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

where

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 δt 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*

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

where ϵ is a positive parameter. This function can also be written as

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,

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

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. So we should think of $\delta(x)$ as a *mapping* between a function f and a number. Specifically, the unit spike 'picks out' the value of the function f at the location of the spike. It also follows that

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 'sampling' property is as follows. Consider a continuous function $f(x)$ with indefinite integral $g(x)$, i.e. $f(x) = g'(x)$. Then

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

From the definition of the derivative,

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

as required.

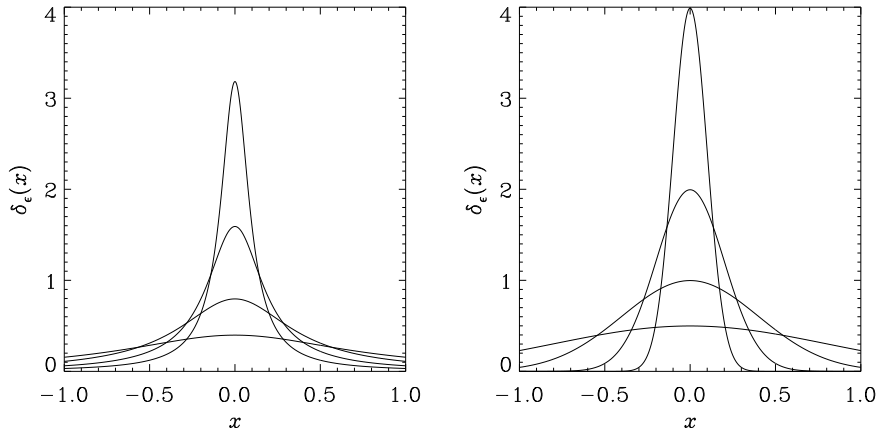
This result (the boxed formula above) is equivalent to the *substitution property* of the Kronecker delta:

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

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

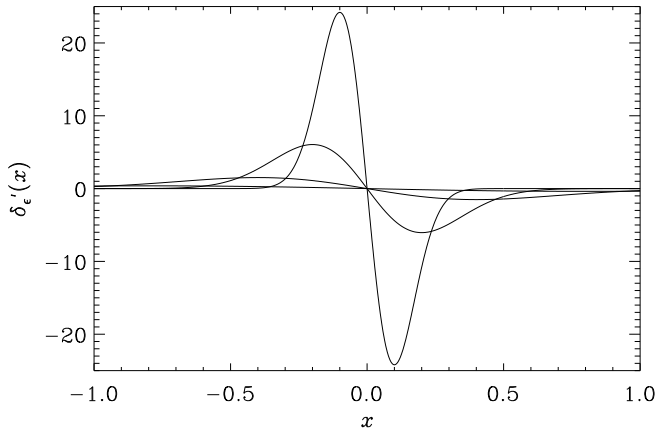
and



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

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

(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?

Consider integrating equation (1) from $x = -\epsilon$ to $x = \epsilon$

and letting $\epsilon \to 0$. If we assume y is bounded the integral term makes no contribution and we get

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

Since y is 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

and

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

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 $y_\mathrm{p}(x)$ is *any* solution of the inhomogeneous equation, i.e. $Ly_\mathrm{p} = f$, then the general solution of the inhomogeneous equation is

since

$$Ly = ALy_1 + BLy_2 + Ly_p$$
$$= $$

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 equa-

tion 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 α_1, α_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

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

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

(3)

subject to the homogeneous BCs

(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

(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 ξ 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:

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

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

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

So

. . . . . .

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

$$\tag{4}$$

$$\tag{5}$$

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

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 as linear combinations of y_1 and y_2.) Since the right-hand side of equation (3) vanishes for $x < \xi$ and $x > \xi$ separately, the solution must be of the form

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

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

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.

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

$$W = y_a y_b' - y_b y_a' =$$

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

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

$$=$$

. . . . . .

3.6 Unlectured remarks

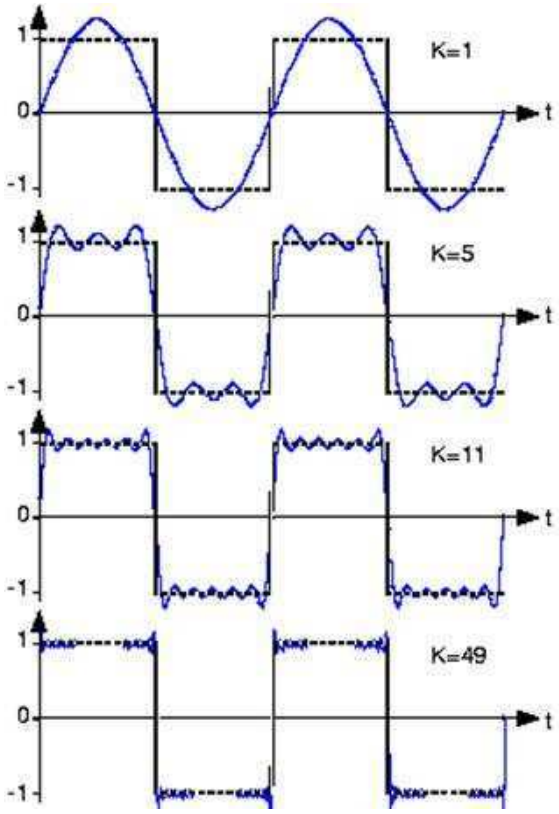
1. Note that the solution y to a 2nd order differential equation of the form $Ly(x) = \delta(x - x_0)$ is continuous because of the properties of the Dirac δ-function, specifically because its integral is finite (assuming the limits of integration include x_0).

2. So far we only considered problems with homogeneous boundary conditions. One can also use Green's functions to solve problems with inhomogeneous boundary conditions. The trick is to solve the homogenous equation $Ly_p = 0$ for a function y_p which satisfies the *inhomogenous* boundary condtions. Then solve the inhomogeneous equation $Ly_g = f$, perhaps using the Green's function method discussed in this chapter, imposing *homogenous* boundary conditions on y_g. Then linearity means that $y_p + y_g$ satisfies the inhomogenous equation with inhomogenous boundary conditions.

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 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*

where

is the wavenumber of the nth 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

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*

where, after multiplying the preceding equation by $\exp(-\mathrm{i}k_m x)$ and integrating we find (recall $k_m = 2\pi m/P$)

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

This expression for c_m (equivalently c_n, relabelling $m \to n$) 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.

4.3 Approaching the Fourier transform

Let $P \to \infty$ so that the function $f(x)$ above is defined on the entire real line without any periodicity. The discrete wavenumbers $k_n = 2\pi n/P$ are replaced by a continuous variable k, because

Consider the definition of the Fourier series

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

In the limit of $P \to \infty$ this looks like the Riemann definition of an integral over k.

In this limit, $P \to \infty$

And thus

$$f(x) \to \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(k) \mathrm{e}^{\mathrm{i}kx} dk$$

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

and the *inverse Fourier transform* (Fourier synthesis)

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 ω rather than x and k (time $\leftrightarrow$ angular frequency vs. position $\leftrightarrow$ wavenumber)

- 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 2. *Several different definitions of the Fourier transform are in use. They differ in the placement of the 2π factor and in the signs of the exponents. The definition used here is probably the most conventional.*

How to remember this convention:

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

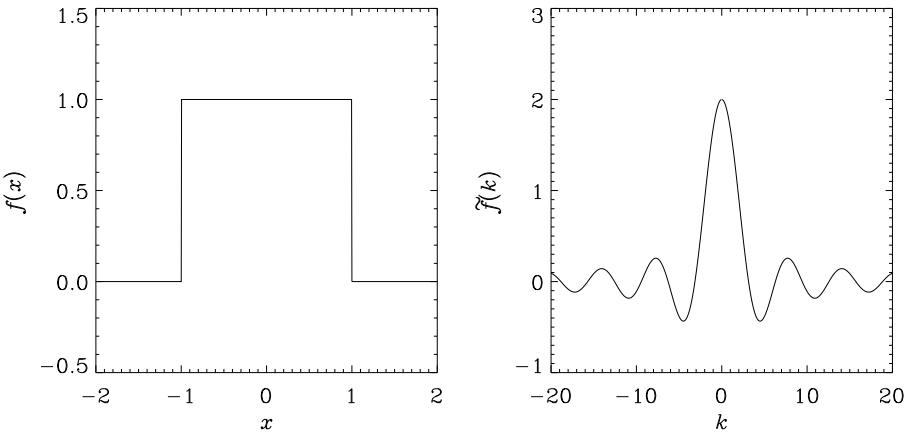
- the inverse transform means that the function $f(x)$ is synthesized from a linear combination of basis functions $\mathrm{e}^{\mathrm{i}kx}$
- the division by 2π always accompanies integration with respect to k

4.4 Examples

Example (1): top-hat function:

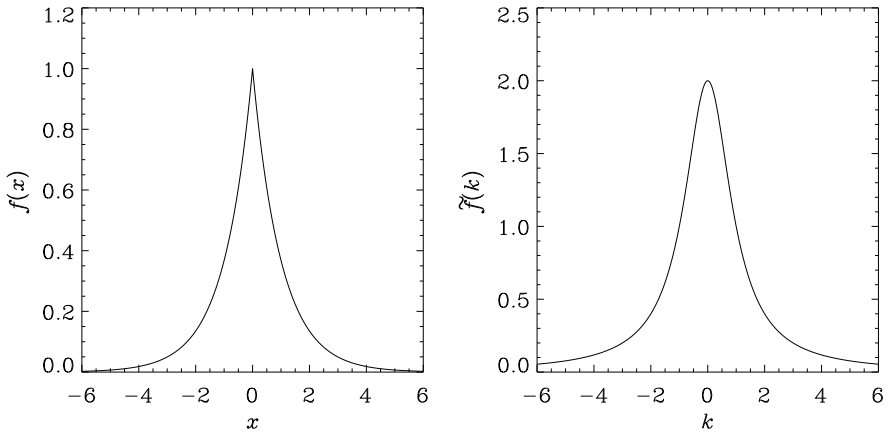
$$f(x) = \begin{cases} c, & a < x < b \\ 0, & \text{otherwise} \end{cases}$$

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



Example (2):

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



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

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

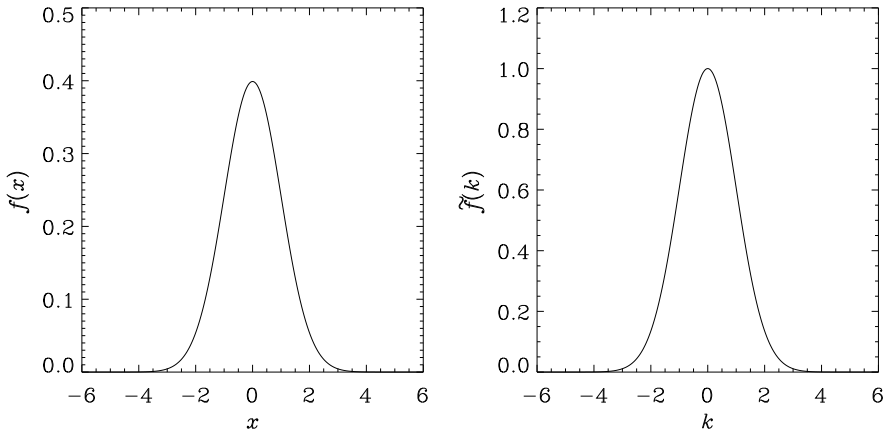
Change variable to

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

so that

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

Then



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) σ_k related to σ_x by

$$\sigma_k = \frac{1}{\sigma_x}$$

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

4.5 Basic properties of the Fourier transform

Linearity:

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

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

Rescaling (for real α):

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

Shift/exponential (for real α):

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

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

Differentiation/multiplication:

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

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

Duality:

$$g(x) = \tilde{f}(x) \qquad \Leftrightarrow \qquad \tilde{g}(k) = 2\pi f(-k) \tag{8}$$

i.e. transforming twice returns (almost) the same function

Complex conjugation and parity inversion (for real x and k):

$$g(x) = [f(x)]^* \qquad \Leftrightarrow \qquad \tilde{g}(k) = [\tilde{f}(-k)]^* \tag{9}$$

Symmetry:

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

Sample derivations: property (3):

Property (4):

Property (6):

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):

Property (8):

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

4.6 The delta function and the Fourier transform

Consider the Gaussian function of example (3):

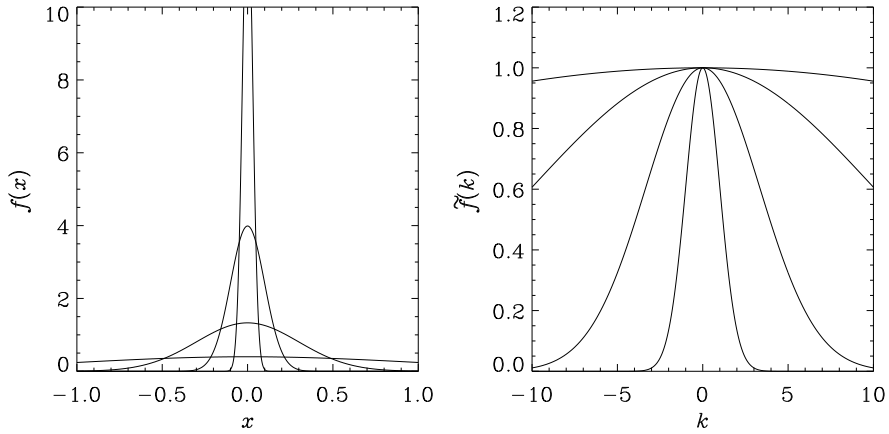
$$f(x) = (2\pi\sigma_x^2)^{-1/2} \exp\left(-\frac{x^2}{2\sigma_x^2}\right)$$

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

The Gaussian is normalized such that

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

As the width σ_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 f approaches the Dirac delta function, $\delta(x)$.

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

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

Now formally apply the inverse transform:

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

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

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.

4.7 The convolution theorem

4.7.1 Definition of convolution

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

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

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

4.7.2 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 δx.

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 $h(z)$. (E.g. let y be the height of a pair of shoes drawn at random. Then z is the height of a random person while wearing a random pair of shoes.)

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

which is $g(z_0 - x)\delta z$. That's for a fixed x. But the probability that z lies in this same range *for all* x is then

which implies

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 $\Phi_p(\boldsymbol{r}) = -GM/|\boldsymbol{r} - \boldsymbol{R}|$. A continuous mass density $\rho(\boldsymbol{r})$ can be thought

of as a sum of infinitely many point masses $\rho(\boldsymbol{R})\,\mathrm{d}^3\boldsymbol{R}$ at positions $\boldsymbol{R}$. The resulting gravitational potential is

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

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

4.7.3 The convolution theorem

The Fourier transform of a convolution is

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.

4.7.4 Correlation

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

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.

For example, consider an array of microphones that if fed a signal $f(y)$ outputs a signal $g(y)$ that is identical to f except for a small unknown time delay α. By computing the correlation $h(x)$ we can find out what the time delay is.

Let $f(y)$ be the real part of the localised signal $\mathrm{e}^{\mathrm{i}ky-y^2}$. The correlation is then

The maximum of h occurs when $x = \alpha$.

The Fourier transform of a correlation is

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.

4.8 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 $g = f$:

Note that division by 2π 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:

4.9 Power spectra

The quantity

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

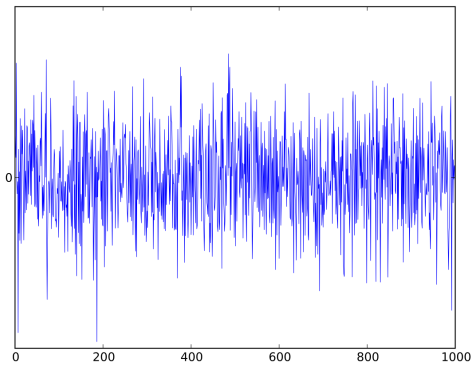
appearing in the Wiener–Khinchin theorem and Parseval's theorem is the *(power) spectrum* or *(power) spectral density* of the function $f(x)$. The WK theorem states that the FT of the autocorrelation function is the power spectrum.

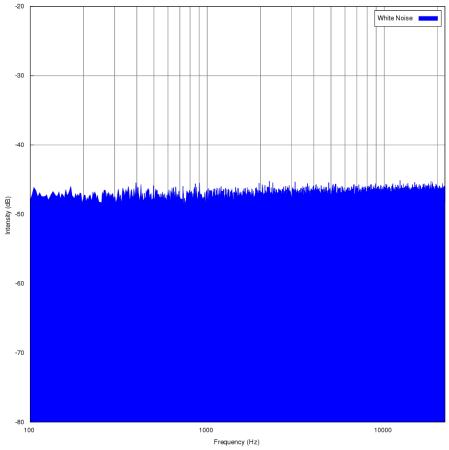
This concept is often used to quantify the spectral content (as a function of angular frequency ω) of a signal $f(t)$.

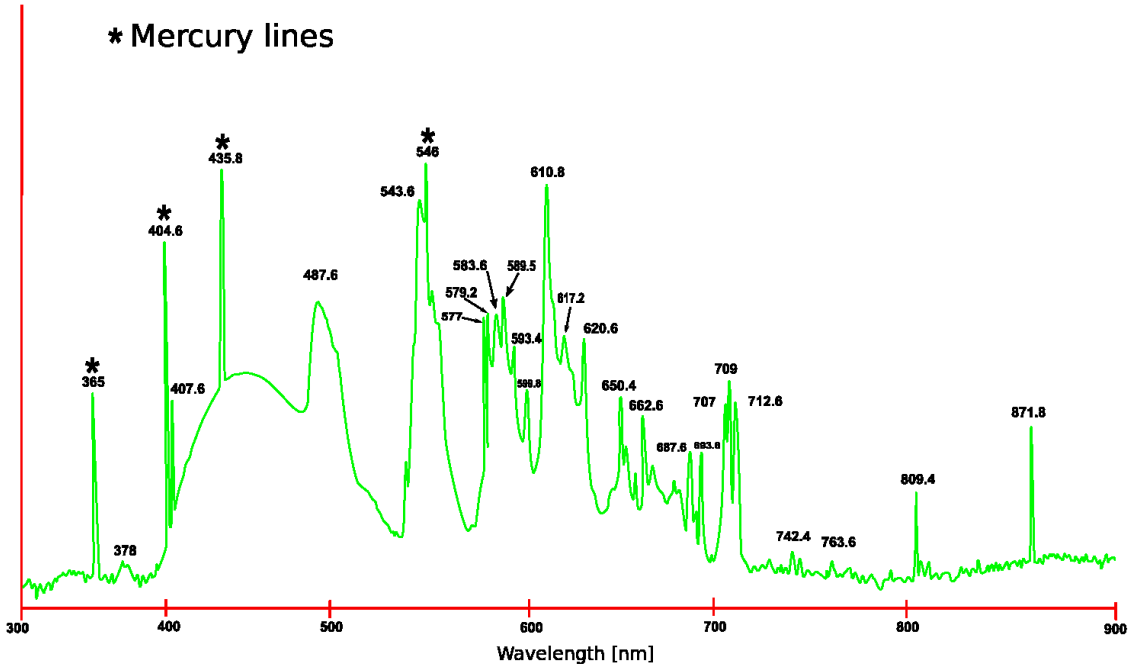
The spectrum of a perfectly periodic signal consists of a series of delta functions at the principal frequency and its harmonics, if present. Its autocorrelation function does not decay as $t \to \infty$.

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

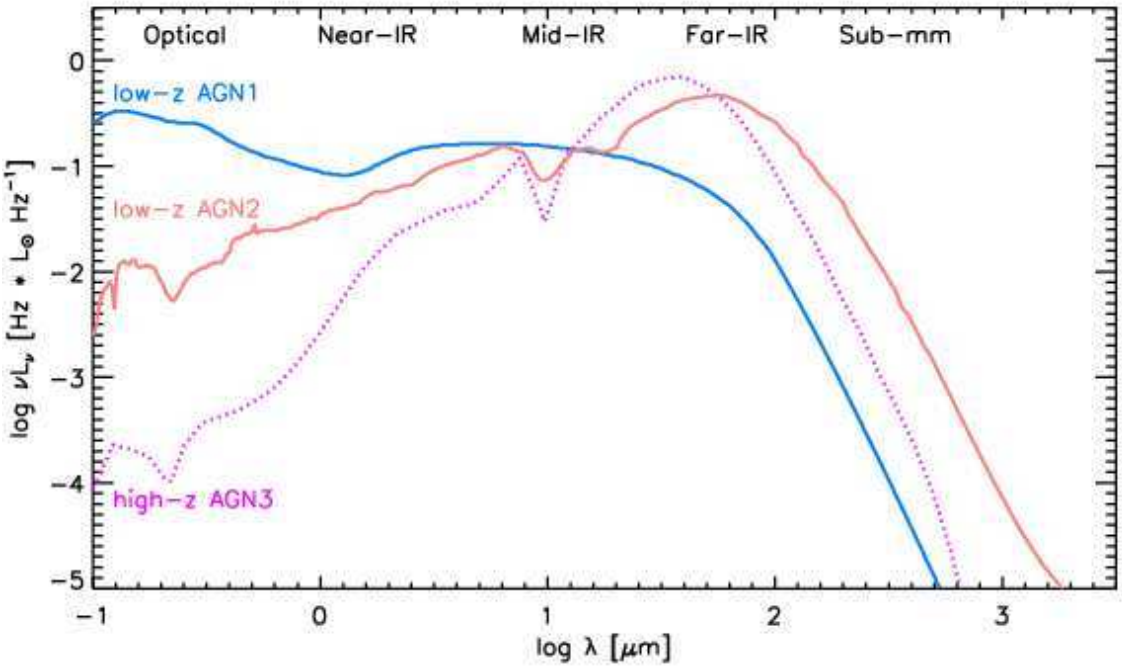
Less idealized signals may have spectra that are peaked at certain frequencies but also contain a general noise component.







Spectrum from a 48" Philips F32T8 natural sunshine fluorescent light



Spectrum of three active galactic nuclei at different red shifts

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:

•

•

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 α 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:

Hence we have $\mathbb{R}^n$ and $\mathbb{C}^n$.

Notes:

- vector multiplication is not defined in general
- $\mathbb{R}^2$ is not quite the same as $\mathbb{C}$ because $\mathbb{C}$ has a rule for multiplication
- $\mathbb{R}^3$ is not quite the same as physical space because physical space has a rule for the distance between two points (i.e. Pythagoras's theorem, if physical space is approximated as Euclidean)

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

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:

Linear independence therefore means that none of the vectors is a linear combination of the others.

Notes:

- if an additional vector is included in 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 of V 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 be written in a unique way as

  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

Here $f(x)$ is the 'vector' and f_n are its 'components' with respect to the 'basis' of functions $\mathrm{e}^{\mathrm{i}nx}$. *Functional analysis* deals with such infinite-dimensional vector spaces.

5.2.4 Examples

▷ Example (1): three-dimensional real space, $\mathbb{R}^3$:

vectors: triples (x, y, z) of real numbers

possible basis: $\{(1, 0, 0), (0, 1, 0), (0, 0, 1)\}$

▷ Example (2): the complex plane, $\mathbb{C}$:

vectors: complex numbers z

EITHER (a) a one-dimensional vector space over $\mathbb{C}$

possible basis: $\{1\}$

OR (b) a two-dimensional vector space over $\mathbb{R}$ (supplemented by a multiplication rule)

possible basis: $\{1, \mathrm{i}\}$

▷ Example (3): real 2×2 symmetric matrices:

vectors: matrices of the form

$$\begin{bmatrix} x & y \\ y & z \end{bmatrix}, \qquad x, y, z \in \mathbb{R}$$

three-dimensional vector space over $\mathbb{R}$

possible basis:

$$\left\{ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \right\}$$

5.2.5 Change of basis

The same vector has different components with respect to different bases. Consider two bases $\{\boldsymbol{e}_i\}$ and $\{\boldsymbol{e}'_i\}$. 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):

The $n \times n$ array of numbers R_{ij} is the *transformation matrix* between the two bases. R_{ij} is the ith component of the vector $\boldsymbol{e}_j$ with respect to the primed basis.

The representation of a vector $\boldsymbol{x}$ in the two bases is

$$\boldsymbol{x} = \boldsymbol{e}_j x_j = \boldsymbol{e}'_i x'_i$$

where x_i and x'_i are the components. Thus

$$\boldsymbol{e}'_i x'_i = \boldsymbol{e}_j x_j = \boldsymbol{e}'_i R_{ij} x_j$$

from which we deduce the transformation law for vector components:

Note that the transformation laws for basis vectors and vector components are 'opposite' so that the vector $\boldsymbol{x}$ is unchanged by the transformation.

Example: in $\mathbb{R}^3$, two bases are $\{\boldsymbol{e}_i\} = \{(1,0,0),(0,1,0),(0,0,1)\}$ and $\{\boldsymbol{e}'_i\} = \{(0,1,0),(0,0,1),(1,0,0)\}$. 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:

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:

The superscript 'T' denotes the *transpose*. In the typed notes, we will use sans serif fonts (A, x) to denote matrices, to distinguish them from linear operators and vectors (see next subsection) which we will denote with bold fonts ($\mathbf{A}$, $\boldsymbol{x}$). In handwritten notes, I will do my best to draw a distinction where one is necessary.

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

and the rules for matrix addition and multiplication are

The transpose of an $m \times n$ matrix is the $n \times m$ matrix

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:

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 those basis vectors:

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 $\boldsymbol{x}$:

$$\mathbf{A}\boldsymbol{x} = \mathbf{A}(\boldsymbol{e}_j x_j) = x_j(\mathbf{A}\boldsymbol{e}_j) = x_j(\boldsymbol{e}_i A_{ij}) = \boldsymbol{e}_i A_{ij} x_j$$

or

This corresponds to the rule for multiplying a matrix by a vector.

The sum of two linear operators is defined by

The product, or composition, of two linear operators has the action

The components therefore satisfy the rules of matrix addition and multiplication:

Recall that matrix multiplication is not commutative, so $\mathbf{BA} \neq \mathbf{AB}$ 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 S is the matrix of the inverse transformation. Substituting one relation into the other (and relabelling indices where required), we obtain

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 R and 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

with the inverse relation

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 x', we have

These transformation laws are consistent, e.g.

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:

- have *Hermitian symmetry*:

- be *positive definite*:

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:

The standard (Euclidean) inner product on $\mathbb{R}^n$ is the 'dot product'

$$\langle \boldsymbol{x}|\boldsymbol{y}\rangle = \boldsymbol{x}\cdot\boldsymbol{y} = x_i y_i$$

which is generalized to $\mathbb{C}^n$ 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 $\mathbb{R}^n$ or $\mathbb{C}^n$ 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

or equivalently

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

$$\begin{aligned}\langle \boldsymbol{x} - \alpha\boldsymbol{y} | \boldsymbol{x} - \alpha\boldsymbol{y}\rangle &= \langle \boldsymbol{x} - \alpha\boldsymbol{y} | \boldsymbol{x}\rangle - \alpha\langle \boldsymbol{x} - \alpha\boldsymbol{y} | \boldsymbol{y}\rangle \\ &= \langle \boldsymbol{x} | \boldsymbol{x}\rangle - \alpha^*\langle \boldsymbol{y} | \boldsymbol{x}\rangle - \alpha\langle \boldsymbol{x} | \boldsymbol{y}\rangle + \alpha\alpha^*\langle \boldsymbol{y} | \boldsymbol{y}\rangle \\ &= \langle \boldsymbol{x} | \boldsymbol{x}\rangle + \alpha\alpha^*\langle \boldsymbol{y} | \boldsymbol{y}\rangle - \alpha\langle \boldsymbol{x} | \boldsymbol{y}\rangle - \alpha^*\langle \boldsymbol{x} | \boldsymbol{y}\rangle^* \\ &= |\boldsymbol{x}|^2 + |\alpha|^2|\boldsymbol{y}|^2 - 2\,\mathrm{Re}\,(\alpha\langle \boldsymbol{x} | \boldsymbol{y}\rangle)\end{aligned}$$

This result holds for any scalar α. First choose the *phase* of α 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

Now choose the *modulus* of α 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 θ between two vectors through

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 3. *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

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

$$\langle \boldsymbol{y} | \boldsymbol{x} \rangle = G_{ij} y_i^* x_j$$

is equal to

$$(\langle \boldsymbol{x} | \boldsymbol{y} \rangle)^* = G_{ij}^* x_i y_j^* = G_{ji}^* y_i^* x_j$$

(in the last step we exchanged the summation indices $i \leftrightarrow j$) for all vectors $\boldsymbol{x}$ and $\boldsymbol{y}$, and therefore

We say that the matrix 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

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:

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

The Hermitian conjugate of a product of matrices is

because

$$[(\mathsf{AB})^\dagger]_{ij} = [(\mathsf{AB})_{ji}]^* \\ = (A_{jk}B_{ki})^* = (A^*_{jk}B^*_{ki}) = B^*_{ki}A^*_{jk} = (\mathsf{B}^\dagger)_{ik}(\mathsf{A}^\dagger)_{kj} = (\mathsf{B}^\dagger\mathsf{A}^\dagger)_{ij}$$

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.

In the latter example, if x and 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.

which is satisfied for all vectors x and y provided that 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

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 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:

$$\mathsf{A}^{\mathrm{T}} = \mathsf{A} \qquad \text{or}$$

An *antisymmetric* (or *skew-symmetric*) matrix satisfies

$$\mathsf{A}^{\mathrm{T}} = -\mathsf{A} \qquad \text{or}$$

An *orthogonal* matrix is one whose transpose is equal to its inverse:

$$\mathsf{A}^{\mathrm{T}} = \mathsf{A}^{-1} \qquad \text{or}$$

These ideas generalize to a complex vector space as follows.

An *Hermitian* matrix is equal to its Hermitian conjugate:

$$\mathsf{A}^{\dagger} = \mathsf{A} \qquad \text{or}$$

An *anti-Hermitian* (or *skew-Hermitian*) matrix satisfies

$$\mathsf{A}^{\dagger} = -\mathsf{A} \qquad \text{or}$$

A *unitary* matrix is one whose Hermitian conjugate is equal to its inverse:

$$\mathsf{A}^{\dagger} = \mathsf{A}^{-1} \qquad \text{or}$$

In addition, a *normal* matrix is one that commutes with its Hermitian conjugate:

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

for some scalar λ, the corresponding *eigenvalue*.

The equivalent statement in a matrix representation is

where A is an $n \times n$ square matrix.

This equation states that a non-trivial linear combination of the columns of the matrix $(\mathrm{A} - \lambda 1)$ is equal to zero, i.e. that the columns of the matrix are linearly dependent. This is equivalent to the statement

which is the *characteristic equation* of the matrix A.

To compute the eigenvalues and eigenvectors, we first solve the characteristic equation. This is a polynomial equation of degree n in λ and therefore has n roots, although not necessarily distinct. These are the eigenvalues of A, and are complex in general. The corresponding eigenvectors are obtained by solving the simultaneous equations found in the rows of $\mathrm{Ax} = \lambda \mathrm{x}$.

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 λ occurs m times, there may be any number between 1 and m of linearly independent eigenvectors corresponding to it. Any linear combination of these is also an eigenvector and the space spanned by such vectors is called an *eigenspace*.

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 $\mathsf{A}^\dagger = \mathsf{A}$. In quantum mechanics, Hermitian matrices (or operators) represent observable quantities.

We consider two eigenvectors x and y corresponding to eigenvalues λ and μ:

$$\mathsf{A}\mathsf{x} = \lambda\mathsf{x} \tag{1}$$

$$\mathsf{A}\mathsf{y} = \mu\mathsf{y} \tag{2}$$

The Hermitian conjugate of equation (2) is (since $\mathsf{A}^\dagger = \mathsf{A}$)

$$\mathsf{y}^\dagger\mathsf{A} = \mu^*\mathsf{y}^\dagger \tag{3}$$

Using equations (1) and (3) we can construct two expressions for $\mathsf{y}^\dagger\mathsf{A}\mathsf{x}$:

(4)

First suppose that x and y are the *same* eigenvector. Then $\mathsf{y} = \mathsf{x}$ and $\mu = \lambda$, so equation (4) becomes

Since $\mathsf{x} \neq 0$, $\mathsf{x}^\dagger\mathsf{x} \neq 0$ and so $\lambda^* = \lambda$. Therefore *the eigenvalues of an Hermitian matrix are real*.

Equation (4) simplifies to

If x and y are now *different* eigenvectors, we deduce that $\mathsf{y}^\dagger\mathsf{x} = 0$, provided that $\mu \neq \lambda$. Therefore *the eigenvectors of an Hermitian matrix corresponding to distinct eigenvalues are orthogonal* (in the standard inner product on $\mathbb{C}^n$).

5.6.3 Related results

Normal matrices (including all Hermitian, anti-Hermitian and unitary matrices) satisfy $\mathsf{A}\mathsf{A}^\dagger = \mathsf{A}^\dagger\mathsf{A}$. 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: $\mathsf{A}^\dagger = \mathsf{A}^{-1}$

.....

Note that:

- real symmetric matrices are Hermitian
- real antisymmetric matrices are anti-Hermitian
- real orthogonal matrices are unitary

Note also that a 1×1 matrix is just a number, λ, which is the eigenvalue of the matrix. To be Hermitian, anti-Hermitian or unitary λ must satisfy

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 A is Hermitian then iA is anti-Hermitian (and vice versa)
- if A is Hermitian then

$$\exp(\mathrm{iA}) = \sum_{n=0}^{\infty} \frac{(\mathrm{iA})^n}{n!} \qquad \text{is unitary}$$

[Compare the following two statements: If z is a real number then $\mathrm{i}z$ is imaginary (and vice versa). If z is a real number then $\exp(\mathrm{i}z)$ is of unit modulus.]

5.6.4 The degenerate case

Suppose we have an n by n matrix A. If a repeated eigenvalue λ occurs m times, it can be shown (with some difficulty) that there are exactly m corresponding linearly independent eigenvectors if A 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*

$$\begin{bmatrix} 0 & \mathrm{i} & 0 \\ -\mathrm{i} & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Characteristic equation:

$$(\lambda^2 - 1)(1 - \lambda) = 0$$

$$\lambda = 1, -1, 1$$

Eigenvector for $\lambda = -1$:

Normalized eigenvector:

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \mathrm{i} \\ 0 \end{bmatrix}$$

Eigenvectors for $\lambda = 1$:

Normalized eigenvectors:

$$\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-\mathrm{i}\\0\end{bmatrix}, \quad \begin{bmatrix}0\\0\\1\end{bmatrix}$$

. . . . . .

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

$$\mathsf{A}' = \mathsf{R}\mathsf{A}\mathsf{R}^{-1} \qquad \text{or equivalently} \qquad \mathsf{A} = \mathsf{R}^{-1}\mathsf{A}'\mathsf{R}$$

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

$$\mathsf{B} = \mathsf{S}^{-1}\mathsf{A}\mathsf{S} \tag{1}$$

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

$$\mathsf{S}^{-1}\mathsf{A}\mathsf{S} = \Lambda$$

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, denoted $\mathsf{x}^{(j)}$. The diagonal entries of the matrix Λ are just the eigenvalues of A, λ_j:

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 $\mathsf{U}^\dagger\mathsf{U} = 1$):

Therefore *a normal matrix can be diagonalized by a unitary transformation*:

where U is a unitary matrix whose columns are the orthonormal eigenvectors of A, and Λ 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*

$$\begin{bmatrix} 0 & \mathrm{i} & 0 \\ -\mathrm{i} & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Using the previously obtained eigenvalues and eigenvectors,

$$\begin{bmatrix} 1/\sqrt{2} & -\mathrm{i}/\sqrt{2} & 0 \\ 1/\sqrt{2} & \mathrm{i}/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & \mathrm{i} & 0 \\ -\mathrm{i} & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ \mathrm{i}/\sqrt{2} & -\mathrm{i}/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} =$$

.....

5.7.4 Orthogonal and unitary transformations

The transformation matrix between two bases $\{\mathsf{e}_i\}$ and $\{\mathsf{e}'_i\}$ has components R_{ij} defined by

$$\mathsf{e}_j = \mathsf{e}'_i R_{ij}$$

The condition for the first basis $\{\mathsf{e}_i\}$ to be orthonormal is

(In going from the second to the third line, note R_{ki} is a number, so $R^\dagger_{ki} = R^*_{ki}$.) If the second basis is also orthonormal, then $\mathsf{e}'^\dagger_k \mathsf{e}'_l = \delta_{kl}$ and the condition becomes

$$R^*_{ki} R_{kj} = \delta_{ij}$$

Therefore *the transformation between orthonormal bases is described by a unitary matrix*.

In a real vector space, an *orthogonal* matrix performs this task. In $\mathbb{R}^2$ or $\mathbb{R}^3$ 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:

$\mathsf{A}^m =$

$\det(\mathsf{A}) =$

$\mathrm{tr}(\mathsf{A}) =$

$\mathrm{tr}(\mathsf{A}^m) =$

Here we use the properties of the determinant and trace:

$$\det(\mathsf{AB}) = \det(\mathsf{A})\det(\mathsf{B})$$

$$\mathrm{tr}(\mathsf{AB}) = (\mathsf{AB})_{ii} = \mathsf{A}_{ij}\mathsf{B}_{ji} = \mathsf{B}_{ji}\mathsf{A}_{ij} = (\mathsf{BA})_{jj} = \mathrm{tr}(\mathsf{BA})$$

Note that diagonal matrices are multiplied very easily (i.e. componentwise). Also the determinant and trace of a diagonal matrix are just the product and sum, respectively, of its elements. Therefore

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

$$\det(\mathsf{A} - \lambda\mathsf{1}) = \det(\mathsf{A}) + \cdots + \mathrm{tr}(\mathsf{A})(-\lambda)^{n-1} + (-\lambda)^n = 0$$

5.8 Quadratic and Hermitian forms

5.8.1 Quadratic form

The *quadratic form* associated with a real symmetric matrix A is

$$Q(\mathsf{x}) = \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x} =$$

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.

$$Q = 2x^2 + 4xy + 5y^2 =$$

The xy term is split equally between the off-diagonal matrix elements. A can be diagonalized by a real orthogonal transformation:

$$\mathsf{S}^{\mathrm{T}}\mathsf{A}\mathsf{S} = \Lambda \qquad \text{with} \quad \mathsf{S}^{\mathrm{T}} = \mathsf{S}^{-1}$$

The vector x transforms according to $\mathsf{x} = \mathsf{S}\mathsf{x}'$, so

$$Q = \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x} = (\mathsf{x}'^{\mathrm{T}}\mathsf{S}^{\mathrm{T}})(\mathsf{S}\Lambda\mathsf{S}^{\mathrm{T}})(\mathsf{S}\mathsf{x}') = \mathsf{x}'^{\mathrm{T}}\Lambda\mathsf{x}'$$

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* $Q = 2x^2 + 4xy + 5y^2$.

$$Q = \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x}$$

The eigenvalues of 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 $\mathsf{S}^{\mathrm{T}}\mathsf{A}\mathsf{S} = \Lambda$ with

Therefore

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 $Q(\mathrm{x}) > 0$ for all $\mathrm{x} \neq 0$, 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

$$Q(\mathrm{x}) = k = \text{constant}$$

In the eigenvector basis this equation simplifies to

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

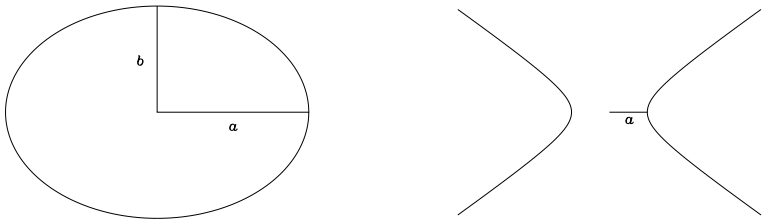
$$\frac{x'^2}{a^2} + \frac{y'^2}{b^2} - \frac{z'^2}{c^2} = \pm 1$$

The quadrics of a definite quadratic form are therefore ellipsoids.

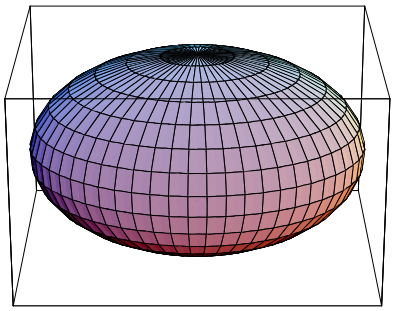
Some special cases:

- 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

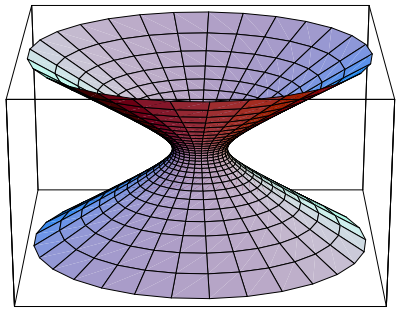


ellipse $\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$ hyperbola $\frac{x^2}{a^2} - \frac{y^2}{b^2} = 1$



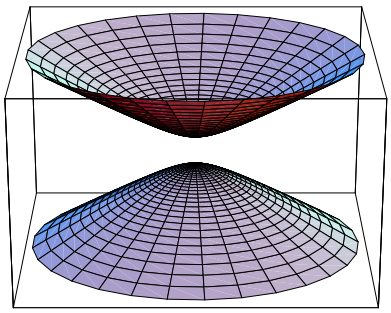
ellipsoid

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



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 $\boldsymbol{r}=\mathbf{0}$. Then its Taylor expansion has the form

$$V(\boldsymbol{r})=V(\mathbf{0})+V_{ij}x_ix_j+O(\boldsymbol{x}^3)$$

where

$$V_{ij}=\frac{1}{2}\frac{\partial^2 V}{\partial x_i\partial x_j}\bigg|_{\boldsymbol{r}=\mathbf{0}}$$

The equipotential surfaces near the origin are therefore given approximately by the quadrics $V_{ij}x_ix_j=$ 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 A is

$$H(\mathsf{x}) = \mathsf{x}^\dagger \mathsf{A}\mathsf{x} =$$

H is a real scalar because

We have seen that 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

$$H = \mathsf{x}^\dagger(\mathsf{U}\Lambda\mathsf{U}^\dagger)\mathsf{x} = (\mathsf{U}^\dagger\mathsf{x})^\dagger\Lambda(\mathsf{U}^\dagger\mathsf{x}) = \mathsf{x}'^\dagger\Lambda\mathsf{x}' =$$

5.9 Stationary property of the eigenvalues

The *Rayleigh quotient* associated with an Hermitian matrix 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 x is an eigenvector of A, then $\lambda(\mathsf{x})$ is the corresponding eigenvalue

In fact, the eigenvalues of A are the stationary values of the function $\lambda(\mathsf{x})$. This is the *Rayleigh–Ritz variational principle*.

Proof:

$$\begin{aligned}
\delta\lambda &= \lambda(\mathsf{x}+\delta\mathsf{x}) - \lambda(\mathsf{x}) \\
&= \frac{(\mathsf{x}+\delta\mathsf{x})^\dagger \mathsf{A}(\mathsf{x}+\delta\mathsf{x})}{(\mathsf{x}+\delta\mathsf{x})^\dagger(\mathsf{x}+\delta\mathsf{x})} - \lambda(\mathsf{x}) \\
&= \frac{\mathsf{x}^\dagger\mathsf{A}\mathsf{x} + (\delta\mathsf{x})^\dagger\mathsf{A}\mathsf{x} + \mathsf{x}^\dagger\mathsf{A}(\delta\mathsf{x}) + O(\delta\mathsf{x}^2)}{\mathsf{x}^\dagger\mathsf{x} + (\delta\mathsf{x})^\dagger\mathsf{x} + \mathsf{x}^\dagger(\delta\mathsf{x}) + O(\delta\mathsf{x}^2)} - \lambda(\mathsf{x}) \\
&= \frac{(\delta\mathsf{x})^\dagger\mathsf{A}\mathsf{x} + \mathsf{x}^\dagger\mathsf{A}(\delta\mathsf{x}) - \lambda(\mathsf{x})[(\delta\mathsf{x})^\dagger\mathsf{x} + \mathsf{x}^\dagger(\delta\mathsf{x})] + O(\delta\mathsf{x}^2)}{\mathsf{x}^\dagger\mathsf{x} + (\delta\mathsf{x})^\dagger\mathsf{x} + \mathsf{x}^\dagger(\delta\mathsf{x}) + O(\delta\mathsf{x}^2)} \\
&= \frac{(\delta\mathsf{x})^\dagger[\mathsf{A}\mathsf{x} - \lambda(\mathsf{x})\mathsf{x}] + [\mathsf{x}^\dagger\mathsf{A} - \lambda(\mathsf{x})\mathsf{x}^\dagger](\delta\mathsf{x})}{\mathsf{x}^\dagger\mathsf{x}} + O(\delta\mathsf{x}^2) \\
&= \frac{(\delta\mathsf{x})^\dagger[\mathsf{A}\mathsf{x} - \lambda(\mathsf{x})\mathsf{x}]}{\mathsf{x}^\dagger\mathsf{x}} + \text{c.c.} + O(\delta\mathsf{x}^2)
\end{aligned}$$

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 x is an eigenvector of A, and the value of $\lambda(\mathsf{x})$ is the corresponding eigenvalue.