathsf{C} \qquad A_{ij} = B_{ik} C_{kj}$$

Transpose of a matrix:

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

Trace of a matrix:

$$\mathrm{tr}\,\mathsf{A} = A_{ii}$$

Determinant of a $(3 \times 3)$ matrix:

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

(or many equivalent expressions).

### 1.2.7   Product of two epsilons

The general identity

$$\epsilon_{ijk}\epsilon_{lmn} = \begin{vmatrix} \delta_{il} & \delta_{im} & \delta_{in} \\ \delta_{jl} & \delta_{jm} & \delta_{jn} \\ \delta_{kl} & \delta_{km} & \delta_{kn} \end{vmatrix}$$

can be established by the following argument. The value of both the LHS and the RHS:

- is 0 when any of $(i, j, k)$ are equal or when any of $(l, m, n)$ are equal

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

- changes sign when any of $(i, j, k)$ are interchanged or when any of $(l, m, n)$ are interchanged

These properties ensure that the LHS and RHS are equal for any choices of the indices. Note that the first property is in fact implied by the third.

We contract the identity once by setting $l = i$:

$$\epsilon_{ijk}\epsilon_{imn} = \begin{vmatrix} \delta_{ii} & \delta_{im} & \delta_{in} \\ \delta_{ji} & \delta_{jm} & \delta_{jn} \\ \delta_{ki} & \delta_{km} & \delta_{kn} \end{vmatrix}$$
$$= \delta_{ii}(\delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}) + \delta_{im}(\delta_{jn}\delta_{ki} - \delta_{ji}\delta_{kn})$$
$$\quad + \delta_{in}(\delta_{ji}\delta_{km} - \delta_{jm}\delta_{ki})$$
$$= 3(\delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}) + (\delta_{jn}\delta_{km} - \delta_{jm}\delta_{kn})$$
$$\quad + (\delta_{jn}\delta_{km} - \delta_{jm}\delta_{kn})$$
$$= \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}$$

This is the most useful form to remember:

$$\boxed{\epsilon_{ijk}\epsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}}$$

Given any product of two epsilons with one common index, the indices can be permuted cyclically into this form, e.g.:

$$\epsilon_{\alpha\beta\gamma}\epsilon_{\mu\nu\beta} = \epsilon_{\beta\gamma\alpha}\epsilon_{\beta\mu\nu} = \delta_{\gamma\mu}\delta_{\alpha\nu} - \delta_{\gamma\nu}\delta_{\alpha\mu}$$

Further contractions of the identity:

$$\epsilon_{ijk}\epsilon_{ijn} = \delta_{jj}\delta_{kn} - \delta_{jn}\delta_{kj}$$
$$= 3\delta_{kn} - \delta_{kn}$$
$$= 2\delta_{kn}$$

$$\epsilon_{ijk}\epsilon_{ijk} = 6$$

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Show that* $(\boldsymbol{a} \times \boldsymbol{b}) \cdot (\boldsymbol{c} \times \boldsymbol{d}) = (\boldsymbol{a} \cdot \boldsymbol{c})(\boldsymbol{b} \cdot \boldsymbol{d}) - (\boldsymbol{a} \cdot \boldsymbol{d})(\boldsymbol{b} \cdot \boldsymbol{c}).$

$$(\boldsymbol{a} \times \boldsymbol{b}) \cdot (\boldsymbol{c} \times \boldsymbol{d}) = (\boldsymbol{a} \times \boldsymbol{b})_i (\boldsymbol{c} \times \boldsymbol{d})_i$$
$$= (\epsilon_{ijk}a_j b_k)(\epsilon_{ilm}c_l d_m)$$
$$= \epsilon_{ijk}\epsilon_{ilm}a_j b_k c_l d_m$$
$$= (\delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl})a_j b_k c_l d_m$$
$$= a_j b_k c_j d_k - a_j b_k c_k d_j$$
$$= (a_j c_j)(b_k d_k) - (a_j d_j)(b_k c_k)$$
$$= (\boldsymbol{a} \cdot \boldsymbol{c})(\boldsymbol{b} \cdot \boldsymbol{d}) - (\boldsymbol{a} \cdot \boldsymbol{d})(\boldsymbol{b} \cdot \boldsymbol{c})$$

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## 1.3 Vector differential operators

### 1.3.1 The gradient operator

We consider a scalar field (function of position, e.g. temperature)

$$\Phi(x, y, z) = \Phi(\boldsymbol{r})$$

Taylor's theorem for a function of three variables:

$$\Phi(x + \delta x, y + \delta y, z + \delta z) = \Phi(x, y, z)$$
$$+ \frac{\partial \Phi}{\partial x}\delta x + \frac{\partial \Phi}{\partial y}\delta y + \frac{\partial \Phi}{\partial z}\delta z + O(\delta x^2, \delta x \delta y, \dots)$$

Equivalently

$$\Phi(\boldsymbol{r} + \delta \boldsymbol{r}) = \Phi(\boldsymbol{r}) + (\boldsymbol{\nabla}\Phi) \cdot \delta \boldsymbol{r} + O(|\delta \boldsymbol{r}|^2)$$

where the *gradient* of the scalar field is

$$\boldsymbol{\nabla}\Phi = \boldsymbol{e}_x \frac{\partial \Phi}{\partial x} + \boldsymbol{e}_y \frac{\partial \Phi}{\partial y} + \boldsymbol{e}_z \frac{\partial \Phi}{\partial z}$$

also written $\operatorname{grad}\Phi$. In suffix notation

$$\boxed{\boldsymbol{\nabla}\Phi = \boldsymbol{e}_i \frac{\partial \Phi}{\partial x_i}}$$

For an *infinitesimal* increment we can write

$$d\Phi = (\boldsymbol{\nabla}\Phi) \cdot d\boldsymbol{r}$$

We can consider $\boldsymbol{\nabla}$ (*del*, *grad* or *nabla*) as a *vector differential operator*

$$\boldsymbol{\nabla} = \boldsymbol{e}_x \frac{\partial}{\partial x} + \boldsymbol{e}_y \frac{\partial}{\partial y} + \boldsymbol{e}_z \frac{\partial}{\partial z} = \boldsymbol{e}_i \frac{\partial}{\partial x_i}$$

which acts on $\Phi$ to produce $\boldsymbol{\nabla}\Phi$.

*Example* ........................................................

▷ *Find $\boldsymbol{\nabla}f$, where $f(r)$ is a function of $r = |\boldsymbol{r}|$.*

$$\boldsymbol{\nabla}f = \boldsymbol{e}_x \frac{\partial f}{\partial x} + \boldsymbol{e}_y \frac{\partial f}{\partial y} + \boldsymbol{e}_z \frac{\partial f}{\partial z}$$

$$\frac{\partial f}{\partial x} = \frac{df}{dr}\frac{\partial r}{\partial x}$$

$$r^2 = x^2 + y^2 + z^2$$

$$2r\frac{\partial r}{\partial x} = 2x$$

$$\frac{\partial f}{\partial x} = \frac{df}{dr}\frac{x}{r}, \text{ etc.}$$

$$\boldsymbol{\nabla}f = \frac{df}{dr}\left(\frac{x}{r}, \frac{y}{r}, \frac{z}{r}\right) = \frac{df}{dr}\frac{\boldsymbol{r}}{r}$$

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### 1.3.2 Geometrical meaning of the gradient

The rate of change of $\Phi$ with distance $s$ in the direction of the unit vector $\boldsymbol{t}$, evaluated at the point $\boldsymbol{r}$, is

$$\frac{d}{ds}\left[\Phi(\boldsymbol{r} + \boldsymbol{t}s) - \Phi(\boldsymbol{r})\right]\bigg|_{s=0}$$

$$= \frac{d}{ds}\left[(\boldsymbol{\nabla}\Phi) \cdot (\boldsymbol{t}s) + O(s^2)\right]\bigg|_{s=0}$$

$$= \boldsymbol{t} \cdot \boldsymbol{\nabla}\Phi$$

This is known as a *directional derivative*.

Notes:

- the derivative is maximal in the direction $\boldsymbol{t} \parallel \boldsymbol{\nabla}\Phi$

- the derivative is zero in directions such that $\boldsymbol{t} \perp \boldsymbol{\nabla}\Phi$

- the directions $t \perp \nabla\Phi$ therefore lie in the plane tangent to the surface $\Phi = \text{constant}$

We conclude that:

- $\nabla\Phi$ is a vector field, pointing in the direction of increasing $\Phi$

- the unit vector normal to the surface $\Phi = \text{constant}$ is $\boldsymbol{n} = \nabla\Phi/|\nabla\Phi|$

- the rate of change of $\Phi$ with arclength $s$ along a curve is $\mathrm{d}\Phi/\mathrm{d}s = \boldsymbol{t} \cdot \nabla\Phi$, where $\boldsymbol{t} = \mathrm{d}\boldsymbol{r}/\mathrm{d}s$ is the unit tangent vector to the curve

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Find the unit normal at the point $\boldsymbol{r} = (x, y, z)$ to the surface*

$$\Phi(\boldsymbol{r}) \equiv xy + yz + zx = -c^2$$

*where $c$ is a constant. Hence find the points where the plane tangent to the surface is parallel to the $(x, y)$ plane.*

$$\nabla\Phi = (y + z, x + z, y + x)$$

$$\boldsymbol{n} = \frac{\nabla\Phi}{|\nabla\Phi|} = \frac{(y + z, x + z, y + x)}{\sqrt{2(x^2 + y^2 + z^2 + xy + xz + yz)}}$$

$$\boldsymbol{n} \parallel \boldsymbol{e}_z \quad \text{when} \quad y + z = x + z = 0$$

$$\Rightarrow -z^2 = -c^2 \quad \Rightarrow z = \pm c$$

solutions $\quad (-c, -c, c), \quad (c, c, -c)$

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### 1.3.3 Related vector differential operators

We now consider a general vector field (e.g. electric field)

$$\boldsymbol{F}(\boldsymbol{r}) = \boldsymbol{e}_x F_x(\boldsymbol{r}) + \boldsymbol{e}_y F_y(\boldsymbol{r}) + \boldsymbol{e}_z F_z(\boldsymbol{r}) = \boldsymbol{e}_i F_i(\boldsymbol{r})$$

The *divergence* of a vector field is the scalar field

$$\nabla \cdot \boldsymbol{F} = \left(\boldsymbol{e}_x \frac{\partial}{\partial x} + \boldsymbol{e}_y \frac{\partial}{\partial y} + \boldsymbol{e}_z \frac{\partial}{\partial z}\right) \cdot (\boldsymbol{e}_x F_x + \boldsymbol{e}_y F_y + \boldsymbol{e}_z F_z)$$

$$= \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$$

also written div $\boldsymbol{F}$. Note that the Cartesian unit vectors are independent of position and do not need to be differentiated. In suffix notation

$$\boxed{\nabla \cdot \boldsymbol{F} = \frac{\partial F_i}{\partial x_i}}$$

The *curl* of a vector field is the vector field

$$\nabla \times \boldsymbol{F} = \left(\boldsymbol{e}_x \frac{\partial}{\partial x} + \boldsymbol{e}_y \frac{\partial}{\partial y} + \boldsymbol{e}_z \frac{\partial}{\partial z}\right) \times (\boldsymbol{e}_x F_x + \boldsymbol{e}_y F_y + \boldsymbol{e}_z F_z)$$

$$= \boldsymbol{e}_x \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z}\right) + \boldsymbol{e}_y \left(\frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x}\right)$$

$$+ \boldsymbol{e}_z \left(\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y}\right)$$

$$= \begin{vmatrix} \boldsymbol{e}_x & \boldsymbol{e}_y & \boldsymbol{e}_z \\ \partial/\partial x & \partial/\partial y & \partial/\partial z \\ F_x & F_y & F_z \end{vmatrix}$$

also written curl $\boldsymbol{F}$. In suffix notation

$$\boxed{\nabla \times \boldsymbol{F} = \boldsymbol{e}_i \epsilon_{ijk} \frac{\partial F_k}{\partial x_j}} \qquad \text{or} \quad (\nabla \times \boldsymbol{F})_i = \epsilon_{ijk} \frac{\partial F_k}{\partial x_j}$$

The *Laplacian* of a scalar field is the scalar field

$$\nabla^2 \Phi = \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}\Phi) = \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} + \frac{\partial^2 \Phi}{\partial z^2} = \frac{\partial^2 \Phi}{\partial x_i \partial x_i}$$

The Laplacian differential operator (*del squared*) is

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{\partial^2}{\partial x_i \partial x_i}$$

It appears very commonly in partial differential equations. The Laplacian of a vector field can also be defined. In suffix notation

$$\nabla^2 \boldsymbol{F} = \boldsymbol{e}_i \frac{\partial^2 F_i}{\partial x_j \partial x_j}$$

because the Cartesian unit vectors are independent of position.

The *directional derivative* operator is

$$\boldsymbol{t} \cdot \boldsymbol{\nabla} = t_x \frac{\partial}{\partial x} + t_y \frac{\partial}{\partial y} + t_z \frac{\partial}{\partial z} = t_i \frac{\partial}{\partial x_i}$$

$\boldsymbol{t} \cdot \boldsymbol{\nabla}\Phi$ is the rate of change of $\Phi$ with distance in the direction of the unit vector $\boldsymbol{t}$. This can be thought of either as $\boldsymbol{t} \cdot (\boldsymbol{\nabla}\Phi)$ or as $(\boldsymbol{t} \cdot \boldsymbol{\nabla})\Phi$.

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

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

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

$$\boldsymbol{\nabla} \times \boldsymbol{F} = \begin{vmatrix} \boldsymbol{e}_x & \boldsymbol{e}_y & \boldsymbol{e}_z \\ \partial/\partial x & \partial/\partial y & \partial/\partial z \\ x^2 y & y^2 z & z^2 x \end{vmatrix} = (-y^2, -z^2, -x^2)$$

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▷ *Find* $\nabla^2 r^n$.

$$\boldsymbol{\nabla} r^n = \left( \frac{\partial r^n}{\partial x}, \frac{\partial r^n}{\partial y}, \frac{\partial r^n}{\partial z} \right)$$

$$= nr^{n-2}(x, y, z) \qquad \left(\text{recall } \frac{\partial r}{\partial x} = \frac{x}{r}, \text{ etc.}\right)$$

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$$\nabla^2 r^n = \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} r^n = \frac{\partial}{\partial x}(nr^{n-2}x) + \frac{\partial}{\partial y}(nr^{n-2}y) + \frac{\partial}{\partial z}(nr^{n-2}z)$$

$$= nr^{n-2} + n(n-2)r^{n-4}x^2 + \cdots$$

$$= 3nr^{n-2} + n(n-2)r^{n-2}$$

$$= n(n+1)r^{n-2}$$

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### 1.3.4 Vector invariance

A scalar is *invariant* under a change of basis, while vector components transform in a particular way under a rotation.

Fields constructed using $\boldsymbol{\nabla}$ share these properties, e.g.:

- $\boldsymbol{\nabla}\Phi$ and $\boldsymbol{\nabla} \times \boldsymbol{F}$ are vector fields and their components depend on the basis

- $\boldsymbol{\nabla} \cdot \boldsymbol{F}$ and $\nabla^2 \Phi$ are scalar fields and are invariant under a rotation

grad, div and $\nabla^2$ can be defined in spaces of any dimension, but curl (like the vector product) is a three-dimensional concept.

### 1.3.5 Vector differential identities

Here $\Phi$ and $\Psi$ are arbitrary scalar fields, and $\boldsymbol{F}$ and $\boldsymbol{G}$ are arbitrary vector fields.

Two operators, one field:

$$\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}\Phi) = \nabla^2 \Phi$$
$$\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \times \boldsymbol{F}) = 0$$
$$\boldsymbol{\nabla} \times (\boldsymbol{\nabla}\Phi) = \boldsymbol{0}$$
$$\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \boldsymbol{F}) = \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{F}) - \nabla^2 \boldsymbol{F}$$

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One operator, two fields:

$$\boldsymbol{\nabla}(\Phi\Psi) = \Psi\boldsymbol{\nabla}\Phi + \Phi\boldsymbol{\nabla}\Psi$$

$$\boldsymbol{\nabla}(\boldsymbol{F}\cdot\boldsymbol{G}) = (\boldsymbol{G}\cdot\boldsymbol{\nabla})\boldsymbol{F} + \boldsymbol{G}\times(\boldsymbol{\nabla}\times\boldsymbol{F}) + (\boldsymbol{F}\cdot\boldsymbol{\nabla})\boldsymbol{G} + \boldsymbol{F}\times(\boldsymbol{\nabla}\times\boldsymbol{G})$$

$$\boldsymbol{\nabla}\cdot(\Phi\boldsymbol{F}) = (\boldsymbol{\nabla}\Phi)\cdot\boldsymbol{F} + \Phi\boldsymbol{\nabla}\cdot\boldsymbol{F}$$

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

$$\boldsymbol{\nabla}\times(\Phi\boldsymbol{F}) = (\boldsymbol{\nabla}\Phi)\times\boldsymbol{F} + \Phi\boldsymbol{\nabla}\times\boldsymbol{F}$$

$$\boldsymbol{\nabla}\times(\boldsymbol{F}\times\boldsymbol{G}) = (\boldsymbol{G}\cdot\boldsymbol{\nabla})\boldsymbol{F} - \boldsymbol{G}(\boldsymbol{\nabla}\cdot\boldsymbol{F}) - (\boldsymbol{F}\cdot\boldsymbol{\nabla})\boldsymbol{G} + \boldsymbol{F}(\boldsymbol{\nabla}\cdot\boldsymbol{G})$$

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Show that $\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\times\boldsymbol{F}) = 0$ for any (twice-differentiable) vector field $\boldsymbol{F}$.*

$$\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\times\boldsymbol{F}) = \frac{\partial}{\partial x_i}\left(\epsilon_{ijk}\frac{\partial F_k}{\partial x_j}\right) = \epsilon_{ijk}\frac{\partial^2 F_k}{\partial x_i \partial x_j} = 0$$

(since $\epsilon_{ijk}$ is antisymmetric on $(i,j)$ while $\partial^2 F_k/\partial x_i \partial x_j$ is symmetric)

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Show that $\boldsymbol{\nabla}\times(\boldsymbol{F}\times\boldsymbol{G}) = (\boldsymbol{G}\cdot\boldsymbol{\nabla})\boldsymbol{F} - \boldsymbol{G}(\boldsymbol{\nabla}\cdot\boldsymbol{F}) - (\boldsymbol{F}\cdot\boldsymbol{\nabla})\boldsymbol{G} + \boldsymbol{F}(\boldsymbol{\nabla}\cdot\boldsymbol{G})$.*

$$\begin{aligned}
\boldsymbol{\nabla}\times(\boldsymbol{F}\times\boldsymbol{G}) &= \boldsymbol{e}_i\epsilon_{ijk}\frac{\partial}{\partial x_j}(\epsilon_{klm}F_l G_m) \\
&= \boldsymbol{e}_i\epsilon_{kij}\epsilon_{klm}\frac{\partial}{\partial x_j}(F_l G_m) \\
&= \boldsymbol{e}_i(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl})\left(G_m\frac{\partial F_l}{\partial x_j} + F_l\frac{\partial G_m}{\partial x_j}\right) \\
&= \boldsymbol{e}_i G_j\frac{\partial F_i}{\partial x_j} - \boldsymbol{e}_i G_i\frac{\partial F_j}{\partial x_j} + \boldsymbol{e}_i F_i\frac{\partial G_j}{\partial x_j} - \boldsymbol{e}_i F_j\frac{\partial G_i}{\partial x_j} \\
&= (\boldsymbol{G}\cdot\boldsymbol{\nabla})\boldsymbol{F} - \boldsymbol{G}(\boldsymbol{\nabla}\cdot\boldsymbol{F}) + \boldsymbol{F}(\boldsymbol{\nabla}\cdot\boldsymbol{G}) - (\boldsymbol{F}\cdot\boldsymbol{\nabla})\boldsymbol{G}
\end{aligned}$$

. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

Notes:

- be clear about which terms to the right an operator is acting on (use brackets if necessary)

- you cannot simply apply standard vector identities to expressions involving $\boldsymbol{\nabla}$, e.g. $\boldsymbol{\nabla}\cdot(\boldsymbol{F}\times\boldsymbol{G}) \neq (\boldsymbol{\nabla}\times\boldsymbol{F})\cdot\boldsymbol{G}$

Related results:

- if a vector field $\boldsymbol{F}$ is *irrotational* ($\boldsymbol{\nabla}\times\boldsymbol{F} = \boldsymbol{0}$) in a region of space, it can be written as the gradient of a *scalar potential*: $\boldsymbol{F} = \boldsymbol{\nabla}\Phi$. e.g. a 'conservative' force field such as gravity

- if a vector field $\boldsymbol{F}$ is *solenoidal* ($\boldsymbol{\nabla}\cdot\boldsymbol{F} = 0$) in a region of space, it can be written as the curl of a *vector potential*: $\boldsymbol{F} = \boldsymbol{\nabla}\times\boldsymbol{G}$. e.g. the magnetic field

## 1.4 Integral theorems

These very important results derive from the *fundamental theorem of calculus* (integration is the inverse of differentiation):

$$\int_a^b \frac{\mathrm{d}f}{\mathrm{d}x}\,\mathrm{d}x = f(b) - f(a)$$

### 1.4.1 The gradient theorem

$$\boxed{\int_C (\boldsymbol{\nabla}\Phi)\cdot\mathrm{d}\boldsymbol{r} = \Phi(\boldsymbol{r}_2) - \Phi(\boldsymbol{r}_1)}$$

where $C$ is any curve from $\boldsymbol{r}_1$ to $\boldsymbol{r}_2$.

Outline proof:

$$\begin{aligned}
\int_C (\boldsymbol{\nabla}\Phi)\cdot\mathrm{d}\boldsymbol{r} &= \int_C \mathrm{d}\Phi \\
&= \Phi(\boldsymbol{r}_2) - \Phi(\boldsymbol{r}_1)
\end{aligned}$$

### 1.4.2 The divergence theorem (Gauss's theorem)

$$\boxed{\int_V (\boldsymbol{\nabla} \cdot \boldsymbol{F})\, \mathrm{d}V = \int_S \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{S}}$$

where $V$ is a volume bounded by the closed surface $S$ (also called $\partial V$). The right-hand side is the *flux* of $\boldsymbol{F}$ through the surface $S$. The vector surface element is $\mathrm{d}\boldsymbol{S} = \boldsymbol{n}\,\mathrm{d}S$, where $\boldsymbol{n}$ is the outward unit normal vector.

Outline proof: first prove for a cuboid:

$$\int_V (\boldsymbol{\nabla} \cdot \boldsymbol{F})\, \mathrm{d}V = \int_{z_1}^{z_2} \int_{y_1}^{y_2} \int_{x_1}^{x_2} \left( \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} \right) \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

$$= \int_{z_1}^{z_2} \int_{y_1}^{y_2} [F_x(x_2, y, z) - F_x(x_1, y, z)]\, \mathrm{d}y\,\mathrm{d}z$$

$$+ \text{ two similar terms}$$

$$= \int_S \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{S}$$

An arbitrary volume $V$ can be subdivided into small cuboids to any desired accuracy. When the integrals are added together, the fluxes through internal surfaces cancel out, leaving only the flux through $S$.

A *simply connected* volume (e.g. a ball) is one with no holes. It has only an outer surface. For a *multiply connected* volume (e.g. a spherical shell), all the surfaces must be considered.

Related results:

$$\int_V (\boldsymbol{\nabla}\Phi)\, \mathrm{d}V = \int_S \Phi\, \mathrm{d}\boldsymbol{S}$$

$$\int_V (\boldsymbol{\nabla} \times \boldsymbol{F})\, \mathrm{d}V = \int_S \mathrm{d}\boldsymbol{S} \times \boldsymbol{F}$$

The rule is to replace $\boldsymbol{\nabla}$ in the volume integral with $\boldsymbol{n}$ in the surface integral, and $\mathrm{d}V$ with $\mathrm{d}S$ (note that $\mathrm{d}\boldsymbol{S} = \boldsymbol{n}\,\mathrm{d}S$).

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *A submerged body is acted on by a hydrostatic pressure $p = -\rho g z$, where $\rho$ is the density of the fluid, $g$ is the gravitational acceleration and $z$ is the vertical coordinate. Find a simplified expression for the pressure force acting on the body.*

$$\boldsymbol{F} = -\int_S p \, \mathrm{d}\boldsymbol{S}$$

$$F_z = \boldsymbol{e}_z \cdot \boldsymbol{F} = \int_S (-\boldsymbol{e}_z p) \cdot \mathrm{d}\boldsymbol{S}$$

$$= \int_V \boldsymbol{\nabla} \cdot (-\boldsymbol{e}_z p) \, \mathrm{d}V$$

$$= \int_V \frac{\partial}{\partial z}(\rho g z) \, \mathrm{d}V$$

$$= \rho g \int_V \mathrm{d}V$$

$$= Mg \qquad (M \text{ is the mass of fluid displaced by the body})$$

Similarly

$$F_x = \int_V \frac{\partial}{\partial x}(\rho g z) \, \mathrm{d}V = 0$$

$$F_y = 0$$

$$\boldsymbol{F} = \boldsymbol{e}_z \, Mg$$

Archimedes' principle: buoyancy force equals weight of displaced fluid

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### 1.4.3   The curl theorem (Stokes's theorem)

$$\boxed{\int_S (\boldsymbol{\nabla} \times \boldsymbol{F}) \cdot \mathrm{d}\boldsymbol{S} = \int_C \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{r}}$$

where $S$ is an open surface bounded by the closed curve $C$ (also called $\partial S$). The right-hand side is the *circulation* of $\boldsymbol{F}$ around the curve $C$. Whichever way the unit normal $\boldsymbol{n}$ is defined on $S$, the line integral follows the direction of a right-handed screw around $\boldsymbol{n}$.

Special case: for a planar surface in the $(x, y)$ plane, we have *Green's theorem in the plane*:

$$\iint_A \left( \frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y = \int_C (F_x \, \mathrm{d}x + F_y \, \mathrm{d}y)$$

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

Outline proof: first prove Green's theorem for a rectangle:

$$\int_{y_1}^{y_2} \int_{x_1}^{x_2} \left( \frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \right) \, \mathrm{d}x \, \mathrm{d}y$$

$$= \int_{y_1}^{y_2} [F_y(x_2, y) - F_y(x_1, y)] \, \mathrm{d}y$$

$$\quad - \int_{x_1}^{x_2} [F_x(x, y_2) - F_x(x, y_1)] \, \mathrm{d}x$$

$$= \int_{x_1}^{x_2} F_x(x, y_1) \, \mathrm{d}x + \int_{y_1}^{y_2} F_y(x_2, y) \, \mathrm{d}y$$

$$\quad + \int_{x_2}^{x_1} F_x(x, y_2) \, \mathrm{d}x + \int_{y_2}^{y_1} F_y(x_1, y) \, \mathrm{d}y$$

$$= \int_C (F_x \, \mathrm{d}x + F_y \, \mathrm{d}y)$$

An arbitrary surface $S$ can be subdivided into small planar rectangles to any desired accuracy. When the integrals are added together, the circulations along internal curve segments cancel out, leaving only the circulation around $C$.

Notes:

- in Stokes's theorem $S$ is an open surface, while in Gauss's theorem it is closed

- many different surfaces are bounded by the same closed curve, while only one volume is bounded by a closed surface

- a multiply connected surface (e.g. an annulus) may have more than one bounding curve

### 1.4.4   Geometrical definitions of grad, div and curl

The integral theorems can be used to assign coordinate-independent meanings to grad, div and curl.

Apply the gradient theorem to an arbitrarily small line segment $\delta \boldsymbol{r} = \boldsymbol{t} \, \delta s$ in the direction of any unit vector $\boldsymbol{t}$. Since the variation of $\boldsymbol{\nabla}\Phi$ and $\boldsymbol{t}$ along the line segment is negligible,

$$(\boldsymbol{\nabla}\Phi) \cdot \boldsymbol{t} \, \delta s \approx \delta\Phi$$

and so

$$\boldsymbol{t} \cdot (\boldsymbol{\nabla}\Phi) = \lim_{\delta s \to 0} \frac{\delta\Phi}{\delta s}$$

This definition can be used to determine the component of $\boldsymbol{\nabla}\Phi$ in any desired direction.

Similarly, by applying the divergence theorem to an arbitrarily small volume $\delta V$ bounded by a surface $\delta S$, we find that

$$\boldsymbol{\nabla} \cdot \boldsymbol{F} = \lim_{\delta V \to 0} \frac{1}{\delta V} \int_{\delta S} \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{S}$$

Finally, by applying the curl theorem to an arbitrarily small open surface $\delta S$ with unit normal vector $\boldsymbol{n}$ and bounded by a curve $\delta C$, we find that

$$\boldsymbol{n} \cdot (\boldsymbol{\nabla} \times \boldsymbol{F}) = \lim_{\delta S \to 0} \frac{1}{\delta S} \int_{\delta C} \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{r}$$

The gradient therefore describes the rate of change of a scalar field with distance. The divergence describes the net source or efflux of a vector field per unit volume. The curl describes the circulation or rotation of a vector field per unit area.

## 1.5 Orthogonal curvilinear coordinates

Cartesian coordinates can be replaced with any independent set of co-ordinates $q_1(x_1, x_2, x_3)$, $q_2(x_1, x_2, x_3)$, $q_3(x_1, x_2, x_3)$, e.g. cylindrical or spherical polar coordinates.

*Curvilinear* (as opposed to rectilinear) means that the coordinate 'axes' are curves. Curvilinear coordinates are useful for solving problems in curved geometry (e.g. geophysics).

### 1.5.1 Line element

The infinitesimal *line element* in Cartesian coordinates is

$$\mathrm{d}\boldsymbol{r} = \boldsymbol{e}_x \, \mathrm{d}x + \boldsymbol{e}_y \, \mathrm{d}y + \boldsymbol{e}_z \, \mathrm{d}z$$

In general curvilinear coordinates we have

$$\boxed{\mathrm{d}\boldsymbol{r} = \boldsymbol{h}_1 \, \mathrm{d}q_1 + \boldsymbol{h}_2 \, \mathrm{d}q_2 + \boldsymbol{h}_3 \, \mathrm{d}q_3}$$

where

$$\boxed{\boldsymbol{h}_i = \boldsymbol{e}_i h_i = \frac{\partial \boldsymbol{r}}{\partial q_i}} \qquad \text{(no sum)}$$

determines the displacement associated with an increment of the coordinate $q_i$.

$h_i = |\boldsymbol{h}_i|$ is the *scale factor* (or *metric coefficient*) associated with the coordinate $q_i$. It converts a coordinate increment into a length. Any point at which $h_i = 0$ is a *coordinate singularity* at which the coordinate system breaks down.

$\boldsymbol{e}_i$ is the corresponding unit vector. This notation generalizes the use of $\boldsymbol{e}_i$ for a Cartesian unit vector. For Cartesian coordinates, $h_i = 1$ and $\boldsymbol{e}_i$ are constant, but in general both $h_i$ and $\boldsymbol{e}_i$ *depend on position*.

The summation convention does not work well with orthogonal curvilinear coordinates.

### 1.5.2 The Jacobian

The *Jacobian* of $(x, y, z)$ with respect to $(q_1, q_2, q_3)$ is defined as

$$J = \frac{\partial(x, y, z)}{\partial(q_1, q_2, q_3)} = \begin{vmatrix} \partial x/\partial q_1 & \partial x/\partial q_2 & \partial x/\partial q_3 \\ \partial y/\partial q_1 & \partial y/\partial q_2 & \partial y/\partial q_3 \\ \partial z/\partial q_1 & \partial z/\partial q_2 & \partial z/\partial q_3 \end{vmatrix}$$

This is the determinant of the *Jacobian matrix* of the transformation from coordinates $(q_1, q_2, q_3)$ to $(x_1, x_2, x_3)$. The columns of the above matrix are the vectors $\boldsymbol{h}_i$ defined above. Therefore the Jacobian is equal to the scalar triple product

$$J = [\boldsymbol{h}_1, \boldsymbol{h}_2, \boldsymbol{h}_3] = \boldsymbol{h}_1 \cdot \boldsymbol{h}_2 \times \boldsymbol{h}_3$$

Given a point with curvilinear coordinates $(q_1, q_2, q_3)$, consider three small displacements $\delta \boldsymbol{r}_1 = \boldsymbol{h}_1 \, \delta q_1$, $\delta \boldsymbol{r}_2 = \boldsymbol{h}_2 \, \delta q_2$ and $\delta \boldsymbol{r}_3 = \boldsymbol{h}_3 \, \delta q_3$ along

the three coordinate directions. They span a parallelepiped of volume

$$\delta V = |[\delta \boldsymbol{r}_1, \delta \boldsymbol{r}_2, \delta \boldsymbol{r}_3]| = |J| \, \delta q_1 \, \delta q_2 \, \delta q_3$$

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

$$\mathrm{d}V = \left| \frac{\partial(x, y, z)}{\partial(q_1, q_2, q_3)} \right| \mathrm{d}q_1 \, \mathrm{d}q_2 \, \mathrm{d}q_3$$

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

$$\int \Phi(\boldsymbol{r}) \, \mathrm{d}V = \iiint \Phi \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z = \iiint \Phi \left| \frac{\partial(x, y, z)}{\partial(q_1, q_2, q_3)} \right| \mathrm{d}q_1 \, \mathrm{d}q_2 \, \mathrm{d}q_3$$

The limits on the integrals also need to be considered.

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

$$\mathrm{d}A = |J| \, \mathrm{d}q_1 \, \mathrm{d}q_2$$

with

$$J = \frac{\partial(x, y)}{\partial(q_1, q_2)} = \begin{vmatrix} \partial x / \partial q_1 & \partial x / \partial q_2 \\ \partial y / \partial q_1 & \partial y / \partial q_2 \end{vmatrix}$$

The equivalent rule for a one-dimensional integral is

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

The modulus sign appears here if the integrals are carried out over a positive range (the upper limits are greater than the lower limits).

### 1.5.3 Properties of Jacobians

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

$$\frac{\partial \alpha_i}{\partial \gamma_j} = \sum_{k=1}^{n} \frac{\partial \alpha_i}{\partial \beta_k} \frac{\partial \beta_k}{\partial \gamma_j}$$

(Under the summation convention we may omit the $\Sigma$ sign.) The left-hand side is the $ij$-component of the Jacobian matrix of the transformation from $\gamma_i$ to $\alpha_i$, and the equation states that this matrix is the product of the Jacobian matrices of the transformations from $\gamma_i$ to $\beta_i$ and from $\beta_i$ to $\alpha_i$. Taking the determinant of this matrix equation, we find

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

This is the *chain rule for Jacobians*: the Jacobian of a composite transformation is the product of the Jacobians of the transformations of which is it composed.

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

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

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

### 1.5.4 Orthogonality of coordinates

Calculus in general curvilinear coordinates is difficult. We can make things easier by choosing the coordinates to be orthogonal:

$$\boldsymbol{e}_i \cdot \boldsymbol{e}_j = \delta_{ij}$$

and right-handed:

$$\boldsymbol{e}_1 \times \boldsymbol{e}_2 = \boldsymbol{e}_3$$

The squared line element is then

$$
\begin{aligned}
|\mathrm{d}\boldsymbol{r}|^2 &= |\boldsymbol{e}_1\, h_1\, \mathrm{d}q_1 + \boldsymbol{e}_2\, h_2\, \mathrm{d}q_2 + \boldsymbol{e}_3\, h_3\, \mathrm{d}q_3|^2 \\
&= h_1^2\, \mathrm{d}q_1^2 + h_2^2\, \mathrm{d}q_2^2 + h_3^2\, \mathrm{d}q_3^2
\end{aligned}
$$

There are no cross terms such as $\mathrm{d}q_1\, \mathrm{d}q_2$.

When oriented along the coordinate directions:

- line element $\mathrm{d}\boldsymbol{r} = \boldsymbol{e}_1\, h_1\, \mathrm{d}q_1$

- surface element $\mathrm{d}\boldsymbol{S} = \boldsymbol{e}_3\, h_1 h_2\, \mathrm{d}q_1\, \mathrm{d}q_2$,

- volume element $\mathrm{d}V = h_1 h_2 h_3\, \mathrm{d}q_1\, \mathrm{d}q_2\, \mathrm{d}q_3$

Note that, for orthogonal coordinates, $J = \boldsymbol{h}_1 \cdot \boldsymbol{h}_2 \times \boldsymbol{h}_3 = h_1 h_2 h_3$

## 1.5.5 Commonly used orthogonal coordinate systems

*Cartesian coordinates* $(x, y, z)$:

$$-\infty < x < \infty, \qquad -\infty < y < \infty, \qquad -\infty < z < \infty$$

$$\boldsymbol{r} = (x, y, z)$$

$$\boldsymbol{h}_x = \frac{\partial \boldsymbol{r}}{\partial x} = (1, 0, 0)$$

$$\boldsymbol{h}_y = \frac{\partial \boldsymbol{r}}{\partial y} = (0, 1, 0)$$

$$\boldsymbol{h}_z = \frac{\partial \boldsymbol{r}}{\partial z} = (0, 0, 1)$$

$$
\begin{aligned}
h_x &= 1, & \boldsymbol{e}_x &= (1, 0, 0) \\
h_y &= 1, & \boldsymbol{e}_y &= (0, 1, 0) \\
h_z &= 1, & \boldsymbol{e}_z &= (0, 0, 1)
\end{aligned}
$$

$$\boldsymbol{r} = x\, \boldsymbol{e}_x + y\, \boldsymbol{e}_y + z\, \boldsymbol{e}_z$$

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

Orthogonal. No singularities.

*Cylindrical polar coordinates $(\rho, \phi, z)$:*

$$0 < \rho < \infty, \qquad 0 \leqslant \phi < 2\pi, \qquad -\infty < z < \infty$$

$$\boldsymbol{r} = (x, y, z) = (\rho \cos \phi, \rho \sin \phi, z)$$

$$\boldsymbol{h}_\rho = \frac{\partial \boldsymbol{r}}{\partial \rho} = (\cos \phi, \sin \phi, 0)$$

$$\boldsymbol{h}_\phi = \frac{\partial \boldsymbol{r}}{\partial \phi} = (-\rho \sin \phi, \rho \cos \phi, 0)$$

$$\boldsymbol{h}_z = \frac{\partial \boldsymbol{r}}{\partial z} = (0, 0, 1)$$

$$h_\rho = 1, \qquad \boldsymbol{e}_\rho = (\cos \phi, \sin \phi, 0)$$
$$h_\phi = \rho, \qquad \boldsymbol{e}_\phi = (-\sin \phi, \cos \phi, 0)$$
$$h_z = 1, \qquad \boldsymbol{e}_z = (0, 0, 1)$$

$$\boldsymbol{r} = \rho \, \boldsymbol{e}_\rho + z \, \boldsymbol{e}_z$$

$$\mathrm{d}V = \rho \, \mathrm{d}\rho \, \mathrm{d}\phi \, \mathrm{d}z$$

Orthogonal. Singular on the axis $\rho = 0$.

**Warning.** *Many authors use $r$ for $\rho$ and $\theta$ for $\phi$. This is confusing because $r$ and $\theta$ then have different meanings in cylindrical and spherical polar coordinates. Instead of $\rho$, which is useful for other things, some authors use $R$, $s$ or $\varpi$.*

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*Spherical polar coordinates $(r, \theta, \phi)$:*

$$0 < r < \infty, \qquad 0 < \theta < \pi, \qquad 0 \leqslant \phi < 2\pi$$

$$\boldsymbol{r} = (x, y, z) = (r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta)$$

$$\boldsymbol{h}_r = \frac{\partial \boldsymbol{r}}{\partial r} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$$

$$\boldsymbol{h}_\theta = \frac{\partial \boldsymbol{r}}{\partial \theta} = (r \cos \theta \cos \phi, r \cos \theta \sin \phi, -r \sin \theta)$$

$$\boldsymbol{h}_\phi = \frac{\partial \boldsymbol{r}}{\partial \phi} = (-r \sin \theta \sin \phi, r \sin \theta \cos \phi, 0)$$

$$h_r = 1, \qquad \boldsymbol{e}_r = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$$
$$h_\theta = r, \qquad \boldsymbol{e}_\theta = (\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta)$$
$$h_\phi = r \sin \theta, \qquad \boldsymbol{e}_\phi = (-\sin \phi, \cos \phi, 0)$$

$$\boldsymbol{r} = r \, \boldsymbol{e}_r$$

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

Orthogonal. Singular on the axis $r = 0$, $\theta = 0$ and $\theta = \pi$.

Notes:

- cylindrical and spherical are related by $\rho = r \sin \theta$, $z = r \cos \theta$

- *plane polar coordinates* are the restriction of cylindrical coordinates to a plane $z = $ constant

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### 1.5.6 Vector calculus in orthogonal coordinates

A scalar field $\Phi(\boldsymbol{r})$ can be regarded as function of $(q_1, q_2, q_3)$:

$$
\begin{aligned}
\mathrm{d}\Phi &= \frac{\partial \Phi}{\partial q_1}\,\mathrm{d}q_1 + \frac{\partial \Phi}{\partial q_2}\,\mathrm{d}q_2 + \frac{\partial \Phi}{\partial q_3}\,\mathrm{d}q_3 \\
&= \left( \frac{\boldsymbol{e}_1}{h_1}\frac{\partial \Phi}{\partial q_1} + \frac{\boldsymbol{e}_2}{h_2}\frac{\partial \Phi}{\partial q_2} + \frac{\boldsymbol{e}_3}{h_3}\frac{\partial \Phi}{\partial q_3} \right) \\
&\qquad \cdot (\boldsymbol{e}_1\,h_1\,\mathrm{d}q_1 + \boldsymbol{e}_2\,h_2\,\mathrm{d}q_2 + \boldsymbol{e}_3\,h_3\,\mathrm{d}q_3) \\
&= (\boldsymbol{\nabla}\Phi) \cdot \mathrm{d}\boldsymbol{r}
\end{aligned}
$$

We identify

$$
\boxed{\boldsymbol{\nabla}\Phi = \frac{\boldsymbol{e}_1}{h_1}\frac{\partial \Phi}{\partial q_1} + \frac{\boldsymbol{e}_2}{h_2}\frac{\partial \Phi}{\partial q_2} + \frac{\boldsymbol{e}_3}{h_3}\frac{\partial \Phi}{\partial q_3}}
$$

Thus

$$
\boldsymbol{\nabla}q_i = \frac{\boldsymbol{e}_i}{h_i} \qquad \text{(no sum)}
$$

We now consider a vector field in orthogonal coordinates:

$$
\boldsymbol{F} = \boldsymbol{e}_1 F_1 + \boldsymbol{e}_2 F_2 + \boldsymbol{e}_3 F_3
$$

Finding the divergence and curl are non-trivial because both $F_i$ and $\boldsymbol{e}_i$ depend on position. Consider

$$
\boldsymbol{\nabla} \times (q_2 \boldsymbol{\nabla} q_3) = (\boldsymbol{\nabla} q_2) \times (\boldsymbol{\nabla} q_3) = \frac{\boldsymbol{e}_2}{h_2} \times \frac{\boldsymbol{e}_3}{h_3} = \frac{\boldsymbol{e}_1}{h_2 h_3}
$$

which implies

$$
\boldsymbol{\nabla} \cdot \left( \frac{\boldsymbol{e}_1}{h_2 h_3} \right) = 0
$$

as well as cyclic permutations of this result. Also

$$
\boldsymbol{\nabla} \times \left( \frac{\boldsymbol{e}_1}{h_1} \right) = \boldsymbol{\nabla} \times (\boldsymbol{\nabla} q_1) = \boldsymbol{0}, \qquad \text{etc.}
$$

To work out $\boldsymbol{\nabla} \cdot \boldsymbol{F}$, write

$$
\boldsymbol{F} = \left( \frac{\boldsymbol{e}_1}{h_2 h_3} \right)(h_2 h_3 F_1) + \cdots
$$

$$
\begin{aligned}
\boldsymbol{\nabla} \cdot \boldsymbol{F} &= \left( \frac{\boldsymbol{e}_1}{h_2 h_3} \right) \cdot \boldsymbol{\nabla}(h_2 h_3 F_1) + \cdots \\
&= \left( \frac{\boldsymbol{e}_1}{h_2 h_3} \right) \cdot \left[ \frac{\boldsymbol{e}_1}{h_1}\frac{\partial}{\partial q_1}(h_2 h_3 F_1) + \frac{\boldsymbol{e}_2}{h_2}\frac{\partial}{\partial q_2}(h_2 h_3 F_1) \right. \\
&\qquad \left. + \frac{\boldsymbol{e}_3}{h_3}\frac{\partial}{\partial q_3}(h_2 h_3 F_1) \right] + \cdots \\
&= \frac{1}{h_1 h_2 h_3}\frac{\partial}{\partial q_1}(h_2 h_3 F_1) + \cdots
\end{aligned}
$$

Similarly, to work out $\boldsymbol{\nabla} \times \boldsymbol{F}$, write

$$
\boldsymbol{F} = \left( \frac{\boldsymbol{e}_1}{h_1} \right)(h_1 F_1) + \cdots
$$

$$
\begin{aligned}
\boldsymbol{\nabla} \times \boldsymbol{F} &= \boldsymbol{\nabla}(h_1 F_1) \times \left( \frac{\boldsymbol{e}_1}{h_1} \right) + \cdots \\
&= \left[ \frac{\boldsymbol{e}_1}{h_1}\frac{\partial}{\partial q_1}(h_1 F_1) + \frac{\boldsymbol{e}_2}{h_2}\frac{\partial}{\partial q_2}(h_1 F_1) + \frac{\boldsymbol{e}_3}{h_3}\frac{\partial}{\partial q_3}(h_1 F_1) \right] \\
&\qquad \times \left( \frac{\boldsymbol{e}_1}{h_1} \right) + \cdots \\
&= \left[ \frac{\boldsymbol{e}_2}{h_1 h_3}\frac{\partial}{\partial q_3}(h_1 F_1) - \frac{\boldsymbol{e}_3}{h_1 h_2}\frac{\partial}{\partial q_2}(h_1 F_1) \right] + \cdots
\end{aligned}
$$

The appearance of the scale factors inside the derivatives can be understood with reference to the geometrical definitions of grad, div and curl:

$$
\boldsymbol{t} \cdot (\boldsymbol{\nabla}\Phi) = \lim_{\delta s \to 0} \frac{\delta \Phi}{\delta s}
$$

$$
\boldsymbol{\nabla} \cdot \boldsymbol{F} = \lim_{\delta V \to 0} \frac{1}{\delta V} \int_{\delta S} \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{S}
$$

$$
\boldsymbol{n} \cdot (\boldsymbol{\nabla} \times \boldsymbol{F}) = \lim_{\delta S \to 0} \frac{1}{\delta S} \int_{\delta C} \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{r}
$$

To summarize:

$$\nabla \Phi = \frac{e_1}{h_1}\frac{\partial \Phi}{\partial q_1} + \frac{e_2}{h_2}\frac{\partial \Phi}{\partial q_2} + \frac{e_3}{h_3}\frac{\partial \Phi}{\partial q_3}$$

$$\nabla \cdot F = \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial q_1}(h_2 h_3 F_1) + \frac{\partial}{\partial q_2}(h_3 h_1 F_2) + \frac{\partial}{\partial q_3}(h_1 h_2 F_3)\right]$$

$$\nabla \times F = \frac{e_1}{h_2 h_3}\left[\frac{\partial}{\partial q_2}(h_3 F_3) - \frac{\partial}{\partial q_3}(h_2 F_2)\right]$$
$$+ \frac{e_2}{h_3 h_1}\left[\frac{\partial}{\partial q_3}(h_1 F_1) - \frac{\partial}{\partial q_1}(h_3 F_3)\right]$$
$$+ \frac{e_3}{h_1 h_2}\left[\frac{\partial}{\partial q_1}(h_2 F_2) - \frac{\partial}{\partial q_2}(h_1 F_1)\right]$$
$$= \frac{1}{h_1 h_2 h_3}\begin{vmatrix} h_1\,e_1 & h_2\,e_2 & h_3\,e_3 \\ \partial/\partial q_1 & \partial/\partial q_2 & \partial/\partial q_3 \\ h_1 F_1 & h_2 F_2 & h_3 F_3 \end{vmatrix}$$

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

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Determine the Laplacian operator in spherical polar coordinates.*

$$h_r = 1, \qquad h_\theta = r, \qquad h_\phi = r\sin\theta$$

$$\nabla^2 \Phi = \frac{1}{r^2 \sin\theta}\left[\frac{\partial}{\partial r}\left(r^2 \sin\theta\frac{\partial \Phi}{\partial r}\right) + \frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial \Phi}{\partial \theta}\right) + \frac{\partial}{\partial \phi}\left(\frac{1}{\sin\theta}\frac{\partial \Phi}{\partial \phi}\right)\right]$$
$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \Phi}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial \Phi}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 \Phi}{\partial \phi^2}$$

. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

### 1.5.7 Grad, div, curl and $\nabla^2$ in cylindrical and spherical polar coordinates

Cylindrical polar coordinates:

$$\nabla\Phi = e_\rho \frac{\partial\Phi}{\partial\rho} + \frac{e_\phi}{\rho}\frac{\partial\Phi}{\partial\phi} + e_z\frac{\partial\Phi}{\partial z}$$

$$\nabla\cdot F = \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho F_\rho) + \frac{1}{\rho}\frac{\partial F_\phi}{\partial\phi} + \frac{\partial F_z}{\partial z}$$

$$\nabla\times F = \frac{1}{\rho}\begin{vmatrix} e_\rho & \rho\,e_\phi & e_z \\ \partial/\partial\rho & \partial/\partial\phi & \partial/\partial z \\ F_\rho & \rho F_\phi & F_z \end{vmatrix}$$

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

Spherical polar coordinates:

$$\nabla\Phi = e_r\frac{\partial\Phi}{\partial r} + \frac{e_\theta}{r}\frac{\partial\Phi}{\partial\theta} + \frac{e_\phi}{r\sin\theta}\frac{\partial\Phi}{\partial\phi}$$

$$\nabla\cdot F = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 F_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\,F_\theta) + \frac{1}{r\sin\theta}\frac{\partial F_\phi}{\partial\phi}$$

$$\nabla\times F = \frac{1}{r^2\sin\theta}\begin{vmatrix} e_r & r\,e_\theta & r\sin\theta\,e_\phi \\ \partial/\partial r & \partial/\partial\theta & \partial/\partial\phi \\ F_r & rF_\theta & r\sin\theta\,F_\phi \end{vmatrix}$$

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

*Example* .........................................................

▷ *Evaluate* $\nabla\cdot r$, $\nabla\times r$ *and* $\nabla^2 r^n$ *using spherical polar coordinates.*

$$r = e_r r$$

$$\nabla\cdot r = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\cdot r) = 3$$

$$\nabla\times r = \frac{1}{r^2\sin\theta}\begin{vmatrix} e_r & r\,e_\theta & r\sin\theta\,e_\phi \\ \partial/\partial r & \partial/\partial\theta & \partial/\partial\phi \\ r & 0 & 0 \end{vmatrix} = 0$$

$$\nabla^2 r^n = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial r^n}{\partial r}\right) = n(n+1)r^{n-2}$$

.........................................................

# 2 Partial differential equations

## 2.1 Motivation

The variation in space and time of scientific quantities is usually described by differential equations. If the quantities depend on space and time, or on more than one spatial coordinate, then the governing equations are *partial differential equations* (PDEs).

Many of the most important PDEs are *linear* and classical methods of analysis can be applied. The techniques developed for linear equations are also useful in the study of nonlinear PDEs.

## 2.2 Linear PDEs of second order

### 2.2.1 Definition

We consider an unknown function $u(x, y)$ (the *dependent variable*) of two *independent variables* $x$ and $y$. A *partial differential equation* is any equation of the form

$$F\left(u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial^2 u}{\partial x^2}, \frac{\partial^2 u}{\partial x \partial y}, \frac{\partial^2 u}{\partial y^2}, \ldots, x, y\right) = 0$$

involving $u$ and any of its derivatives evaluated at the same point.

- the *order* of the equation is the highest order of derivative that appears
- the equation is *linear* if $F$ depends linearly on $u$ and its derivatives

A linear PDE of second order has the general form

$$Lu = f$$

where $L$ is a differential operator such that

$$Lu = a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x} + e\frac{\partial u}{\partial y} + gu$$

where $a, b, c, d, e, f, g$ are functions of $x$ and $y$.

- if $f = 0$ the equation is said to be *homogeneous*
- if $a, b, c, d, e, g$ are independent of $x$ and $y$ the equation is said to have *constant coefficients*

These ideas can be generalized to more than two independent variables, or to systems of PDEs with more than one dependent variable.

### 2.2.2 Principle of superposition

$L$ defined above is an example of a *linear operator*:

$$L(\alpha u) = \alpha Lu$$

$$L(u + v) = Lu + Lv$$

where $u$ and $v$ any functions of $x$ and $y$, and $\alpha$ is any constant.

The principle of superposition:

- if $u$ and $v$ satisfy the homogeneous equation $Lu = 0$, then $\alpha u$ and $u + v$ also satisfy the homogeneous equation
- similarly, any linear combination of solutions of the homogeneous equation is also a solution
- if the *particular integral* $u_{\mathrm{p}}$ satisfies the inhomogeneous equation $Lu = f$ and the *complementary function* $u_{\mathrm{c}}$ satisfies the homogeneous equation $Lu = 0$, then $u_{\mathrm{p}} + u_{\mathrm{c}}$ also satisfies the inhomogeneous equation:

$$L(u_{\mathrm{p}} + u_{\mathrm{c}}) = Lu_{\mathrm{p}} + Lu_{\mathrm{c}} = f + 0 = f$$

The same principle applies to any other type of linear equation (e.g. algebraic, ordinary differential, integral).

### 2.2.3 Classic examples

Laplace's equation:

$$\nabla^2 u = 0$$

Diffusion equation (heat equation):

$$\frac{\partial u}{\partial t} = \lambda \nabla^2 u, \qquad \lambda = \text{diffusion coefficient (or } \textit{diffusivity}\text{)}$$

Wave equation:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u, \qquad c = \text{wave speed}$$

All involve the vector-invariant operator $\nabla^2$, the form of which depends on the number of active dimensions.

Inhomogeneous versions of these equations are also found. The inhomogeneous term usually represents a 'source' or 'force' that generates or drives the quantity $u$.

## 2.3 Physical examples of occurrence

### 2.3.1 Examples of Laplace's (or Poisson's) equation

Gravitational acceleration is related to gravitational potential by

$$\boldsymbol{g} = -\boldsymbol{\nabla}\Phi$$

The source (divergence) of the gravitational field is mass:

$$\boldsymbol{\nabla} \cdot \boldsymbol{g} = -4\pi G\rho$$

where $G$ is Newton's constant and $\rho$ is the mass density. Combine:

$$\nabla^2\Phi = 4\pi G\rho$$

External to the mass distribution, we have Laplace's equation $\nabla^2\Phi = 0$. With the source term the inhomogeneous equation is called *Poisson's equation*.

Analogously, in electrostatics, the electric field is related to the electrostatic potential by

$$\boldsymbol{E} = -\boldsymbol{\nabla}\Phi$$

The source of the electric field is electric charge:

$$\boldsymbol{\nabla} \cdot \boldsymbol{E} = \frac{\rho}{\epsilon_0}$$

where $\rho$ is the charge density and $\epsilon_0$ is the permittivity of free space. Combine to obtain Poisson's equation:

$$\nabla^2\Phi = -\frac{\rho}{\epsilon_0}$$

The vector field ($\boldsymbol{g}$ or $\boldsymbol{E}$) is said to be *generated* by the potential $\Phi$. A scalar potential is easier to work with because it does not have multiple components and its value is independent of the coordinate system. The potential is also directly related to the energy of the system.

### 2.3.2 Examples of the diffusion equation

A conserved quantity with density (amount per unit volume) $Q$ and flux density (flux per unit area) $\boldsymbol{F}$ satisfies the *conservation equation*:

$$\frac{\partial Q}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{F} = 0$$

This is more easily understood when integrated over the volume $V$ bounded by any (fixed) surface $S$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V Q\,\mathrm{d}V = \int_V \frac{\partial Q}{\partial t}\,\mathrm{d}V = -\int_V \boldsymbol{\nabla} \cdot \boldsymbol{F}\,\mathrm{d}V = -\int_S \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{S}$$

The amount of $Q$ in the volume $V$ changes only as the result of a net flux through $S$.

Often the flux of $Q$ is directed down the gradient of $Q$ through the linear relation (Fick's law)

$$\boldsymbol{F} = -\lambda \boldsymbol{\nabla} Q$$

Combine to obtain the diffusion equation (if $\lambda$ is independent of $\boldsymbol{r}$):

$$\frac{\partial Q}{\partial t} = \lambda \nabla^2 Q$$

In a steady state $Q$ satisfies Laplace's equation.

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Heat conduction in a solid.* Conserved quantity: energy. Heat per unit volume: $CT$ ($C$ is heat capacity per unit volume, $T$ is temperature. Heat flux density: $-K\boldsymbol{\nabla}T$ ($K$ is thermal conductivity). Thus

$$\frac{\partial}{\partial t}(CT) + \boldsymbol{\nabla} \cdot (-K\boldsymbol{\nabla}T) = 0$$

$$\frac{\partial T}{\partial t} = \lambda \nabla^2 T, \qquad \lambda = \frac{K}{C}$$

e.g. copper: $\lambda \approx 1\,\mathrm{cm^2\,s^{-1}}$ . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

Further example: concentration of a contaminant in a gas. $\lambda \approx 0.2\,\mathrm{cm^2\,s^{-1}}$

### 2.3.3 Examples of the wave equation

*Waves on a string.* The string has uniform mass per unit length $\rho$ and uniform tension $T$. The transverse displacement $y(x,t)$ is small ($|\partial y/\partial x| \ll 1$) and satisfies Newton's second law for an element $\delta x$ of the string:

$$(\rho\,\delta x)\frac{\partial^2 y}{\partial t^2} = \delta F_y \approx \frac{\partial F_y}{\partial x}\delta x$$

Now

$$F_y = T\sin\theta \approx T\frac{\partial y}{\partial x}$$

where $\theta$ is the angle between the $x$-axis and the tangent to the string. Combine to obtain the one-dimensional wave equation

$$\frac{\partial^2 y}{\partial t^2} = c^2\frac{\partial^2 y}{\partial x^2}, \qquad c = \sqrt{\frac{T}{\rho}}$$

e.g. violin (D-)string: $T \approx 40\,\mathrm{N}$, $\rho \approx 1\,\mathrm{g\,m^{-1}}$: $c \approx 200\,\mathrm{m\,s^{-1}}$

*Electromagnetic waves.* Maxwell's equations for the electromagnetic field in a vacuum:

$$\boldsymbol{\nabla} \cdot \boldsymbol{E} = 0$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$$

$$\boldsymbol{\nabla} \times \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = \boldsymbol{0}$$

$$\frac{1}{\mu_0}\boldsymbol{\nabla} \times \boldsymbol{B} - \epsilon_0\frac{\partial \boldsymbol{E}}{\partial t} = \boldsymbol{0}$$

where $\boldsymbol{E}$ is electric field, $\boldsymbol{B}$ is magnetic field, $\mu_0$ is the permeability of free space and $\epsilon_0$ is the permittivity of free space. Eliminate $\boldsymbol{E}$:

$$\frac{\partial^2 \boldsymbol{B}}{\partial t^2} = -\boldsymbol{\nabla} \times \frac{\partial \boldsymbol{E}}{\partial t} = -\frac{1}{\mu_0\epsilon_0}\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \boldsymbol{B})$$

Now use the identity $\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \boldsymbol{B}) = \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{B}) - \nabla^2\boldsymbol{B}$ and Maxwell's equation $\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$ to obtain the (vector) wave equation

$$\frac{\partial^2 \boldsymbol{B}}{\partial t^2} = c^2\nabla^2\boldsymbol{B}, \qquad c = \sqrt{\frac{1}{\mu_0\epsilon_0}}$$

$\boldsymbol{E}$ obeys the same equation. $c$ is the speed of light. $c \approx 3 \times 10^8\,\mathrm{m\,s^{-1}}$

Further example: sound waves in a gas. $c \approx 300\,\mathrm{m\,s^{-1}}$

## 2.3.4 Examples of other second-order linear PDEs

Schrödinger's equation (quantum-mechanical wavefunction of a particle of mass $m$ in a potential $V$):

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\boldsymbol{r})\psi$$

Helmholtz equation (arises in wave problems):

$$\nabla^2 u + k^2 u = 0$$

Klein–Gordon equation (arises in quantum mechanics):

$$\frac{\partial^2 u}{\partial t^2} = c^2(\nabla^2 u - m^2 u)$$

## 2.3.5 Examples of nonlinear PDEs

Burgers' equation (describes shock waves):

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \lambda\nabla^2 u$$

Nonlinear Schrödinger equation (describes solitons, e.g. in optical fibre communication):

$$i\frac{\partial\psi}{\partial t} = -\nabla^2\psi - |\psi|^2\psi$$

These equations require different methods of analysis.

## 2.4 Separation of variables (Cartesian coordinates)

### 2.4.1 Diffusion equation

We consider the one-dimensional diffusion equation (e.g. conduction of heat along a metal bar):

$$\frac{\partial u}{\partial t} = \lambda\frac{\partial^2 u}{\partial x^2}$$

The bar could be considered *finite* (having two ends), *semi-infinite* (having one end) or *infinite* (having no end). Typical *boundary conditions* at an end are:

- $u$ is specified (*Dirichlet* boundary condition)

- $\partial u/\partial x$ is specified (*Neumann* boundary condition)

If a boundary is removed to infinity, we usually require instead that $u$ be *bounded* (i.e. remain finite) as $x \to \pm\infty$. This condition is needed to eliminate unphysical solutions.

To determine the solution fully we also require *initial conditions*. For the diffusion equation this means specifying $u$ as a function of $x$ at some initial time (usually $t = 0$).

Try a solution in which the variables appear in separate factors:

$$u(x, t) = X(x)T(t)$$

Substitute this into the PDE:

$$X(x)T'(t) = \lambda X''(x)T(t)$$

(recall that a prime denotes differentiation of a function with respect to its argument). Divide through by $\lambda XT$ to *separate the variables*:

$$\frac{T'(t)}{\lambda T(t)} = \frac{X''(x)}{X(x)}$$

The LHS depends only on $t$, while the RHS depends only on $x$. Both must therefore equal a constant, which we call $-k^2$ (for later convenience). The PDE is separated into two *ordinary differential equations* (ODEs)

$$T' + \lambda k^2 T = 0$$

$$X'' + k^2 X = 0$$

with general solutions

$$T = A\exp(-\lambda k^2 t)$$

$$X = B\sin(kx) + C\cos(kx)$$

*Finite bar*: suppose the Neumann boundary conditions $\partial u/\partial x = 0$ (i.e. zero heat flux) apply at the two ends $x = 0, L$. Then the admissible solutions of the $X$ equation are

$$X = C\cos(kx), \qquad k = \frac{n\pi}{L}, \qquad n = 0, 1, 2, \dots$$

Combine the factors to obtain the *elementary solution* (let $C = 1$ WLOG)

$$u = A\cos\left(\frac{n\pi x}{L}\right)\exp\left(-\frac{n^2\pi^2\lambda t}{L^2}\right)$$

Each elementary solution represents a 'decay mode' of the bar. The decay rate is proportional to $n^2$. The $n = 0$ mode represents a uniform temperature distribution and does not decay.

The principle of superposition allows us to construct a *general solution* as a linear combination of elementary solutions:

$$u(x, t) = \sum_{n=0}^{\infty} A_n \cos\left(\frac{n\pi x}{L}\right)\exp\left(-\frac{n^2\pi^2\lambda t}{L^2}\right)$$

The coefficients $A_n$ can be determined from the *initial conditions*. If the temperature at time $t = 0$ is specified, then

$$u(x, 0) = \sum_{n=0}^{\infty} A_n \cos\left(\frac{n\pi x}{L}\right)$$

is known. The coefficients $A_n$ are just the Fourier coefficients of the initial temperature distribution.

*Semi-infinite bar*: The solution $X \propto \cos(kx)$ is valid for any real value of $k$ so that $u$ is bounded as $x \to \pm\infty$. We may assume $k \geqslant 0$ WLOG. The solution decays in time unless $k = 0$. The general solution is a linear combination in the form of an integral:

$$u = \int_0^{\infty} A(k)\cos(kx)\exp(-\lambda k^2 t)\,\mathrm{d}k$$

This is an example of a Fourier integral, studied in section 4.

Notes:

- separation of variables doesn't work for all linear equations, by any means, but it does for some of the most important examples

- it is not supposed to be obvious that the most general solution can be written as a linear combination of separated solutions

### 2.4.2 Wave equation (example)

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \qquad 0 < x < L$$

Boundary conditions:

$$u = 0 \qquad \text{at } x = 0, L$$

Initial conditions:

$$u, \frac{\partial u}{\partial t} \qquad \text{specified at } t = 0$$

Trial solution:

$$u(x, t) = X(x)T(t)$$

$$X(x)T''(t) = c^2 X''(x)T(t)$$

$$\frac{T''(t)}{c^2 T(t)} = \frac{X''(x)}{X(x)} = -k^2$$

$$T'' + c^2 k^2 T = 0$$

$$X'' + k^2 X = 0$$

$$T = A\sin(ckt) + B\cos(ckt)$$

$$X = C\sin(kx), \qquad k = \frac{n\pi}{L}, \qquad n = 1, 2, 3, \dots$$

Elementary solution:

$$u = \left[A\sin\left(\frac{n\pi ct}{L}\right) + B\cos\left(\frac{n\pi ct}{L}\right)\right]\sin\left(\frac{n\pi x}{L}\right)$$

General solution:

$$u = \sum_{n=1}^{\infty}\left[A_n\sin\left(\frac{n\pi ct}{L}\right) + B_n\cos\left(\frac{n\pi ct}{L}\right)\right]\sin\left(\frac{n\pi x}{L}\right)$$

At $t = 0$:

$$u = \sum_{n=1}^{\infty} B_n\sin\left(\frac{n\pi x}{L}\right)$$

$$\frac{\partial u}{\partial t} = \sum_{n=1}^{\infty}\left(\frac{n\pi c}{L}\right)A_n\sin\left(\frac{n\pi x}{L}\right)$$

The Fourier series for the initial conditions determine all the coefficients $A_n, B_n$.

### 2.4.3 Helmholtz equation (example)

A three-dimensional example in a cube:

$$\nabla^2 u + k^2 u = 0, \qquad 0 < x, y, z < L$$

Boundary conditions:

$$u = 0 \qquad \text{on the boundaries}$$

Trial solution:

$$u(x, y, z) = X(x)Y(y)Z(z)$$

$$X''(x)Y(y)Z(z) + X(x)Y''(y)Z(z) + X(x)Y(y)Z''(z)$$
$$+ k^2 X(x)Y(y)Z(z) = 0$$

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} + k^2 = 0$$

The variables are separated: each term must equal a constant. Call the constants $-k_x^2, -k_y^2, -k_z^2$:

$$X'' + k_x^2 X = 0$$

$$Y'' + k_y^2 Y = 0$$

$$Z'' + k_z^2 Z = 0$$

$$k^2 = k_x^2 + k_y^2 + k_z^2$$

$$X \propto \sin(k_x x), \qquad k_x = \frac{n_x\pi}{L}, \qquad n_x = 1, 2, 3, \ldots$$

$$Y \propto \sin(k_y y), \qquad k_y = \frac{n_y\pi}{L}, \qquad n_y = 1, 2, 3, \ldots$$

$$Z \propto \sin(k_z z), \qquad k_z = \frac{n_z\pi}{L}, \qquad n_z = 1, 2, 3, \ldots$$

Elementary solution:

$$u = A\sin\left(\frac{n_x\pi x}{L}\right)\sin\left(\frac{n_y\pi y}{L}\right)\sin\left(\frac{n_z\pi z}{L}\right)$$

The solution is possible only if $k^2$ is one of the discrete values

$$k^2 = (n_x^2 + n_y^2 + n_z^2)\frac{\pi^2}{L^2}$$

These are the eigenvalues of the problem.

# 3 Green's functions

## 3.1 Impulses and the delta function

### 3.1.1 Physical motivation

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

$$\frac{\mathrm{d}p}{\mathrm{d}t} = F$$

where

$$p = m\frac{\mathrm{d}x}{\mathrm{d}t}$$

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

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

and is called the *impulse*.

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

In other applications we may wish to represent an idealized point charge or point mass, or a localized source of heat, waves, etc. Here we need a mathematical object of infinite density and zero spatial extension but having a non-zero integral effect.

The delta function is introduced to meet these requirements.

### 3.1.2 Step function and delta function

We start by defining the *Heaviside unit step function*

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

The value of $H(0)$ does not matter for most purposes. It is sometimes taken to be $1/2$. An alternative notation for $H(x)$ is $\theta(x)$.

$H(x)$ can be used to construct other discontinuous functions. Consider the particular 'top-hat' function

$$\delta_\epsilon(x) = \begin{cases} 1/\epsilon, & 0 < x < \epsilon \\ 0, & \text{otherwise} \end{cases}$$

where $\epsilon$ is a positive parameter. This function can also be written as

$$\delta_\epsilon(x) = \frac{H(x) - H(x - \epsilon)}{\epsilon}$$

The area under the curve is equal to one. In the limit $\epsilon \to 0$, we obtain a 'spike' of infinite height, vanishing width and unit area localized at $x = 0$. This limit is the *Dirac delta function*, $\delta(x)$.

The indefinite integral of $\delta_\epsilon(x)$ is

$$\int_{-\infty}^{x} \delta_\epsilon(\xi)\,\mathrm{d}\xi = \begin{cases} 0, & x \leqslant 0 \\ x/\epsilon, & 0 \leqslant x \leqslant \epsilon \\ 1, & x \geqslant \epsilon \end{cases}$$

In the limit $\epsilon \to 0$, we obtain

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

or, equivalently,

$$\boxed{\delta(x) = H'(x)}$$

Our idealized impulsive force (section 3.1.1) can be represented as

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

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

$$p = I\,H(t).$$

In other physical applications $\delta(x)$ is used to represent an idealized point charge or localized source. It can be placed anywhere: $q\,\delta(x - \xi)$ represents a 'spike' of strength $q$ located at $x = \xi$.

## 3.2   Other definitions

We might think of defining the delta function as

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

but this is not specific enough to describe it. It is not a function in the usual sense but a 'generalized function' or 'distribution'.

Instead, the defining property of $\delta(x)$ can be taken to be

$$\int_{-\infty}^{\infty} f(x)\delta(x)\,\mathrm{d}x = f(0)$$

where $f(x)$ is any continuous function. This is because the unit spike picks out the value of the function at the location of the spike. It also follows that

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

Since $\delta(x - \xi) = 0$ for $x \neq \xi$, the integral can be taken over *any* interval that includes the point $x = \xi$.

One way to justify this result is as follows. Consider a continuous function $f(x)$ with indefinite integral $g(x)$, i.e. $f(x) = g'(x)$. Then

$$\int_{-\infty}^{\infty} f(x)\delta_\epsilon(x - \xi)\,\mathrm{d}x = \frac{1}{\epsilon}\int_{\xi}^{\xi+\epsilon} f(x)\,\mathrm{d}x$$
$$= \frac{g(\xi + \epsilon) - g(\xi)}{\epsilon}$$

From the definition of the derivative,

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

as required.

This result (the boxed formula above) is equivalent to the *substitution property* of the Kronecker delta:

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

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

$\delta(x)$ can also be seen as the limit of localized functions other than our top-hat example. Alternative, smooth choices for $\delta_\epsilon(x)$ include

$$\delta_\epsilon(x) = \frac{\epsilon}{\pi(x^2 + \epsilon^2)}$$

$$\delta_\epsilon(x) = (2\pi\epsilon^2)^{-1/2} \exp\left(-\frac{x^2}{2\epsilon^2}\right)$$
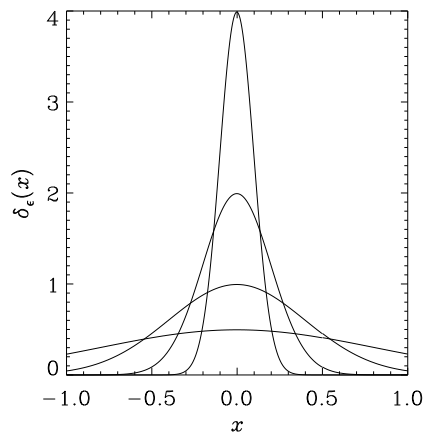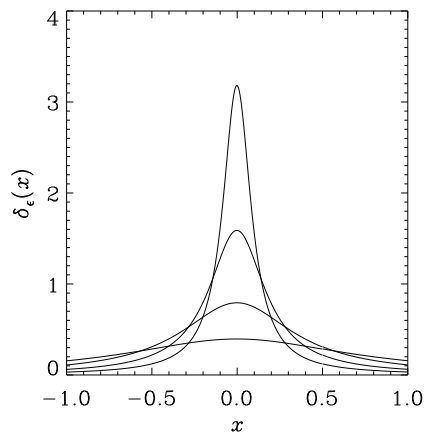


## 3.3   More on generalized functions

Derivatives of the delta function can also be defined as the limits of sequences of functions. The generating functions for $\delta'(x)$ are the derivatives of (smooth) functions (e.g. Gaussians) that generate $\delta(x)$, and have both positive and negative 'spikes' localized at $x = 0$. The defining property of $\delta'(x)$ can be taken to be

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

where $f(x)$ is any differentiable function. This follows from an integration by parts before the limit is taken.
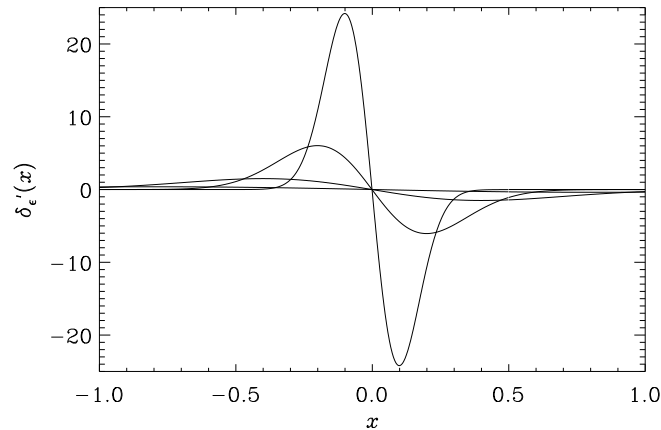


Not all operations are permitted on generalized functions. In particular, two generalized functions of the same variable cannot be multiplied together. e.g. $H(x)\delta(x)$ is meaningless. However $\delta(x)\delta(y)$ is permissible and represents a point source in a two-dimensional space.

## 3.4   Differential equations containing delta functions

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

Consider, as an example, the linear second-order ODE

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + y = \delta(x) \tag{1}$$

If $x$ represents time, this equation could represent the behaviour of a simple harmonic oscillator in response to an impulsive force.

In each of the regions $x < 0$ and $x > 0$ separately, the right-hand side vanishes and the general solution is a linear combination of $\cos x$ and $\sin x$. We may write

$$y = \begin{cases} A\cos x + B\sin x, & x < 0 \\ C\cos x + D\sin x, & x > 0 \end{cases}$$

Since the general solution of a second-order ODE should contain only two arbitrary constants, it must be possible to relate $C$ and $D$ to $A$ and $B$.

What is the nature of the non-smoothness in $y$? It can be helpful to think of a sequence of functions related by differentiation:

$y$ must be of the same class as $xH(x)$: it is continuous but has a jump in its first derivative. The size of the jump can be found by integrating equation (1) from $x = -\epsilon$ to $x = \epsilon$ and letting $\epsilon \to 0$:

$$\left[\frac{\mathrm{d}y}{\mathrm{d}x}\right] \equiv \lim_{\epsilon \to 0} \left[\frac{\mathrm{d}y}{\mathrm{d}x}\right]_{x=-\epsilon}^{x=\epsilon} = 1$$

Since $y$ is bounded it makes no contribution under this procedure. Since $y$ is continuous, the jump conditions are

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

Applying these, we obtain

$$C - A = 0$$

$$D - B = 1$$

and so the general solution is

$$y = \begin{cases} A\cos x + B\sin x, & x < 0 \\ A\cos x + (B+1)\sin x, & x > 0 \end{cases}$$

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

## 3.5 Inhomogeneous linear second-order ODEs

### 3.5.1 Complementary functions and particular integral

The general linear second-order ODE with constant coefficients has the form

$$y''(x) + py'(x) + qy(x) = f(x) \qquad \text{or} \qquad Ly = f$$

where $L$ is a linear operator such that $Ly = y'' + py' + qy$.

The equation is *homogeneous* (unforced) if $f = 0$, otherwise it is *inhomogeneous* (forced).

The principle of superposition applies to linear ODEs as to all linear equations.

Suppose that $y_1(x)$ and $y_2(x)$ are linearly independent solutions of the homogeneous equation, i.e. $Ly_1 = Ly_2 = 0$ and $y_2$ is not simply a constant multiple of $y_1$. Then the general solution of the homogeneous equation is $Ay_1 + By_2$.

If $y_p(x)$ is *any* solution of the inhomogeneous equation, i.e. $Ly_p = f$, then the general solution of the inhomogeneous equation is

$$y = Ay_1 + By_2 + y_p$$

Here $y_1$ and $y_2$ are known as *complementary functions* and $y_p$ as a *particular integral*.

### 3.5.2 Initial-value and boundary-value problems

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

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

$$\alpha_1 y'(a) + \alpha_2 y(a) = \alpha_3$$

where $\alpha_1, \alpha_2, \alpha_3$ are constants and $\alpha_1, \alpha_2$ are not both zero. If $\alpha_3 = 0$ the BC is *homogeneous*.

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

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

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

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

### 3.5.3 Green's function for an initial-value problem

Suppose we want to solve the inhomogeneous ODE

$$y''(x) + py'(x) + qy(x) = f(x) \quad \text{for } x \geqslant 0 \tag{1}$$

subject to the homogeneous BCs

$$y(0) = y'(0) = 0 \tag{2}$$

Green's function $G(x, \xi)$ for this problem is the solution of

$$\boxed{\frac{\partial^2 G}{\partial x^2} + p\frac{\partial G}{\partial x} + qG = \delta(x - \xi)} \tag{3}$$

subject to the homogeneous BCs

$$G(0, \xi) = \frac{\partial G}{\partial x}(0, \xi) = 0 \tag{4}$$

Notes:

- $G(x, \xi)$ is defined for $x \geqslant 0$ and $\xi \geqslant 0$

- $G(x, \xi)$ satisfies the same equation and boundary conditions with respect to $x$ as $y$ does

- however, it is the *response to forcing that is localized at a point* $x = \xi$, rather than a distributed forcing $f(x)$

If Green's function can be found, the solution of equation (1) is then

$$\boxed{y(x) = \int_0^\infty G(x, \xi) f(\xi) \, \mathrm{d}\xi} \tag{5}$$

To verify this, let $L$ be the differential operator

$$L = \frac{\partial^2}{\partial x^2} + p \frac{\partial}{\partial x} + q$$

Then equations (1) and (3) read $Ly = f$ and $LG = \delta(x - \xi)$ respectively. Applying $L$ to equation (5) gives

$$Ly(x) = \int_0^\infty LG \, f(\xi) \, \mathrm{d}\xi = \int_0^\infty \delta(x - \xi) f(\xi) \, \mathrm{d}\xi = f(x)$$

as required. It also follows from equation (4) that $y$ satisfies the boundary conditions (2) as required.

The meaning of equation (5) is that the response to distributed forcing (i.e. the solution of $Ly = f$) is obtained by summing the responses to forcing at individual points, weighted by the force distribution. This works because the ODE is linear and the BCs are homogeneous.

To find Green's function, note that equation (3) is just an ODE involving a delta function, in which $\xi$ appears as a parameter. To satisfy this equation, $G$ must be continuous but have a discontinuous first derivative. The jump conditions can be found by integrating equation (3) from $x = \xi - \epsilon$ to $x = \xi + \epsilon$ and letting $\epsilon \to 0$:

$$\left[ \frac{\partial G}{\partial x} \right] \equiv \lim_{\epsilon \to 0} \left[ \frac{\partial G}{\partial x} \right]_{x = \xi - \epsilon}^{x = \xi + \epsilon} = 1$$

Since $p \, \partial G / \partial x$ and $qG$ are bounded they make no contribution under this procedure. Since $G$ is continuous, the jump conditions are

$$[G] = 0, \qquad \left[ \frac{\partial G}{\partial x} \right] = 1 \qquad \text{at } x = \xi \tag{6}$$

Suppose that two complementary functions $y_1, y_2$ are known. The *Wronskian* $W(x)$ of two solutions $y_1(x)$ and $y_2(x)$ of a second-order ODE is the determinant of the Wronskian matrix:

$$\boxed{W[y_1, y_2] = \begin{vmatrix} y_1 & y_2 \\ y_1' & y_2' \end{vmatrix} = y_1 y_2' - y_2 y_1'}$$

The Wronskian is non-zero unless $y_1$ and $y_2$ are linearly dependent (one is a constant multiple of the other).

Since the right-hand side of equation (3) vanishes for $x < \xi$ and $x > \xi$ separately, the solution must be of the form

$$G(x, \xi) = \begin{cases} A(\xi) y_1(x) + B(\xi) y_2(x), & 0 \leqslant x < \xi \\ C(\xi) y_1(x) + D(\xi) y_2(x), & x > \xi \end{cases}$$

To determine $A, B, C, D$ we apply the boundary conditions (4) and the jump conditions (6).

Boundary conditions at $x = 0$:

$$A(\xi) y_1(0) + B(\xi) y_2(0) = 0$$

$$A(\xi) y_1'(0) + B(\xi) y_2'(0) = 0$$

In matrix form:

$$\begin{bmatrix} y_1(0) & y_2(0) \\ y_1'(0) & y_2'(0) \end{bmatrix} \begin{bmatrix} A(\xi) \\ B(\xi) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Since the determinant $W(0)$ of the matrix is non-zero the only solution is $A(\xi) = B(\xi) = 0$.

Jump conditions at $x = \xi$:

$$C(\xi)y_1(\xi) + D(\xi)y_2(\xi) = 0$$

$$C(\xi)y_1'(\xi) + D(\xi)y_2'(\xi) = 1$$

In matrix form:

$$\begin{bmatrix} y_1(\xi) & y_2(\xi) \\ y_1'(\xi) & y_2'(\xi) \end{bmatrix} \begin{bmatrix} C(\xi) \\ D(\xi) \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Solution:

$$\begin{bmatrix} C(\xi) \\ D(\xi) \end{bmatrix} = \frac{1}{W(\xi)} \begin{bmatrix} y_2'(\xi) & -y_2(\xi) \\ -y_1'(\xi) & y_1(\xi) \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -y_2(\xi)/W(\xi) \\ y_1(\xi)/W(\xi) \end{bmatrix}$$

Green's function is therefore

$$G(x, \xi) = \begin{cases} 0, & 0 \leqslant x \leqslant \xi \\ \frac{y_1(\xi)y_2(x) - y_1(x)y_2(\xi)}{W(\xi)}, & x \geqslant \xi \end{cases}$$

### 3.5.4   Green's function for a boundary-value problem

We now consider a similar equation

$$Ly = f$$

for $a \leqslant x \leqslant b$, subject to the two-point homogeneous BCs

$$\alpha_1 y'(a) + \alpha_2 y(a) = 0 \tag{1}$$

$$\beta_1 y'(b) + \beta_2 y(b) = 0 \tag{2}$$

Green's function $G(x, \xi)$ for this problem is the solution of

$$LG = \delta(x - \xi) \tag{3}$$

subject to the homogeneous BCs

$$\alpha_1 \frac{\partial G}{\partial x}(a, \xi) + \alpha_2 G(a, \xi) = 0 \tag{4}$$

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$$\beta_1 \frac{\partial G}{\partial x}(b, \xi) + \beta_2 G(b, \xi) = 0 \tag{5}$$

and is defined for $a \leqslant x \leqslant b$ and $a \leqslant \xi \leqslant b$.

By a similar argument, the solution of $Ly = f$ subject to the BCs (1) and (2) is then

$$\boxed{y(x) = \int_a^b G(x, \xi) f(\xi) \, d\xi}$$

We find Green's function by a similar method. Let $y_a(x)$ be a complementary function satisfying the left-hand BC (1), and let $y_b(x)$ be a complementary function satisfying the right-hand BC (2). (These can always be found.) Since the right-hand side of equation (3) vanishes for $x < \xi$ and $x > \xi$ separately, the solution must be of the form

$$G(x, \xi) = \begin{cases} A(\xi)y_a(x), & a \leqslant x < \xi \\ B(\xi)y_b(x), & \xi < x \leqslant b \end{cases}$$

satisfying the BCs (4) and (5). To determine $A, B$ we apply the jump conditions $[G] = 0$ and $[\partial G/\partial x] = 1$ at $x = \xi$:

$$B(\xi)y_b(\xi) - A(\xi)y_a(\xi) = 0$$

$$B(\xi)y_b'(\xi) - A(\xi)y_a'(\xi) = 1$$

In matrix form:

$$\begin{bmatrix} y_a(\xi) & y_b(\xi) \\ y_a'(\xi) & y_b'(\xi) \end{bmatrix} \begin{bmatrix} -A(\xi) \\ B(\xi) \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Solution:

$$\begin{bmatrix} -A(\xi) \\ B(\xi) \end{bmatrix} = \frac{1}{W(\xi)} \begin{bmatrix} y_b'(\xi) & -y_b(\xi) \\ -y_a'(\xi) & y_a(\xi) \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -y_b(\xi)/W(\xi) \\ y_a(\xi)/W(\xi) \end{bmatrix}$$

Green's function is therefore

$$G(x, \xi) = \begin{cases} \frac{y_a(x)y_b(\xi)}{W(\xi)}, & a \leqslant x \leqslant \xi \\ \frac{y_a(\xi)y_b(x)}{W(\xi)}, & \xi \leqslant x \leqslant b \end{cases}$$

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This method fails if the Wronskian $W[y_a, y_b]$ vanishes. This happens if $y_a$ is proportional to $y_b$, i.e. if there is a complementary function that happens to satisfy both homogeneous BCs. In this (exceptional) case the equation $Ly = f$ may not have a solution satisfying the BCs; if it does, the solution will not be unique.

### 3.5.5  Examples of Green's function

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Find Green's function for the initial-value problem*

$$y''(x) + y(x) = f(x), \qquad y(0) = y'(0) = 0$$

Complementary functions $y_1 = \cos x$, $y_2 = \sin x$.

Wronskian

$$W = y_1 y_2' - y_2 y_1' = \cos^2 x + \sin^2 x = 1$$

Now

$$y_1(\xi) y_2(x) - y_1(x) y_2(\xi) = \cos \xi \sin x - \cos x \sin \xi = \sin(x - \xi)$$

Thus

$$G(x, \xi) = \begin{cases} 0, & 0 \leqslant x \leqslant \xi \\ \sin(x - \xi), & x \geqslant \xi \end{cases}$$

So

$$y(x) = \int_0^x \sin(x - \xi) f(\xi) \, d\xi$$

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*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Find Green's function for the two-point boundary-value problem*

$$y''(x) + y(x) = f(x), \qquad y(0) = y(1) = 0$$

Complementary functions $y_a = \sin x$, $y_b = \sin(x - 1)$ satisfying left and right BCs respectively.

Wronskian

$$W = y_a y_b' - y_b y_a' = \sin x \cos(x - 1) - \sin(x - 1) \cos x = \sin 1$$

Thus

$$G(x, \xi) = \begin{cases} \sin x \sin(\xi - 1) / \sin 1, & 0 \leqslant x \leqslant \xi \\ \sin \xi \sin(x - 1) / \sin 1, & \xi \leqslant x \leqslant 1 \end{cases}$$

So

$$y(x) = \int_0^1 G(x, \xi) f(\xi) \, d\xi$$

$$= \frac{\sin(x - 1)}{\sin 1} \int_0^x \sin \xi \, f(\xi) \, d\xi + \frac{\sin x}{\sin 1} \int_x^1 \sin(\xi - 1) f(\xi) \, d\xi$$

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# 4 The Fourier transform

## 4.1 Motivation

A periodic signal can be analysed into its harmonic components by calculating its Fourier series. If the period is $P$, then the harmonics have frequencies $n/P$ where $n$ is an integer.

The Fourier transform generalizes this idea to functions that are not periodic. The 'harmonics' can then have any frequency.

The Fourier transform provides a complementary way of looking at a function. Certain operations on a function are more easily computed 'in the Fourier domain'. This idea is particularly useful in solving certain kinds of differential equation.

Furthermore, the Fourier transform has innumerable applications in diverse fields such as astronomy, optics, signal processing, data analysis, statistics and number theory.

## 4.2 Relation to Fourier series

A function $f(x)$ has period $P$ if $f(x + P) = f(x)$ for all $x$. It can then be written as a *Fourier series*

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos(k_n x) + \sum_{n=1}^{\infty} b_n \sin(k_n x)$$

where

$$k_n = \frac{2\pi n}{P}$$

is the wavenumber of the $n$th harmonic.

Such a series is also used to write any function that is defined only on an interval of length $P$, e.g. $-P/2 < x < P/2$. The Fourier series gives the extension of the function by periodic repetition.

The Fourier coefficients are found from

$$a_n = \frac{2}{P} \int_{-P/2}^{P/2} f(x) \cos(k_n x) \, dx$$

$$b_n = \frac{2}{P} \int_{-P/2}^{P/2} f(x) \sin(k_n x) \, dx$$

Define

$$c_n = \begin{cases} (a_{-n} + \mathrm{i}b_{-n})/2, & n < 0 \\ a_0/2, & n = 0 \\ (a_n - \mathrm{i}b_n)/2, & n > 0 \end{cases}$$

Then the same result can be expressed more simply and compactly in the notation of the *complex Fourier series*

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \, \mathrm{e}^{\mathrm{i}k_n x}$$

$$c_n = \frac{1}{P} \int_{-P/2}^{P/2} f(x) \, \mathrm{e}^{-\mathrm{i}k_n x} \, \mathrm{d}x$$

This expression for $c_n$ can be verified using the *orthogonality relation*

$$\frac{1}{P} \int_{-P/2}^{P/2} \mathrm{e}^{\mathrm{i}(k_n - k_m)x} \, \mathrm{d}x = \delta_{mn}$$

which follows from an elementary integration.

To approach the Fourier transform, let $P \to \infty$ so that the function is defined on the entire real line without any periodicity. The wavenumbers $k_n$ are replaced by a continuous variable $k$. We define

$$\tilde{f}(k) = \int_{-\infty}^{\infty} f(x) \, \mathrm{e}^{-\mathrm{i}kx} \, \mathrm{d}x$$

corresponding to $P c_n$. The Fourier sum becomes an integral

$$f(x) = \int_{-\infty}^{\infty} \frac{1}{P} \tilde{f}(k) \, \mathrm{e}^{\mathrm{i}kx} \, \frac{\mathrm{d}n}{\mathrm{d}k_n} \, \mathrm{d}k$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(k) \, \mathrm{e}^{\mathrm{i}kx} \, \mathrm{d}k$$

We therefore have the *forward Fourier transform* (Fourier analysis)

$$\boxed{\tilde{f}(k) = \int_{-\infty}^{\infty} f(x) \, \mathrm{e}^{-\mathrm{i}kx} \, \mathrm{d}x}$$

and the *inverse Fourier transform* (Fourier synthesis)

$$\boxed{f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(k) \, \mathrm{e}^{\mathrm{i}kx} \, \mathrm{d}k}$$

Notes:

- the Fourier transform operation is sometimes denoted by

$$\tilde{f}(k) = \mathcal{F}[f(x)], \qquad f(x) = \mathcal{F}^{-1}[\tilde{f}(k)]$$

- the variables are often called $t$ and $\omega$ rather than $x$ and $k$

- it is sometimes useful to consider complex values of $k$

- for a rigorous proof, certain technical conditions on $f(x)$ are required

A necessary condition for $\tilde{f}(k)$ to exist for all real values of $k$ (in the sense of an ordinary function) is that $f(x) \to 0$ as $x \to \pm\infty$. Otherwise the Fourier integral does not converge (e.g. for $k = 0$).

A set of sufficient conditions for $\tilde{f}(k)$ to exist is that $f(x)$ have 'bounded variation', have a finite number of discontinuities and be 'absolutely integrable', i.e.

$$\int_{-\infty}^{\infty} |f(x)| \, \mathrm{d}x < \infty.$$

However, we will see that Fourier transforms can be assigned in a wider sense to some functions that do not satisfy all of these conditions, e.g. $f(x) = 1$.

**Warning.** *Several different definitions of the Fourier transform are in use. They differ in the placement of the $2\pi$ factor and in the signs of the exponents. The definition used here is probably the most common.*

How to remember this definition:

- the sign of the exponent is different in the forward and inverse transforms

- the inverse transform means that the function $f(x)$ is synthesized from a linear combination of basis functions $\mathrm{e}^{\mathrm{i}kx}$

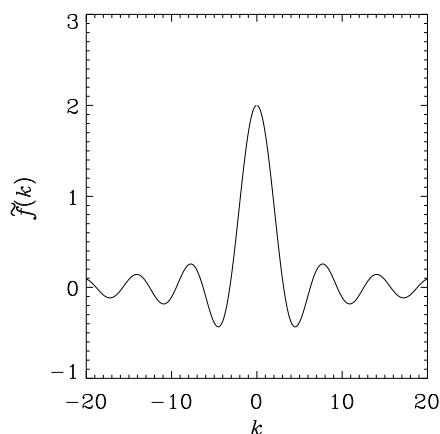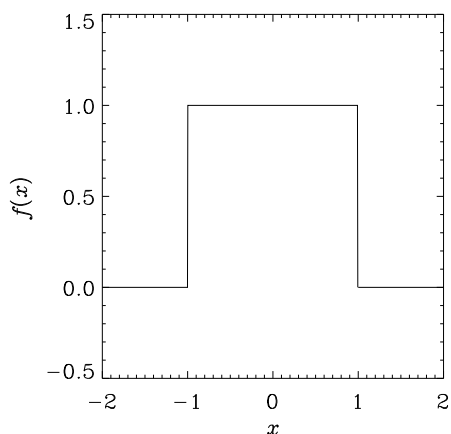- the division by $2\pi$ always accompanies an integration with respect to $k$

## 4.3 Examples

Example (1): top-hat function:

$$f(x) = \begin{cases} c, & a < x < b \\ 0, & \text{otherwise} \end{cases}$$

$$\tilde{f}(k) = \int_a^b c\,\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x = \frac{\mathrm{i}c}{k}\left(\mathrm{e}^{-\mathrm{i}kb} - \mathrm{e}^{-\mathrm{i}ka}\right)$$

e.g. if $a = -1$, $b = 1$ and $c = 1$:

$$\tilde{f}(k) = \frac{\mathrm{i}}{k}\left(\mathrm{e}^{-\mathrm{i}k} - \mathrm{e}^{\mathrm{i}k}\right) = \frac{2\sin k}{k}$$



Example (2):

$$f(x) = \mathrm{e}^{-|x|}$$

$$\tilde{f}(k) = \int_{-\infty}^{0} \mathrm{e}^{x}\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x + \int_{0}^{\infty} \mathrm{e}^{-x}\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x$$

$$= \frac{1}{1 - \mathrm{i}k}\left[\mathrm{e}^{(1-\mathrm{i}k)x}\right]_{-\infty}^{0} - \frac{1}{1 + \mathrm{i}k}\left[\mathrm{e}^{-(1+\mathrm{i}k)x}\right]_{0}^{\infty}$$

$$= \frac{1}{1 - \mathrm{i}k} + \frac{1}{1 + \mathrm{i}k}$$

$$= \frac{2}{1 + k^2}$$
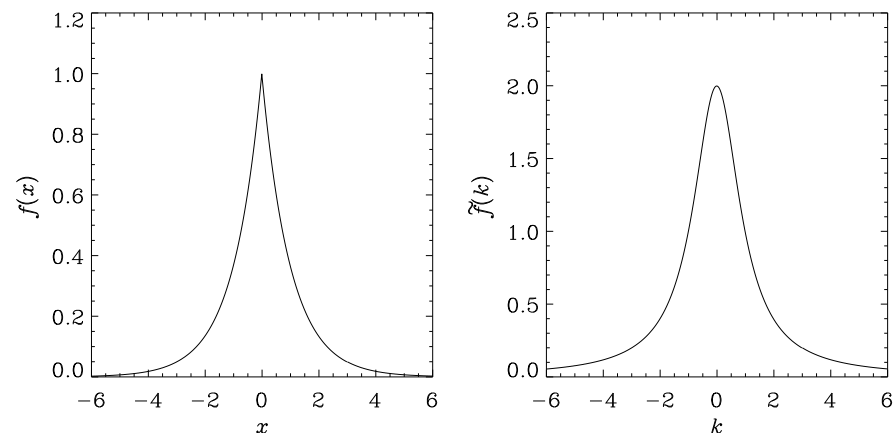


Example (3): Gaussian function (normal distribution):

$$f(x) = (2\pi\sigma_x^2)^{-1/2}\exp\left(-\frac{x^2}{2\sigma_x^2}\right)$$

$$\tilde{f}(k) = (2\pi\sigma_x^2)^{-1/2}\int_{-\infty}^{\infty}\exp\left(-\frac{x^2}{2\sigma_x^2} - \mathrm{i}kx\right)\,\mathrm{d}x$$

Change variable to

$$z = \frac{x}{\sigma_x} + \mathrm{i}\sigma_x k$$

so that

$$-\frac{z^2}{2} = -\frac{x^2}{2\sigma_x^2} - \mathrm{i}kx + \frac{\sigma_x^2 k^2}{2}$$

Then

$$\tilde{f}(k) = (2\pi\sigma_x^2)^{-1/2}\int_{-\infty}^{\infty}\exp\left(-\frac{z^2}{2}\right)\,\mathrm{d}z\,\sigma_x\exp\left(-\frac{\sigma_x^2 k^2}{2}\right)$$

$$= \exp\left(-\frac{\sigma_x^2 k^2}{2}\right)$$
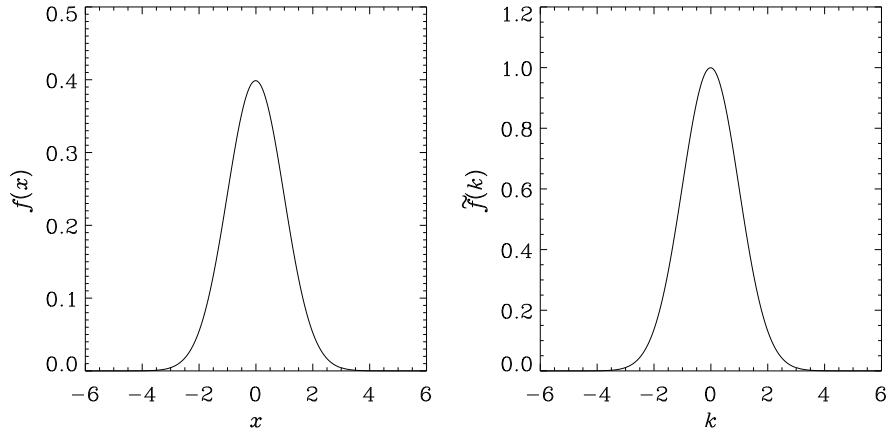
where we use the standard Gaussian integral

$$\int_{-\infty}^{\infty} \exp\left(-\frac{z^2}{2}\right) \, \mathrm{d}z = (2\pi)^{1/2}$$

Actually there is a slight cheat here because $z$ has an imaginary part. This will be explained next term.

The result is proportional to a standard Gaussian function of $k$:

$$\tilde{f}(k) \propto (2\pi\sigma_k^2)^{-1/2} \exp\left(-\frac{k^2}{2\sigma_k^2}\right)$$

of width (standard deviation) $\sigma_k$ related to $\sigma_x$ by

$$\sigma_x \sigma_k = 1$$

This illustrates a property of the Fourier transform: the narrower the function of $x$, the wider the function of $k$.

## 4.4  Basic properties of the Fourier transform

Linearity:

$$g(x) = \alpha f(x) \qquad \Leftrightarrow \qquad \tilde{g}(k) = \alpha \tilde{f}(k) \qquad (1)$$
$$h(x) = f(x) + g(x) \qquad \Leftrightarrow \qquad \tilde{h}(k) = \tilde{f}(k) + \tilde{g}(k) \qquad (2)$$

Rescaling (for real $\alpha$):

$$g(x) = f(\alpha x) \qquad \Leftrightarrow \qquad \tilde{g}(k) = \frac{1}{|\alpha|}\tilde{f}\left(\frac{k}{\alpha}\right) \qquad (3)$$

Shift/exponential (for real $\alpha$):

$$g(x) = f(x - \alpha) \qquad \Leftrightarrow \qquad \tilde{g}(k) = \mathrm{e}^{-\mathrm{i}k\alpha}\tilde{f}(k) \qquad (4)$$
$$g(x) = \mathrm{e}^{\mathrm{i}\alpha x} f(x) \qquad \Leftrightarrow \qquad \tilde{g}(k) = \tilde{f}(k - \alpha) \qquad (5)$$

Differentiation/multiplication:

$$g(x) = f'(x) \qquad \Leftrightarrow \qquad \tilde{g}(k) = \mathrm{i}k\tilde{f}(k) \qquad (6)$$
$$g(x) = xf(x) \qquad \Leftrightarrow \qquad \tilde{g}(k) = \mathrm{i}\tilde{f}'(k) \qquad (7)$$

Duality:

$$g(x) = \tilde{f}(x) \qquad \Leftrightarrow \qquad \tilde{g}(k) = 2\pi f(-k) \qquad (8)$$
i.e. transforming twice returns (almost) the same function

Complex conjugation and parity inversion (for real $x$ and $k$):
$$g(x) = [f(x)]^* \qquad \Leftrightarrow \qquad \tilde{g}(k) = [\tilde{f}(-k)]^* \qquad (9)$$

Symmetry:

$$f(-x) = \pm f(x) \qquad \Leftrightarrow \qquad \tilde{f}(-k) = \pm\tilde{f}(k) \qquad (10)$$

Sample derivations: property (3):

$$g(x) = f(\alpha x)$$

$$\tilde{g}(k) = \int_{-\infty}^{\infty} f(\alpha x)\, \mathrm{e}^{-\mathrm{i}kx}\, \mathrm{d}x$$

$$= \mathrm{sgn}(\alpha) \int_{-\infty}^{\infty} f(y)\, \mathrm{e}^{-\mathrm{i}ky/\alpha}\, \frac{\mathrm{d}y}{\alpha}$$

$$= \frac{1}{|\alpha|} \int_{-\infty}^{\infty} f(y)\, \mathrm{e}^{-\mathrm{i}(k/\alpha)y}\, \mathrm{d}y$$

$$= \frac{1}{|\alpha|} \tilde{f}\left(\frac{k}{\alpha}\right)$$

Property (4):

$$g(x) = f(x - \alpha)$$

$$\tilde{g}(k) = \int_{-\infty}^{\infty} f(x - \alpha)\, \mathrm{e}^{-\mathrm{i}kx}\, \mathrm{d}x$$

$$= \int_{-\infty}^{\infty} f(y)\, \mathrm{e}^{-\mathrm{i}k(y+\alpha)}\, \mathrm{d}y$$

$$= \mathrm{e}^{-\mathrm{i}k\alpha} \tilde{f}(k)$$

Property (6):

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

$$\tilde{g}(k) = \int_{-\infty}^{\infty} f'(x)\, \mathrm{e}^{-\mathrm{i}kx}\, \mathrm{d}x$$

$$= \left[ f(x)\, \mathrm{e}^{-\mathrm{i}kx} \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f(x)(-\mathrm{i}k)\mathrm{e}^{-\mathrm{i}kx}\, \mathrm{d}x$$

$$= \mathrm{i}k\, \tilde{f}(k)$$

The integrated part vanishes because $f(x)$ must tend to zero as $x \to \pm\infty$ in order to possess a Fourier transform.

Property (7):

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

$$\tilde{g}(k) = \int_{-\infty}^{\infty} x f(x)\, \mathrm{e}^{-\mathrm{i}kx}\, \mathrm{d}x$$

$$= \mathrm{i} \int_{-\infty}^{\infty} f(x)(-\mathrm{i}x)\mathrm{e}^{-\mathrm{i}kx}\, \mathrm{d}x$$

$$= \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}k} \int_{-\infty}^{\infty} f(x)\, \mathrm{e}^{-\mathrm{i}kx}\, \mathrm{d}x$$

$$= \mathrm{i}\tilde{f}'(k)$$

Property (8):

$$g(x) = \tilde{f}(x)$$

$$\tilde{g}(k) = \int_{-\infty}^{\infty} \tilde{f}(x)\, \mathrm{e}^{-\mathrm{i}kx}\, \mathrm{d}x$$

$$= 2\pi f(-k)$$

Property (10): if $f(-x) = \pm f(x)$, i.e. $f$ is even or odd, then

$$\tilde{f}(-k) = \int_{-\infty}^{\infty} f(x)\, \mathrm{e}^{+\mathrm{i}kx}\, \mathrm{d}x$$

$$= \int_{-\infty}^{\infty} \pm f(-x)\, \mathrm{e}^{\mathrm{i}kx}\, \mathrm{d}x$$

$$= \pm \int_{-\infty}^{\infty} f(y)\, \mathrm{e}^{-\mathrm{i}ky}\, \mathrm{d}y$$

$$= \pm \tilde{f}(k)$$

## 4.5 The delta function and the Fourier transform

Consider the Gaussian function of example (3):

$$f(x) = (2\pi\sigma_x^2)^{-1/2} \exp\left(-\frac{x^2}{2\sigma_x^2}\right)$$

$$\tilde{f}(k) = \exp\left(-\frac{\sigma_x^2 k^2}{2}\right)$$

The Gaussian is normalized such that

$$\int_{-\infty}^{\infty} f(x)\,\mathrm{d}x = 1$$

As the width $\sigma_x$ tends to zero, the Gaussian becomes taller and narrower, but the area under the curve remains the same. The value of $f(x)$ tends to zero for any non-zero value of $x$. At the same time, the value of $\tilde{f}(k)$ tends to unity for any finite value of $k$.
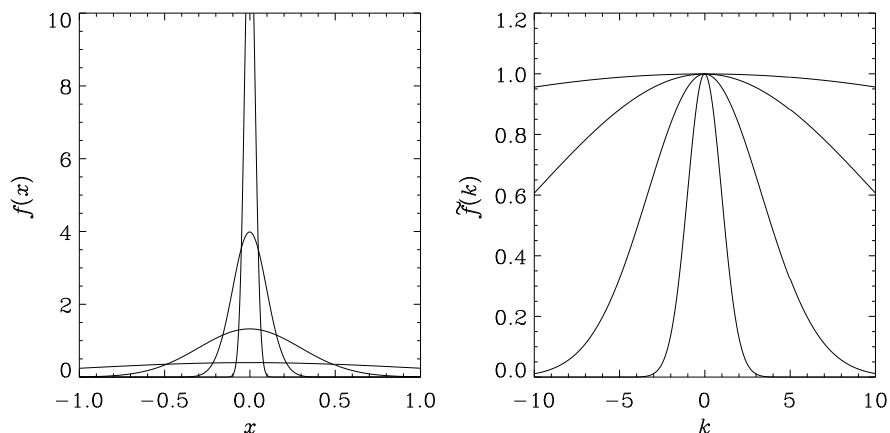


In this limit we approach the Dirac delta function, $\delta(x)$.

The substitution property allows us to verify the Fourier transform of the delta function:

$$\tilde{\delta}(k) = \int_{-\infty}^{\infty} \delta(x)\,\mathrm{e}^{-ikx}\,\mathrm{d}x = \mathrm{e}^{-ik0} = 1$$

Now formally apply the inverse transform:

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} 1\,\mathrm{e}^{ikx}\,\mathrm{d}k$$

Relabel the variables and rearrange (the exponent can have either sign):

$$\boxed{\int_{-\infty}^{\infty} \mathrm{e}^{\pm ikx}\,\mathrm{d}x = 2\pi\delta(k)}$$

Therefore the Fourier transform of a unit constant (1) is $2\pi\delta(k)$. Note that a constant function does not satisfy the necessary condition for the existence of a (regular) Fourier transform. But it does have a Fourier transform in the space of generalized functions.

## 4.6 The convolution theorem

### 4.6.1 Definition of convolution

The *convolution* of two functions, $h = f * g$, is defined by

$$h(x) = \int_{-\infty}^{\infty} f(y)g(x-y)\,\mathrm{d}y$$

Note that the sum of the arguments of $f$ and $g$ is the argument of $h$. Convolution is a symmetric operation:

$$[g * f](x) = \int_{-\infty}^{\infty} g(y)f(x-y)\,\mathrm{d}y$$

$$= \int_{-\infty}^{\infty} f(z)g(x-z)\,\mathrm{d}z$$

$$= [f * g](x)$$

### 4.6.2 Interpretation and examples

In statistics, a continuous random variable $x$ (e.g. the height of a person drawn at random from the population) has a *probability distribution* (or *density*) *function* $f(x)$. The probability of $x$ lying in the range $x_0 < x < x_0 + \delta x$ is $f(x_0)\delta x$, in the limit of small $\delta x$.

If $x$ and $y$ are independent random variables with distribution functions $f(x)$ and $g(y)$, then let the distribution function of their sum, $z = x+y$, be $h(z)$.

Now, for any given value of $x$, the probability that $z$ lies in the range

$$z_0 < z < z_0 + \delta z$$

is just the probability that $y$ lies in the range

$$z_0 - x < y < z_0 - x + \delta z$$

which is $g(z_0 - x)\delta z$. Therefore

$$h(z_0)\delta z = \int_{-\infty}^{\infty} f(x)g(z_0 - x)\delta z \, dx$$

which implies

$$h = f * g$$

The effect of measuring, observing or processing scientific data can often be described as a convolution of the data with a certain function.

e.g. when a point source is observed by a telescope, a broadened image is seen, known as the *point spread function* of the telescope. When an extended source is observed, the image that is seen is the convolution of the source with the point spread function.

In this sense convolution corresponds to a broadening or distortion of the original data.

A point mass $M$ at position $\boldsymbol{R}$ gives rise to a gravitational potential $\Phi(\boldsymbol{r}) = -GM/|\boldsymbol{r} - \boldsymbol{R}|$. A continuous mass density $\rho(\boldsymbol{r})$ can be thought of as a sum of infinitely many point masses $\rho(\boldsymbol{R})\,d^3\boldsymbol{R}$ at positions $\boldsymbol{R}$. The resulting gravitational potential is

$$\Phi(\boldsymbol{r}) = -G \int \frac{\rho(\boldsymbol{R})}{|\boldsymbol{r} - \boldsymbol{R}|}\,d^3\boldsymbol{R}$$

which is the (3D) convolution of the mass density $\rho(\boldsymbol{r})$ with the potential of a unit point charge at the origin, $-G/|\boldsymbol{r}|$.

### 4.6.3 The convolution theorem

The Fourier transform of a convolution is

$$\begin{aligned}
\tilde{h}(k) &= \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} f(y)g(x - y)\,dy \right] e^{-ikx}\,dx \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(y)g(x - y)\,e^{-ikx}\,dx\,dy \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(y)g(z)\,e^{-iky}\,e^{-ikz}\,dz\,dy \qquad (z = x - y) \\
&= \int_{-\infty}^{\infty} f(y)\,e^{-iky}\,dy \int_{-\infty}^{\infty} g(z)\,e^{-ikz}\,dz \\
&= \tilde{f}(k)\tilde{g}(k)
\end{aligned}$$

Similarly, the Fourier transform of $f(x)g(x)$ is $\frac{1}{2\pi}[\tilde{f} * \tilde{g}](k)$.

This means that:

- convolution is an operation best carried out as a multiplication in the Fourier domain

- the Fourier transform of a product is a complicated object

- convolution can be undone (*deconvolution*) by a division in the Fourier domain. If $g$ is known and $f * g$ is measured, then $f$ can be obtained, in principle.

### 4.6.4 Correlation

The *correlation* of two functions, $h = f \otimes g$, is defined by

$$h(x) = \int_{-\infty}^{\infty} [f(y)]^* g(x+y) \, \mathrm{d}y$$

Now the argument of $h$ is the shift between the arguments of $f$ and $g$.

Correlation is a way of quantifying the relationship between two (typically oscillatory) functions. If two signals (oscillating about an average value of zero) oscillate in phase with each other, their correlation will be positive. If they are out of phase, the correlation will be negative. If they are completely unrelated, their correlation will be zero.

The Fourier transform of a correlation is

$$\tilde{h}(k) = \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} [f(y)]^* g(x+y) \, \mathrm{d}y \right] \mathrm{e}^{-\mathrm{i}kx} \, \mathrm{d}x$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [f(y)]^* g(x+y) \, \mathrm{e}^{-\mathrm{i}kx} \, \mathrm{d}x \, \mathrm{d}y$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [f(y)]^* g(z) \, \mathrm{e}^{\mathrm{i}ky} \, \mathrm{e}^{-\mathrm{i}kz} \, \mathrm{d}z \, \mathrm{d}y \qquad (z = x + y)$$

$$= \left[ \int_{-\infty}^{\infty} f(y) \, \mathrm{e}^{-\mathrm{i}ky} \, \mathrm{d}y \right]^* \int_{-\infty}^{\infty} g(z) \, \mathrm{e}^{-\mathrm{i}kz} \, \mathrm{d}z$$

$$= [\tilde{f}(k)]^* \tilde{g}(k)$$

This result (or the special case $g = f$) is the *Wiener–Khinchin theorem*.

The *autoconvolution* and *autocorrelation* of $f$ are $f * f$ and $f \otimes f$. Their Fourier transforms are $\tilde{f}^2$ and $|\tilde{f}|^2$, respectively.

### 4.7 Parseval's theorem

If we apply the inverse transform to the WK theorem we find

$$\int_{-\infty}^{\infty} [f(y)]^* g(x+y) \, \mathrm{d}y = \frac{1}{2\pi} \int_{-\infty}^{\infty} [\tilde{f}(k)]^* \tilde{g}(k) \, \mathrm{e}^{\mathrm{i}kx} \, \mathrm{d}k$$

Now set $x = 0$ and relabel $y \mapsto x$ to obtain *Parseval's theorem*

$$\int_{-\infty}^{\infty} [f(x)]^* g(x) \, \mathrm{d}x = \frac{1}{2\pi} \int_{-\infty}^{\infty} [\tilde{f}(k)]^* \tilde{g}(k) \, \mathrm{d}k$$

The special case used most frequently is when $g = f$:

$$\boxed{\int_{-\infty}^{\infty} |f(x)|^2 \, \mathrm{d}x = \frac{1}{2\pi} \int_{-\infty}^{\infty} |\tilde{f}(k)|^2 \, \mathrm{d}k}$$

Note that division by $2\pi$ accompanies the integration with respect to $k$.

Parseval's theorem means that the Fourier transform is a 'unitary transformation' that preserves the 'inner product' between two functions (see later!), in the same way that a rotation preserves lengths and angles.

Alternative derivation using the delta function:

$$\int_{-\infty}^{\infty} [f(x)]^* g(x) \, \mathrm{d}x$$

$$= \int_{-\infty}^{\infty} \left[ \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(k) \, \mathrm{e}^{\mathrm{i}kx} \, \mathrm{d}k \right]^* \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{g}(k') \, \mathrm{e}^{\mathrm{i}k'x} \, \mathrm{d}k' \, \mathrm{d}x$$

$$= \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [\tilde{f}(k)]^* \tilde{g}(k') \, \mathrm{e}^{\mathrm{i}(k'-k)x} \, \mathrm{d}x \, \mathrm{d}k' \, \mathrm{d}k$$

$$= \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [\tilde{f}(k)]^* \tilde{g}(k') \, 2\pi \delta(k' - k) \, \mathrm{d}k' \, \mathrm{d}k$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} [\tilde{f}(k)]^* \tilde{g}(k) \, \mathrm{d}k$$

## 4.8 Power spectra

The quantity

$$\Phi(k) = |\tilde{f}(k)|^2$$

appearing in the Wiener–Khinchin theorem and Parseval's theorem is the *(power) spectrum* or *(power) spectral density* of the function $f(x)$. The WK theorem states that the FT of the autocorrelation function is the power spectrum.

This concept is often used to quantify the spectral content (as a function of angular frequency $\omega$) of a signal $f(t)$.

The spectrum of a perfectly periodic signal consists of a series of delta functions at the principal frequency and its harmonics, if present. Its autocorrelation function does not decay as $t \to \infty$.

*White noise* is an ideal random signal with autocorrelation function proportional to $\delta(t)$: the signal is perfectly decorrelated. It therefore has a flat spectrum ($\Phi = $ constant).

Less idealized signals may have spectra that are peaked at certain frequencies but also contain a general noise component.

# 5 Matrices and linear algebra

## 5.1 Motivation

Many scientific quantities are vectors. A linear relationship between two vectors is described by a *matrix*. This could be either

- a *physical* relationship, e.g. that between the angular velocity and angular momentum vectors of a rotating body

- a relationship between the *components* of (physically) the same vector in different coordinate systems

*Linear algebra* deals with the addition and multiplication of scalars, vectors and matrices.

*Eigenvalues* and *eigenvectors* are the characteristic numbers and directions associated with matrices, which allow them to be expressed in the simplest form. The matrices that occur in scientific applications usually have special *symmetries* that impose conditions on their eigenvalues and eigenvectors.

Vectors do not necessarily live in physical space. In some applications (notably quantum mechanics) we have to deal with *complex spaces* of various dimensions.

## 5.2 Vector spaces

### 5.2.1 Abstract definition of scalars and vectors

We are used to thinking of scalars as numbers, and vectors as directed line segments. For many purposes it is useful to define scalars and vectors in a more general (and abstract) way.

*Scalars* are the elements of a *number field*, of which the most important examples are:

- **R**, the set of real numbers

- **C**, the set of complex numbers

A number field $F$:

- is a set of elements on which the operations of *addition* and *multiplication* are defined and satisfy the usual laws of arithmetic (commutative, associative and distributive)

- is *closed* under addition and multiplication

- includes *identity* elements (the numbers 0 and 1) for addition and multiplication

- includes *inverses* (negatives and reciprocals) for addition and multiplication for every element, except that 0 has no reciprocal

*Vectors* are the elements of a *vector space* (or *linear space*) defined over a number field $F$.

A vector space $V$:

- is a set of elements on which the operations of *vector addition* and *scalar multiplication* are defined and satisfy certain axioms

- is closed under these operations

- includes an identity element (the vector $\mathbf{0}$) for vector addition

We will write vectors in bold italic face (or underlined in handwriting).

Scalar multiplication means multiplying a vector $\boldsymbol{x}$ by a scalar $\alpha$ to obtain the vector $\alpha\boldsymbol{x}$. Note that $0\boldsymbol{x} = \mathbf{0}$ and $1\boldsymbol{x} = \boldsymbol{x}$.

The basic example of a vector space is $F^n$. An element of $F^n$ is a list of $n$ scalars, $(x_1, \ldots, x_n)$, where $x_i \in F$. This is called an *n-tuple*. Vector addition and scalar multiplication are defined componentwise:

$$(x_1, \ldots, x_n) + (y_1, \ldots, y_n) = (x_1 + y_1, \ldots, x_n + y_n)$$

$$\alpha(x_1, \ldots, x_n) = (\alpha x_1, \ldots, \alpha x_n)$$

Hence we have $\mathbf{R}^n$ and $\mathbf{C}^n$.

Notes:

- vector multiplication is not defined in general

- $\mathbf{R}^2$ is not quite the same as $\mathbf{C}$ because $\mathbf{C}$ has a rule for multiplication

- $\mathbf{R}^3$ is not quite the same as physical space because physical space has a rule for the distance between two points (i.e. Pythagoras's theorem, if physical space is approximated as Euclidean)

The formal axioms of number fields and vector spaces can be found in books on linear algebra.

### 5.2.2   Span and linear dependence

Let $S = \{\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_m\}$ be a subset of vectors in $V$.

A *linear combination* of $S$ is any vector of the form $\boldsymbol{e}_1 x_1 + \boldsymbol{e}_2 x_2 + \cdots + \boldsymbol{e}_m x_m$, where $x_1, x_2, \ldots, x_m$ are scalars.

The *span* of $S$ is the set of all vectors that are linear combinations of $S$. If the span of $S$ is the entire vector space $V$, then $S$ is said to span $V$.

The vectors of $S$ are said to be *linearly independent* if no non-trivial linear combination of $S$ equals zero, i.e. if

$$\boldsymbol{e}_1 x_1 + \boldsymbol{e}_2 x_2 + \cdots + \boldsymbol{e}_m x_m = \mathbf{0} \quad \text{implies} \quad x_1 = x_2 = \cdots = x_m = 0$$

If, on the other hand, the vectors are linearly dependent, then such an equation holds for some non-trivial values of the coefficients $x_1, \ldots, x_m$. Suppose that $x_k$ is one of the non-zero coefficients. Then $\boldsymbol{e}_k$ can be expressed as a linear combination of the other vectors:

$$\boldsymbol{e}_k = -\sum_{i \neq k} \boldsymbol{e}_i \frac{x_i}{x_k}$$

Linear independence therefore means that none of the vectors is a linear combination of the others.

Notes:

- if an additional vector is added to a spanning set, it remains a spanning set

- if a vector is removed from a linearly independent set, the set remains linearly independent

### 5.2.3 Basis and dimension

A *basis* for a vector space $V$ is a subset of vectors $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_n\}$ that spans $V$ and is linearly independent. The properties of bases (proved in books on linear algebra) are:

- all bases have the same number of elements, $n$, which is called the *dimension* of $V$

- any $n$ linearly independent vectors in $V$ form a basis for $V$

- any vector $\boldsymbol{x} \in V$ can written in a unique way as

$$\boldsymbol{x} = \boldsymbol{e}_1 x_1 + \cdots + \boldsymbol{e}_n x_n$$

and the scalars $x_i$ are called the *components* of $\boldsymbol{x}$ with respect to the basis $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_n\}$

Vector spaces can have *infinite* dimension, e.g. the set of functions defined on the interval $0 < x < 2\pi$ and having Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \, \mathrm{e}^{inx}$$

Here $f(x)$ is the 'vector' and $f_n$ are its 'components' with respect to the 'basis' of functions $\mathrm{e}^{inx}$. *Functional analysis* deals with such infinite-dimensional vector spaces.

### 5.2.4 Examples

▷ Example (1): three-dimensional real space, $\mathbf{R}^3$:

vectors: triples $(x, y, z)$ of real numbers

possible basis: $\{(1, 0, 0), (0, 1, 0), (0, 0, 1)\}$

$(x, y, z) = (1, 0, 0)x + (0, 1, 0)y + (0, 0, 1)z$

▷ Example (2): the complex plane, $\mathbf{C}$:

vectors: complex numbers $z$

EITHER (a) a one-dimensional vector space over $\mathbf{C}$

possible basis: $\{1\}$

$z = 1 \cdot z$

OR (b) a two-dimensional vector space over $\mathbf{R}$ (supplemented by a multiplication rule)

possible basis: $\{1, \mathrm{i}\}$

$z = 1 \cdot x + \mathrm{i} \cdot y$

▷ Example (3): real $2 \times 2$ symmetric matrices:

vectors: matrices of the form

$$\begin{bmatrix} x & y \\ y & z \end{bmatrix}, \qquad x, y, z \in \mathbf{R}$$

three-dimensional vector space over $\mathbf{R}$

possible basis:

$$\left\{ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \right\}$$

$$\begin{bmatrix} x & y \\ y & z \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} x + \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} y + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} z$$

### 5.2.5 Change of basis

The same vector has different components with respect to different bases.

Consider two bases $\{e_i\}$ and $\{e_i'\}$. Since they are bases, we can write the vectors of one set in terms of the other, using the summation convention (sum over $i$ from 1 to $n$):

$$\boxed{e_j = e_i' R_{ij}}$$

The $n \times n$ array of numbers $R_{ij}$ is the *transformation matrix* between the two bases. $R_{ij}$ is the $i$th component of the vector $e_j$ with respect to the primed basis.

The representation of a vector $x$ in the two bases is

$$x = e_j x_j = e_i' x_i'$$

where $x_i$ and $x_i'$ are the components. Thus

$$e_i' x_i' = e_j x_j = e_i' R_{ij} x_j$$

from which we deduce the transformation law for vector components:

$$\boxed{x_i' = R_{ij} x_j}$$

Note that the transformation laws for basis vectors and vector components are 'opposite' so that the vector $x$ is unchanged by the transformation.

Example: in $\mathbf{R}^3$, two bases are $\{e_i\} = \{(1,0,0),(0,1,0),(0,0,1)\}$ and $\{e_i'\} = \{(0,1,0),(0,0,1),(1,0,0)\}$. Then

$$R_{ij} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

There is no need for a basis to be either orthogonal or normalized. In fact, we have not yet defined what these terms mean.

### 5.3 Matrices

#### 5.3.1 Array viewpoint

A matrix can be regarded simply as a rectangular array of numbers:

$$\mathsf{A} = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix}$$

This viewpoint is equivalent to thinking of a vector as an $n$-tuple, or, more correctly, as either a column matrix or a row matrix:

$$\mathsf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \qquad \mathsf{x}^{\mathrm{T}} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix}$$

We will write matrices and vectors in sans serif face when adopting this viewpoint. The superscript 'T' denotes the *transpose*.

The transformation matrix $R_{ij}$ described above is an example of a square matrix $(m = n)$.

Using the suffix notation and the summation convention, the familiar rules for multiplying a matrix by a vector on the right or left are

$$\boxed{(\mathsf{Ax})_i = A_{ij} x_j} \qquad \boxed{(\mathsf{x}^{\mathrm{T}}\mathsf{A})_j = x_i A_{ij}}$$

and the rules for matrix addition and multiplication are

$$\boxed{(\mathsf{A} + \mathsf{B})_{ij} = A_{ij} + B_{ij}} \qquad \boxed{(\mathsf{AB})_{ij} = A_{ik} B_{kj}}$$

The transpose of an $m \times n$ matrix is the $n \times m$ matrix

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

### 5.3.2 Linear operators

A *linear operator* $\mathbf{A}$ on a vector space $V$ acts on elements of $V$ to produce other elements of $V$. The action of $\mathbf{A}$ on $\boldsymbol{x}$ is written $\mathbf{A}(\boldsymbol{x})$ or just $\mathbf{A}\boldsymbol{x}$. The property of linearity means:

$$\mathbf{A}(\alpha\boldsymbol{x}) = \alpha\mathbf{A}\boldsymbol{x} \qquad \text{for scalar } \alpha$$

$$\mathbf{A}(\boldsymbol{x} + \boldsymbol{y}) = \mathbf{A}\boldsymbol{x} + \mathbf{A}\boldsymbol{y}$$

Notes:

- a linear operator has an existence without reference to any basis

- the operation can be thought of as a *linear transformation* or *mapping* of the space $V$ (a simple example is a rotation of three-dimensional space)

- a more general idea, not considered here, is that a linear operator can act on vectors of one space $V$ to produce vectors of another space $V'$, possibly of a different dimension

The components of $\mathbf{A}$ with respect to a basis $\{\boldsymbol{e}_i\}$ are defined by the action of $\mathbf{A}$ on the basis vectors:

$$\mathbf{A}\boldsymbol{e}_j = \boldsymbol{e}_i A_{ij}$$

The components form a square matrix. We write $(\mathbf{A})_{ij} = A_{ij}$ and $(\boldsymbol{x})_i = x_i$.

Since $\mathbf{A}$ is a linear operator, a knowledge of its action on a basis is sufficient to determine its action on any vector $\mathbf{x}$:

$$\mathbf{A}\boldsymbol{x} = \mathbf{A}(\boldsymbol{e}_j x_j) = x_j(\mathbf{A}\boldsymbol{e}_j) = x_j(\boldsymbol{e}_i A_{ij}) = \boldsymbol{e}_i A_{ij} x_j$$

or

$$(\mathbf{A}\boldsymbol{x})_i = A_{ij} x_j$$

This corresponds to the rule for multiplying a matrix by a vector.

The sum of two linear operators is defined by

$$(\mathbf{A} + \mathbf{B})\boldsymbol{x} = \mathbf{A}\boldsymbol{x} + \mathbf{B}\boldsymbol{x} = \boldsymbol{e}_i(A_{ij} + B_{ij})x_j$$

The product, or composition, of two linear operators has the action

$$(\mathbf{A}\mathbf{B})\boldsymbol{x} = \mathbf{A}(\mathbf{B}\boldsymbol{x}) = \mathbf{A}(\boldsymbol{e}_i B_{ij} x_j) = (\mathbf{A}\boldsymbol{e}_k)B_{kj} x_j = \boldsymbol{e}_i A_{ik} B_{kj} x_j$$

The components therefore satisfy the rules of matrix addition and multiplication:

$$(\mathbf{A} + \mathbf{B})_{ij} = A_{ij} + B_{ij} \qquad (\mathbf{A}\mathbf{B})_{ij} = A_{ik} B_{kj}$$

Recall that matrix multiplication is not commutative, so $\mathbf{B}\mathbf{A} \neq \mathbf{A}\mathbf{B}$ in general.

Therefore a matrix can be thought of as the components of a linear operator with respect to a given basis, just as a column matrix or $n$-tuple can be thought of as the components of a vector with respect to a given basis.

### 5.3.3 Change of basis again

When changing basis, we wrote one set of basis vectors in terms of the other:

$$\boldsymbol{e}_j = \boldsymbol{e}'_i R_{ij}$$

We could equally have written

$$\boldsymbol{e}'_j = \boldsymbol{e}_i S_{ij}$$

where $\mathsf{S}$ is the matrix of the inverse transformation. Substituting one relation into the other (and relabelling indices where required), we obtain

$$\boldsymbol{e}'_j = \boldsymbol{e}'_k R_{ki} S_{ij}$$

$$\boldsymbol{e}_j = \boldsymbol{e}_k S_{ki} R_{ij}$$

This can only be true if

$$R_{ki} S_{ij} = S_{ki} R_{ij} = \delta_{kj}$$

or, in matrix notation,

$$\mathsf{RS} = \mathsf{SR} = 1$$

Therefore $\mathsf{R}$ and $\mathsf{S}$ are inverses: $\mathsf{R} = \mathsf{S}^{-1}$ and $\mathsf{S} = \mathsf{R}^{-1}$.

The transformation law for vector components, $x_i' = R_{ij} x_j$, can be written in matrix notation as

$$\boxed{\mathsf{x}' = \mathsf{R}\mathsf{x}}$$

with the inverse relation

$$\mathsf{x} = \mathsf{R}^{-1}\mathsf{x}'$$

How do the components of a linear operator $\mathbf{A}$ transform under a change of basis? We require, for any vector $\boldsymbol{x}$,

$$\mathbf{A}\boldsymbol{x} = \boldsymbol{e}_i A_{ij} x_j = \boldsymbol{e}_i' A_{ij}' x_j'$$

Using $\boldsymbol{e}_j = \boldsymbol{e}_i' R_{ij}$ and relabelling indices, we find

$$\boldsymbol{e}_k' R_{ki} A_{ij} x_j = \boldsymbol{e}_k' A_{kj}' x_j'$$

$$R_{ki} A_{ij} x_j = A_{kj}' x_j'$$

$$\mathsf{RA}(\mathsf{R}^{-1}\mathsf{x}') = \mathsf{A}'\mathsf{x}'$$

Since this is true for any $\mathsf{x}'$, we have

$$\boxed{\mathsf{A}' = \mathsf{RAR}^{-1}}$$

These transformation laws are consistent, e.g.

$$\mathsf{A}'\mathsf{x}' = \mathsf{RAR}^{-1}\mathsf{Rx} = \mathsf{RAx} = (\mathsf{Ax})'$$

$$\mathsf{A}'\mathsf{B}' = \mathsf{RAR}^{-1}\mathsf{RBR}^{-1} = \mathsf{RABR}^{-1} = (\mathsf{AB})'$$

## 5.4  Inner product (scalar product)

This is used to give a meaning to lengths and angles in a vector space.

### 5.4.1  Definition

An *inner product* (or *scalar product*) is a scalar function $\langle \boldsymbol{x} | \boldsymbol{y} \rangle$ of two vectors $\boldsymbol{x}$ and $\boldsymbol{y}$. Other common notations are $(\boldsymbol{x}, \boldsymbol{y})$, $\langle \boldsymbol{x}, \boldsymbol{y} \rangle$ and $\boldsymbol{x} \cdot \boldsymbol{y}$. An inner product must:

- be linear in the second argument:

$$\langle \boldsymbol{x} | \alpha \boldsymbol{y} \rangle = \alpha \langle \boldsymbol{x} | \boldsymbol{y} \rangle \qquad \text{for scalar } \alpha$$

$$\langle \boldsymbol{x} | \boldsymbol{y} + \boldsymbol{z} \rangle = \langle \boldsymbol{x} | \boldsymbol{y} \rangle + \langle \boldsymbol{x} | \boldsymbol{z} \rangle$$

- have *Hermitian symmetry*:

$$\langle \boldsymbol{y} | \boldsymbol{x} \rangle = \langle \boldsymbol{x} | \boldsymbol{y} \rangle^*$$

- be *positive definite*:

$$\langle \boldsymbol{x} | \boldsymbol{x} \rangle \geqslant 0 \qquad \text{with equality if and only if } \boldsymbol{x} = \mathbf{0}$$

Notes:

- an inner product has an existence without reference to any basis

- the star is needed to ensure that $\langle \boldsymbol{x} | \boldsymbol{x} \rangle$ is real

- the star is not needed in a real vector space

- it follows that the inner product is *antilinear* in the first argument:

$$\langle \alpha \boldsymbol{x} | \boldsymbol{y} \rangle = \alpha^* \langle \boldsymbol{x} | \boldsymbol{y} \rangle \qquad \text{for scalar } \alpha$$

$$\langle \boldsymbol{x} + \boldsymbol{y} | \boldsymbol{z} \rangle = \langle \boldsymbol{x} | \boldsymbol{z} \rangle + \langle \boldsymbol{y} | \boldsymbol{z} \rangle$$

The standard (Euclidean) inner product on $\mathbf{R}^n$ is the 'dot product'

$$\langle \boldsymbol{x} | \boldsymbol{y} \rangle = \boldsymbol{x} \cdot \boldsymbol{y} = x_i y_i$$

which is generalized to $\mathbf{C}^n$ as

$$\langle \boldsymbol{x} | \boldsymbol{y} \rangle = x_i^* y_i$$

The star is needed for Hermitian symmetry. We will see later that any other inner product on $\mathbf{R}^n$ or $\mathbf{C}^n$ can be reduced to this one by a suitable choice of basis.

$\langle \boldsymbol{x} | \boldsymbol{x} \rangle^{1/2}$ is the 'length' or 'norm' of the vector $\boldsymbol{x}$, written $|\boldsymbol{x}|$ or $\|\boldsymbol{x}\|$. In one dimension this agrees with the meaning of 'absolute value' if we are using the dot product.

### 5.4.2 The Cauchy–Schwarz inequality

$$\boxed{|\langle \boldsymbol{x} | \boldsymbol{y} \rangle|^2 \leqslant \langle \boldsymbol{x} | \boldsymbol{x} \rangle \langle \boldsymbol{y} | \boldsymbol{y} \rangle}$$

or equivalently

$$\boxed{|\langle \boldsymbol{x} | \boldsymbol{y} \rangle| \leqslant |\boldsymbol{x}||\boldsymbol{y}|}$$

with equality if and only if $\boldsymbol{x} = \alpha \boldsymbol{y}$ (i.e. the vectors are parallel or antiparallel).

Proof: We assume that $\boldsymbol{x} \neq \boldsymbol{0}$ and $\boldsymbol{y} \neq \boldsymbol{0}$, otherwise the inequality is trivial. We consider the non-negative quantity

$$
\begin{aligned}
\langle \boldsymbol{x} - \alpha \boldsymbol{y} | \boldsymbol{x} - \alpha \boldsymbol{y} \rangle &= \langle \boldsymbol{x} - \alpha \boldsymbol{y} | \boldsymbol{x} \rangle - \alpha \langle \boldsymbol{x} - \alpha \boldsymbol{y} | \boldsymbol{y} \rangle \\
&= \langle \boldsymbol{x} | \boldsymbol{x} \rangle - \alpha^* \langle \boldsymbol{y} | \boldsymbol{x} \rangle - \alpha \langle \boldsymbol{x} | \boldsymbol{y} \rangle + \alpha \alpha^* \langle \boldsymbol{y} | \boldsymbol{y} \rangle \\
&= \langle \boldsymbol{x} | \boldsymbol{x} \rangle + \alpha \alpha^* \langle \boldsymbol{y} | \boldsymbol{y} \rangle - \alpha \langle \boldsymbol{x} | \boldsymbol{y} \rangle - \alpha^* \langle \boldsymbol{x} | \boldsymbol{y} \rangle^* \\
&= |\boldsymbol{x}|^2 + |\alpha|^2 |\boldsymbol{y}|^2 - 2 \operatorname{Re}(\alpha \langle \boldsymbol{x} | \boldsymbol{y} \rangle)
\end{aligned}
$$

This result holds for any scalar $\alpha$. First choose the *phase* of $\alpha$ such that $\alpha \langle \boldsymbol{x} | \boldsymbol{y} \rangle$ is real and non-negative and therefore equal to $|\alpha||\langle \boldsymbol{x} | \boldsymbol{y} \rangle|$. Then

$$|\boldsymbol{x}|^2 + |\alpha|^2 |\boldsymbol{y}|^2 - 2|\alpha||\langle \boldsymbol{x} | \boldsymbol{y} \rangle| \geqslant 0$$

$$(|\boldsymbol{x}| - |\alpha||\boldsymbol{y}|)^2 + 2|\alpha||\boldsymbol{x}||\boldsymbol{y}| - 2|\alpha||\langle \boldsymbol{x} | \boldsymbol{y} \rangle| \geqslant 0$$

Now choose the *modulus* of $\alpha$ such that $|\alpha| = |\boldsymbol{x}|/|\boldsymbol{y}|$, which is finite and non-zero. Then divide the inequality by $2|\alpha|$ to obtain

$$|\boldsymbol{x}||\boldsymbol{y}| - |\langle \boldsymbol{x} | \boldsymbol{y} \rangle| \geqslant 0$$

as required.

In a real vector space, the Cauchy–Schwarz inequality allows us to define the angle $\theta$ between two vectors through

$$\langle \boldsymbol{x} | \boldsymbol{y} \rangle = |\boldsymbol{x}||\boldsymbol{y}| \cos \theta$$

If $\langle \boldsymbol{x} | \boldsymbol{y} \rangle = 0$ (in any vector space) the vectors are said to be *orthogonal*.

### 5.4.3 Inner product and bases

The inner product is *bilinear*: it is antilinear in the first argument and linear in the second argument.

**Warning.** *This is the usual convention in physics and applied mathematics. In pure mathematics it is usually the other way around.*

A knowledge of the inner product of the basis vectors is therefore sufficient to determine the inner product of any two vectors $\boldsymbol{x}$ and $\boldsymbol{y}$. Let

$$\langle \boldsymbol{e}_i | \boldsymbol{e}_j \rangle = G_{ij}$$

Then

$$\langle \boldsymbol{x} | \boldsymbol{y} \rangle = \langle \boldsymbol{e}_i x_i | \boldsymbol{e}_j y_j \rangle = x_i^* y_j \langle \boldsymbol{e}_i | \boldsymbol{e}_j \rangle = G_{ij} x_i^* y_j$$

The $n \times n$ array of numbers $G_{ij}$ are the *metric coefficients* of the basis $\{\boldsymbol{e}_i\}$. The Hermitian symmetry of the inner product implies that

$$G_{ij} y_i^* x_j = (G_{ij} x_i^* y_j)^* = G_{ij}^* x_i y_j^* = G_{ji}^* y_i^* x_j$$

for all vectors $\boldsymbol{x}$ and $\boldsymbol{y}$, and therefore

$$G_{ji} = G_{ij}^*$$

We say that the matrix $\mathsf{G}$ is *Hermitian*.

An *orthonormal* basis is one for which

$$\langle \boldsymbol{e}_i | \boldsymbol{e}_j \rangle = \delta_{ij}$$

in which case the inner product is the standard one

$$\langle \boldsymbol{x} | \boldsymbol{y} \rangle = x_i^* y_i$$

We will see later that it is possible to transform any basis into an orthonormal one.

## 5.5 Hermitian conjugate

### 5.5.1 Definition and simple properties

We define the *Hermitian conjugate* of a matrix to be the complex conjugate of its transpose:

$$\boxed{\mathsf{A}^\dagger = (\mathsf{A}^{\mathrm{T}})^*} \qquad \boxed{(\mathsf{A}^\dagger)_{ij} = A_{ji}^*}$$

This applies to general rectangular matrices, e.g.

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \end{bmatrix}^\dagger = \begin{bmatrix} A_{11}^* & A_{21}^* \\ A_{12}^* & A_{22}^* \\ A_{13}^* & A_{23}^* \end{bmatrix}$$

The Hermitian conjugate of a column matrix is

$$\mathsf{x}^\dagger = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}^\dagger = \begin{bmatrix} x_1^* & x_2^* & \cdots & x_n^* \end{bmatrix}$$

Note that

$$\boxed{(\mathsf{A}^\dagger)^\dagger = \mathsf{A}}$$

The Hermitian conjugate of a product of matrices is

$$\boxed{(\mathsf{AB})^\dagger = \mathsf{B}^\dagger \mathsf{A}^\dagger}$$

because

$$(\mathsf{AB})_{ij}^\dagger = (\mathsf{AB})_{ji}^* = (A_{jk}B_{ki})^* = B_{ki}^* A_{jk}^* = (\mathsf{B}^\dagger)_{ik}(\mathsf{A}^\dagger)_{kj} = (\mathsf{B}^\dagger \mathsf{A}^\dagger)_{ij}$$

Note the reversal of the order of the product, as also occurs with the transpose or inverse of a product of matrices. This result extends to arbitrary products of matrices and vectors, e.g.

$$(\mathsf{ABCx})^\dagger = \mathsf{x}^\dagger \mathsf{C}^\dagger \mathsf{B}^\dagger \mathsf{A}^\dagger$$

$$(\mathsf{x}^\dagger \mathsf{A} \mathsf{y})^\dagger = \mathsf{y}^\dagger \mathsf{A}^\dagger \mathsf{x}$$

In the latter example, if $\mathsf{x}$ and $\mathsf{y}$ are vectors, each side of the equation is a scalar (a complex number). The Hermitian conjugate of a scalar is just the complex conjugate.

### 5.5.2 Relationship with inner product

We have seen that the inner product of two vectors is

$$\langle \boldsymbol{x} | \boldsymbol{y} \rangle = G_{ij} x_i^* y_j = x_i^* G_{ij} y_j$$

where $G_{ij}$ are the metric coefficients. This can also be written

$$\langle \boldsymbol{x} | \boldsymbol{y} \rangle = \mathsf{x}^\dagger \mathsf{G} \mathsf{y}$$

and the Hermitian conjugate of this equation is

$$\langle \boldsymbol{x} | \boldsymbol{y} \rangle^* = \mathsf{y}^\dagger \mathsf{G}^\dagger \mathsf{x}$$

Similarly

$$\langle \boldsymbol{y}|\boldsymbol{x}\rangle = \mathsf{y}^\dagger \mathsf{G}\mathsf{x}$$

The Hermitian symmetry of the inner product requires $\langle \boldsymbol{y}|\boldsymbol{x}\rangle = \langle \boldsymbol{x}|\boldsymbol{y}\rangle^*$, i.e.

$$\mathsf{y}^\dagger \mathsf{G}\mathsf{x} = \mathsf{y}^\dagger \mathsf{G}^\dagger \mathsf{x}$$

which is satisfied for all vectors $\mathsf{x}$ and $\mathsf{y}$ provided that $\mathsf{G}$ is an Hermitian matrix:

$$\mathsf{G}^\dagger = \mathsf{G}$$

If the basis is orthonormal, then $G_{ij} = \delta_{ij}$ and we have simply

$$\langle \boldsymbol{x}|\boldsymbol{y}\rangle = \mathsf{x}^\dagger \mathsf{y}$$

### 5.5.3 Adjoint operator

A further relationship between the Hermitian conjugate and the inner product is as follows.

The *adjoint* of a linear operator $\mathbf{A}$ with respect to a given inner product is a linear operator $\mathbf{A}^\dagger$ satisfying

$$\langle \mathbf{A}^\dagger \boldsymbol{x}|\boldsymbol{y}\rangle = \langle \boldsymbol{x}|\mathbf{A}\boldsymbol{y}\rangle$$

for all vectors $\boldsymbol{x}$ and $\boldsymbol{y}$. With the standard inner product this implies

$$\left[ (\mathbf{A}^\dagger)_{ij} x_j \right]^* y_i = x_i^* A_{ij} y_j$$
$$(\mathbf{A}^\dagger)_{ij}^* x_j^* y_i = A_{ji} x_j^* y_i$$
$$(\mathbf{A}^\dagger)_{ij}^* = A_{ji}$$
$$(\mathbf{A}^\dagger)_{ij} = A_{ji}^*$$

The components of the operator $\mathbf{A}$ with respect to a basis are given by a square matrix $\mathsf{A}$. The components of the adjoint operator (with respect to the standard inner product) are given by the Hermitian conjugate matrix $\mathsf{A}^\dagger$.

### 5.5.4 Special square matrices

The following types of special matrices arise commonly in scientific applications.

A *symmetric* matrix is equal to its transpose:

$$\mathsf{A}^\mathrm{T} = \mathsf{A} \qquad \text{or} \qquad A_{ji} = A_{ij}$$

An *antisymmetric* (or *skew-symmetric*) matrix satisfies

$$\mathsf{A}^\mathrm{T} = -\mathsf{A} \qquad \text{or} \qquad A_{ji} = -A_{ij}$$

An *orthogonal* matrix is one whose transpose is equal to its inverse:

$$\mathsf{A}^\mathrm{T} = \mathsf{A}^{-1} \qquad \text{or} \qquad \mathsf{A}\mathsf{A}^\mathrm{T} = \mathsf{A}^\mathrm{T}\mathsf{A} = 1$$

These ideas generalize to a complex vector space as follows.

An *Hermitian* matrix is equal to its Hermitian conjugate:

$$\mathsf{A}^\dagger = \mathsf{A} \qquad \text{or} \qquad A_{ji}^* = A_{ij}$$

An *anti-Hermitian* (or *skew-Hermitian*) matrix satisfies

$$\mathsf{A}^\dagger = -\mathsf{A} \qquad \text{or} \qquad A_{ji}^* = -A_{ij}$$

A *unitary* matrix is one whose Hermitian conjugate is equal to its inverse:

$$\mathsf{A}^\dagger = \mathsf{A}^{-1} \qquad \text{or} \qquad \mathsf{A}\mathsf{A}^\dagger = \mathsf{A}^\dagger\mathsf{A} = 1$$

In addition, a *normal* matrix is one that commutes with its Hermitian conjugate:

$$\mathsf{A}\mathsf{A}^\dagger = \mathsf{A}^\dagger\mathsf{A}$$

It is easy to verify that Hermitian, anti-Hermitian and unitary matrices are all normal.

## 5.6   Eigenvalues and eigenvectors

### 5.6.1   Basic properties

An *eigenvector* of a linear operator $\mathbf{A}$ is a non-zero vector $\boldsymbol{x}$ satisfying

$$\mathbf{A}\boldsymbol{x} = \lambda\boldsymbol{x}$$

for some scalar $\lambda$, the corresponding *eigenvalue*.

The equivalent statement in a matrix representation is

$$\boxed{\mathsf{A}\mathsf{x} = \lambda\mathsf{x}} \qquad \text{or} \qquad (\mathsf{A} - \lambda\mathbf{1})\mathsf{x} = \mathsf{0}$$

where $\mathsf{A}$ is an $n \times n$ square matrix.

This equation states that a non-trivial linear combination of the columns of the matrix $(\mathsf{A} - \lambda\mathbf{1})$ is equal to zero, i.e. that the columns of the matrix are linearly dependent. This is equivalent to the statement

$$\boxed{\det(\mathsf{A} - \lambda\mathbf{1}) = 0}$$

which is the *characteristic equation* of the matrix $\mathsf{A}$.

To compute the eigenvalues and eigenvectors, we first solve the characteristic equation. This a polynomial equation of degree $n$ in $\lambda$ and therefore has $n$ roots, although not necessarily distinct. These are the eigenvalues of $\mathsf{A}$, and are complex in general. The corresponding eigenvectors are obtained by solving the simultaneous equations found in the rows of $\mathsf{A}\mathsf{x} = \lambda\mathsf{x}$.

If the $n$ roots are distinct, then there are $n$ linearly independent eigenvectors, each of which is determined uniquely up to an arbitrary multiplicative constant.

If the roots are not all distinct, the repeated eigenvalues are said to be *degenerate*. If an eigenvalue $\lambda$ occurs $m$ times, there may be any number between 1 and $m$ of linearly independent eigenvectors corresponding to

it. Any linear combination of these is also an eigenvector and the space spanned by such vectors is called an *eigenspace*.

Example (1):

$$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

characteristic equation $\begin{vmatrix} 0 - \lambda & 0 \\ 0 & 0 - \lambda \end{vmatrix} = \lambda^2 = 0$

eigenvalues $0, 0$

eigenvectors: $\begin{bmatrix} 0 - \lambda & 0 \\ 0 & 0 - \lambda \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Rightarrow \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

two linearly independent eigenvectors, e.g. $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$

two-dimensional eigenspace corresponding to eigenvalue 0

Example (2):

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

characteristic equation $\begin{vmatrix} 0 - \lambda & 1 \\ 0 & 0 - \lambda \end{vmatrix} = \lambda^2 = 0$

eigenvalues $0, 0$

eigenvectors: $\begin{bmatrix} 0 - \lambda & 1 \\ 0 & 0 - \lambda \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Rightarrow \begin{bmatrix} y \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

only one linearly independent eigenvector $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$

one-dimensional eigenspace corresponding to eigenvalue 0

### 5.6.2 Eigenvalues and eigenvectors of Hermitian matrices

The matrices most often encountered in physical applications are real symmetric or, more generally, Hermitian matrices satisfying $A^\dagger = A$. In quantum mechanics, Hermitian matrices (or operators) represent observable quantities.

We consider two eigenvectors $x$ and $y$ corresponding to eigenvalues $\lambda$ and $\mu$:

$$Ax = \lambda x \tag{1}$$

$$Ay = \mu y \tag{2}$$

The Hermitian conjugate of equation (2) is (since $A^\dagger = A$)

$$y^\dagger A = \mu^* y^\dagger \tag{3}$$

Using equations (1) and (3) we can construct two expressions for $y^\dagger A x$:

$$y^\dagger A x = \lambda y^\dagger x = \mu^* y^\dagger x$$

$$(\lambda - \mu^*) y^\dagger x = 0 \tag{4}$$

First suppose that $x$ and $y$ are the *same* eigenvector. Then $y = x$ and $\mu = \lambda$, so equation (4) becomes

$$(\lambda - \lambda^*) x^\dagger x = 0$$

Since $x \neq 0$, $x^\dagger x \neq 0$ and so $\lambda^* = \lambda$. Therefore *the eigenvalues of an Hermitian matrix are real.*

Equation (4) simplifies to

$$(\lambda - \mu) y^\dagger x = 0$$

If $x$ and $y$ are now *different* eigenvectors, we deduce that $y^\dagger x = 0$, provided that $\mu \neq \lambda$. Therefore *the eigenvectors of an Hermitian matrix corresponding to distinct eigenvalues are orthogonal* (in the standard inner product on $\mathbf{C}^n$).

### 5.6.3 Related results

Normal matrices (including all Hermitian, anti-Hermitian and unitary matrices) satisfy $AA^\dagger = A^\dagger A$. It can be shown that:

- the eigenvectors of normal matrices corresponding to distinct eigenvalues are orthogonal

- the eigenvalues of Hermitian, anti-Hermitian and unitary matrices are real, imaginary and of unit modulus, respectively

These results can all be proved in a similar way.

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Show that the eigenvalues of a unitary matrix are of unit modulus and the eigenvectors corresponding to distinct eigenvalues are orthogonal.*

Let $A$ be a unitary matrix: $\qquad A^\dagger = A^{-1}$

$$Ax = \lambda x$$

$$Ay = \mu y$$

$$y^\dagger A^\dagger = \mu^* y^\dagger$$

$$y^\dagger A^\dagger A x = \mu^* \lambda y^\dagger x$$

$$(\mu^* \lambda - 1) y^\dagger x = 0$$

$$y = x: \qquad |\lambda|^2 - 1 = 0 \qquad \text{since } x \neq 0$$

$$\Rightarrow |\lambda| = 1$$

$$y \neq x: \qquad \left(\frac{\lambda}{\mu} - 1\right) y^\dagger x = 0$$

$$\mu \neq \lambda: \qquad y^\dagger x = 0$$

. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

Note that:

- real symmetric matrices are Hermitian

- real antisymmetric matrices are anti-Hermitian

- real orthogonal matrices are unitary

Note also that a $1 \times 1$ matrix is just a number, $\lambda$, which is the eigenvalue of the matrix. To be Hermitian, anti-Hermitian or unitary $\lambda$ must satisfy

$$\lambda^* = \lambda, \qquad \lambda^* = -\lambda \qquad \text{or} \qquad \lambda^* = \lambda^{-1}$$

respectively. Hermitian, anti-Hermitian and unitary matrices therefore correspond to real, imaginary and unit-modulus numbers, respectively.

There are direct correspondences between Hermitian, anti-Hermitian and unitary matrices:

- if $\mathsf{A}$ is Hermitian then $i\mathsf{A}$ is anti-Hermitian (and vice versa)

- if $\mathsf{A}$ is Hermitian then

$$\exp(i\mathsf{A}) = \sum_{n=0}^{\infty} \frac{(i\mathsf{A})^n}{n!} \qquad \text{is unitary}$$

[Compare the following two statements: If $z$ is a real number then $iz$ is imaginary (and vice versa). If $z$ is a real number then $\exp(iz)$ is of unit modulus.]

### 5.6.4 The degenerate case

If a repeated eigenvalue $\lambda$ occurs $m$ times, it can be shown (with some difficulty) that there are exactly $m$ corresponding linearly independent eigenvectors *if the matrix is normal.*

It is always possible to construct an orthogonal basis within this $m$-dimensional eigenspace (e.g. by the Gram–Schmidt procedure: see Example Sheet 3, Question 2). Therefore, even if the eigenvalues are

degenerate, it is always possible to find $n$ mutually orthogonal eigenvectors, which form a basis for the vector space. In fact, this is possible if and only if the matrix is normal.

Orthogonal eigenvectors can be normalized (divide by their norm) to make them orthonormal. Therefore *an orthonormal basis can always be constructed from the eigenvectors of a normal matrix.* This is called an *eigenvector basis.*

*Example* ........................................................

▷ *Find an orthonormal set of eigenvectors of the Hermitian matrix*

$$\begin{bmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Characteristic equation:

$$\begin{vmatrix} -\lambda & i & 0 \\ -i & -\lambda & 0 \\ 0 & 0 & 1-\lambda \end{vmatrix} = 0$$

$$(\lambda^2 - 1)(1 - \lambda) = 0$$

$$\lambda = 1, -1, 1$$

Eigenvector for $\lambda = -1$:

$$\begin{bmatrix} 1 & i & 0 \\ -i & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$x + iy = 0, \quad z = 0$$

Normalized eigenvector:

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix}$$

Eigenvectors for $\lambda = 1$:

$$\begin{bmatrix} -1 & i & 0 \\ -i & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$-x + iy = 0$$

Normalized eigenvectors:

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

.........................................................................

## 5.7  Diagonalization of a matrix

### 5.7.1  Similarity

We have seen that the matrices $A$ and $A'$ representing a linear operator in two different bases are related by

$$A' = RAR^{-1} \qquad \text{or equivalently} \qquad A = R^{-1}A'R$$

where $R$ is the transformation matrix between the two bases.

Two square matrices $A$ and $B$ are said to be *similar* if they are related by

$$B = S^{-1}AS \tag{1}$$

where $S$ is some invertible matrix. This means that $A$ and $B$ are representations of the same linear operator in different bases. The relation (1) is called a *similarity transformation*. $S$ is called the *similarity matrix*.

A square matrix $A$ is said to be *diagonalizable* if it is similar to a diagonal matrix, i.e. if

$$S^{-1}AS = \Lambda$$

for some invertible matrix $S$ and some *diagonal matrix*

$$\Lambda = \begin{bmatrix} \Lambda_1 & 0 & \cdots & 0 \\ 0 & \Lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Lambda_n \end{bmatrix}$$

### 5.7.2  Diagonalization

An $n \times n$ matrix $A$ can be diagonalized if and only if it has $n$ linearly independent eigenvectors. The columns of the similarity matrix $S$ are just the eigenvectors of $A$. The diagonal entries of the matrix $\Lambda$ are just the eigenvalues of $A$:

The meaning of diagonalization is that the matrix is expressed in its simplest form by transforming it to its eigenvector basis.

### 5.7.3 Diagonalization of a normal matrix

An $n \times n$ normal matrix always has $n$ linearly independent eigenvectors and is therefore diagonalizable. Furthermore, the eigenvectors can be chosen to be orthonormal. In this case the similarity matrix is *unitary*, because a unitary matrix is precisely one whose columns are orthonormal vectors (consider $U^\dagger U = 1$):

Therefore *a normal matrix can be diagonalized by a unitary transformation*:

$$\boxed{U^\dagger A U = \Lambda}$$

where $U$ is a unitary matrix whose columns are the orthonormal eigenvectors of $A$, and $\Lambda$ is a diagonal matrix whose entries are the eigenvalues of $A$.

In particular, this result applies to the important cases of real symmetric and, more generally, Hermitian matrices.

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Diagonalize the Hermitian matrix*

$$\begin{bmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Using the previously obtained eigenvalues and eigenvectors,

$$\begin{bmatrix} 1/\sqrt{2} & -i/\sqrt{2} & 0 \\ 1/\sqrt{2} & i/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ i/\sqrt{2} & -i/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

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### 5.7.4 Orthogonal and unitary transformations

The transformation matrix between two bases $\{e_i\}$ and $\{e'_i\}$ has components $R_{ij}$ defined by

$$e_j = e'_i R_{ij}$$

The condition for the first basis $\{e_i\}$ to be orthonormal is

$$e_i^\dagger e_j = \delta_{ij}$$

$$(e'_k R_{ki})^\dagger e'_l R_{lj} = \delta_{ij}$$

$$R_{ki}^* R_{lj} e_k'^\dagger e'_l = \delta_{ij}$$

If the second basis is also orthonormal, then $e_k'^\dagger e'_l = \delta_{kl}$ and the condition becomes

$$R_{ki}^* R_{kj} = \delta_{ij}$$

$$R^\dagger R = 1$$

Therefore *the transformation between orthonormal bases is described by a unitary matrix.*

In a real vector space, an *orthogonal* matrix performs this task. In $\mathbf{R}^2$ or $\mathbf{R}^3$ an orthogonal matrix corresponds to a rotation and/or reflection.

A real symmetric matrix is normal and has real eigenvalues and real orthogonal eigenvectors. Therefore *a real symmetric matrix can be diagonalized by a real orthogonal transformation.*

Note that this is not generally true of real antisymmetric or orthogonal matrices because their eigenvalues and eigenvectors are not generally real. They can, however, be diagonalized by complex unitary transformations.

### 5.7.5   Uses of diagonalization

Certain operations on (diagonalizable) matrices are more easily carried out using the representation

$$\mathsf{S}^{-1}\mathsf{A}\mathsf{S} = \Lambda \qquad \text{or} \qquad \mathsf{A} = \mathsf{S}\Lambda\mathsf{S}^{-1}$$

Examples:

$$\mathsf{A}^m = \left(\mathsf{S}\Lambda\mathsf{S}^{-1}\right)\left(\mathsf{S}\Lambda\mathsf{S}^{-1}\right)\cdots\left(\mathsf{S}\Lambda\mathsf{S}^{-1}\right) = \mathsf{S}\Lambda^m\mathsf{S}^{-1}$$

$$\det(\mathsf{A}) = \det\left(\mathsf{S}\Lambda\mathsf{S}^{-1}\right) = \det(\mathsf{S})\det(\Lambda)\det(\mathsf{S}^{-1}) = \det(\Lambda)$$

$$\mathrm{tr}(\mathsf{A}) = \mathrm{tr}\left(\mathsf{S}\Lambda\mathsf{S}^{-1}\right) = \mathrm{tr}\left(\Lambda\mathsf{S}^{-1}\mathsf{S}\right) = \mathrm{tr}(\Lambda)$$

$$\mathrm{tr}(\mathsf{A}^m) = \mathrm{tr}\left(\mathsf{S}\Lambda^m\mathsf{S}^{-1}\right) = \mathrm{tr}\left(\Lambda^m\mathsf{S}^{-1}\mathsf{S}\right) = \mathrm{tr}(\Lambda^m)$$

Here we use the properties of the determinant and trace:

$$\det(\mathsf{A}\mathsf{B}) = \det(\mathsf{A})\det(\mathsf{B})$$

$$\mathrm{tr}(\mathsf{A}\mathsf{B}) = (\mathsf{A}\mathsf{B})_{ii} = \mathsf{A}_{ij}\mathsf{B}_{ji} = \mathsf{B}_{ji}\mathsf{A}_{ij} = (\mathsf{B}\mathsf{A})_{jj} = \mathrm{tr}(\mathsf{B}\mathsf{A})$$

Note that diagonal matrices are multiplied very easily (i.e. component-wise). Also the determinant and trace of a diagonal matrix are just the product and sum, respectively, of its elements. Therefore

$$\det(\mathsf{A}) = \prod_{i=1}^{n}\lambda_i$$

$$\mathrm{tr}(\mathsf{A}) = \sum_{i=1}^{n}\lambda_i$$

In fact these two statements are true for all matrices (whether or not they are diagonalizable), as follows from the product and sum of roots in the characteristic equation

$$\det(\mathsf{A} - \lambda\mathbf{1}) = \det(\mathsf{A}) + \cdots + \mathrm{tr}(\mathsf{A})(-\lambda)^{n-1} + (-\lambda)^n = 0$$

### 5.8   Quadratic and Hermitian forms

#### 5.8.1   Quadratic form

The *quadratic form* associated with a real symmetric matrix $\mathsf{A}$ is

$$Q(\mathsf{x}) = \mathsf{x}^\mathsf{T}\mathsf{A}\mathsf{x} = x_i A_{ij} x_j = A_{ij} x_i x_j$$

$Q$ is a homogeneous quadratic function of $(x_1, x_2, \ldots, x_n)$, i.e. $Q(\alpha\mathsf{x}) = \alpha^2 Q(\mathsf{x})$. In fact, any homogeneous quadratic function is the quadratic form of a symmetric matrix, e.g.

$$Q = 2x^2 + 4xy + 5y^2 = \begin{bmatrix} x & y \end{bmatrix}\begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix}$$

The $xy$ term is split equally between the off-diagonal matrix elements.

$\mathsf{A}$ can be diagonalized by a real orthogonal transformation:

$$\mathsf{S}^\mathsf{T}\mathsf{A}\mathsf{S} = \Lambda \qquad \text{with} \quad \mathsf{S}^\mathsf{T} = \mathsf{S}^{-1}$$

The vector $\mathsf{x}$ transforms according to $\mathsf{x} = \mathsf{S}\mathsf{x}'$, so

$$Q = \mathsf{x}^\mathsf{T}\mathsf{A}\mathsf{x} = (\mathsf{x}'^\mathsf{T}\mathsf{S}^\mathsf{T})(\mathsf{S}\Lambda\mathsf{S}^\mathsf{T})(\mathsf{S}\mathsf{x}') = \mathsf{x}'^\mathsf{T}\Lambda\mathsf{x}'$$

The quadratic form is therefore reduced to a sum of squares,

$$Q = \sum_{i=1}^{n}\lambda_i x_i'^2$$

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Diagonalize the quadratic form $Q = 2x^2 + 4xy + 5y^2$.*

$$Q = \begin{bmatrix} x & y \end{bmatrix}\begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \mathsf{x}^\mathsf{T}\mathsf{A}\mathsf{x}$$

The eigenvalues of $\mathsf{A}$ are 1 and 6 and the corresponding normalized eigenvectors are

$$\frac{1}{\sqrt{5}}\begin{bmatrix} 2 \\ -1 \end{bmatrix}, \qquad \frac{1}{\sqrt{5}}\begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

(calculation omitted). The diagonalization of $A$ is $S^T A S = \Lambda$ with

$$S = \begin{bmatrix} 2/\sqrt{5} & 1/\sqrt{5} \\ -1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix}, \qquad \Lambda = \begin{bmatrix} 1 & 0 \\ 0 & 6 \end{bmatrix}$$

Therefore

$$Q = x'^2 + 6y'^2 = \left[\frac{1}{\sqrt{5}}(2x - y)\right]^2 + 6\left[\frac{1}{\sqrt{5}}(x + 2y)\right]^2$$

. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

The eigenvectors of $A$ define the *principal axes* of the quadratic form. In diagonalizing $A$ by transforming to its eigenvector basis, we are rotating the coordinates to reduce the quadratic form to its simplest form.

A *positive definite* matrix is one for which all the eigenvalues are positive ($\lambda > 0$). Similarly:

- *negative definite* means $\lambda < 0$
- *positive (negative) semi-definite* means $\lambda \geqslant 0$ ($\lambda \leqslant 0$)
- *definite* means positive definite or negative definite

In the above example, the diagonalization shows that $Q(\mathsf{x}) > 0$ for all $\mathsf{x} \neq 0$, and we say that the quadratic form is positive definite.


### 5.8.2  Quadratic surfaces

The *quadratic surfaces* (or *quadrics*) associated with a real quadratic form in three dimensions are the family of surfaces

$$Q(\mathsf{x}) = k = \text{constant}$$

In the eigenvector basis this equation simplifies to

$$\lambda_1 x_1'^2 + \lambda_2 x_2'^2 + \lambda_3 x_3'^2 = k$$

The equivalent equation in two dimensions is related to the standard form for a *conic section*, i.e. an *ellipse* (if $\lambda_1 \lambda_2 > 0$)

$$\frac{x'^2}{a^2} + \frac{y'^2}{b^2} = 1$$

or a *hyperbola* (if $\lambda_1 \lambda_2 < 0$)

$$\frac{x'^2}{a^2} - \frac{y'^2}{b^2} = \pm 1$$

The semi-axes (distances of the curve from the origin along the principal axes) are $a = \sqrt{|k/\lambda_1|}$ and $b = \sqrt{|k/\lambda_2|}$.

Notes:

- the scale of the ellipse (e.g.) is determined by the constant $k$
- the shape of the ellipse is determined by the eigenvalues
- the orientation of the ellipse is determined by the eigenvectors

In three dimensions, the quadratic surfaces are *ellipsoids* (if the eigenvalues all have the same sign) of standard form

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

or *hyperboloids* (if the eigenvalues differ in sign) of standard form

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

The quadrics of a definite quadratic form are therefore ellipsoids.

Some special cases:

- if $\lambda_1 = \lambda_2 = \lambda_3$ we have a sphere
- if (e.g.) $\lambda_1 = \lambda_2$ we have a surface of revolution about the $z'$-axis
- if (e.g.) $\lambda_3 = 0$ we have the translation of a conic section along the $z'$-axis (an elliptic or hyperbolic cylinder)

## Conic sections and quadric surfaces
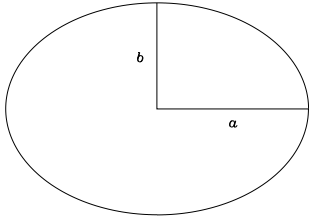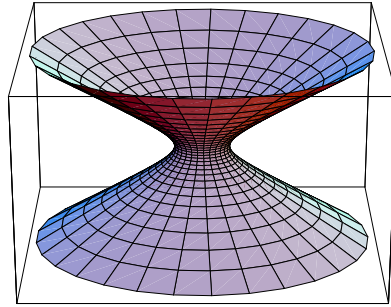


ellipse     $\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$
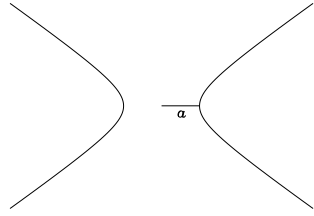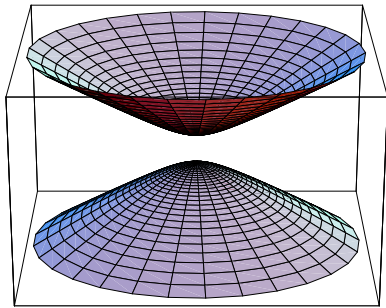
hyperbola     $\frac{x^2}{a^2} - \frac{y^2}{b^2} = 1$
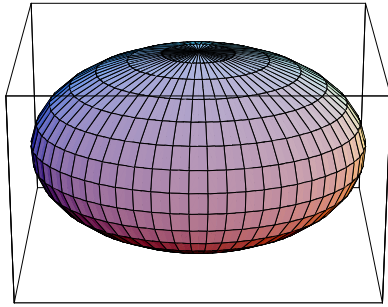
ellipsoid

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

hyperboloid of one sheet

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

hyperboloid of two sheets     $\frac{x^2}{a^2} + \frac{y^2}{b^2} - \frac{z^2}{c^2} = -1$

Example:

Let $V(\boldsymbol{r})$ be a potential with a stationary point at the origin $\boldsymbol{r} = \boldsymbol{0}$. Then its Taylor expansion has the form

$$V(\boldsymbol{r}) = V(\boldsymbol{0}) + V_{ij}x_i x_j + O(\boldsymbol{x}^3)$$

where

$$V_{ij} = \frac{1}{2}\left.\frac{\partial^2 V}{\partial x_i \partial x_j}\right|_{\boldsymbol{r}=\boldsymbol{0}}$$

The equipotential surfaces near the origin are therefore given approximately by the quadrics $V_{ij}x_i x_j = $ constant. These are ellipsoids or hyperboloids with principal axes given by the eigenvectors of the symmetric matrix $V_{ij}$.

### 5.8.3 Hermitian form

In a complex vector space, the *Hermitian form* associated with an Hermitian matrix $\mathsf{A}$ is

$$H(\mathsf{x}) = \mathsf{x}^\dagger \mathsf{A}\mathsf{x} = x_i^* A_{ij} x_j$$

$H$ is a real scalar because

$$H^* = (\mathsf{x}^\dagger \mathsf{A}\mathsf{x})^\dagger = \mathsf{x}^\dagger \mathsf{A}^\dagger \mathsf{x} = \mathsf{x}^\dagger \mathsf{A}\mathsf{x} = H$$

We have seen that $\mathsf{A}$ can be diagonalized by a unitary transformation:

$$\mathsf{U}^\dagger \mathsf{A}\mathsf{U} = \Lambda \qquad \text{with} \quad \mathsf{U}^\dagger = \mathsf{U}^{-1}$$

and so

$$H = \mathsf{x}^\dagger (\mathsf{U}\Lambda\mathsf{U}^\dagger)\mathsf{x} = (\mathsf{U}^\dagger \mathsf{x})^\dagger \Lambda (\mathsf{U}^\dagger \mathsf{x}) = \mathsf{x}'^\dagger \Lambda \mathsf{x}' = \sum_{i=1}^{n} \lambda_i x_i'^2$$

Therefore an Hermitian form can be reduced to a real quadratic form by transforming to the eigenvector basis.

## 5.9 Stationary property of the eigenvalues

The *Rayleigh quotient* associated with an Hermitian matrix $\mathsf{A}$ is the normalized Hermitian form

$$\lambda(\mathsf{x}) = \frac{\mathsf{x}^\dagger \mathsf{A}\mathsf{x}}{\mathsf{x}^\dagger \mathsf{x}}$$

Notes:

- $\lambda(\mathsf{x})$ is a real scalar

- $\lambda(\alpha \mathsf{x}) = \lambda(\mathsf{x})$

- if $\mathsf{x}$ is an eigenvector of $\mathsf{A}$, then $\lambda(\mathsf{x})$ is the corresponding eigenvalue

In fact, the eigenvalues of $\mathsf{A}$ are the stationary values of the function $\lambda(\mathsf{x})$. This is the *Rayleigh–Ritz variational principle.*

Proof:

$$\delta\lambda = \lambda(\mathsf{x} + \delta\mathsf{x}) - \lambda(\mathsf{x})$$

$$= \frac{(\mathsf{x} + \delta\mathsf{x})^\dagger \mathsf{A}(\mathsf{x} + \delta\mathsf{x})}{(\mathsf{x} + \delta\mathsf{x})^\dagger(\mathsf{x} + \delta\mathsf{x})} - \lambda(\mathsf{x})$$

$$= \frac{\mathsf{x}^\dagger \mathsf{A}\mathsf{x} + (\delta\mathsf{x})^\dagger \mathsf{A}\mathsf{x} + \mathsf{x}^\dagger \mathsf{A}(\delta\mathsf{x}) + O(\delta\mathsf{x}^2)}{\mathsf{x}^\dagger \mathsf{x} + (\delta\mathsf{x})^\dagger \mathsf{x} + \mathsf{x}^\dagger(\delta\mathsf{x}) + O(\delta\mathsf{x}^2)} - \lambda(\mathsf{x})$$

$$= \frac{(\delta\mathsf{x})^\dagger \mathsf{A}\mathsf{x} + \mathsf{x}^\dagger \mathsf{A}(\delta\mathsf{x}) - \lambda(\mathsf{x})[(\delta\mathsf{x})^\dagger \mathsf{x} + \mathsf{x}^\dagger(\delta\mathsf{x})] + O(\delta\mathsf{x}^2)}{\mathsf{x}^\dagger \mathsf{x} + (\delta\mathsf{x})^\dagger \mathsf{x} + \mathsf{x}^\dagger(\delta\mathsf{x}) + O(\delta\mathsf{x}^2)}$$

$$= \frac{(\delta\mathsf{x})^\dagger[\mathsf{A}\mathsf{x} - \lambda(\mathsf{x})\mathsf{x}] + [\mathsf{x}^\dagger \mathsf{A} - \lambda(\mathsf{x})\mathsf{x}^\dagger](\delta\mathsf{x})}{\mathsf{x}^\dagger \mathsf{x}} + O(\delta\mathsf{x}^2)$$

$$= \frac{(\delta\mathsf{x})^\dagger[\mathsf{A}\mathsf{x} - \lambda(\mathsf{x})\mathsf{x}]}{\mathsf{x}^\dagger \mathsf{x}} + \text{c.c.} + O(\delta\mathsf{x}^2)$$

where 'c.c.' denotes the complex conjugate. Therefore the first-order variation of $\lambda(\mathsf{x})$ vanishes for *all* perturbations $\delta\mathsf{x}$ if and only if $\mathsf{A}\mathsf{x} = \lambda(\mathsf{x})\mathsf{x}$. In that case $\mathsf{x}$ is an eigenvector of $\mathsf{A}$, and the value of $\lambda(\mathsf{x})$ is the corresponding eigenvalue.

## 6 Elementary analysis

### 6.1 Motivation

Analysis is the careful study of infinite processes such as limits, convergence, differential and integral calculus, and is one of the foundations of mathematics. This section covers some of the basic concepts including the important problem of the convergence of infinite series. It also introduces the remarkable properties of analytic functions of a complex variable.

### 6.2 Sequences

#### 6.2.1 Limits of sequences

We first consider a *sequence* of real or complex numbers $f_n$, defined for all integers $n \geqslant n_0$. Possible behaviours as $n$ increases are:

- $f_n$ tends towards a particular value

- $f_n$ does not tend to any value but remains limited in magnitude

- $f_n$ is unlimited in magnitude

**Definition.** *The sequence $f_n$ converges to the limit $L$ as $n \to \infty$ if, for any positive number $\epsilon$, $|f_n - L| < \epsilon$ for sufficiently large $n$.*

In other words *the members of the sequence are eventually contained within an arbitrarily small disk centred on $L$.* We write this as

$$\boxed{\lim_{n\to\infty} f_n = L} \qquad \text{or} \qquad \boxed{f_n \to L \quad \text{as } n \to \infty}$$

Note that $L$ here is a finite number.

To say that a property holds *for sufficiently large $n$* means that there exists an integer $N$ such that the property is true for all $n \geqslant N$.

Example:

$$\lim_{n\to\infty} n^{-\alpha} = 0 \qquad \text{for any } \alpha > 0$$

Proof: $|n^{-\alpha} - 0| < \epsilon$ holds for all $n > \epsilon^{-1/\alpha}$.

If $f_n$ does not tend to a limit it may nevertheless be *bounded*.

**Definition.** *The sequence $f_n$ is bounded as $n \to \infty$ if there exists a positive number $K$ such that $|f_n| < K$ for sufficiently large $n$.*

Example:

$$\left(\frac{n+1}{n}\right) e^{in\alpha} \quad \text{is bounded as } n \to \infty \text{ for any real number } \alpha$$

Proof:

$$\left|\left(\frac{n+1}{n}\right) e^{in\alpha}\right| = \frac{n+1}{n} < 2 \quad \text{for all } n \geqslant 2$$

### 6.2.2  Cauchy's principle of convergence

A necessary and sufficient condition for the sequence $f_n$ to converge is that, for any positive number $\epsilon$, $|f_{n+m} - f_n| < \epsilon$ for all positive integers $m$, for sufficiently large $n$. Note that this condition does not require a knowledge of the value of the limit $L$.

## 6.3  Convergence of series

### 6.3.1  Meaning of convergence

What is the meaning of an infinite series such as

$$\sum_{n=n_0}^{\infty} u_n$$

involving the addition of an infinite number of terms?

We define the *partial sum*

$$S_N = \sum_{n=n_0}^{N} u_n$$

The infinite series $\sum u_n$ is said to *converge* if the sequence of partial sums $S_N$ tends to a limit $S$ as $N \to \infty$. The value of the series is then $S$. Otherwise the series *diverges*.

Note that whether a series converges or diverges does not depend on the value of $n_0$ (i.e. on when the series begins) but only on the behaviour of the terms for large $n$.

According to Cauchy's principle of convergence, a necessary and sufficient condition for $\sum u_n$ to converge is that, for any positive number $\epsilon$, $|u_{n+1} + u_{n+2} + \cdots + u_{n+m}| < \epsilon$ for all positive integers $m$, for sufficiently large $n$.

### 6.3.2  Classic examples

The *geometric series* $\sum z^n$ has the partial sum

$$\sum_{n=0}^{N} z^n = \begin{cases} \frac{1-z^{N+1}}{1-z}, & z \neq 1 \\ N+1, & z = 1 \end{cases}$$

Therefore $\sum z^n$ converges if $|z| < 1$, and the sum is $1/(1-z)$. If $|z| \geqslant 1$ the series diverges.

The *harmonic series* $\sum n^{-1}$ diverges. Consider the partial sum

$$S_N = \sum_{n=1}^{N} \frac{1}{n} > \int_1^{N+1} \frac{\mathrm{d}x}{x} = \ln(N+1)$$

Therefore $S_N$ increases without bound and does not tend to a limit as $N \to \infty$.

### 6.3.3   Absolute and conditional convergence

If $\sum |u_n|$ converges, then $\sum u_n$ also converges. $\sum u_n$ is then said to converge *absolutely*.

If $\sum |u_n|$ diverges, then $\sum u_n$ may or may not converge. If it does, it is said to converge *conditionally*.

[Proof of the first statement above: If $\sum |u_n|$ converges then, for any positive number $\epsilon$,

$$|u_{n+1}| + |u_{n+2}| + \cdots + |u_{n+m}| < \epsilon$$

for all positive integers $m$, for sufficiently large $n$. But then

$$|u_{n+1} + u_{n+2} + \cdots + u_{n+m}| \leqslant |u_{n+1}| + |u_{n+2}| + \cdots + |u_{n+m}|$$
$$< \epsilon$$

and so $\sum u_n$ also converges.]

### 6.3.4   Necessary condition for convergence

A necessary condition for $\sum u_n$ to converge is that $u_n \to 0$ as $n \to \infty$. Formally, this can be shown by noting that $u_n = S_n - S_{n-1}$. If the series converges then $\lim S_n = \lim S_{n-1} = S$, and therefore $\lim u_n = 0$.

This condition is *not* sufficient for convergence, as exemplified by the harmonic series.

### 6.3.5   The comparison test

This refers to series of non-negative real numbers. We write these as $|u_n|$ because the comparison test is most often applied in assessing the absolute convergence of a series of real or complex numbers.

If $\sum |v_n|$ converges and $|u_n| \leqslant |v_n|$ for all $n$, then $\sum |u_n|$ also converges. This follows from the fact that

$$\sum_{n=n_0}^{N} |u_n| \leqslant \sum_{n=n_0}^{N} |v_n|$$

and each partial sum is a non-decreasing sequence, which must either tend to a limit or increase without bound.

More generally, if $\sum |v_n|$ converges and $|u_n| \leqslant K|v_n|$ for sufficiently large $n$, where $K$ is a constant, then $\sum |u_n|$ also converges.

Conversely, if $\sum |v_n|$ diverges and $|u_n| \geqslant K|v_n|$ for sufficiently large $n$, where $K$ is a positive constant, then $\sum |u_n|$ also diverges.

In particular, if $\sum |v_n|$ converges (diverges) and $|u_n|/|v_n|$ tends to a non-zero limit as $n \to \infty$, then $\sum |u_n|$ also converges (diverges).

### 6.3.6   D'Alembert's ratio test

This uses a comparison between a given series $\sum u_n$ of complex terms and a geometric series $\sum v_n = \sum r^n$, where $r > 0$.

The *absolute ratio of successive terms* is

$$r_n = \left| \frac{u_{n+1}}{u_n} \right|$$

Suppose that $r_n$ tends to a limit $r$ as $n \to \infty$. Then

- if $r < 1$, $\sum u_n$ converges absolutely
- if $r > 1$, $\sum u_n$ diverges ($u_n$ does not tend to zero)
- if $r = 1$, a different test is required

Even if $r_n$ does not tend to a limit, if $r_n \leqslant r$ for sufficiently large $n$, where $r < 1$ is a constant, then $\sum u_n$ converges absolutely.

Example: for the harmonic series $\sum n^{-1}$, $r_n = n/(n+1) \to 1$ as $n \to \infty$. A different test is required, such as the integral comparison test used above.

The ratio test is useless for series in which some of the terms are zero. However, it can easily be adapted by relabelling the series to remove the vanishing terms.

### 6.3.7 Cauchy's root test

The same conclusions as for the ratio test apply when instead

$$r_n = |u_n|^{1/n}$$

This result also follows from a comparison with a geometric series. It is more powerful than the ratio test but usually harder to apply.

## 6.4 Functions of a continuous variable

### 6.4.1 Limits and continuity

We now consider how a real or complex function $f(z)$ of a real or complex variable $z$ behaves near a point $z_0$.

**Definition.** *The function $f(z)$ tends to the limit $L$ as $z \to z_0$ if, for any positive number $\epsilon$, there exists a positive number $\delta$, depending on $\epsilon$, such that $|f(z) - L| < \epsilon$ for all $z$ such that $|z - z_0| < \delta$.*

We write this as

$$\boxed{\lim_{z \to z_0} f(z) = L} \qquad \text{or} \qquad \boxed{f(z) \to L \quad \text{as } z \to z_0}$$

The value of $L$ would normally be $f(z_0)$. However, cases such as

$$\lim_{z \to 0} \frac{\sin z}{z} = 1$$

must be expressed as limits because $\sin 0/0 = 0/0$ is indeterminate.

**Definition.** *The function $f(z)$ is continuous at the point $z = z_0$ if $f(z) \to f(z_0)$ as $z \to z_0$.*

**Definition.** *The function $f(z)$ is bounded as $z \to z_0$ if there exist positive numbers $K$ and $\delta$ such that $|f(z)| < K$ for all $z$ with $|z - z_0| < \delta$.*

**Definition.** *The function $f(z)$ tends to the limit $L$ as $z \to \infty$ if, for any positive number $\epsilon$, there exists a positive number $R$, depending on $\epsilon$, such that $|f(z) - L| < \epsilon$ for all $z$ with $|z| > R$.*

We write this as

$$\boxed{\lim_{z \to \infty} f(z) = L} \qquad \text{or} \qquad \boxed{f(z) \to L \quad \text{as } z \to \infty}$$

**Definition.** *The function $f(z)$ is bounded as $z \to \infty$ if there exist positive numbers $K$ and $R$ such that $|f(z)| < K$ for all $z$ with $|z| > R$.*

There are different ways in which $z$ can approach $z_0$ or $\infty$, especially in the complex plane. Sometimes the limit or bound applies only if approached in a particular way, e.g.

$$\lim_{x \to +\infty} \tanh x = 1, \qquad \lim_{x \to -\infty} \tanh x = -1$$

This notation implies that $x$ is approaching positive or negative real infinity along the real axis. In the context of real variables $x \to \infty$ usually means specifically $x \to +\infty$. A related notation for one-sided limits is exemplified by

$$\lim_{x \to 0+} \frac{x(1+x)}{|x|} = 1, \qquad \lim_{x \to 0-} \frac{x(1+x)}{|x|} = -1$$

### 6.4.2 The $O$ notation

The useful symbols $O$, $o$ and $\sim$ are used to compare the rates of growth or decay of different functions.

- $f(z) = O(g(z))$ as $z \to z_0$ means that $\frac{f(z)}{g(z)}$ is bounded as $z \to z_0$

- $f(z) = o(g(z))$ as $z \to z_0$ means that $\frac{f(z)}{g(z)} \to 0$ as $z \to z_0$

- $f(z) \sim g(z)$ as $z \to z_0$ means that $\frac{f(z)}{g(z)} \to 1$ as $z \to z_0$

If $f(z) \sim g(z)$ we say that $f$ is *asymptotically equal* to $g$. This should *not* be written as $f(z) \to g(z)$.

Notes:

- these definitions also apply when $z_0 = \infty$

- $f(z) = O(1)$ means that $f(z)$ is bounded

- either $f(z) = o(g(z))$ or $f(z) \sim g(z)$ implies $f(z) = O(g(z))$

- only $f(z) \sim g(z)$ is a symmetric relation

Examples:

$$A \cos z = O(1) \quad \text{as } z \to 0$$
$$A \sin z = O(z) = o(1) \quad \text{as } z \to 0$$
$$\ln x = o(x) \quad \text{as } x \to +\infty$$
$$\cosh x \sim \tfrac{1}{2}\mathrm{e}^x \quad \text{as } x \to +\infty$$

## 6.5 Taylor's theorem for functions of a real variable

Let $f(x)$ be a (real or complex) function of a real variable $x$, which is differentiable at least $n$ times in the interval $x_0 \leqslant x \leqslant x_0 + h$. Then

$$\boxed{\begin{aligned} f(x_0 + h) = &f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \cdots \\ &\cdots + \frac{h^{n-1}}{(n-1)!}f^{(n-1)}(x_0) + R_n \end{aligned}}$$

where

$$R_n = \int_{x_0}^{x_0+h} \frac{(x_0 + h - x)^{n-1}}{(n-1)!} f^{(n)}(x)\,\mathrm{d}x$$

is the remainder after $n$ terms of the Taylor series.

[Proof: integrate $R_n$ by parts $n$ times.]

The remainder term can be expressed in various ways. Lagrange's expression for the remainder is

$$R_n = \frac{h^n}{n!} f^{(n)}(\xi)$$

where $\xi$ is an unknown number in the interval $x_0 < \xi < x_0 + h$. So

$$R_n = O(h^n)$$

If $f(x)$ is infinitely differentiable in $x_0 \leqslant x \leqslant x_0 + h$ (it is a *smooth* function) we can write an infinite Taylor series

$$\boxed{f(x_0 + h) = \sum_{n=0}^{\infty} \frac{h^n}{n!} f^{(n)}(x_0)}$$

which converges for sufficiently small $h$ (as discussed below).

## 6.6 Analytic functions of a complex variable

### 6.6.1 Complex differentiability

**Definition.** *The derivative of the function $f(z)$ at the point $z = z_0$ is*

$$f'(z_0) = \lim_{z \to z_0} \frac{f(z) - f(z_0)}{z - z_0}$$

*If this exists, the function $f(z)$ is differentiable at $z = z_0$.*

Another way to write this is

$$\frac{df}{dz} \equiv f'(z) = \lim_{\delta z \to 0} \frac{f(z + \delta z) - f(z)}{\delta z}$$

Requiring a function of a *complex* variable to be differentiable is a surprisingly strong constraint. The limit must be the same when $\delta z \to 0$ in any direction in the complex plane.

### 6.6.2 The Cauchy–Riemann equations

Separate $f = u + iv$ and $z = x + iy$ into their real and imaginary parts:

$$f(z) = u(x, y) + iv(x, y)$$

If $f'(z)$ exists we can calculate it by assuming that $\delta z = \delta x + i\,\delta y$ approaches 0 along the real axis, so $\delta y = 0$:

$$
\begin{aligned}
f'(z) &= \lim_{\delta x \to 0} \frac{f(z + \delta x) - f(z)}{\delta x} \\
&= \lim_{\delta x \to 0} \frac{u(x + \delta x, y) + iv(x + \delta x, y) - u(x, y) - iv(x, y)}{\delta x} \\
&= \lim_{\delta x \to 0} \frac{u(x + \delta x, y) - u(x, y)}{\delta x} + i \lim_{\delta x \to 0} \frac{v(x + \delta x, y) - v(x, y)}{\delta x} \\
&= \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x}
\end{aligned}
$$

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The derivative should have the same value if $\delta z$ approaches 0 along the imaginary axis, so $\delta x = 0$:

$$
\begin{aligned}
f'(z) &= \lim_{\delta y \to 0} \frac{f(z + i\,\delta y) - f(z)}{i\,\delta y} \\
&= \lim_{\delta y \to 0} \frac{u(x, y + \delta y) + iv(x, y + \delta y) - u(x, y) - iv(x, y)}{i\,\delta y} \\
&= -i \lim_{\delta y \to 0} \frac{u(x, y + \delta y) - u(x, y)}{\delta y} + \lim_{\delta y \to 0} \frac{v(x, y + \delta y) - v(x, y)}{\delta y} \\
&= -i \frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}
\end{aligned}
$$

Comparing the real and imaginary parts of these expressions, we deduce the *Cauchy–Riemann equations*

$$\boxed{\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \qquad \frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y}}$$

These are necessary conditions for $f(z)$ to have a complex derivative. They are also sufficient conditions, provided that the partial derivatives are also continuous.

### 6.6.3 Analytic functions

If a function $f(z)$ has a complex derivative at every point $z$ in a region $R$ of the complex plane, it is said to be *analytic* in $R$. To be analytic at a point $z = z_0$, $f(z)$ must be differentiable throughout some neighbourhood $|z - z_0| < \epsilon$ of that point.

Examples of functions that are analytic in the whole complex plane (known as *entire functions*):

- $f(z) = c$, a complex constant

- $f(z) = z$, for which $u = x$ and $v = y$, and we easily verify the CR equations

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- $f(z) = z^n$, where $n$ is a positive integer

- $f(z) = P(z) = c_n z^n + c_{n-1} z^{n-1} + \cdots + c_0$, a general polynomial function with complex coefficients

- $f(z) = \exp(z)$

In the case of the exponential function we have

$$f(z) = e^z = e^x e^{iy} = e^x \cos y + i \, e^x \sin y = u + iv$$

The CR equations are satisfied for all $x$ and $y$:

$$\frac{\partial u}{\partial x} = e^x \cos y = \frac{\partial v}{\partial y}$$

$$\frac{\partial v}{\partial x} = e^x \sin y = -\frac{\partial u}{\partial y}$$

The derivative of the exponential function is

$$f'(z) = \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x} = e^x \cos y + i \, e^x \sin y = e^z$$

as expected.

Sums, products and compositions of analytic functions are also analytic, e.g.

$$f(z) = z \exp(iz^2) + z^3$$

The usual product, quotient and chain rules apply to complex derivatives of analytic functions. Familiar relations such as

$$\frac{d}{dz} z^n = n z^{n-1}, \qquad \frac{d}{dz} \sin z = \cos z, \qquad \frac{d}{dz} \cosh z = \sinh z$$

apply as usual.

Many complex functions are analytic everywhere in the complex plane except at isolated points, which are called the *singular points* or *singularities* of the function.

Examples:

- $f(z) = P(z)/Q(z)$, where $P(z)$ and $Q(z)$ are polynomials. This is called a *rational function* and is analytic except at points where $Q(z) = 0$.

- $f(z) = z^c$, where $c$ is a complex constant, is analytic except at $z = 0$ (unless $c$ is a non-negative integer)

- $f(z) = \ln z$ is also analytic except at $z = 0$

The last two examples are in fact *multiple-valued functions*, which require special treatment (see next term).

Examples of non-analytic functions:

- $f(z) = \text{Re}(z)$, for which $u = x$ and $v = 0$, so the CR equations are not satisfied anywhere

- $f(z) = z^*$, for which $u = x$ and $v = -y$

- $f(z) = |z|$, for which $u = (x^2 + y^2)^{1/2}$ and $v = 0$

- $f(z) = |z|^2$, for which $u = x^2 + y^2$ and $v = 0$

In the last case the CR equations are satisfied only at $x = y = 0$ and we can say that $f'(0) = 0$. However, $f(z)$ is not analytic even at $z = 0$ because it is not differentiable throughout any neighbourhood $|z| < \epsilon$ of 0.

### 6.6.4 Consequences of the Cauchy–Riemann equations

If we know the real part of an analytic function in some region, we can find its imaginary part (or vice versa) up to an additive constant by integrating the CR equations.

Example:

$$u(x, y) = x^2 - y^2$$

$$\frac{\partial v}{\partial y} = \frac{\partial u}{\partial x} = 2x \quad \Rightarrow \quad v = 2xy + g(x)$$

$$\frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y} \quad \Rightarrow \quad 2y + g'(x) = 2y \quad \Rightarrow \quad g'(x) = 0$$

Therefore $v(x,y) = 2xy + c$, where $c$ is a real constant, and we recognize

$$f(z) = x^2 - y^2 + \mathrm{i}(2xy + c) = (x + \mathrm{i}y)^2 + \mathrm{i}c = z^2 + \mathrm{i}c$$

The real and imaginary parts of an analytic function satisfy Laplace's equation (they are *harmonic functions*):

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\partial u}{\partial y}\right)$$
$$= \frac{\partial}{\partial x}\left(\frac{\partial v}{\partial y}\right) + \frac{\partial}{\partial y}\left(-\frac{\partial v}{\partial x}\right)$$
$$= 0$$

The proof that $\nabla^2 v = 0$ is similar. This provides a useful method for solving Laplace's equation in two dimensions. Furthermore,

$$\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v = \frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial v}{\partial y}$$
$$= \frac{\partial v}{\partial y}\frac{\partial v}{\partial x} - \frac{\partial v}{\partial x}\frac{\partial v}{\partial y}$$
$$= 0$$

and so the curves of constant $u$ and those of constant $v$ intersect at right angles. $u$ and $v$ are said to be *conjugate harmonic functions*.

## 6.7   Taylor series for analytic functions

If a function of a complex variable is analytic in a region $R$ of the complex plane, not only is it differentiable everywhere in $R$, it is also differentiable any number of times. If $f(z)$ is analytic at $z = z_0$, it has an infinite Taylor series

$$f(z) = \sum_{n=0}^{\infty} a_n(z - z_0)^n, \qquad a_n = \frac{f^{(n)}(z_0)}{n!}$$

which converges within some neighbourhood of $z_0$ (as discussed below). In fact this can be taken as a definition of analyticity.

## 6.8   Zeros, poles and essential singularities

### 6.8.1   Zeros of complex functions

The zeros of $f(z)$ are the points $z = z_0$ in the complex plane where $f(z_0) = 0$. A zero is of order $N$ if

$$f(z_0) = f'(z_0) = f''(z_0) = \cdots = f^{(N-1)}(z_0) = 0 \qquad \text{but} \quad f^{(N)}(z_0) \neq 0$$

The first non-zero term in the Taylor series of $f(z)$ about $z = z_0$ is then proportional to $(z - z_0)^N$. Indeed

$$f(z) \sim a_N(z - z_0)^N \qquad \text{as} \quad z \to z_0$$

A *simple zero* is a zero of order 1. A *double zero* is one of order 2, etc.

Examples:

- $f(z) = z$ has a simple zero at $z = 0$
- $f(z) = (z - \mathrm{i})^2$ has a double zero at $z = \mathrm{i}$
- $f(z) = z^2 - 1 = (z - 1)(z + 1)$ has simple zeros at $z = \pm 1$

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Find and classify the zeros of $f(z) = \sinh z$.*

$$0 = \sinh z = \frac{1}{2}(\mathrm{e}^z - \mathrm{e}^{-z})$$

$$e^z = e^{-z}$$

$$e^{2z} = 1$$

$$2z = 2n\pi i$$

$$z = n\pi i, \qquad n \in \mathbf{Z}$$

$$f'(z) = \cosh z = \cos(n\pi) \neq 0 \quad \text{at these points}$$

$$\Rightarrow \quad \text{all simple zeros}$$

......................................................................

### 6.8.2 Poles

If $g(z)$ is analytic and non-zero at $z = z_0$ then it has an expansion (locally, at least) of the form

$$g(z) = \sum_{n=0}^{\infty} b_n (z - z_0)^n \qquad \text{with} \quad b_0 \neq 0$$

Consider the function

$$f(z) = (z - z_0)^{-N} g(z) = \sum_{n=-N}^{\infty} a_n (z - z_0)^n$$

with $a_n = b_{n+N}$ and so $a_{-N} \neq 0$. This is not a Taylor series because it includes negative powers of $z - z_0$, and $f(z)$ is not analytic at $z = z_0$. We say that $f(z)$ has a pole of order $N$. Note that

$$f(z) \sim a_{-N}(z - z_0)^{-N} \qquad \text{as} \quad z \to z_0$$

A *simple pole* is a pole of order 1. A *double pole* is one of order 2, etc.

Notes:

- if $f(z)$ has a zero of order $N$ at $z = z_0$, then $1/f(z)$ has a pole of order $N$ there, and vice versa

- if $f(z)$ is analytic and non-zero at $z = z_0$ and $g(z)$ has a zero of order $N$ there, then $f(z)/g(z)$ has a pole of order $N$ there

Example:

$$f(z) = \frac{2z}{(z+1)(z-i)^2}$$

has a simple pole at $z = -1$ and a double pole at $z = i$ (as well as a simple zero at $z = 0$). The expansion about the double pole can be carried out by letting $z = i + w$ and expanding in $w$:

$$f(z) = \frac{2(i+w)}{(i+w+1)w^2}$$

$$= \frac{2i(1-iw)}{(i+1)\left[1 + \frac{1}{2}(1-i)w\right]w^2}$$

$$= \frac{2i}{(i+1)w^2}(1-iw)\left[1 - \frac{1}{2}(1-i)w + O(w^2)\right]$$

$$= (1+i)w^{-2}\left[1 - \frac{1}{2}(1+i)w + O(w^2)\right]$$

$$= (1+i)(z-i)^{-2} - i(z-i)^{-1} + O(1) \qquad \text{as} \quad z \to i$$

### 6.8.3 Essential singularities

It can be shown that any function that is analytic (and single-valued) throughout an annulus $a < |z - z_0| < b$ centred on a point $z = z_0$ has a unique *Laurent series*

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n$$

which converges for all values of $z$ within the annulus.

If $a = 0$, then $f(z)$ is analytic throughout the disk $|z - z_0| < b$ except possibly at $z = z_0$ itself, and the Laurent series determines the behaviour of $f(z)$ near $z = z_0$. There are three possibilities:

- if the first non-zero term in the Laurent series has $n \geqslant 0$, then $f(z)$ is analytic at $z = z_0$ and the series is just a Taylor series

- if the first non-zero term in the Laurent series has $n = -N < 0$, then $f(z)$ has a pole of order $N$ at $z = z_0$

- otherwise, if the Laurent series involves an infinite number of terms with $n < 0$, then $f(z)$ has an *essential singularity* at $z = z_0$

A classic example of an essential singularity is $f(z) = \mathrm{e}^{1/z}$ at $z = 0$. Here we can generate the Laurent series from a Taylor series in $1/z$:

$$\mathrm{e}^{1/z} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{z}\right)^n = \sum_{n=-\infty}^{0} \frac{1}{(-n)!} z^n$$

The behaviour of a function near an essential singularity is remarkably complicated. *Picard's theorem* states that, in any neighbourhood of an essential singularity, the function takes all possible complex values (possibly with one exception) at infinitely many points. (In the case of $f(z) = \mathrm{e}^{1/z}$, the exceptional value 0 is never attained.)

### 6.8.4 Behaviour at infinity

We can examine the behaviour of a function $f(z)$ as $z \to \infty$ by defining a new variable $\zeta = 1/z$ and a new function $g(\zeta) = f(z)$. Then $z = \infty$ maps to a single point $\zeta = 0$, the *point at infinity*.

If $g(\zeta)$ has a zero, pole or essential singularity at $\zeta = 0$, then we can say that $f(z)$ has the corresponding property at $z = \infty$.

Examples: $f_1(z) = \mathrm{e}^z = \mathrm{e}^{1/\zeta} = g_1(\zeta)$ has an essential singularity at $z = \infty$. $f_2(z) = z^2 = 1/\zeta^2 = g_2(\zeta)$ has a double pole at $z = \infty$. $f_3(z) = \mathrm{e}^{1/z} = \mathrm{e}^{\zeta} = g_3(\zeta)$ is analytic at $z = \infty$.

### 6.9 Convergence of power series

#### 6.9.1 Circle of convergence

If the power series

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n$$

converges for $z = z_1$, then it converges absolutely for all $z$ such that $|z - z_0| < |z_1 - z_0|$.

[Proof: The necessary condition for convergence, $\lim a_n(z_1 - z_0)^n = 0$, implies that $|a_n(z_1 - z_0)^n| < \epsilon$ for sufficiently large $n$, for any $\epsilon > 0$. Therefore $|a_n(z - z_0)^n| < \epsilon r^n$ for sufficiently large $n$, with $r = |(z - z_0)/(z_1 - z_0)| < 1$. By comparison with the geometric series $\sum r^n$, $\sum |a_n(z - z_0)^n|$ converges.]

It follows that, if the power series diverges for $z = z_2$, then it diverges for all $z$ such that $|z - z_0| > |z_2 - z_0|$.

Therefore the series converges for $|z - z_0| < R$ and diverges for $|z - z_0| > R$. $R$ is called the *radius of convergence* and may be zero (exceptionally), positive or infinite.

$|z - z_0| = R$ is the *circle of convergence*. The series converges inside it and diverges outside. On the circle, it may either converge or diverge.

### 6.9.2 Determination of the radius of convergence

The absolute ratio of successive terms in a power series is

$$r_n = \left| \frac{a_{n+1}}{a_n} \right| |z - z_0|$$

Suppose that $|a_{n+1}/a_n| \to L$ as $n \to \infty$. Then $r_n \to r = L|z - z_0|$. According to the ratio test, the series converges for $L|z - z_0| < 1$ and diverges for $L|z - z_0| > 1$. The radius of convergence is $R = 1/L$.

The same result, $R = 1/L$, follows from Cauchy's root test if instead $|a_n|^{1/n} \to L$ as $n \to \infty$.

The radius of convergence of the Taylor series of a function $f(z)$ about the point $z = z_0$ is equal to the distance of the nearest singular point of the function $f(z)$ from $z_0$. Since a convergent power series defines an analytic function, no singularity can lie inside the circle of convergence.

### 6.9.3 Examples

The following examples are generated from familiar Taylor series.

$$\ln(1 - z) = -z - \frac{z^2}{2} - \frac{z^3}{3} - \cdots = -\sum_{n=1}^{\infty} \frac{z^n}{n}$$

Here $|a_{n+1}/a_n| = n/(n + 1) \to 1$ as $n \to \infty$, so $R = 1$. The series converges for $|z| < 1$ and diverges for $|z| > 1$. (In fact, on the circle $|z| = 1$, the series converges except at the point $z = 1$.) The function has a singularity at $z = 1$ that limits the radius of convergence.

$$\arctan z = z - \frac{z^3}{3} + \frac{z^5}{5} - \frac{z^7}{7} + \cdots = z \sum_{n=0}^{\infty} \frac{1}{2n + 1} (-z^2)^n$$

Thought of as a power series in $(-z^2)$, this has $|a_{n+1}/a_n| = (2n + 1)/(2n + 3) \to 1$ as $n \to \infty$. Therefore $R = 1$ in terms of $(-z^2)$. But

since $|-z^2| = 1$ is equivalent to $|z| = 1$, the series converges for $|z| < 1$ and diverges for $|z| > 1$.

$$e^z = 1 + z + \frac{z^2}{2} + \frac{z^3}{6} + \cdots = \sum_{n=0}^{\infty} \frac{z^n}{n!}$$

Here $|a_{n+1}/a_n| = 1/(n + 1) \to 0$ as $n \to \infty$, so $R = \infty$. The series converges for all $z$; this is an entire function.

# 7 Ordinary differential equations

## 7.1 Motivation

Very many scientific problems are described by differential equations. Even if these are partial differential equations, they can often be reduced to ordinary differential equations (ODEs), e.g. by the method of separation of variables.

The ODEs encountered most frequently are linear and of either first or second order. In particular, second-order equations describe oscillatory phenomena.

Part IA dealt with first-order ODEs and also with linear second-order ODEs with constant coefficients. Here we deal with general linear second-order ODEs.

The general linear inhomogeneous first-order ODE

$$y'(x) + p(x)y(x) = f(x)$$

can be solved using the integrating factor $g = \exp \int p \, dx$ to obtain the general solution

$$y = \frac{1}{g} \int g f \, dx$$

Provided that the integrals can be evaluated, the problem is completely solved. An equivalent method does not exist for second-order ODEs, but an extensive theory can still be developed.

## 7.2 Classification

The general second-order ODE is an equation of the form

$$F(y'', y', y, x) = 0$$

for an unknown function $y(x)$, where $y' = dy/dx$ and $y'' = d^2y/dx^2$.

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The general linear second-order ODE has the form

$$Ly = f$$

where $L$ is a linear operator such that

$$Ly = ay'' + by' + cy$$

where $a, b, c, f$ are functions of $x$.

The equation is *homogeneous* (unforced) if $f = 0$, otherwise it is *inhomogeneous* (forced).

The principle of superposition applies to linear ODEs as to all linear equations.

Although the solution may be of interest only for real $x$, it is often informative to analyse the solution in the complex domain.

## 7.3 Homogeneous linear second-order ODEs

### 7.3.1 Linearly independent solutions

Divide through by the coefficient of $y''$ to obtain a standard form

$$\boxed{y''(x) + p(x)y'(x) + q(x)y(x) = 0}$$

Suppose that $y_1(x)$ and $y_2(x)$ are two solutions of this equation. They are *linearly independent* if

$$Ay_1(x) + By_2(x) = 0 \quad \text{(for all } x\text{)} \qquad \text{implies} \quad A = B = 0$$

i.e. if one is not simply a constant multiple of the other.

If $y_1(x)$ and $y_2(x)$ are linearly independent solutions, then the *general solution* of the ODE is

$$y(x) = Ay_1(x) + By_2(x)$$

where $A$ and $B$ are arbitrary constants. There are two arbitrary constants because the equation is of second order.

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### 7.3.2 The Wronskian

The *Wronskian* $W(x)$ of two solutions $y_1(x)$ and $y_2(x)$ of a second-order ODE is the determinant of the Wronskian matrix:

$$W[y_1, y_2] = \begin{vmatrix} y_1 & y_2 \\ y_1' & y_2' \end{vmatrix} = y_1 y_2' - y_2 y_1'$$

Suppose that $Ay_1(x) + By_2(x) = 0$ in some interval of $x$. Then also $Ay_1'(x) + By_2'(x) = 0$, and so

$$\begin{bmatrix} y_1 & y_2 \\ y_1' & y_2' \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

If this is satisfied for non-trivial $A$, $B$ then $W = 0$ (in that interval of $x$). Therefore the solutions are linearly independent if $W \neq 0$.

### 7.3.3 Calculation of the Wronskian

Consider

$$\begin{aligned} W' &= y_1 y_2'' - y_2 y_1'' \\ &= y_1(-py_2' - qy_2) - y_2(-py_1' - qy_1) \\ &= -pW \end{aligned}$$

since both $y_1$ and $y_2$ solve the ODE. This first-order ODE for $W$ has the solution

$$W = \exp\left(-\int p \, \mathrm{d}x\right)$$

This expression involves an indefinite integral and could be written more fussily as

$$W(x) = \exp\left[-\int^x p(\xi) \, \mathrm{d}\xi\right]$$

Notes:

- the indefinite integral involves an arbitrary additive constant, so $W$ involves an arbitrary multiplicative constant

- apart from that, $W$ is the same for any two solutions $y_1$ and $y_2$

- $W$ is therefore an intrinsic property of the ODE

- if $W \neq 0$ for one value of $x$ (and $p$ is integrable) then $W \neq 0$ for all $x$, so linear independence need be checked at only one value of $x$

### 7.3.4 Finding a second solution

Suppose that one solution $y_1(x)$ is known. Then a second solution $y_2(x)$ can be found as follows.

First find $W$ as described above. The definition of $W$ then provides a first-order linear ODE for the unknown $y_2$:

$$y_1 y_2' - y_2 y_1' = W$$

$$\frac{y_2'}{y_1} - \frac{y_2 y_1'}{y_1^2} = \frac{W}{y_1^2}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{y_2}{y_1}\right) = \frac{W}{y_1^2}$$

$$y_2 = y_1 \int \frac{W}{y_1^2} \, \mathrm{d}x$$

Again, this result involves an indefinite integral and could be written more fussily as

$$y_2(x) = y_1(x) \int^x \frac{W(\xi)}{[y_1(\xi)]^2} \, \mathrm{d}\xi$$

Notes:

- the indefinite integral involves an arbitrary additive constant, since any amount of $y_1$ can be added to $y_2$

- $W$ involves an arbitrary multiplicative constant, since $y_2$ can be multiplied by any constant

- this expression for $y_2$ therefore provides the general solution of the ODE

Example . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Given that $y = x^n$ is a solution of $x^2 y'' - (2n-1)xy' + n^2 y = 0$, find the general solution.* Standard form

$$y'' - \left(\frac{2n-1}{x}\right)y' + \left(\frac{n^2}{x^2}\right)y = 0$$

Wronskian

$$W = \exp\left(-\int p\,\mathrm{d}x\right) = \exp\int\left(\frac{2n-1}{x}\right)\mathrm{d}x$$

$$= \exp\left[(2n-1)\ln x + \text{constant}\right]$$

$$= A x^{2n-1}$$

Second solution

$$y_2 = y_1 \int \frac{W}{y_1^2}\,\mathrm{d}x = x^n\left(\int A x^{-1}\,\mathrm{d}x\right)$$

$$= A x^n \ln x + B x^n$$

. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

The same result can be obtained by writing $y_2(x) = y_1(x)u(x)$ and obtaining a first-order linear ODE for $u'$. This method applies to higher-order linear ODEs and is reminiscent of the factorization of polynomial equations.

## 7.4 Series solutions

### 7.4.1 Ordinary and singular points

We consider a homogeneous linear second-order ODE in standard form:

$$y''(x) + p(x)y'(x) + q(x)y(x) = 0$$

A point $x = x_0$ is an *ordinary point* of the ODE if:

$$p(x) \text{ and } q(x) \text{ are both analytic at } x = x_0$$

Otherwise it is a *singular point*.

A singular point $x = x_0$ is *regular* if:

$$(x - x_0)p(x) \text{ and } (x - x_0)^2 q(x) \text{ are both analytic at } x = x_0$$

Example . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Identify the singular points of Legendre's equation*

$$(1 - x^2)y'' - 2xy' + \ell(\ell + 1)y = 0$$

*where $\ell$ is a constant, and determine their nature.* Divide through by $(1 - x^2)$ to obtain the standard form with

$$p(x) = -\frac{2x}{1 - x^2}, \qquad q(x) = \frac{\ell(\ell + 1)}{1 - x^2}$$

Both $p(x)$ and $q(x)$ are analytic for all $x$ except $x = \pm 1$. These are the singular points. They are both regular:

$$(x - 1)p(x) = \frac{2x}{1 + x}, \qquad (x - 1)^2 q(x) = \ell(\ell + 1)\left(\frac{1 - x}{1 + x}\right)$$

are both analytic at $x = 1$, and similarly for $x = -1$. . . . . . . . . . . . . . .

### 7.4.2 Series solutions about an ordinary point

Wherever $p(x)$ and $q(x)$ are analytic, the ODE has two linearly independent solutions that are also analytic. If $x = x_0$ is an ordinary point, the ODE has two linearly independent solutions of the form

$$y = \sum_{n=0}^{\infty} a_n (x - x_0)^n$$

The coefficients $a_n$ can be determined by substituting the series into the ODE and comparing powers of $(x - x_0)$. The radius of convergence of the series solutions is the distance to the nearest singular point of the ODE in the complex plane.

Since $p(x)$ and $q(x)$ are analytic at $x = x_0$,

$$p(x) = \sum_{n=0}^{\infty} p_n (x - x_0)^n, \qquad q(x) = \sum_{n=0}^{\infty} q_n (x - x_0)^n$$

inside some circle centred on $x = x_0$. Let

$$y = \sum_{n=0}^{\infty} a_n (x - x_0)^n$$

$$y' = \sum_{n=0}^{\infty} n a_n (x - x_0)^{n-1} = \sum_{n=0}^{\infty} (n+1) a_{n+1} (x - x_0)^n$$

$$y'' = \sum_{n=0}^{\infty} n(n-1) a_n (x - x_0)^{n-2} = \sum_{n=0}^{\infty} (n+2)(n+1) a_{n+2} (x - x_0)^n$$

Note the following rule for multiplying power series:

$$pq = \sum_{\ell=0}^{\infty} p_\ell (x - x_0)^\ell \sum_{m=0}^{\infty} q_m (x - x_0)^m$$

$$= \sum_{n=0}^{\infty} \left[ \sum_{r=0}^{n} p_{n-r} q_r \right] (x - x_0)^n$$

Thus

$$py' = \sum_{n=0}^{\infty} \left[ \sum_{r=0}^{n} p_{n-r} (r+1) a_{r+1} \right] (x - x_0)^n$$

$$qy = \sum_{n=0}^{\infty} \left[ \sum_{r=0}^{n} q_{n-r} a_r \right] (x - x_0)^n$$

The coefficient of $(x - x_0)^n$ in the ODE $y'' + py' + qy = 0$ is therefore

$$(n+2)(n+1) a_{n+2} + \sum_{r=0}^{n} p_{n-r} (r+1) a_{r+1} + \sum_{r=0}^{n} q_{n-r} a_r = 0$$

This is a *recurrence relation* that determines $a_{n+2}$ (for $n \geqslant 0$) in terms of the preceding coefficients $a_0, a_1, \ldots, a_{n+1}$. The first two coefficients $a_0$ and $a_1$ are not determined: they are the two arbitrary constants in the general solution.

The above procedure is rarely followed in practice. If $p$ and $q$ are *rational functions* (i.e. ratios of polynomials) it is a much better idea to multiply the ODE through by a suitable factor to clear denominators *before* substituting in the power series for $y$, $y'$ and $y''$.

*Example* ............................................................

▷ *Find series solutions about $x = 0$ of Legendre's equation*

$$(1 - x^2) y'' - 2xy' + \ell(\ell + 1) y = 0$$

$x = 0$ is an ordinary point, so let

$$y = \sum_{n=0}^{\infty} a_n x^n, \qquad y' = \sum_{n=0}^{\infty} n a_n x^{n-1}, \qquad y'' = \sum_{n=0}^{\infty} n(n-1) a_n x^{n-2}$$

Substitute these expressions into the ODE to obtain

$$\sum_{n=0}^{\infty} n(n-1) a_n x^{n-2} + \sum_{n=0}^{\infty} \left[ -n(n-1) - 2n + \ell(\ell+1) \right] a_n x^n = 0$$

The coefficient of $x^n$ (for $n \geqslant 0$) is

$$(n+1)(n+2)a_{n+2} + \left[-n(n+1) + \ell(\ell+1)\right]a_n = 0$$

The recurrence relation is therefore

$$\frac{a_{n+2}}{a_n} = \frac{n(n+1) - \ell(\ell+1)}{(n+1)(n+2)} = \frac{(n-\ell)(n+\ell+1)}{(n+1)(n+2)}$$

$a_0$ and $a_1$ are the arbitrary constants. The other coefficients follow from the recurrence relation. .............................................

Notes:

- an even solution is obtained by choosing $a_0 = 1$ and $a_1 = 0$

- an odd solution is obtained by choosing $a_0 = 0$ and $a_1 = 1$

- these solutions are obviously linearly independent since one is not a constant multiple of the other

- since $|a_{n+2}/a_n| \to 1$ as $n \to \infty$, the even and odd series converge for $|x^2| < 1$, i.e. for $|x| < 1$

- the radius of convergence is the distance to the singular points of Legendre's equation at $x = \pm 1$

- if $\ell \geqslant 0$ is an even integer, then $a_{\ell+2}$ and all subsequent even coefficients vanish, so the even solution is a *polynomial* (terminating power series) of degree $\ell$

- if $\ell \geqslant 1$ is an odd integer, then $a_{\ell+2}$ and all subsequent odd coefficients vanish, so the odd solution is a polynomial of degree $\ell$

The polynomial solutions are called *Legendre polynomials*, $P_\ell(x)$. They are conventionally normalized (i.e. $a_0$ or $a_1$ is chosen) such that $P_\ell(1) = 1$, e.g.

$$P_0(x) = 1, \qquad P_1(x) = x, \qquad P_2(x) = \tfrac{1}{2}(3x^2 - 1)$$
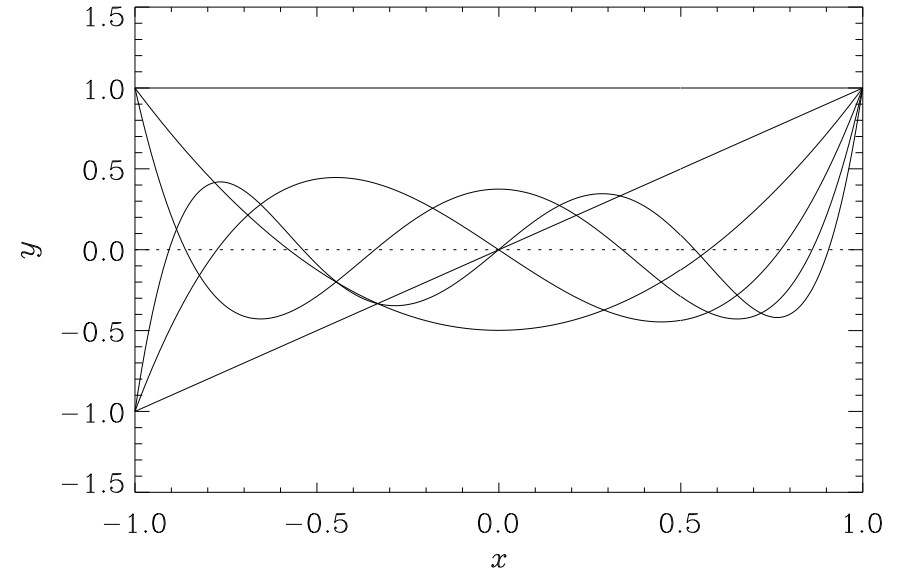


### 7.4.3 Series solutions about a regular singular point

If $x = x_0$ is a regular singular point, *Fuchs's theorem* guarantees that the ODE has at least one solution of the form

$$\boxed{y = \sum_{n=0}^{\infty} a_n (x - x_0)^{n+\sigma}, \qquad a_0 \neq 0}$$

i.e. a Taylor series multiplied by a power $(x - x_0)^\sigma$, where the index $\sigma$ is a (generally complex) number to be determined.

Notes:

- this is a Taylor series only if $\sigma$ is a non-negative integer

- there may be one or two solutions of this form (see below)

- the condition $a_0 \neq 0$ is required to define $\sigma$ uniquely

To understand in simple terms why the solutions behave in this way, recall that

$$P(x) \equiv (x - x_0)p(x) = \sum_{n=0}^{\infty} P_n(x - x_0)^n$$

$$Q(x) \equiv (x - x_0)^2 q(x) = \sum_{n=0}^{\infty} Q_n(x - x_0)^n$$

are analytic at the regular singular point $x = x_0$. Near $x = x_0$ the ODE can be approximated using the leading approximations to $p$ and $q$:

$$y'' + \frac{P_0 y'}{x - x_0} + \frac{Q_0 y}{(x - x_0)^2} \approx 0$$

The exact solutions of this approximate equation are of the form $y = (x - x_0)^\sigma$, where $\sigma$ satisfies the *indicial equation*

$$\sigma(\sigma - 1) + P_0 \sigma + Q_0 = 0$$

with two (generally complex) roots. [If the roots are equal, the solutions are $(x - x_0)^\sigma$ and $(x - x_0)^\sigma \ln(x - x_0)$.] It is reasonable that the solutions of the full ODE should resemble the solutions of the approximate ODE near the singular point.

*Frobenius's method* is used to find the series solutions about a regular singular point. This is best demonstrated by example.

*Example* . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .

▷ *Find series solutions about $x = 0$ of Bessel's equation*

$$x^2 y'' + x y' + (x^2 - \nu^2) y = 0$$

*where $\nu$ is a constant.* $x = 0$ is a regular singular point because $p = 1/x$ and $q = 1 - \nu^2/x^2$ are singular there but $xp = 1$ and $x^2 q = x^2 - \nu^2$ are both analytic there.

Seek a solution of the form

$$y = \sum_{n=0}^{\infty} a_n x^{n+\sigma}, \qquad a_0 \neq 0$$

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Then

$$y' = \sum_{n=0}^{\infty} (n + \sigma) a_n x^{n+\sigma-1},$$

$$y'' = \sum_{n=0}^{\infty} (n + \sigma)(n + \sigma - 1) a_n x^{n+\sigma-2}$$

Bessel's equation requires

$$\sum_{n=0}^{\infty} \left[ (n + \sigma)(n + \sigma - 1) + (n + \sigma) - \nu^2 \right] a_n x^{n+\sigma} + \sum_{n=0}^{\infty} a_n x^{n+\sigma+2} = 0$$

Relabel the second series:

$$\sum_{n=0}^{\infty} \left[ (n + \sigma)^2 - \nu^2 \right] a_n x^{n+\sigma} + \sum_{n=2}^{\infty} a_{n-2} x^{n+\sigma} = 0$$

Now compare powers of $x^{n+\sigma}$:

$$n = 0: \qquad \left[ \sigma^2 - \nu^2 \right] a_0 = 0 \tag{1}$$

$$n = 1: \qquad \left[ (1 + \sigma)^2 - \nu^2 \right] a_1 = 0 \tag{2}$$

$$n \geqslant 2: \qquad \left[ (n + \sigma)^2 - \nu^2 \right] a_n + a_{n-2} = 0 \tag{3}$$

Since $a_0 \neq 0$ by assumption, equation (1) provides the *indicial equation*

$$\sigma^2 - \nu^2 = 0$$

with roots $\sigma = \pm\nu$. Equation (2) then requires that $a_1 = 0$ (except possibly in the case $\nu = \pm\frac{1}{2}$, but even then $a_1$ can be *chosen* to be 0). Equation (3) provides the *recurrence relation*

$$a_n = -\frac{a_{n-2}}{n(n + 2\sigma)}$$

Since $a_1 = 0$, all the odd coefficients vanish. Since $|a_n/a_{n-2}| \to 0$ as $n \to \infty$, the radius of convergence of the series is infinite.

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For most values of $\nu$ we therefore obtain two linearly independent solutions (choosing $a_0 = 1$):

$$y_1 = x^\nu \left[ 1 - \frac{x^2}{4(1+\nu)} + \frac{x^4}{32(1+\nu)(2+\nu)} + \cdots \right]$$

$$y_2 = x^{-\nu} \left[ 1 - \frac{x^2}{4(1-\nu)} + \frac{x^4}{32(1-\nu)(2-\nu)} + \cdots \right]$$

However, if $\nu = 0$ there is clearly only one solution of this form. Furthermore, if $\nu$ is a non-zero integer one of the recurrence relations will fail at some point and the corresponding series is invalid. In these cases the second solution is of a different form (see below). ................

A general analysis shows that:

- *if the roots of the indicial equation are equal*, there is only one solution of the form $\sum a_n (x - x_0)^{n+\sigma}$

- *if the roots differ by an integer*, there is generally only one solution of this form because the recurrence relation for the smaller value of $\mathrm{Re}(\sigma)$ will usually (but not always) fail

- otherwise, there are two solutions of the form $\sum a_n (x - x_0)^{n+\sigma}$

- the radius of convergence of the series is the distance from the point of expansion to the nearest singular point of the ODE

If the roots $\sigma_1, \sigma_2$ of the indicial equation are equal or differ by an integer, one solution is of the form

$$y_1 = \sum_{n=0}^{\infty} a_n (x - x_0)^{n+\sigma_1}, \qquad \mathrm{Re}(\sigma_1) \geqslant \mathrm{Re}(\sigma_2)$$

and the other is of the form

$$y_2 = \sum_{n=0}^{\infty} b_n (x - x_0)^{n+\sigma_2} + c y_1 \ln(x - x_0)$$

The coefficients $b_n$ and $c$ can be determined (with some difficulty) by substituting this form into the ODE and comparing coefficients of $(x - x_0)^n$ and $(x - x_0)^n \ln(x - x_0)$. In exceptional cases $c$ may vanish.

Alternatively, $y_2$ can be found (also with some difficulty) using the Wronskian method (section 7.3.4).

Example: Bessel's equation of order $\nu = 0$:

$$y_1 = 1 - \frac{x^2}{4} + \frac{x^4}{64} + \cdots$$

$$y_2 = y_1 \ln x + \frac{x^2}{4} - \frac{3x^4}{128} + \cdots$$

Example: Bessel's equation of order $\nu = 1$:

$$y_1 = x - \frac{x^3}{8} + \frac{x^5}{192} + \cdots$$

$$y_2 = y_1 \ln x - \frac{2}{x} + \frac{3x^3}{32} + \cdots$$

These examples illustrate a feature that is commonly encountered in scientific applications: one solution is regular (i.e. analytic) and the other is singular. Usually only the regular solution is an acceptable solution of the scientific problem.

### 7.4.4 Irregular singular points

If either $(x - x_0)p(x)$ or $(x - x_0)^2 q(x)$ is not analytic at the point $x = x_0$, it is an *irregular* singular point of the ODE. The solutions can have worse kinds of singular behaviour there.

Example: the equation $x^4 y'' + 2x^2 y' - y = 0$ has an irregular singular point at $x = 0$. Its solutions are $\exp(\pm x^{-1})$, both of which have an essential singularity at $x = 0$.

In fact this example is just the familiar equation $\mathrm{d}^2 y / \mathrm{d}z^2 = y$ with the substitution $x = 1/z$. Even this simple ODE has an irregular singular point at $z = \infty$.