Summary of Concepts in Methods

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1 Fourier series

Real Fourier series Let m, n be nonnegative integers. The following integrals are constantly useful:

$$\int_0^L \cos\frac{2\pi mx}{L}\cos\frac{2\pi nx}{L}\,dx = \frac{L}{2}\delta_{mn} \tag{1}$$

$$\int_0^L \cos\frac{2\pi mx}{L}\sin\frac{2\pi nx}{L}\,dx = 0 \tag{2}$$

$$\int_0^L \sin\frac{2\pi mx}{L}\sin\frac{2\pi nx}{L}\,dx = \frac{L}{2}\delta_{mn}. \tag{3}$$

These are called *orthogonality relations*.

Let f be a nice function, periodic with period L. f has a *Fourier expansion*, that is,

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty}\left(a_n\cos\frac{2\pi nx}{L} + b_n\sin\frac{2\pi nx}{L}\right), \tag{4}$$

where

$$a_n = \frac{2}{L}\int_0^L f(x)\cos\frac{2\pi nx}{L}\,dx \tag{5}$$

$$b_n = \frac{2}{L}\int_0^L f(x)\sin\frac{2\pi nx}{L}\,dx. \tag{6}$$

The equals sign in (4) should be interpreted as actual equality if f is continuous at x, and $(f(x+) + f(x-))/2$ (i.e. the mean value) if f has a jump discontinuity at x.

We can equally well write all of these integrals over the period $[-L/2, L/2]$.

Since sine is odd and cosine is even,

- if f is even, all the sine coefficients b_n vanish
- if f is odd, all the cosine coefficients a_n vanish

Fourier sine and cosine series Given a function on $[0, L/2]$, there are two easy ways to extend f to a periodic function on $[-L/2, L/2]$: the even extension

$$f_e(x) = \begin{cases} f(x) & x \geqslant 0 \\ f(-x) & x < 0 \end{cases}$$

and the odd extension

$$f_o(x) = \begin{cases} f(x) & x > 0 \\ -f(-x) & x < 0 \\ 0 & x = 0 \end{cases}$$

Given the previous paragraph, the former has a Fourier series containing only cosines, the latter a Fourier series containing only sines. In particular,

$$f_e(x) = \frac{A_0}{2} + \sum_{n=1}^{\infty} A_n\cos\frac{2\pi nx}{L}, \tag{7}$$

where

$$A_n = \frac{4}{L}\int_0^{L/2} f(x)\cos\frac{2\pi nx}{L}\,dx \tag{8}$$

the *Fourier cosine series* of f, and

$$f_o(x) = \sum_{n=1}^{\infty} B_n\sin\frac{2\pi nx}{L}, \tag{9}$$

where

$$B_n = \frac{4}{L}\int_0^{L/2} f(x)\sin\frac{2\pi nx}{L}\,dx \tag{10}$$

the *Fourier sine series* of f.

Complex Fourier series Sometimes it is easier to calculate integrals using $e^{2\pi inx/L}$ than the trigonometric functions. These exponentials satisfy the orthogonality relation

$$\frac{1}{L}\int_0^L \exp\left(\frac{2\pi imx}{L}\right)\exp\left(-\frac{2\pi inx}{L}\right)dx = \delta_{mn}. \tag{11}$$

There is then an expansion

$$f(x) = \sum_{n=-\infty}^{\infty} c_n\exp\left(\frac{2\pi inx}{L}\right), \tag{12}$$

where

$$c_n = \frac{1}{L}\int_0^L f(x)e^{-2\pi inx/L}\,dx \tag{13}$$

An advantage of this is that we only have to calculate one thing, the disadvantage is that any boundary conditions cannot be inserted freely, and evenness and oddness cannot be exploited to reduce the calculation.

Parseval's theorem The orthogonality of the expansion functions allows us to derive a formula for the integral of the square of f. First, if f is real,

$$\frac{2}{L}\int_0^L f(x)^2\,dx = \frac{a_0^2}{2} + \sum_{n=1}^{\infty}(a_n^2 + b_n^2) \tag{14}$$

while for a possibly complex f with a complex Fourier series,

$$\frac{1}{L}\int_0^L |f(x)|^2\,dx = \sum_{n=-\infty}^{\infty}|c_n|^2. \tag{15}$$

This expresses quantities like the "energy" that the function has.

Convergence Convergence of Fourier series is subtle: it is quite easy to show that the Fourier series converges to f in mean square (that is, $\int_0^L |f - S_N|^2 \to 0$), but the sort of convergence you actually want, namely *pointwise convergence* is a different matter. The standard set of conditions is due to Dirichlet: if

1. f is absolutely integrable,
2. f has a finite number of extrema, and
3. f has a finite number of discontinuities,

then the Fourier series expansion converges to f in the sense described above.

As a rule of thumb, if $f^{(k)}$ are continuous for $k < K$ and $f^{(K)}$ is continuous apart from jump discontinuities, the Fourier coefficients decay as $O(n^{-K-1})$.

2 Self-adjoint differential equations

2.1 Sturm–Liouville equations

Recall that in a vector space V with an inner product, a linear operator[1] L has an adjoint $L^\dagger$ if

$$\langle Lu, v\rangle = \langle u, L^\dagger v\rangle$$

for every $u, v \in V$. We want to apply this to a vector space V of functions on an interval $[a, b]$, and an inner product given by an integral:

$$\langle u, v\rangle = \int_a^b \overline{u(x)} v(x) w(x)\, dx,$$

where $w(x) > 0$ for $a < x < b$ is some fixed nonnegative weighting function. We suppose that L is a differential operator.[2] Then integration by parts allows us to write

$$\int_a^b \overline{Lu(x)} v(x) w(x)\, dx = \int_a^b \overline{u(x)} (L^\dagger v(x)) w(x)\, dx + [\text{boundary terms}],$$

and if the space of functions can be restricted so that the boundary terms always vanish, $L^\dagger$ really is the adjoint of L.

The best-behaved linear operators on a vector space are those which are *self-adjoint*: i.e. those with $L^\dagger = L$, and this section is about the most common type of self-adjoint differential operator, namely *Sturm–Liouville operators*.

The most general self-adjoint second-order differential operator is

$$L_x = \frac{1}{w(x)}\left(-\frac{d}{dx} p(x) \frac{d}{dx} + q(x)\right)$$

where $p(x), w(x) > 0$ for $a < x < b$, and an operator that can be put in this form is called a *Sturm–Liouville operator*. Integrating by parts, we find we need

$$\Big[p(x)(u(x)v'(x) - u'(x)v(x))\Big]_a^b = 0$$

for the boundary terms to vanish.

Common suitable boundary conditions include:

Dirichlet $y(a) = y(b) = 0$

Neumann $y'(a) = y'(b) = 0$

Robin $y(a) + \mu y'(a) = y(b) + \mu y'(b) = 0$

Mixed Some combination of the above

Periodic $y(a) = y(b), y'(a) = y'(b)$

An equation of the form

$$L_x y(x) = \lambda y(x),$$

is called a *Sturm–Liouville equation*. If y satisfies the boundary conditions and this equation, it is called an *eigenfunction*. λ is called the *eigenvalue*.[3] It is also common to multiply through by the weight function, giving the alternative equation

$$(py')' + qy = \lambda w y$$

A general second-order equation can be put in Sturm–Liouville form using an integrating factor: if

$$A(x)y'' + B(x)y' + C(x)y = 0,$$

then writing

$$0 = -y'' - (B/A)y' - (C/A)y = -e^{-\mu}(e^\mu y')' - (C/A)y$$

we see $\mu = \int (B/A)$ is the appropriate integrating factor.

2.2 General results

Under these conditions, there are very strong results about the eigenvalues and eigenfunctions:

1. There are infinitely many eigenvalues, which form an increasing sequence of real numbers,
$$\lambda_1 < \lambda_2 < \lambda_3 < \cdots$$
2. The eigenfunctions with a certain eigenvalue form a vector subspace (the *eigenspace*).
3. Eigenfunctions corresponding to different eigenvalues are orthogonal, in the sense that if u, v have different eigenvalues,
$$\langle u, v\rangle := \int_a^b \overline{u(x)} v(x) w(x)\, dx = 0$$

Non-degeneracy For Dirichlet or Neumann boundary conditions, the eigenvalues are non-degenerate: each eigenspace is one-dimensional, so eigenfunctions with the same eigenvalue are proportional.

Zeros The nth eigenfunction has $n - 1$ zeros in (a, b), and eigenfunctions with different eigenvalues have distinct zeros.

[1] That is, a linear map $V \to V$.

[2] In the rest of this course, we are mostly concerned with real differential operators and functions, but IB Quantum Mechanics requires the complex version, so we give the general results here.

[3] Which terminology is by analogy with the language of linear algebra, as one might expect given the preceding discussion.

Completeness Any function satisfying the boundary conditions can be written as an *eigenfunction expansion*:

$$y(x) = \sum_{n=1}^{\infty} a_n u_n(x),$$

where

$$a_n = \frac{\langle u_n, y\rangle}{\langle u_n, u_n\rangle}.$$

Parseval's theorem Suppose that y has an expansion as in the previous section. Then

$$\langle y, y\rangle = \sum_{n=1}^{\infty} |a_n|^2 \langle u_n, u_n\rangle. \tag{16}$$

This follows immediately from orthogonality.

Since this is the case, $S_N = \sum_{n=1}^{N} a_n u_n$ satisfies

$$\langle y - S_N, y - S_N\rangle \to 0, \tag{17}$$

i.e. S_N converges to y in mean square.

2.3 Examples

Simple harmonic motion on $[0, L]$ (for example)

$$-y'' = \lambda y \tag{18}$$

is a Sturm–Liouville equation when appropriate boundary conditions are applied: Sturm–Liouville eigenfunctions are a significant generalisation of the trigonometric solutions of this equation.

- If the boundary conditions are periodic, all eigenspaces but that corresponding to $\lambda = 0$ have dimension 2, which is why we obtain both the sine and cosine solutions.
- On the other hand, if $y(0) = y(L) = 0$, the eigenvalues are $(2\pi n)^2$, with eigenfunctions $\sin(2\pi mx/L)$, and the eigenvalues are nondegenerate.

Bessel's equation on $[0, 1]$

$$x^2y'' + xy' + (\alpha^2x^2 - \nu^2)y = 0. \tag{19}$$

or in Sturm–Liouville form,

$$-(xy')' + \frac{n^2}{x}y = \alpha^2 xy,$$

α^2 the eigenvalue. This equation has the unusual feature, shared with the trigonometric equation, that the eigenfunctions are all formed from a common function by rescaling its argument, with each eigenvalue corresponding to a zero of this function.[4]

Legendre's equation on $[-1, 1]$

$$(1 - x^2)y'' - 2xy' - n(n+1)y = 0, \tag{20}$$

or in Sturm–Liouville form,

$$-((1 - x^2)y')' = n(n+1)y,$$

Hermite equation on $(-\infty, \infty)$

$$y'' - 2xy' + 2ny = 0, \tag{21}$$

or in Sturm–Liouville form,

$$-(e^{-x^2}y')' = 2ne^{-x^2}y$$

Laguerre equation on $(0, \infty)$

$$xy'' + (a + 1 - x)y' + ny = 0, \tag{22}$$

or in Sturm–Liouville form,

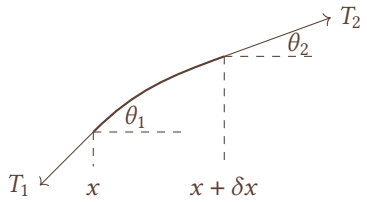
$$-(x^{a+1}e^{-x}y')' = nx^a e^{-x}y$$

All three of these have polynomial eigenfunctions. The Legendre polynomials are covered below, the other two in IB Quantum Mechanics.

3 PDEs on bounded domains

3.1 Derivation of some physically-significant PDEs

Wave equation Suppose we have a uniform inelastic string of mass density μ, fixed at two endpoints and with a constant horizontal tension T through it (the horizontal tension needs to be constant because of the inelasticity). Write the displacement of the string from straight as y, assumed small. We also assume that the string only moves vertically, and consider a chunk of string of length δx.



Resolving forces horizontally, we find

$$T_1 \cos\theta_1 = T_2 \cos\theta_2 = T, \tag{23}$$

θ being the angle of the string to the horizontal. Applying $F = ma$ vertically and using (23), we have

$$\begin{aligned}\mu\delta x \frac{\partial^2 y}{\partial t^2} &= T_2 \sin\theta_2 - T_1 \sin\theta_1 \\ &= T\tan\theta_2 - T\tan\theta_2 \\ &= T\left(\frac{\partial y}{\partial x}(x + \delta x, t) - \frac{\partial y}{\partial x}(x, t)\right)\end{aligned}$$

Now dividing by $\mu\delta x$ and taking the limit as $\delta x \to 0$, we obtain by definition

$$\frac{\partial^2 y}{\partial t^2} = \frac{T}{\mu}\frac{\partial^2 y}{\partial x^2},$$

the *wave equation*. We usually set $T/\mu = c^2$, and write $\partial u/\partial v = u_v$, and then this equation is written

$$y_{tt} = c^2 y_{xx} \tag{24}$$

[4] It turns out that the trigonometric functions *are* very closely related to solutions to Bessel's equation: put $y = x^{-1/2}u$ and the equation becomes $-u'' = (1 + (n^2 - 1/4)/x^2)u$, and then if $n = 1/2$ this is the SHM equation.

Diffusion equation To derive the diffusion equation, we combine two principles, "stuff wants to be where there is less of it", and "stuff is conserved". Let θ be the quantity of interest, $\mathbf{J}$ the flux. The first of these, called variously Fick's law (for diffusion), Fourier's law (for heat), or Ohm's law (for electricity), says more concretely that *flux is proportional to the negative of the gradient of the concentration*:

$$\mathbf{J} = -k\nabla\theta.$$

(We have been quite vague because this principle applies in the same form to many different systems, as seen by the number of names it has).

The second principle, conservation of stuff, says that the concentration in a region increases when stuff flows in. In particular,

$$\int_V \frac{\partial\theta}{\partial t}\,dt \propto -\int_{\partial V} \mathbf{J}\cdot\mathbf{n}\,dS = -\int_V \nabla\cdot\mathbf{J}\,dV :$$

since both of these integrands are the same and the volume is arbitrary, we conclude that

$$\frac{\partial\theta}{\partial t} = -\mu\nabla\cdot\mathbf{J},$$

"local" conservation of stuff. Combining this with the other equation, we obtain

$$\frac{\partial\theta}{\partial t} = \nabla\cdot(D\nabla\theta)$$

for some function D, the diffusion coefficient. If D is constant and we are in one dimension, we get the *diffusion equation* that we study in this course:

$$\frac{\partial\theta}{\partial t} = D\frac{\partial^2\theta}{\partial x^2}. \tag{25}$$

Laplace's equation Laplace's equation can be thought of as the steady-state version of the diffusion equation, although it also occurs in a number of other static systems, such as Maxwell's equations in a vacuum with no charges.

$$\nabla^2 u = 0. \tag{26}$$

3.2 Separation of variables

Thanks to uniqueness theorems for solutions of differential equations, *how* we find a solution does not matter: if it satisfies the equation and its boundary conditions, it is *the* solution.

The following method is one way of finding a solution, by reducing the PDE to a number of ODEs by hypothesising that it is a (sum of) product(s) of functions of one variable. It uses the idea that if a function of one variable is equal to a function of a different, independent variable, both must be constant. The general procedure is:

1. Choose a coordinate system (Cartesian, polar, spherical, ...) so tha the boundary conditions are nice curves (x constant, or r constant, for example).
2. Write the function as a product of functions of each separate variable, and rearrange to obtain terms that are functions of only one variable.
3. Put each variable's term equal to a constant.
4. Find the eigenvalues and eigenfunctions of the equations separately, one by one, until all the variables' functions are determined. (Generally you want to solve the ones with bounded domains and/or homogeneous boundary conditions first, because they are easier and will have only a discrete set of solutions. The last constant is determined by the others.)
5. Multiply the compatible functions together, discarding any unimportant multiplicative constants.
6. Form a(n infinite) sum of the possible functions thus obtained, with arbitrary coefficients.
7. Use the other boundary conditions to determine the coefficients in this series.

Generally, time is a good separating variable if the region is static. Only a few co-ordinate systems allow us to separate variables, of which the ones we care about in this course are Cartesians, polars, sphericals and cylindricals, all of which.

3.3 Spherical coordinates: Legendre's equation

Separating variables, $u = R(r)\Theta(\theta)\Phi(\phi)$,

$$0 = \frac{1}{r^2}\left(\frac{(r^2R')'}{R} + \frac{1}{\sin^2\theta}\left(\frac{\sin\theta((\sin\theta)\Theta')'}{\Theta} + \frac{\Phi''}{\Phi}\right)\right).$$

The first term is a function of R, the second of θ,ϕ, so we must have

$$(r^2R')' = n(n+1)r^2R$$

This is a homogeneous equation, solved by r^n and r^{-n-1}. Likewise, the second term is a constant, but the bracket is the sum of a function of θ and a function of ϕ, so we obtain

$$\Phi'' = -m^2\Phi$$
$$-(\sin\theta)((\sin\theta)\Theta')' + m^2\Theta = \lambda(\sin\theta)^2\Theta$$

Since Φ must be periodic, m is an integer, and we have solutions $e^{\pm mi\phi}$.

The equation for Θ does not in general have elementary solutions. Putting $\cos\theta = x$ (so $x \in [-1,1]$) and $y = \Theta(\arccos x)$, it becomes

$$-((1-x^2)y')' + \frac{m^2}{1-x^2}y = n(n+1)y, \tag{27}$$

the *associated Legendre equation*. In this course, we only care about axisymmetric solutions, that is, those with $m = 0$; in fact, the solutions for other m can be derived from these. The simpler equation

$$-((1-x^2)y')' = n(n+1)y, \tag{28}$$

is called the *Legendre equation*.

A Frobenius expansion reveals that to be finite at ±1, we need n to be an integer as well, and the solution will then be a polynomial of degree n. These are denoted by P_n, with the normalisation $P_n(1) = 1$. The Legendre equation is a Sturm–Liouville equation with weight 1, so the P_n are orthogonal polynomials on $[-1,1]$.

3.4 Cylindrical coordinates: Bessel's equation

Separating variables, $u = R(r)\Phi(\phi)Z(z)$, so

$$\frac{1}{r^2}\left(\frac{r(rR')'}{R} + \frac{\Phi''}{\Phi}\right) + \frac{Z''}{Z} = 0$$

As before, we obtain three equations, namely

$$Z'' = \lambda^2 Z$$
$$\Phi'' = -m^2\Phi$$
$$(rR')' + \lambda^2 rR - \frac{m^2}{r}R = 0.$$

Φ is periodic, so m is an integer. λ is not constrained, and can be eliminated from the last equation by putting $\lambda r = x$. We obtain *Bessel's equation*, which is usually written as

$$r^2R'' + rR' + (r^2 - m^2)R = 0. \tag{29}$$

Bessel's equation is not solved by a elementary function unless m is a half-integer. The rest of the time, it has two independent solutions which are new functions. The one regular at the origin is $J_m(x)$, sometimes called the *Bessel function of the first kind* which, by the method of Frobenius, is given by the series

$$\sum_{n=0}^{\infty} \frac{(-1)^k}{k!\Gamma(m+k+1)}\left(\frac{x}{2}\right)^{m+2k}; \tag{30}$$

this series remains valid even if m is not an integer.

The linearly independent solution is singular at 0: for non-integer m, we could take J_{-m} as an independent solution, but for integer m, $J_{\pm m}$ are actually proportional, so instead we have to use Y_m, the *Bessel function of the second kind*, given by

$$Y_m = J_m \cot m\pi - J_{-m}\csc m\pi$$

when m is not an integer, and the limit of this when m is an integer.

Once again Bessel's equation is a Sturm–Liouville equation. This implies that the solutions with different λ are orthogonal with weight x:

$$\int_0^1 J_m(j_{m,k}x)J_m(j_{m,l}x)x\,dx = 0$$

where $j_{m,k}$ is the kth zero of J_m.

3.5 Examples

Wave equation with no boundary conditions

$$u_{tt} = c^2 u_{xx}$$

Suppose that $u = T(t)X(x)$. Then

$$\frac{T''}{T} = c^2\frac{X''}{X}$$

These are functions of different variables, so they are both constant. Put $X'' = -k^2X$, and we have solution $X = Ae^{ikx} + Be^{-ikx}$). Then $T'' = -c^2k^2T$, so $T = Ce^{ikct} + De^{ikct}$. Therefore any solution to the wave equation can be written as a sum of *plane waves*: functions of the form $e^{ik(\pm x \pm ct)}$, where each $\pm$ is independent.

Laplace's equation in a rectangle Consider the system

$$\begin{aligned} u_{xx} + u_{yy} &= 0 \qquad 0 < x < a, 0 < y < b \\ u(0,y) = u(a,y) &= 0 \\ u(x,0) &= f(x) \\ u(x,b) &= g(x) \end{aligned}$$

Separating variables as $u = X(x)Y(y)$ gives

$$\frac{X''}{X} + \frac{Y''}{Y} = 0.$$

Each term is a function of different variables, so they must both be constant. Noting that X has to vanish at $x = 0$ and $x = a$, we choose the constant so that

$$X'' = -k^2X,$$

which has solutions $X = \sin(kx)$, where k is a multiple of π/a, i.e. the eigenfunctions are $X = \sin(n\pi x/a)$ (if $k = 0$, we get $X = Ax + B$, which only satisfies both boundary conditions if $A = B = 0$, so we do ignore this term).

Then we have

$$Y'' = -(n\pi/a)^2 Y.$$

There are various options for what the sensible form of solution is to write down here. Since we need to match two non-trivial boundary conditions, it is advantageous to choose the functions so that each vanishes on one boundary, and is 1 on the opposite one. Thankfully this is possible: since $\sinh ky$ and $\sinh k(b-y)$ are linearly independent, we can take

$$Y = A\frac{\sinh(n\pi y/a)}{\sinh(n\pi b/a)} + B\frac{\sinh(n\pi(b-y)/a)}{\sinh(n\pi b/a)}$$

Therefore in general the solution is of the form

$$u(x,y) = \sum_{n=1}^{\infty}\left(A_n\sinh(n\pi y/a) + B_n\sinh(n\pi(b-y)/a)\right)\frac{\sin(n\pi x/a)}{\sinh(n\pi b/a)}$$

Putting $y = 0, b$ gives

$$f(x) = u(x,0) = \sum_{n=1}^{\infty} B_n\sin(n\pi x/a)$$
$$g(x) = u(x,b) = \sum_{n=1}^{\infty} A_n\sin(n\pi x/a),$$

and we then find the coefficients using the orthogonality of the expansions: we have

$$B_n = \frac{2}{a}\int_0^a f(x)\sin(n\pi x/a)\,dx$$
$$A_n = \frac{2}{a}\int_0^a g(x)\sin(n\pi x/a)\,dx.$$

4 Inhomogeneous ODEs: Green's functions

4.1 The delta function

As in IA Differential Equations, we define an object δ that we pretend is a function, so that for any continuous function f,

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

Replacing $f(x)$ by $f(x+a)$ and shifting the integration variable,

$$\int_{-\infty}^{\infty} f(x)\delta(x-a)\,dx = f(a).$$

In fact, since values of f away from a do not affect the value of this integral, we have for any $\varepsilon, \eta > 0$

$$\int_{a-\varepsilon}^{a+\eta} f(x)\delta(x-a)\,dx = f(a).$$

No function with these properties can actually exist, but it is a useful mnemonic device for solving differential equations. The attraction is the following: suppose that we can solve the equation

$$L_x G(x;\xi) = \delta(x-\xi). \tag{31}$$

with some particular boundary conditions (usually homogeneous). Then

$$\begin{aligned} L_x \int_a^b G(x;\xi)f(\xi)\,d\xi &= \int_a^b L_x G(x;\xi)f(\xi)\,d\xi \\ &= \int_a^b \delta(x-\xi)f(\xi)\,d\xi = f(x)\,: \end{aligned}$$

the response of the equation to an impulsive forcing can be used to construct the solution to the equation with a general forcing.

The function G is called the *Green's function*[5] of the operator L with the specified boundary conditions.

4.2 Forced equations with fixed boundaries

We want to solve

$$Py'' + Qy' + Ry = f, \tag{32}$$

with the boundary conditions $y(a) = y(b) = 0$. Provided that the coefficients are continuous and P does not vanish, the solution will be of the form

$$\int_a^b G(x;\xi)f(\xi)\,d\xi,$$

where G solves

$$P(x)\frac{d^2}{dx^2}G(x;\xi) + Q(x)\frac{d}{dx}G(x;\xi) + R(x)G(x;\xi) = \delta(x-\xi). \tag{33}$$

To solve this equation,

1. Find a nontrivial solution to $PG'' + QG' + RG = 0$ with $G(a;\xi) = 0$, call it y_a, which will be proportional to G on $[a,\xi)$.
2. Find a nontrivial solution to $PG'' + QG' + RG = 0$ with $G(b;\xi) = 0$, call it y_b, which will be proportional to G on $(\xi, b]$.
3. Integrate (33) over a small interval containing ξ. We find that we need G to be continuous at ξ, and the jump condition $[P\,dG/dx]_{\xi-}^{\xi+} = 1$.
4. For the solutions to match, we therefore require A, B so that
$$\begin{aligned} Ay_b(\xi) - By_a(\xi) &= 0 \\ Ay_b'(\xi) - By_a'(\xi) &= \frac{1}{P(\xi)}. \end{aligned}$$
Provided that the solutions y_a, y_b are linearly independent, this is enough to specify G completely.

The solution in general is

$$G(x;\xi) = \frac{1}{P(\xi)W(y_a,y_b)(\xi)} \begin{cases} y_b(\xi)y_a(x) & a \leqslant x < \xi \\ y_a(\xi)y_b(x) & \xi < x \leqslant b \end{cases}$$

where W is the Wronskian, but in practice, it is easier to solve the equations directly than apply this formula.

4.3 Forced initial value problems

Suppose that $y = y(t)$, and we want to solve

$$P\ddot{y} + Q\dot{y} + Ry = f, \tag{34}$$

where $y(0) = y'(0) = 0$. Again, we look first at

$$P(t)\frac{d^2}{dt^2}G(t;\tau) + Q(t)\frac{d}{dt}G(t;\tau) + R(t)G(t;\tau) = \delta(t-\tau), \tag{35}$$

but since the initial condition is $G(0;\tau) = \dot{G}(0;\tau) = 0$, the solution for $t < \tau$ is automatically 0. Therefore we only need to solve

$$P\ddot{y} + Q\dot{y} + Ry = 0$$

for $t > \tau$, and integrating over τ implies that G is continuous there and $[\dot{G}]_{\tau-}^{\tau+} = 1/P(\tau)$, so we need to impose the initial conditions

$$\begin{aligned} y(\tau) &= 0 \\ \dot{y}(\tau) &= 1/P(\tau). \end{aligned}$$

4.4 Eigenfunction expansions

What if the equation is a Sturm–Liouville equation? Since the Green's function is continuous and differentiable most of the time, we would expect it to have an eigenfunction expansion.

To be concrete, suppose we want to solve

$$-(py')' - \tilde{\lambda}wy = wf, \tag{36}$$

where $\tilde{\lambda}$ is not an eigenvalue, and $y(a) = y(b) = 0$. Expanding $y = \sum_{n=1}^{\infty} a_n u_n$, since

$$-(pu_n')' - \tilde{\lambda}wu_n = (\lambda_n - \tilde{\lambda})wu_n,$$

[5] The non-grammatical usage is standard: somehow, 'Green function' sounds silly.

we find using linearity that

$$wf = -(py')' - \tilde{\lambda} wy = \sum_{n=1}^{\infty} (\lambda_n - \tilde{\lambda}) a_n w u_n.$$

Multiplying by u_m and integrating, orthogonality implies that

$$a_n = \frac{1}{\lambda_n - \tilde{\lambda}} \frac{\langle u_n, f\rangle}{\langle u_n, u_n\rangle},$$

where again $\langle u, v\rangle = \int_a^b u(x)v(x)w(x)\,dx$. Therefore,

$$\begin{aligned} y(x) &= \sum_{n=1}^{\infty} \frac{u_n(x)}{\lambda_n - \tilde{\lambda}} \frac{\langle u_n, f\rangle}{\langle u_n, u_n\rangle} \\ &= \int_a^b \left(\sum_{n=1}^{\infty} \frac{u_n(x)u_n(\xi)w(\xi)}{\lambda_n - \tilde{\lambda}} \right) f(\xi)\,d\xi, \end{aligned}$$

so we can make the identification

$$G(x;\xi) = w(\xi) \sum_{n=1}^{\infty} \frac{u_n(x)u_n(\xi)}{(\lambda_n - \tilde{\lambda})\langle u_n, u_n\rangle}$$

(whether to include the weight function or not depends on convention).

5 Fourier transforms

5.1 Derivation, definitions and properties

Derivation Consider the complex Fourier series of a function over the period $[-L/2, L/2]$. We have

$$f(x) = \sum_{n\in\mathbb{Z}} \frac{e^{2\pi i n x/L}}{L} \int_{-L/2}^{L/2} f(y) e^{-2\pi i n y/L}\,dy.$$

Writing $k = 2\pi n/L$, this becomes

$$f(x) = \frac{1}{2\pi} \sum_{k\in 2\pi\mathbb{Z}/L} \frac{2\pi}{L} e^{ikx} \int_{-L/2}^{L/2} f(y) e^{-iky}\,dy.$$

This looks like a Riemann sum, albeit somehow for an improper integral, and taking the limit as $L \to \infty$ in a rather casual way,

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} \left(\int_{-\infty}^{\infty} f(y) e^{-iky}\,dy \right) dk.$$

Hence we obtain the transform pair

$$\tilde{f}(k) = \int_{-\infty}^{\infty} f(x) e^{-ikx}\,dx \tag{37}$$

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx}\,dx; \tag{38}$$

and $\tilde{f}$ is called the *Fourier transform* of f.[6] The Fourier transform of f is also denoted by $\mathcal{F}(f)$.

Linearity If λ, μ are constants,

$$\widetilde{\lambda f + \mu g}(k) = \lambda \tilde{f}(k) + \mu \tilde{g}(k) \tag{39}$$

Variable shift

$$\widetilde{f(\cdot - a)}(k) = e^{ika} \tilde{f}(k) \tag{40}$$

Derivatives

$$\widetilde{f'}(k) = -ik\tilde{f}(k) \tag{41}$$

Multiplication by x

$$\widetilde{xf(x)}(k) = -i(\tilde{f})'(k) \tag{42}$$

Parseval/Plancherel

$$\int_{-\infty}^{\infty} \overline{f(x)} g(x)\,dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} \overline{\tilde{f}(k)} \tilde{g}(k)\,dk \tag{43}$$

$$\int_{-\infty}^{\infty} |f(x)|^2\,dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} |\tilde{f}(k)|^2\,dk \tag{44}$$

Since $\mathcal{F}^{-1} = (2\pi)^{-1}\mathcal{F} \circ \mathcal{S}$, where $\mathcal{S}$ is the operation that sends $f(x) \to f(-x)$, the inverse transform has corresponding identities. We do not list them all here, as they ar readily available elsewhere.

One final note: if a function is discontinuous (and the discontinuity is not removable), its Fourier transform will not be integrable (it usually decays too slowly). A workaround when taking the inverse transform is to use the *principal value*:

$$f(x) = \lim_{M\to\infty} \int_{-M}^{M} \tilde{f}(k) e^{ikx}\,dx.$$

(Clearly this will give the same answer as an ordinary integral for integrable $\tilde{f}(k)$, but it also works for some other $\tilde{f}(k)$.)

5.2 Convolution

The *convolution* of two functions $f, g\colon \mathbb{R} \rightrightarrows \mathbb{R}$ is defined by

$$(f \star g)(x) = \int_{-\infty}^{\infty} f(y) g(x-y)\,dy. \tag{45}$$

This has various simple properties:

Symmetric/commutative

$$(f \star g)(x) = (g \star f)(x) \tag{46}$$

Associative

$$\big((f \star g) \star h\big)(x) = \big(f \star (g \star h)\big)(x) \tag{47}$$

Bilinear If λ, μ are constants,

$$\big((\lambda f + \mu g) \star h\big)(x) = \lambda(f \star h)(x) + \mu(g \star h)(x) \tag{48}$$

$$\big(f \star (\lambda g + \mu h)\big)(x) = \lambda(f \star g)(x) + \mu(f \star h)(x) \tag{49}$$

It is easy to show each of the above properties by changing variables.

Translation Writing $\tau_a f(x) = f(x-a)$ etc, we have

$$\big(\tau_a(f \star g)\big)(x) = \big((\tau_a f) \star g\big)(x) = \big(f \star (\tau_a g)\big)(x)$$

[6] There are various conventions in use for where to put the minus sign and the 2π in this formula. See my Fourier Transform handout for details.

Derivatives Due to the translation property, the derivative also has a simple relationship with convolution:

$$(f \star g)'(x) = (f' \star g)(x) = (f \star g')(x) \tag{50}$$

"Identity" The delta function acts like an identity for convolution, although it is not actually a function:

$$(f \star \delta)(x) = (\delta \star f)(x) = f(x)$$

Convolution theorem The Fourier transform interchanges convolution and multiplication:

$$\widetilde{(f \star g)}(k) = \tilde{f}(k) \cdot \tilde{g}(k) \tag{51}$$

$$\widetilde{(f \cdot g)}(k) = \frac{1}{2\pi}(\tilde{f} \star \tilde{g})(k) \tag{52}$$

Notice the $1/2\pi$ in the second! This comes from the inverse Fourier transform's $1/2\pi$.

5.3 Discrete Fourier transform

There is also a Fourier transform on finite sets: we have

$$\frac{1}{N}\sum_{n=0}^{N-1} e^{2\pi i n\omega/N} e^{-2\pi i m\omega/N} = \delta_{mn},$$

which allows us to give a *discrete Fourier transform*, almost universally known as the DFT, which sends a function on $\{0, 1, \ldots, N-1\}$ to another function on $\{0, 1, \ldots, N-1\}$:

$$\tilde{f}(\omega) = \sum_{n=0}^{N-1} f(n) e^{-2\pi i n\omega/N},$$

with inverse

$$f(n) = \frac{1}{N}\sum_{\omega=0}^{N-1} \tilde{f}(\omega) e^{2\pi i n\omega/N}.$$

(As with the normal Fourier transform, the position of the normalisation constant N and the sign of the exponential can be chosen in different ways, although there is less variation here than in the continuum case.)

The DFT has the same shift, convolution and Parseval/Plancherel properties as the continuous Fourier transform, although we do not record them here.

5.4 Applications

Solving constant-coefficient ODEs The Fourier transform of a linear constant-coefficient differential operator L acting on y is $p(k)\tilde{y}(k)$ for some polynomial p, so if $Ly = f$, we have $\tilde{y}(k) = \tilde{f}(k)/p(k)$. We then apply the inverse transform to this to obtain y as a convolution.

In subjects such as electrical engineering, constant-coefficient ODEs are sufficiently prevalent that the object $R(k) = 1/p(k)$ has its own name: it is called the *transfer function*.

Two important remarks:

- The Fourier transform by itself does not have a built-in way to insert boundary conditions. If there are boundary conditions, they must be satisfied by finding the complementary function separately.[7]
- There are functions with the same Fourier transform: for example,

$$\begin{aligned}\frac{1}{-a+ik} &= \int_{-\infty}^{\infty} e^{-ikx} e^{ax} H(x)\,dx \\ &= \int_{-\infty}^{\infty} e^{-ikx}(-e^{ax}H(-x))\,dx,\end{aligned}$$

  and you should choose the appropriate inverse based on either what you know about the value of a so that the integral converges, or appeal to causality: if we expect the solution to only be influenced by past events, the convolution integral should stop at t.

Solving constant-coefficient PDEs The Fourier transform often allows us to turn a PDE, which is generally difficult to solve, into an easier ODE. We will give examples of this later.

N.B. When the coefficients are not constant, the Fourier transform is far less useful: its main power comes from turning the translation symmetry (and hence derivatives) into simple multiplication. (This doesn't mean that it is useless, but it usually no longer solves problems instantly.)

6 PDEs on unbounded domains

6.1 Classification

As we have seen with the wave equation, diffusion equation and Laplace's equation, the signs of the second-order terms in a linear partial differential equation have a significant effect on what the solution looks like (the lower-order terms are most of the time considerably less significant). The generic second-order linear PDE can be written as

$$a_{11}u_{xx} + 2a_{12}u_{xy} + a_{22}u_{yy} + b_1u_x + b_2u_y + cu + d = 0,$$

where u and all of the coefficients are functions of x and y. The appropriate classification turns out to depend on the determinant of the quadratic form $a_{11}\alpha^2 + 2a_{12}\alpha\beta + a_{22}\beta^2$, i.e.

$$\Delta(x, y) \coloneqq a_{11}a_{22} - a_{12}^2.$$

We classify equations based on the sign of this quadratic form: an equation is

Elliptic if $\Delta > 0$ (e.g. Laplace's equation)

Hyperbolic if $\Delta < 0$ (e.g. the wave equation)

Parabolic if $\Delta = 0$ (e.g. the diffusion equation)

It turns out that this classification is, in broad terms, sufficiently granular: every second-order partial differential equation behaves like one of the Laplace's equation, the diffusion equation or the wave equation.

[7] The Laplace Transform $f(x) \mapsto \int_0^\infty f(x)e^{-sx}\,dx$ will be introduced in Complex Methods to tackle problems with initial conditions.

N.B. Since Δ is a function of the variables, it can change sign: an equation can have different classification in different regions.

6.2 Well-posedness

A differential equation is *well-posed* if the solutions are well-behaved in a particular way, namely

- The solution exists and is uniquely determined in the whole domain of interest (this essentially requires having "the right sort" of boundary data).
- A small change in the boundary data causes only small changes in the solution (for eigenfunction expansions, this usually amounts to needing the larger-eigenvalue contributions to not grow faster than the others as we move away from the boundary data, since it is the higher-eigenvalue functions that change most when the boundary data is perturbed locally).[8]

6.3 The method of characteristics

The big idea of this method is to choose a new set of coordinates, in which the equation is very simple. It will often turn out that the value of the solution at a point only depends on one point of the boundary data, and that point is the one that lies on the same line in a family of *characteristic lines*.

6.3.1 Characteristics for first-order equations

Consider the general equation

$$au_x + bu_y + cu + d = 0,$$

where again a, b, c, d are functions of u, and suppose that the equation has a boundary condition $u = f$ on the curve $g(x, y) = 0$. We want to find a coordinate s so that the equation becomes

$$u_s + cu + d = 0,$$

and a coordinate t that parametrises the boundary data, so that $(x, y) \mapsto (s, t)$ is a valid change of coordinates. If we can do that, the equation is easy to solve, since it is just an ODE in s that depends on t parametrically.

The method works as follows:

1. Write down the *characteristic equations*: we want

   $$au_x + bu_y = U_s = \frac{\partial x}{\partial s}U_x + \frac{\partial y}{\partial s}U_y,$$

   so we need

   $$\frac{\partial x}{\partial s} = a \qquad \frac{\partial y}{\partial s} = b. \tag{53}$$

2. Solve the characteristic equations for x, y as functions of s, to obtain the *characteristics*.

3. Parametrise the boundary curve $g(x, y) = 0$ by $x = x_0(t), y = y_0(t)$.

4. Provided that $g(x, y) = 0$ crosses each characteristic exactly once and is never tangent to a characteristic, (x, y) is determined uniquely by (s, t) (go along the boundary until you get to the characteristic through that point, then go along that characteristic, read off the t and the s), the change of coordinates is a bijection so we can invert it and write the original equation as

   $$U_s + C(s, t)U + D(s, t) = 0, \tag{54}$$

   and solve this for $U(s, t)$;

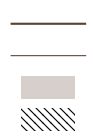
5. Finally, at each point, the initial condition is given by $U(0, t) = f(x_0(t), y_0(t)) = F(t)$.

Notice that the solution to the equation is determined in the region formed by all the characteristics that cross the initial data curve once: even if we can't finish the rest of the calculation, as we may not be able to if the equation is sufficiently nasty, we can at least say where a solution is determined.

6.3.2 Characteristics for second-order equations

Here, our goal differs depending on the type of PDE we are dealing with. It is quite simple to show that a legitimate change of coordinates does not change the sign of the determinant function Δ (just do it!), so the classification is stable under changing coordinates. The idea now is to choose coordinates to make the equation take a canonical form close to that of one of the three archetypal equations we have already considered, so that the second-order terms are $u_{\xi\xi} + u_{\eta\eta}$ for elliptic equations, $u_{\xi\xi}$ for parabolic equations, and $u_{\xi\eta}$ for hyperbolic equations. Where do we find the coordinates to write down these new equations? By solving first-order characteristic equations.

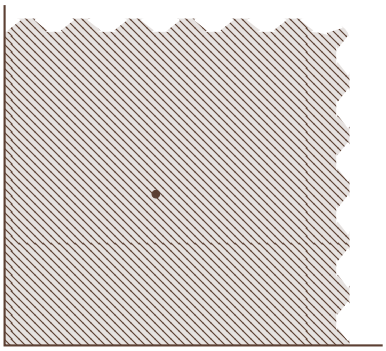
Characteristics can be found by considering eigenvalues of the quadratic form. The following diagrams illustrate each basic case; they all show



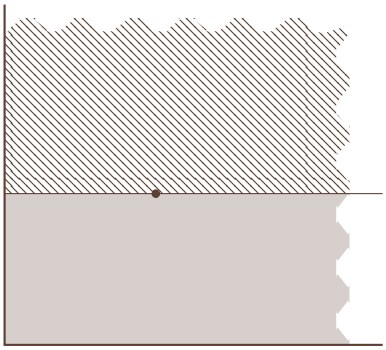
an arbitrary point P
the boundary/initial lines
the characteristics through P
the points that affect P
the points that P affects

Elliptic There are no real eigenvalues, and so no characteristics (there is no "propagation": one condition must be specified on the entire boundary, e.g. the value of the function, or its derivative).

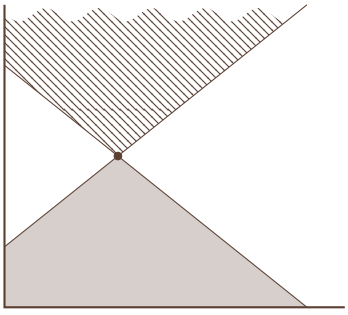
[8] This is a manifestation of the rule of thumb that bulk properties like mass and energy tend to mostly accounted for in the first few eigenfunctions, while the larger-eigenvalue ones are more for taking into account the specific local variations.



Parabolic There is one real eigenvalue, and so one characteristic through a point, along which the propagation speed is infinite. The "time direction" is the vector perpendicular to this. We need one initial condition, and one condition on the boundary. Information moves infinitely fast, and there is a smoothing effect. The direction of time is visible (backward diffusion is ill-posed since the reverse of smoothing is "roughening").



Hyperbolic There are two real eigenvalues, so two characteristics through each point. Information from the boundary propagates in two directions, but at finite speed: a point is influenced by the data given on the boundary *between* the two intersection points of the characteristics. One condition on the boundary and *two* initial conditions must be specified.



The wave equation is same under time-reversal, so forward and backward solutions "look the same" (apart from the boundary conditions' influence). "Time" is relative: you can determine if one point is "before" another, but there need not be a "global" time.

Canonical form of the hyperbolic equation This type is where the characteristics are most significant.

Let $U(\xi(x,y),\eta(x,y)) = u(x,y)$. Then

$$\begin{aligned} u_{xx} &= (\xi_x U_\xi + \eta_x U_\eta)_x \\ &= \xi_x^2 U_{\xi\xi} + 2\xi_x\eta_x U_{\xi\eta} + \eta_x^2 U_{\eta\eta} + \xi_{xx} U_\xi + \eta_{xx} U_\eta, \end{aligned}$$

and so on, so

$$\begin{aligned} &a_{11}u_{xx} + 2a_{12}u_{xy} + a_{22}u_{yy} \\ &\quad = (a_{11}\xi_x^2 + 2a_{12}\xi_x\xi_y + a_{22}\xi_y^2)U_{\xi\xi} \\ &\qquad + 2(a_{11}\xi_x\eta_x + a_{12}(\xi_y\eta_x + \xi_x\eta_y) + a_{22}\xi_y\eta_y)U_{\xi\eta} \\ &\qquad + (a_{11}\eta_x^2 + 2a_{12}\eta_x\eta_y + a_{22}\eta_y^2)U_{\eta\eta} \\ &\qquad + (a_{11}\xi_{xx} + 2a_{12}\xi_{xy} + a_{22}\xi_{yy})U_\xi \\ &\qquad + (a_{11}\eta_{xx} + 2a_{12}\eta_{xy} + a_{22}\eta_{yy})U_\eta. \end{aligned}$$

Therefore we need both ξ and η to satisfy the equation

$$a_{11}v_x^2 + 2a_{12}v_x v_y + a_{22}v_y^2 = 0,$$

i.e.

$$\frac{v_x}{v_y} = \frac{-a_{12} \pm \sqrt{-\Delta}}{a_{11}} = \lambda_\pm.$$

But on the curve $\xi = \text{const}$, we have $0 = \xi_x + (dy/dx)\xi_y$, so $dy/dx = -\xi_x/\xi_y$. Therefore the characteristics are given by curves with

$$\frac{dy}{dx} = -\lambda_\pm;$$

solving these gives a simple way of expressing ξ and η in terms of x and y.

The simplest example of this is the wave equation, $u_{tt} - c^2u_{xx} = 0$. Then we have $\lambda_\pm = \pm c$, so the characteristics are

$$\frac{dx}{dt} = \mp c,$$

so the characteristics are $x \mp ct = \text{const}$.. In this case, this allows us to recover the familiar d'Alembert solution as the sum of a function of $x - ct$ and a function of $x + ct$.

7 Green's functions for PDEs

7.1 Free Green's functions

A *free* Green's function solves the problem $Lu = \delta(x - \xi)$ with no boundary conditions beyond, possibly, decay at ∞. These particular Green's functions are useful for constructing Green's functions for other problems with other types of boundary conditions on more complicated domains, which we do below.

Laplace's equation In three dimensions, we need to solve

$$\nabla^2 G(\mathbf{x};\boldsymbol{\xi}) = \delta(\mathbf{x} - \boldsymbol{\xi}),$$

with the condition that $G \to 0$ as $|\mathbf{x}| \to \infty$.[9] Integrating over the ball of radius r surrounding $\boldsymbol{\xi}$, we have

$$1 = \int_{|\mathbf{x}-\boldsymbol{\xi}|<r} \nabla^2 G(\mathbf{x};\boldsymbol{\xi})\, dV = \int_{|\mathbf{x}-\boldsymbol{\xi}|=r} \frac{\partial G}{\partial r}\, dS.$$

[9] It is worth pointing out that the convention used in this course is not the sensible one: it is generally better to consider $-\nabla^2$, because it is a positive operator, and the Green's function also ends up positive rather than negative.

We now appeal to the symmetry: since the problem has rotational symmetry about $\boldsymbol{\xi}$, we assert that G is only a function of r, and hence this equation becomes

$$1 = 4\pi r^2 \frac{\partial G}{\partial r},$$

and we find immediately that

$$G(\mathbf{x};\boldsymbol{\xi}) = -\frac{1}{4\pi|\mathbf{x}-\boldsymbol{\xi}|}. \tag{55}$$

Suppose we did the same calculation in two dimensions. Then we find that

$$G(\mathbf{x};\boldsymbol{\xi}) = \frac{1}{2\pi}\log|\mathbf{x}-\boldsymbol{\xi}| : \tag{56}$$

it is not possible to have a two-dimensional solution that converges to 0, so this has to do.

Diffusion equation We have

$$G_t - DG_{xx} = \delta(x-\xi)\delta(t-\tau).$$

Taking the Fourier transform in x, we find

$$\tilde{G}_t + Dk^2\tilde{G} = e^{ik\xi}\delta(t-\tau)$$

This is a first-order equation with integrating factor e^{Dk^2t}, so

$$(e^{Dk^2t}\tilde{G})_t = e^{ik\xi+Dk^2t}\delta(t-\tau),$$

and the integrating factor on the right resolves to $e^{Dk^2\tau}$ since the δ will just take the value at $t=\tau$. Integrating, we therefore have

$$\tilde{G} = e^{ik\xi-k^2D(t-\tau)}H(t-\tau),$$

and it remains to invert this. We can write down the inverse of this transform using the rules for Gaussians (thankfully the Heaviside function guarantees the coefficient of k^2 is negative, so the integrals involved all converge), and we find

$$G(x,t;\xi;\tau) = H(t-\tau)\frac{1}{\sqrt{4\pi D(t-\tau)}}\exp\Big(-\frac{(x-\xi)^2}{4D(t-\tau)}\Big) \tag{57}$$

Wave equation We have

$$G_{tt} - c^2G_{xx} = \delta(x-\xi)\delta(t-\tau).$$

Taking the Fourier transform in x, we find

$$\tilde{G}_{tt} + c^2k^2\tilde{G} = e^{ik\xi}\delta(t-\tau)$$

This is a one-dimensional initial value problem Green's function, which we have calculated before: the solution will be $A\sin(ck(t-\tau))$ for some A; in particular, we find that $e^{ik\xi} = ckA$, so

$$\tilde{G} = e^{ik\xi}\frac{\sin ck(t-\tau)}{ck}H(t-\tau).$$

To untransform, notice that the right-hand side is just

$$\frac{1}{2c}\int_{-c(t-\tau)}^{c(t-\tau)} e^{-ik(x-\xi)}\,dx = \frac{1}{2c}\int_{\xi-c(t-\tau)}^{\xi+c(t-\tau)} e^{-iky}\,dy,$$

i.e. the Fourier transform of $H\big(c(t-\tau)-|x-\xi|\big)$. Hence

$$G(x,t;\xi,\tau) = \frac{1}{2c}H(t-\tau)H\big(c(t-\tau)-|x-\xi|\big).$$

7.2 Green's functions for bounded domains

With some adjustments, the free Green's function can usually be used to create Green's functions for more complicated boundary conditions. We shall now do so.

Laplace's equation Recall Green's Second Identity: for any twice-differentiable ϕ,ψ and volume V bounded by a piecewise-differentiable boundary surface, we have

$$\int_V (\phi\nabla^2\psi - \psi\nabla^2\phi)dV = \int_{\partial V}\Big(\phi\frac{\partial\psi}{\partial\nu} - \psi\frac{\partial\phi}{\partial\nu}\Big)\,dS, \tag{58}$$

where $\partial/\partial\nu$ is the derivative in the direction normal to the surface ∂V.

Choose $\phi = u$ to solve Laplace's equation, $\psi = G(\cdot,\boldsymbol{\xi})$ any Green's function for Laplace's equation, and V to be the domain U on which we wish to solve Laplace's equation, with a small ball $B(\varepsilon)$ of radius ε around x removed. Then both functions satisfy Laplace's equation on V, so the left-hand side is 0. Since the small ball is inside V, its boundary has the opposite orientation, so we find that

$$\begin{aligned}\int_{\partial B(\varepsilon)}\Big(u(\boldsymbol{\xi})\frac{\partial G}{\partial\nu}(\mathbf{x};\boldsymbol{\xi}) - G(\mathbf{x};\boldsymbol{\xi})\frac{\partial u}{\partial\nu}(\boldsymbol{\xi})\Big)\,dS \\ = \int_{\partial U}\Big(u(\boldsymbol{\xi})\frac{\partial G}{\partial\nu}(\mathbf{x};\boldsymbol{\xi}) - G(\mathbf{x};\boldsymbol{\xi})\frac{\partial u}{\partial\nu}(\boldsymbol{\xi})\Big)\,dS.\end{aligned}$$

Now, we can expand the left-hand side as a series in ε to find the limit as $\varepsilon\to 0$. By the definition of Green's function, the first term on the left converges to $u(\mathbf{x})$, the second to 0 (since G itself is not sufficiently singular to counteract the area of the sphere converging to 0), and hence we obtain

$$u(\mathbf{x}) = \int_{\partial U}\Big(u(\boldsymbol{\xi})\frac{\partial G}{\partial\nu}(\mathbf{x};\boldsymbol{\xi}) - G(\mathbf{x};\boldsymbol{\xi})\frac{\partial u}{\partial\nu}(\boldsymbol{\xi})\Big)\,dS.$$

This is sometimes called *Green's Third Identity*.

We know that Laplace's equation requires a single boundary condition, so u looks overdetermined in this equation. To get around this, we can choose how G behaves on the boundary to remove the redundancy. In particular, suppose we know u on the boundary (or $\partial u/\partial\nu$), and we have chosen a Green's function so that $\partial G/\partial\nu$ (or G) vanishes on the boundary. Then the formula gives us an expression for u in terms of its values on the boundary. We call the Green's function with vanishing normal derivative G_D ("Dirichlet") and that which itself vanishes G_N ("Neumann"), and thus we have the two formulae

$$\begin{aligned}u(\mathbf{x}) &= \int_{\partial U} u(\boldsymbol{\xi})\frac{\partial G_D}{\partial\nu}(\mathbf{x};\boldsymbol{\xi})\,dS \\ u(\mathbf{x}) &= -\int_{\partial D} G_N(\mathbf{x};\boldsymbol{\xi})\frac{\partial u}{\partial\nu}(\boldsymbol{\xi})\,dS,\end{aligned}$$

where the first is for Dirichlet boundary conditions, the second for Neumann boundary conditions.

The Method of Images For domains where the boundary is simply a straight line, there is a straightforward way to build Dirichlet and Neumann Green's functions: we place an extra point on the other side of the boundary, and add or subtract a copy of the Green's function based at that point to cancel out the appropriate part of the original on the boundary: we can think of it as a reflexion of the source in the boundary. Notice that since the new singularity is outside the domain, in the domain itself, this new term will satisfy the original differential equation with no forcing, and so only affects the boundary value equation, not the defining one. This works in general for equations where the coefficients are independent of time (which forces G to only depend on $|\mathbf{x}-\boldsymbol{\xi}|$): let $R\boldsymbol{\xi}$ be the reflexion of the point $\boldsymbol{\xi}$ in the boundary line. We show that

$$G_D(\mathbf{x};\boldsymbol{\xi}) = G(\mathbf{x};\boldsymbol{\xi}) - G(\mathbf{x};R\boldsymbol{\xi}) \tag{59}$$
$$G_N(\mathbf{x};\boldsymbol{\xi}) = G(\mathbf{x};\boldsymbol{\xi}) + G(\mathbf{x};R\boldsymbol{\xi}). \tag{60}$$

are suitable Dirichlet and Neumann Green's functions respectively.

By the assumption we may write $G(\mathbf{x};\boldsymbol{\xi}) = F(|\mathbf{x}-\boldsymbol{\xi}|^2)$ for some F, while

$$|\mathbf{x}-\boldsymbol{\xi}|^2 + |\mathbf{x}-R\boldsymbol{\xi}|^2 = |\boldsymbol{\xi}-R\boldsymbol{\xi}|^2$$

by Pythagoras's Theorem, and differentiating gives

$$d|\mathbf{x}-\boldsymbol{\xi}|^2 + d|\mathbf{x}-R\boldsymbol{\xi}|^2 = 0;$$

in particular this will hold on the boundary with d replaced by the normal derivative. Thus we find

$$\begin{aligned}\frac{\partial G}{\partial \nu}(\mathbf{x};\boldsymbol{\xi}) &= F'(|\mathbf{x}-\boldsymbol{\xi}|^2)\frac{\partial}{\partial \nu}|\mathbf{x}-\boldsymbol{\xi}|^2\\ &= F'(|\mathbf{x}-\boldsymbol{\xi}|^2)\frac{\partial}{\partial \nu}|\mathbf{x}-R\boldsymbol{\xi}|^2\\ &= -F'(|\mathbf{x}-R\boldsymbol{\xi}|^2)\frac{\partial}{\partial \nu}|\mathbf{x}-R\boldsymbol{\xi}|^2 = -\frac{\partial G}{\partial \nu}(\mathbf{x};R\boldsymbol{\xi}),\end{aligned}$$

where in the last line we have used that on the boundary, $|\mathbf{x}-\boldsymbol{\xi}| = |\mathbf{x}-R\boldsymbol{\xi}|$.

Therefore (59) and its derivative become

$$\begin{aligned}G_D(\mathbf{x};\boldsymbol{\xi}) &= 0,\\ \frac{\partial G_D}{\partial \nu}(\mathbf{x},\boldsymbol{\xi}) &= 2\frac{\partial G}{\partial \nu}(\mathbf{x};\boldsymbol{\xi})\end{aligned}$$

while (60) and its derivative become

$$\begin{aligned}G_N(\mathbf{x};\boldsymbol{\xi}) &= 2G(\mathbf{x};\boldsymbol{\xi})\\ \frac{\partial G_N}{\partial \nu}(\mathbf{x},\boldsymbol{\xi}) &= 0.\end{aligned}$$

More complicated domains (e.g. two boundaries at right-angles) may need more image sources, or images in non-obvious places, but the principle is the same. Notable examples are the sphere, where the image point is the geometrical inverse ("reflexion in a sphere"), and periodic boundary conditions, which require adding in an infinite set of images.[10]

7.3 Huygens's principle

Huygens's principle says that the influence that a point x feels from the initial conditions is found by adding up the influence of each point considered as a source of a particular strength. For example, if we consider the diffusion equation $\theta_t = D\theta_{xx}$ with initial condition $\theta(x,0) = f(x)$, the solution will be

$$\theta(x,t) = \int_{-\infty}^{\infty} G(x,t;\xi,0)f(\xi)\,d\xi,$$

where G is the diffusion Green's function we found above. Proving this is relatively straightforward if we assume that we can use the Fourier transform:

Diffusion equation with an initial condition Taking the Fourier transform of $\theta_t - D\theta_{xx} = 0$, we have

$$\tilde{\theta}_t + Dk^2\tilde{\theta} = 0.$$

The initial condition is $\tilde{\theta}(0,k) = \tilde{f}(k)$. We have then

$$[e^{-Dk^2\tau}\tilde{\theta}(k,\tau)]_0^t = 0,$$

by using integrating factors, so

$$\theta(\tilde{k},t) = e^{-Dk^2t}\tilde{(k,0)} = e^{-Dk^2t}\tilde{f}(k).$$

Now we simply write down the solution using the Convolution Theorem,

$$\theta(x,t) = \int_{-\infty}^{\infty} G(x,t;\xi,0)f(\xi)\,d\xi,$$

since the inverse transform of e^{-Dk^2t} is $G(x,t;0,0)$ and $G(\xi-x,t;0,0) = G(x,t;\xi,0)$.

Wave equation with an initial condition

$$\begin{aligned}u_{tt} - c^2u_{xx} &= 0\\ u(x,0) &= f(x)\\ u_t(x,0) &= g(x)\end{aligned}$$

Something a bit different happens here. Again taking the Fourier transform,

$$\tilde{u}_{tt} + c^2k^2\tilde{u} = 0,$$

with $\tilde{u}(k,0) = \tilde{f}(k)$ and $\tilde{u}_t(k,0) = \tilde{g}(k)$. We calculate that

$$\tilde{u}(k,t) = \tilde{f}(k)\cos(ckt) + \tilde{g}(k)\frac{\sin(ckt)}{ck}.$$

The second term we recognise as the Fourier transform of the convolution $\int_{-\infty}^{\infty} G(x,t;\xi,0)g(\xi)\,d\xi$. The first is new. Staring at it, however, we realise that it is the Fourier transform of $\frac{1}{2}(\delta(x-ct)+\delta(x+ct))$. Applying the Convolution Theorem, we thus find

$$\begin{aligned}u(x,t) &= \frac{1}{2}\big(f(x+ct)+f(x-ct)\big) + \frac{1}{2c}\int_{-\infty}^{\infty} G(x,t;\xi,0)g(\xi)\,d\xi\\ &= \frac{1}{2}\big(f(x+ct)+f(x-ct)\big) + \frac{1}{2c}\int_{x-ct}^{x+ct} g(\xi)\,d\xi,\end{aligned}$$

d'Alembert's solution to the wave equation: the position depends on the *position* on the boundary *at* the intersections with the characteristics, and the velocity *between* the intersections of the characteristics with the boundary.

[10] Of course we already have another way to write the solution to a PDE on a finite interval or in a periodic setting: Fourier series. The relative merits of each approach become clear in applications.

7.4 Forced PDEs

Poisson's equation Poisson's equation is "Laplace's equation with something on the right", i.e.

$$\nabla^2\phi = f, \tag{61}$$

with some boundary condition; in this course we look at the easiest, namely the case where we know $\phi(\mathbf{x}) = g(\mathbf{x})$ on ∂V.

We use a very similar argument to before to find the solution here: set up Green's Second Identity on $V \setminus B(\mathbf{x}, \varepsilon)$:

$$\begin{aligned}\int_V \big(G(\mathbf{x};\boldsymbol{\xi})\nabla^2\phi(\boldsymbol{\xi}) - \phi(\boldsymbol{\xi})\nabla^2 G(\mathbf{x};\boldsymbol{\xi})\big)\,dV \\ = \int_{\partial V}\Big(G(\mathbf{x};\boldsymbol{\xi})\frac{\partial\phi}{\partial\nu}(\boldsymbol{\xi}) - \phi(\boldsymbol{\xi})\frac{\partial G}{\partial\nu}(\mathbf{x};\boldsymbol{\xi})\Big)\,dS \\ - \int_{\partial B(\mathbf{x},\varepsilon)}\Big(G(\mathbf{x};\boldsymbol{\xi})\frac{\partial\phi}{\partial\nu}(\boldsymbol{\xi}) - \phi(\boldsymbol{\xi})\frac{\partial G}{\partial\nu}(\mathbf{x};\boldsymbol{\xi})\Big)\,dS\end{aligned}$$

Using that $\nabla^2 G = \delta$, $\nabla^2\phi = f$, and the previous argument about shrinking the ball, we obtain

$$\begin{aligned}\int_V \Big(G(\mathbf{x};\boldsymbol{\xi})f(\boldsymbol{\xi}) - 0\Big)\,dV \\ = \int_{\partial V}\Big(G(\mathbf{x};\boldsymbol{\xi})\frac{\partial\phi}{\partial\nu}(\boldsymbol{\xi}) - \phi(\boldsymbol{\xi})\frac{\partial G}{\partial\nu}(\mathbf{x};\boldsymbol{\xi})\Big)\,dS \\ + \phi(\mathbf{x}),\end{aligned}$$

and supposing that $G(\mathbf{x};\boldsymbol{\xi}) = 0$ for $\boldsymbol{\xi} \in \partial V$, we obtain

$$\phi(\mathbf{x}) = \int_V G(\mathbf{x};\boldsymbol{\xi})f(\boldsymbol{\xi})\,dV + \int_{\partial V} g(\boldsymbol{\xi})\frac{\partial G}{\partial\nu}(\mathbf{x};\boldsymbol{\xi})\,dS$$

Duhamel's principle for the diffusion equation Roughly, Duhamel's principle says that *a forcing is like having a boundary condition at each time t*. We can realise this easily using the diffusion equation: suppose that we apply a momentary forcing $f(x,\sigma)$ to each point at time σ; this is represented by

$$\theta_t^{(\sigma)} - D\theta_{xx}^{(\sigma)} = f(x,\sigma)\delta(t-\sigma).$$

Integrating over the interval $[\sigma - \delta t/2, \sigma + \delta t/2]$, we have

$$\theta^{(\sigma)}(x,\sigma+\delta t/2) - \theta^{(\sigma)}(x,\sigma-\delta t/2) - 0 = f(x,\sigma).$$

But if we suppose that θ is initially zero, taking the limit of this as $\delta t \to 0$ gives

$$\theta^{(\sigma)}(x,\sigma) = f(x,\sigma),$$

i.e. a boundary condition at $t = \sigma$. We have solved this problem before: its solution is

$$\theta^{(\sigma)}(x,t) = \int_{-\infty}^{\infty} G(x,t;\xi,\sigma)f(\xi,\sigma)\,d\xi.$$

Each σ has a solution of this form, and the solution for all such σ can be found by integrating: we have $f(x,t) = \int_0^\infty f(x,\sigma)\delta(t-\sigma)\,d\sigma$, so the solution to

$$\theta_t - D\theta_{xx} = f$$

with zero initial condition is

$$\begin{aligned}\theta(x,t) &= \int_0^\infty\int_{-\infty}^{\infty} G(x,t;\xi,\sigma)f(\xi,\sigma)\,d\xi\,d\sigma \\ &= \int_0^t\int_{-\infty}^{\infty} G(x,t;\xi,\tau)f(\xi,\tau)\,d\xi\,d\tau,\end{aligned}$$

since the Green's function is zero for $\tau > t$.

This can also be derived using the Fourier transform in the usual way: we just have an ODE forced by $\tilde f(k,t)$ rather than a homogeneous one.

Duhamel's principle for the wave equation We give an example of the calculation using the Fourier Transform. We can equally well argue in the same way as we did in the previous section. Consider the forced wave equation

$$\begin{aligned}u_{tt} - c^2u_{xx} &= h(x,t) && t>0\\ u(x,0) &= f(x)\\ u_t(x,0) &= g(x).\end{aligned}$$

Taking the Fourier transform,

$$\begin{aligned}\tilde u_{tt} - c^2k^2\tilde u &= \tilde h(k,t) && t>0\\ \tilde u(k,0) &= \tilde f(k)\\ \tilde u_t(k,0) &= \tilde g(k).\end{aligned}$$

We have the Green's function for this initial value problem: with homogeneous boundary conditions, it is

$$H(t-\tau)\frac{\sin(ck(t-\tau))}{ck}.$$

Hence the solution is the sum of the integral of this against $h(k,t)$ and the part to account for the boundary terms, which we have calculated before: we find

$$\begin{aligned}\tilde u(k,t) = \tilde f(k)\cos(ckt) + \tilde g(k)\frac{\sin(ck(t-\tau))}{ck} \\ + \int_0^t \frac{\sin(ck(t-\tau))}{ck}\tilde h(k,\tau)\,d\tau.\end{aligned}$$

Taking the inverse Fourier transform and changing the order of integration, we arrive at the general solution, namely

$$\begin{aligned}u(x,t) = \frac12\big(f(x-ct)+f(x+ct)\big) + \frac{1}{2c}\int_{x-ct}^{x+ct} g(\xi)\,d\xi \\ + \int_0^t\int_{x-c(t-\tau)}^{x+c(t-\tau)} h(\xi,\tau)\,d\xi\,d\tau,\end{aligned}$$

or as a clearer expression of Duhamel's principle,

$$\begin{aligned}u(x,t) = \frac12\big(f(x-ct)+f(x+ct)\big) + \int_{-\infty}^{\infty} G(x,t;\xi,0)g(\xi)\,d\xi \\ + \int_0^t\int_{-\infty}^{\infty} G(x,t;\xi,\tau)h(\xi,\tau)\,d\xi\,d\tau\end{aligned}$$

Superposition of solutions satisfying different boundary conditions In more complicated situations, we exploit the linearity of the equation, which enables us to split the solution into several parts, each satisfying a simpler boundary condition. For example, the wave equation on a half-line, where $u(0,t) = v(t)$, together with the other equations:

$$\begin{aligned} u_{tt} - c^2 u_{xx} &= h(x,t) \qquad & 0 < x, 0 < t \\ u(x,0) &= f(x) \\ u_t(x,0) &= g(x) \end{aligned}$$

However, if we instead look at $w(x,t) \coloneqq u(x,t) - v(t)$, we find it satisfies the system of equations

$$\begin{aligned} w_{tt} - c^2 w_{xx} &= h(x,t) - v(t) \qquad & 0 < x, 0 < t \\ w(x,0) &= f(x) - v(0) \\ w_t(x,0) &= g(x) - v'(0) \\ w(0,t) &= 0, \end{aligned}$$

and this we can solve, by using the Dirichlet Green's function $G_D(x,t;\xi,\tau) = G(x,t;\xi,\tau) - G(x,t;-\xi,\tau)$:

$$\begin{aligned} w(x,t) = \frac{1}{2}\big(f(x-ct) + f(x+ct)\big) - v(t) \\ + \int_0^\infty G_D(x,t;\xi,0)\big(g(\xi) - v'(0)\big)\,d\xi \\ + \int_0^t \int_0^\infty G_D(x,t;\xi,\tau)\big(h(\xi,\tau) - v(\tau)\big)\,d\xi\,d\tau, \end{aligned}$$

and adding $v(t)$ to both sides gives us back $u(x,t)$.