Notes on Mathematical Methods

1060-710: Mathematical and Statistical Methods for Astrophysics *

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1 The Gamma Function

See Arfken & Weber, Chapter 8, especially Section 8.1

Something which will come up in the context of several special functions is the Gamma function, defined for positive z as

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt \tag{1.1}$$

To see why this is an interesting quantity, let's step back and look at a few simpler integrals first.

If $\alpha > 0$,

$$\int_0^\infty e^{-\alpha t} dt = -\frac{e^{-\alpha t}}{\alpha} \Big|_0^\infty = \frac{1}{\alpha} .$$
 (1.2)

Next, think about

$$\int_0^\infty t \, e^{-\alpha t} dt \; . \tag{1.3}$$

We could integrate by parts, using $\int u \, dv = uv - \int v \, du$ with u = t and $dv = e^{-\alpha t} dt$ but there's a cute trick due to Richard Feynman. Since

$$\frac{\partial}{\partial \alpha} e^{-\alpha t} = -t \, e^{-\alpha t} \tag{1.4}$$

we can write

$$\int_0^\infty t \, e^{-\alpha t} dt = \int_0^\infty \left(-\frac{\partial}{\partial \alpha} e^{-\alpha t} \right) dt = -\frac{d}{d\alpha} \int_0^\infty e^{-\alpha t} dt = -\frac{d}{d\alpha} \frac{1}{\alpha} = \frac{1}{\alpha^2} \tag{1.5}$$

and similarly

$$\int_{0}^{\infty} t^{2} e^{-\alpha t} dt = \left(-\frac{d}{d\alpha}\right)^{2} \left(\frac{1}{\alpha}\right) = \frac{2}{\alpha^{3}}$$
(1.6)

and

$$\int_0^\infty t^3 e^{-\alpha t} dt = \left(-\frac{d}{d\alpha}\right)^3 \left(\frac{1}{\alpha}\right) = \frac{3 \cdot 2}{\alpha^4}$$
(1.7)

and in general

$$\int_{0}^{\infty} t^{n} e^{-\alpha t} dt = \left(-\frac{d}{d\alpha}\right)^{n} \left(\frac{1}{\alpha}\right) = \frac{n!}{\alpha^{n+1}}$$
(1.8)

for any non-negative integer n. (Note that the factorial is defined so that 0! = 1 and (n+1)! = (n+1)n!.) We can now set α to 1 and see

$$n! = \int_0^\infty t^n e^{-t} dt = \Gamma(n+1) .$$
 (1.9)

The integral definition of the Gamma function extends the meaning of the factorial to noninteger numbers, and the Gamma function satisfies

$$\Gamma(z+1) = z\Gamma(z) \tag{1.10}$$

$$\Gamma(1) = 1 \tag{1.11}$$

You might wonder why the Gamma function is defined so that $\Gamma(n + 1) = n!$ with the troublesome extra +1. This is so that $\Gamma(z)$ is finite for all positive z. We know the integral is well-behaved as $t \to \infty$ because the exponential kills the integrand faster than any power. The integral will be finite if the part near t = 0 is well behaved, i.e., if

$$\lim_{\epsilon \to 0} \int_0^{\epsilon} t^z \, e^{-t} dt = 0 \tag{1.12}$$

but

$$\int_0^{\epsilon} t^z e^{-t} dt \to \int_0^{\epsilon} t^z e^{-t} dt = \frac{t^z}{z} \Big|_0^{\epsilon} = \frac{\epsilon^z}{z} \to 0 \qquad \text{when } z > 0 \qquad (1.13)$$

On the other hand, we know that $\Gamma(0)$ must blow up, since (1.10) tells us

$$1 = \Gamma(1) = 0\Gamma(0) . (1.14)$$

But, for example $\Gamma(1/2)$ should be finite, even though it would seem to be the factorial of a negative number (i.e., -1/2). In fact, we can use the change of variables $x = \sqrt{t}$; $dx = \frac{1}{2} \frac{dt}{\sqrt{t}}$ to calculate

$$\Gamma(1/2) = \int_0^\infty t^{-1/2} e^{-t} dt = 2 \int_0^\infty e^{-x^2} dx = \int_{-\infty}^\infty e^{-x^2} dx .$$
(1.15)

This is another very famous integral, which can be done by another cool trick, using conversion from Cartesian to polar coördinates in the plane:

$$\left(\Gamma(1/2) \right)^2 = \left(\int_{-\infty}^{\infty} e^{-x^2} dx \right) \left(\int_{-\infty}^{\infty} e^{-y^2} dy \right) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-x^2 - y^2} dx \, dy$$

$$= \int_{0}^{2\pi} \int_{0}^{\infty} e^{-r^2} r \, dr \, d\phi = 2\pi \int_{0}^{\infty} e^{-u} \frac{du}{2} = \pi$$

$$(1.16)$$

(where in the last step we've used the substitution $u = r^2$; du = 2r dr) so

$$\Gamma(1/2) = \sqrt{\pi} \tag{1.17}$$

We can also extend the definition of $\Gamma(z)$ to negative values according to

$$\Gamma(z-1) = \frac{\Gamma(z)}{z-1} \tag{1.18}$$

it will blow up for negative integers (because $\Gamma(0)$ blows up) but otherwise be fine. For instance

$$\Gamma(-1/2) = \frac{\Gamma(1/2)}{-1/2} = -2\sqrt{\pi} .$$
(1.19)

For other non-integer arguments the values are tabulated and can be explored on a computer, e.g.,

> ipython -pylab from scipy.special import gamma gamma(1)gamma(2)The result looks like this: gamma(3) gamma(4)gamma(5) gamma(37)/gamma(36)gamma(10.16)/gamma(9.16) gamma(0.5)sqrt(pi) gamma(-0.5)-2.0*sqrt(pi) figure() z=linspace(0.001,5,500) z1=linspace(-0.999,-0.001,100) z2=linspace(-1.999,-1.001,100) z3=linspace(-2.999,-2.001,100) z4=linspace(-3.999,-3.001,100) z5=linspace(-4.999,-4.001,100) plot(z,gamma(z),'k-') plot(z1,gamma(z1),'k-') plot(z2,gamma(z2),'k-')plot(z3,gamma(z3),'k-') plot(z4,gamma(z4),'k-')plot(z5,gamma(z5),'k-')axis([-5,5,-10,10]) xticks(arange(-5,6)) yticks(arange(-10,11,2)) grid(1) xlabel('\$z\$') ylabel('\$\Gamma(z)\$') savefig('gammafcn.eps')

 $\Gamma(z)$ י הי 14 L U ۱ N L ≈ C N ω Þ (7

Differential Equations 2

See Arfken & Weber, Chapter 9

General Properties; Superposition 2.1

Many situations in astrophysics (and physics in general) are described by linear partial differential equations, which we can write schematically as

$$\mathcal{L}\psi(\vec{r}) = 0$$
 (homogeneous PDE) (2.1)

or

$$\mathcal{L}\psi(\vec{r}) = \rho(\vec{r})$$
 (inhomogeneous PDE) (2.2)

the differential operator can depend in potentially complicated ways on the coördinates, but not on the scalar field ψ . If \mathcal{L} is a linear differential operator, it implies the principle of superposition: if ψ_1 and ψ_2 are solutions to the homogeneous PDE (2.1), so is $a\psi_1 + b\psi_2$:

$$\mathcal{L}(c_1\psi_1 + c_2\psi_2) = c_1\mathcal{L}\psi_1^{\bullet} + c_2\mathcal{L}\psi_2^{\bullet} = 0.$$
(2.3)

The typical approach is to find a sufficient set of independent solutions $\{\psi_n\}$ so that an arbitrary solution can be written

$$\psi = \sum_{n} c_n \psi_n \tag{2.4}$$

and then fix the constants $\{c_n\}$ according to the boundary conditions of the problem.

Arfken has a list of differential equations that arise in physics, for example

1. the Laplace equation

$$\nabla^2 \psi = 0 \tag{2.5}$$

2. the Poisson equation (e.g., Newtonian gravity)

$$\nabla^2 \psi = 4\pi\rho \tag{2.6}$$

3. the Helmholtz equation

$$(\nabla^2 + k^2)\psi = 0 (2.7)$$

4. the diffusion equation

$$\left(\nabla^2 - \frac{1}{a^2}\frac{\partial}{\partial t}\right)\psi = 0 \tag{2.8}$$

5. the wave equation

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\psi = 0 \tag{2.9}$$

etc etc. Notice that these all involve the Laplacian ∇^2 . (Some also involve time derivatives, but if we write $\psi(\vec{r},t) = \int_{-\infty}^{\infty} e^{-i\omega t} \psi_{\omega}(\vec{r}) dt$, the wave equation for $\psi(\vec{r},t)$ becomes the Helmholtz equation for $\psi_{\omega}(\vec{r})$ with $k = \omega/c$.) Since our goal is not to develop the full theory of differential equations, but rather to become familiar with some of the solutions that come up all the time in physics and astronomy, let's look more into typical partial differential equations involving the Laplacian in some common coördinate systems.

2.2 The Laplacian; Separation of Variables

Recall from vector calculus that the Laplacian has the following forms in Cartesian coördinates $\{x, y, z\}$, cylindrical coördinates¹ $\{s, \phi, z\}$, and spherical coördinates $\{r, \theta, \phi\}$:

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

$$= \frac{\partial^{2}}{\partial s^{2}} + \frac{1}{s}\frac{\partial}{\partial s} + \frac{1}{s^{2}}\frac{\partial^{2}}{\partial \phi^{2}} + \frac{\partial^{2}}{\partial z^{2}}$$

$$= \frac{\partial^{2}}{\partial r^{2}} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^{2}}\frac{\partial^{2}}{\partial \theta^{2}} + \frac{\cot\theta}{r^{2}}\frac{\partial}{\partial \theta} + \frac{1}{r^{2}\sin^{2}\theta}\frac{\partial^{2}}{\partial \phi^{2}}$$
(2.10)

Note that

- Every term in (2.10) has units of one over length squared.
- I've expanded out some expressions like $\frac{1}{s}\frac{\partial}{\partial s}\left(s\frac{\partial}{\partial s}\right)$ and $\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)$ compared to the forms in Arfken.

2.2.1 Cartesian Coördinates

For concreteness, we'll the Helmholtz equation

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + k^2\right)\psi(x, y, z) = 0.$$
(2.11)

A standard method for converting a partial differential equation into a set of ordinary differential equations is separation of variables, to look for a solution of the form

$$\psi(x, y, z) = X(x)Y(y)Z(z)$$
 . (2.12)

(Remember that we plan to use superposition to combine different solutions, so we're not making such a restrictive assumption on the form of the general solution.) Substituting (2.12) into (2.11) and dividing by ψ gives us

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} + k^2 = 0$$
(2.13)

Since the first term depends only on z, the second only on y and the third only on z, the only way the equation can be satisfied in general is if each of them is a constant:

$$\frac{X''(x)}{X(x)} + \underbrace{\frac{Y''(y)}{Y(y)}}_{=-k_x^2} + \underbrace{\frac{Z''(z)}{Z(z)}}_{=-k_z^2} + k^2 = 0$$
(2.14)

¹What to call the cylindrical radial coördinate $\sqrt{x^2 + y^2}$ is a perpetually troubling issue. It's clearly inappropriate to call it r in a three-dimensional context, since that means something different in spherical coördinates. Arfken calls it ρ , but that can get confusing if ρ is also used as a density. I'll follow the convention of Griffiths's *Introduction to Electrodynamics* and call it s.

so we can solve the original PDE if X, Y, and Z satisfy²

$$X''(x) + k_x^2 X(x) = 0 (2.15a)$$

$$Y''(y) + k_y^2 Y(y) = 0$$
(2.15b)

$$Z''(z) + k_z^2 Z(z) = 0. (2.15c)$$

Each of these, (2.15a) for example, is a pretty simple and familiar ODE. Since it's second order, we know there are two independent solutions for a given k_x , and they are

$$X(x) \equiv \begin{cases} e^{ik_x x} \\ e^{-ik_x x} \end{cases} \text{ or equivalently } \begin{cases} \sin k_x x \\ \cos k_x x \end{cases}$$
(2.16)

What values are allowed for $\{k_x, k_y, k_z\}$ depend on things like the boundary conditions for the problem. Note that k_x , k_y and k_z all have units of inverse length.

2.2.2 Cylindrical Coördinates

Now the PDE is

$$\left(\frac{\partial^2}{\partial s^2} + \frac{1}{s}\frac{\partial}{\partial s} + \frac{1}{s^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} + k^2\right)\psi(s,\phi,z) = 0$$
(2.17)

and guessing a separable solution

$$\psi(s,\phi,z) = S(s)\Phi(\phi)Z(z) \tag{2.18}$$

gives the equations

$$\frac{S''(s)}{S(s)} + \frac{1}{s}\frac{S'(s)}{S(s)} + \frac{1}{s^2}\frac{\Phi''(\phi)}{\Phi(\phi)} + \frac{Z''(z)}{Z(z)} + k^2 = 0$$
(2.19)

The separation is slightly trickier this time. We can handle the z dependence the same as before, and write

$$\frac{Z''(z)}{Z(z)} = -k_z^2 . (2.20)$$

Everything else has some s dependence in it, but if we multiply through by s^2 we get

$$s^{2}\frac{S''(s)}{S(s)} + s\frac{S'(s)}{S(s)} + (k^{2} - k_{z}^{2})s^{2} + \frac{\Phi''(\phi)}{\Phi(\phi)} = 0.$$
(2.21)

Now the last term depends only on ϕ and we can set it to a constant, call it $-m^2$. Again, the simple ODE

$$\Phi''(\phi) + m^2 \Phi(\phi) = 0$$
 (2.22)

has the solution

$$\Phi(\phi) = e^{im\phi} . \tag{2.23}$$

²We've implicitly assumed each constant is negative by writing them as $-k_x^2$ etc. Depending on the problem, we may find that some of them should actually be positive, but this can always be handled by allowing e.g., k_x to be imaginary in the end.

But in a physical problem, ϕ is an angular coördinate with a period of 2π , so if the solution to the PDE is to be single-valued, we have to enforce

$$\Phi(\phi + 2\pi) = \Phi(\phi) . \tag{2.24}$$

This means we know the conditions on m:

m must be an integer

So we're back to the non-trivial ODE for s:

$$s^{2}S''(s) + sS'(s) + \left[(k^{2} - k_{z}^{2})s^{2} - m^{2}\right]S(s) = 0.$$
(2.25)

It looks like the z and ϕ equations have stuck us with a two parameter family of possible ODEs for the s dependence, but that's not really true. m is a dimensionless parameter (in fact we know it has to be an integer in most physical problems) but $k^2 - k_z^2$ has dimensions of inverse length squared. That means it really just sets the scale of the s dependence, and we can get a simpler differential equation by changing variables to $x = s\sqrt{k^2 - k_z^2}$ and defining y(x) = S(s); since this is just a rescaling,

$$s\frac{d}{ds} = x\frac{d}{dx} \tag{2.26}$$

and the differential equation becomes

$$x^{2}y''(x) + xy'(x) + \left[x^{2} - m^{2}\right]y(x) = 0.$$
(2.27)

This is Bessel's equation, and the two independent solutions to it are called Bessel functions $J_m(x)$ and $N_m(x)$.

2.3 Spherical Coördinates

In spherical coördinates, the PDE is

$$\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{\cot\theta}{r^2}\frac{\partial}{\partial \theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2} + k^2\right)\psi(r,\theta,\phi) = 0$$
(2.28)

and the search for a separated solution

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi) \tag{2.29}$$

gives us

$$\frac{R''(r)}{R(r)} + \frac{2}{r}\frac{R'(r)}{R(r)} + \frac{1}{r^2}\frac{\Theta''(\theta)}{\Theta(\theta)} + \frac{\cot\theta}{r^2}\frac{\Theta'(\theta)}{\Theta(\theta)} + \frac{1}{r^2\sin^2\theta}\frac{\Phi''(\phi)}{\Phi(\phi)} + k^2 = 0$$
(2.30)

As before, the ϕ dependence is

$$\Phi(\phi) = e^{im\phi} \qquad m \in \mathbb{Z} \tag{2.31}$$

so multiplying by r^2 gives us

$$\underbrace{r^2 \frac{R''(r)}{R(r)} + 2r \frac{R'(r)}{R(r)} + k^2 r^2}_{\ell(\ell+1)} + \underbrace{\frac{\Theta''(\theta)}{\Theta(\theta)} + \cot\theta \frac{\Theta'(\theta)}{\Theta(\theta)} - \frac{m^2}{\sin^2 \theta}}_{-\ell(\ell+1)} = 0$$
(2.32)

where by separating the left-hand side into a piece depending only on r and a piece depending only on θ we know that each has to be a constant. We've written that constant rather provocatively, but it's because the angular equation

$$\Theta''(\theta) + \cot \theta \,\Theta'(\theta) + \left(\ell(\ell+1) - \frac{m^2}{\sin^2 \theta}\right) \Theta(\theta) = 0 \tag{2.33}$$

turns out to have geometrically sensible solutions only when

$$|m| \le \ell \in \mathbb{Z} \tag{2.34}$$

These are the associated Legendre functions $P_{\ell}^m(\cos\theta)$ (and $Q_{\ell}^m(\cos\theta)$) and they are part of the spherical harmonics $Y_{\ell}^m(\theta,\phi) = P_{\ell}^m(\cos\theta)e^{im\phi}$ which we'll come back to later.

Look instead at the radial equation

$$r^{2}R''(r) + 2rR'(r) + \left[k^{2}r^{2} - \ell(\ell+1)\right]R(r) = 0$$
(2.35)

Again, the dimensionful parameter k can be scaled away, but the dimensionless parameter ℓ cannot. Setting x = kr and y(x) = R(r) gives us

$$x^{2}y''(x) + 2xy'(x) + \left[x^{2} - \ell(\ell+1)\right]y(x) = 0$$
(2.36)

This is not quite Bessel's equation (2.27) but a little bit of algebra shows that if we write

$$\eta(x) = y(x)\sqrt{x} \tag{2.37}$$

then $\eta(x)$ solves the differential equation

$$x^{2}\eta''(x) + x\eta'(x) + \left[x^{2} - \left(\ell + \frac{1}{2}\right)^{2}\right]\eta(x) = 0$$
(2.38)

which is Bessel's equation if we replace the integer m with the non-integer value $\ell + \frac{1}{2}$.

So Bessel functions, thought of now as the solutions to

$$x^{2}y''(x) + xy'(x) + \left[x^{2} - \nu^{2}\right]y(x) = 0.$$
(2.39)

for a particular (not necessarily integer) ν are going to be important!

Thursday, September 10, 2009

3 Bessel Functions

See Arfken & Weber, Chapter 9 (especially sec 9.5-9.6) and Chapter 11 We saw last time that the differential equation

$$x^{2}y''(x) + xy'(x) + \left[x^{2} - \nu^{2}\right]y(x) = 0.$$
(3.1)

comes up in problems involving the Laplacian in cylindrical coördinates, and is also relevant to some problems in cylindrical coördinates. This is the Bessel equation, and its solutions are called *Bessel Functions*. All of the following are defined for any real number ν , and solve (3.1) for that ν :

- $J_{\nu}(x)$ Bessel functions, also known as Bessel functions of the first kind
- $N_{\nu}(x)$ Neumann functions, also known as Bessel functions of the second kind, and also written $Y_{\nu}(x)$

 $H_{\nu}^{(1,2)}(x)$ Hankel functions

Not all of them are independent, but which combinations make a full set depend on the value of $|\nu|$. Note that, for example, $J_{\nu}(x)$ and $J_{-\nu}(x)$ solve the same differential equation, but they are defined differently.

But does naming something really give us any power over it? Many many differential equations have solutions which can be written as hypergeometric functions, but calling something a hypergeometric function doesn't really give us any insight. We gain insight into special functions by studying their properties. For example, we deal with sines and cosines enough that realizing that a result can be written as a trigonometric function tells us a lot about it.

3.1 Power Series Expansions

One of the ways we understand transcendental functions like sines, cosines and exponentials is to write them as power series, like

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} \tag{3.2a}$$

$$\cos x = \sum_{n=0}^{\infty} \left(-1\right)^n \frac{x^{2n}}{(2n)!} \tag{3.2b}$$

$$\sin x = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)!}$$
(3.2c)

these allow us to show, for example, that

$$e^{ix} = \cos x + i \sin x \tag{3.3}$$

So we'll look to write a solution to (3.1) as a power series

$$y(x) = \sum_{n=0}^{\infty} a_n x^{s+n} .$$
 (3.4)

We require $a_0 \neq 0$ so that s is the lowest power of x appearing in the series. By substituting

$$y'(x) = \sum_{n=0}^{\infty} a_n (s+n) x^{s+n-1}$$
(3.5a)

$$y''(x) = \sum_{n=0}^{\infty} a_n (s+n)(s+n-1)x^{s+n-2}$$
(3.5b)

into (3.1) we find

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

= $\sum_{n=0}^{\infty} a_{n} \left\{ x^{s+n} \left[\underbrace{(s+n)(s+n-1) + (s+n)}_{(s+n)^{2}} - \nu^{2} \right] + x^{s+n+2} \right\}$. (3.6)

$$= a_0 x^s (s^2 - \nu^2) + a_1 x^{s+1} [(s+1)^2 - \nu^2] + \sum_{n=2}^{\infty} x^{s+n} \left\{ \left[(s+n)^2 - \nu^2 \right] a_n + a_{n-2} \right\}$$

For (3.4) to be a solution, the coëfficient of each power of x has to vanish.

The lowest term gives us what is known as the *indicial equation*

$$a_0(s^2 - \nu^2) = 0 ; (3.7)$$

since $a_0 \neq 0$ by definition, that means the two possibilities are $s = \nu$ and $s = -\nu$. In principle these can be two different solutions, but that's fine, since we expect a second order ODE to have two independent solutions.

Replacing ν^2 with s^2 and looking at the next term, we get

$$0 = a_1[(s+1)^2 - s^2] = a_1(2s+1)$$
(3.8)

So, except for the special case s = -1/2 (which is only a possible solution if $\nu^2 = 1/4$), we have to have a_1 , which means there is no x^{s+1} term.³

Requiring each of the other terms to vanish gives us a relationship among the a_n s:

$$\left[(s+n)^2 - \nu^2\right]a_n + a_{n-2} = 0 \tag{3.9}$$

This recursion relation can be used to work out the general form of the series:

$$y(x) = \sum_{n=0}^{\infty} (-1)^k \frac{a_0 2^s \,\Gamma(s+1)}{k! \,\Gamma(s+k+1)} \left(\frac{x}{2}\right)^{s+2k} \tag{3.10}$$

³In the case s = -1/2, the lowest term goes like $x^{-1/2}$, and the term which is not ruled out by (3.8). But for $\nu^2 = 1/4$ the other solution starts with the $x^{1/2}$ term, and it turns out allowing $a_1 \neq 0$ for s = -1/2 would just end up mixing in some of the s = 1/2 solution. So even in the one case where we're not forced to have $a_1 = 0$ we can choose to do it anyway, and everything will work out.

Note that we have written

$$\prod_{k=1}^{n} (s+k) = \frac{\Gamma(s+k+1)}{\Gamma(s+1)} ; \qquad (3.11)$$

if s is an integer, this is just (s+k)!/s! but the Gamma function allows us to generalize this to non-integer s.

The standard normalization convention is to choose

$$a_0 = \frac{1}{2^s \,\Gamma(s+1)} \tag{3.12}$$

so that the Bessel Function (of the First Kind) is defined as

$$J_s(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k! \,\Gamma(s+k+1)} \left(\frac{x}{2}\right)^{s+2k} \tag{3.13}$$

This is the definition for any real s. Bessel's equation (3.1) is satisfied for a given ν by both $J_{\nu}(x)$ and $J_{-\nu}(x)$. For non-integer ν these are the two independent solutions to the second-order ODE; one starts at $x^{-\nu}$ and the other at x^{ν} .

For integer ν it turns out that $J_{-\nu}(x)$ is just a multiple of $J_{\nu}(x)$. Why is that? Well, for $\nu = 0, -\nu$ and ν are the same thing. For a positive integer n,

$$J_{-n}(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k! \, \Gamma(k+1-n)} \left(\frac{x}{2}\right)^{2k-n} \,. \tag{3.14}$$

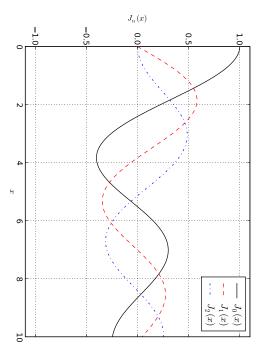
For k = 0, 1, ..., n - 1, the denominator has a Gamma function of a non-positive integer, which we learned the other day blows up, so those coëfficients are actually zero. That means the sum is

$$J_{-n}(x) = \sum_{k=n}^{\infty} \frac{(-1)^k}{k! (k-n)!} \left(\frac{x}{2}\right)^{2k-n} = \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell+n}}{(\ell+n)! \ell!} \left(\frac{x}{2}\right)^{2\ell+n} = (-1)^n J_n(x)$$
(3.15)

3.1.1 Numerical Implementations

As common functions, $J_{\nu}(x)$ are implemented in your favorite mathematical computation environment. For instance, in SciPy's special function package:^{*a*}

```
> ipython -pylab
from scipy.special import *
x=linspace(0.0001,10,1000)
plot(x,jn(0,x),'k-',label='$J_0(x)$')
plot(x,jn(1,x),'r--',label='$J_1(x)$')
plot(x,jn(2,x),'b-.',label='$J_2(x)$')
legend()
xlabel('$x$')
ylabel('$x$')
ylabel('$J_n(x)$')
axis([0,10,-1.1,1.1])
grid(True)
savefig('besselJ.eps',bbox_inches='tigh
```



^aThe list of special function names is at http://docs.scipy.org/doc/scipy/reference/spec

3.2 Neumann Functions

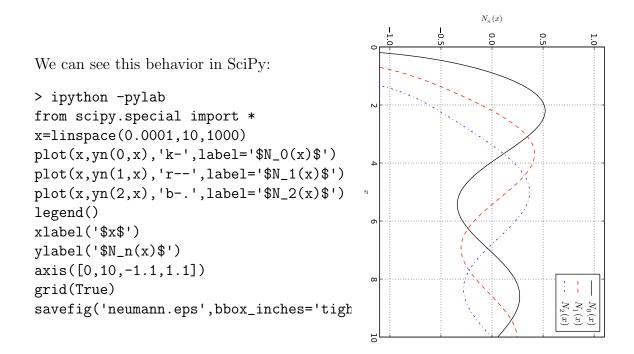
In order to get two independent solutions, one defines the Neumann Functions or Bessel Functions of the Second Kind, written $N_{\nu}(x)$ or sometimes $Y_{\nu}(x)$. The definition is

$$N_{\nu}(x) = \begin{cases} \frac{\cos \pi \nu J_{\nu}(x) - J_{-\nu}(x)}{\sin \pi \nu} & \nu \notin \mathbb{Z} \\ \frac{1}{\pi} \left(\frac{\partial J_{\nu}(x)}{\partial \nu} - (-1)^{\nu} \frac{\partial J_{-\nu}(x)}{\partial \nu} \right) & \nu \in \mathbb{Z} \end{cases}$$
(3.16)

You will explore the properties of these functions further on the homework, in particular showing that

- $N_n(x)$ solves Bessel's equation even for integer n
- $N_n(x)$, for non-negative integer *n*, contains powers of *x* starting at x^{-n} , and also terms involving $\ln x$

It's the presence of the logarithmic terms that explains why we didn't find $N_n(x)$ when we were looking for power series solutions. It also means there's not an explicit form of $N_n(x)$ that's worth writing down, but we do see that $N_n(x)$ diverges at x = 0, logarithmically for n = 0 and like x^{-n} otherwise.



For any $\nu^2 \ge 0$, picking $\nu \ge 0$ for convenience, $J_{\nu}(x)$ and $N_{\nu}(x)$ provide two independent solutions to Bessel's equation.

Tuesday, September 15, 2009

3.3 Example: Wave Equation in 2d Polar Coördinates

Let's start with the wave equation in 2+1 dimensions, written in terms of the polar coördinates (r, ϕ) and of time. (We could do this in cylindrical coördinates [in which case r would be called s] but we'd just be carrying around the extra z dependence.) We know that the wave equation

$$\nabla^2 \psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} = 0 \tag{3.17}$$

has solutions (choose one from each column)

$$\begin{cases} J_m(kr) \\ N_m(kr) \end{cases} \begin{cases} \cos m\phi \\ \sin m\phi \end{cases} \begin{cases} \cos kct \\ \sin kct \end{cases}$$
(3.18)

where m is a non-negative integer and k is non-negative real number.

To figure out what coëfficients go in the superposition, we need to satisfy the boundary conditions of the problem. E.g., consider the case where ψ vanishes on a circular outer boundary r = a

$$\psi(a,\phi,t) = 0 \tag{3.19}$$

and look for the solution for $0 \le r \le a$. This would describe, e.g., the oscillations of a drum of radius a. Since r = 0 is included, we know the coëfficients of any terms involving the Neumann functions have to vanish (or else ψ would blow up at the origin) so we're left with solutions of the form

$$J_m(kr) \begin{cases} \cos m\phi\\ \sin m\phi \end{cases} \begin{cases} \cos kct\\ \sin kct \end{cases}$$
(3.20)

To satisfy the boundary conditions at all ϕ and t, we're not allowed to choose arbitrary k; for a given term in the superposition we need one that has $J_m(ka) = 0$. We know from plotting the Bessel functions that they oscillate, so we define the positive values of their arguments for which they cross zero as γ_{mn} i.e.,

$$J_m(\gamma_{mn}) = 0 ; \qquad (3.21)$$

 γ_{mn} is the *n*th zero of the *m*th Bessel function. There's no closed-form expression for these, but they're tabulated.

The solutions we want are thus superpositions of

$$J_m\left(\frac{\gamma_{mn}}{a}r\right) \left\{ \begin{array}{l} \cos m\phi\\ \sin m\phi \end{array} \right\} \left\{ \begin{array}{l} \cos \frac{\gamma_{mn}}{a}ct\\ \sin \frac{\gamma_{mn}}{a}ct \end{array} \right\} \qquad n = 1, 2, \dots; \qquad m = 0, 1, 2, \dots$$
(3.22)

To nail down all the coëfficients, we need to know initial conditions on the waves, e.g., $\psi(r, \phi, 0)$ and $\dot{\psi}(r, \phi, 0)$; for concreteness, we can assume we deform the drumhead into some shape and then release it, so that

$$\psi(r,\phi,0) = f(r,\phi) \tag{3.23}$$

$$\psi(r,\phi,0) = 0 \tag{3.24}$$

where $f(r, \phi)$ is some specified function. The $\dot{\psi}$ condition means the solutions are of the form

$$J_m\left(\frac{\gamma_{mn}}{a}r\right)\left\{\frac{\cos m\phi}{\sin m\phi}\right\}\cos\frac{\gamma_{mn}}{a}ct \qquad n=1,2,\ldots; \qquad m=0,1,2,\ldots$$
(3.25)

and we can write the solution explicitly as

$$\psi(r,\phi,t) = \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} J_m\left(\frac{\gamma_{mn}}{a}r\right) \left(A_{mn}\cos m\phi + B_{mn}\sin m\phi\right)\cos\frac{\gamma_{mn}}{a}ct$$
(3.26)

and we impose the boundary conditions by choosing $\{A_{mn}\}\$ and $\{B_{mn}\}\$ so that

$$f(r,\phi) = \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} J_m\left(\frac{\gamma_{mn}}{a}r\right) \left(A_{mn}\cos m\phi + B_{mn}\sin m\phi\right)$$
(3.27)

This is called a *Fourier-Bessel series*. The Fourier part is hopefully somewhat familiar and can be inverted by use of identities like

$$\int_{0}^{2\pi} \sin m_1 \phi \, \sin m_2 \phi \, d\phi = \begin{cases} \pi & m_1 = m_2 \neq 0\\ 0 & m_1 \neq m_2 \end{cases} \,. \tag{3.28}$$

The Bessel part turns out to be handled with the identity

$$\int_0^a J_m\left(\frac{\gamma_{mn_1}}{a}r\right) J_m\left(\frac{\gamma_{mn_2}}{a}r\right) dr = 0 \quad \text{if } n_1 \neq n_2 \tag{3.29}$$

which we can deduce from the Bessel equation. Recall that for a given k and m, $J_m(kr)$ satisfies

$$0 = \left[r^2 \frac{d^2}{dr^2} + r \frac{d}{dr} + (k^2 r^2 - m^2)\right] J_m(kr) = r \left[\frac{d}{dr} \left(r \frac{dJ_m(kr)}{dr}\right) + \left(k^2 r - \frac{m}{r}\right) J_m(kr)\right]$$
(3.30)

Taking the equation for $k = k_1$ and multiplying through by $J_m(k_2 r)$ we get

$$0 = J_m(k_2 r) \frac{d}{dr} \left(r \frac{dJ_m(k_1 r)}{dr} \right) + \left(k_1^2 r - \frac{m}{r} \right) J_m(k_2 r) J_m(k_1 r)$$
(3.31)

If we integrate this with respect to r from r = 0 to r = a, we get

$$0 = \left[\left(J_m(k_2 r) \right) r \left(\frac{dJ_m(k_1 r)}{dr} \right) \right]_0^a - \int_0^a \left(\frac{dJ_m(k_2 r)}{dr} \right) r \left(\frac{dJ_m(k_1 r)}{dr} \right) dr + \int_0^a \left(k_1^2 r - \frac{m}{r} \right) J_m(k_2 r) J_m(k_1 r) dr$$
(3.32)

where we've integrated the first term by parts. Switching k_1 and k_2 and subtracting gives us

$$0 = \left[rJ_m(k_2r) \left(\frac{dJ_m(k_1r)}{dr} \right) \right]_0^a - \left[rJ_m(k_1r) \left(\frac{dJ_m(k_2r)}{dr} \right) \right]_0^a + (k_1^2 - k_2^2) \int_0^a J_m(k_1r) J_m(k_2r) dr$$
(3.33)

Now we can specialize to the case where $k_1 = \gamma_{mn_1}/a$ and $k_2 = \gamma_{mn_2}/a$; that makes the contribution to the first two terms from r = a vanish (the contribution from r = 0 already vanishes because of the factor of r) and we get

$$0 = \frac{\gamma_{mn_1}^2 - \gamma_{mn_2}^2}{a^2} \int_0^a J_m\left(\frac{\gamma_{mn_1}}{a}r\right) J_m\left(\frac{\gamma_{mn_2}}{a}r\right) dr$$
(3.34)

and so we see that indeed

$$\int_{0}^{a} J_{m}\left(\frac{\gamma_{mn_{1}}}{a}r\right) J_{m}\left(\frac{\gamma_{mn_{2}}}{a}r\right) dr = 0 \quad \text{if } k_{1} \neq k_{2} \tag{3.35}$$

3.4 Asymptotic Behavior

Bessel functions of half-integer order do have a simpler, more familiar form. Using the identity

$$\Gamma(k+1)\Gamma(k+1/2) = \frac{\Gamma(2k+1)\sqrt{\pi}}{2^{2k}} = \frac{(2k)!\sqrt{\pi}}{2^{2k}}$$
(3.36)

(which is not hard to show starting with $\Gamma(1/2) = \sqrt{\pi}$) we can show

$$J_{-1/2}(x) = \sqrt{\frac{2}{\pi x}} \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} x^{2k} = \sqrt{\frac{2}{\pi x}} \cos x \tag{3.37}$$

and along similar lines

$$J_{1/2}(x) = \sqrt{\frac{2}{\pi x}} \sin x$$
(3.38a)

$$N_{1/2}(x) = -J_{-1/2}(x) = -\sqrt{\frac{2}{\pi x}} \cos x$$
(3.38b)

That turns out to be the key to understanding how the Bessel (and Neumann) functions behave at large x; we can define $\mathcal{J}_{\nu}(x)$ so that

$$J_{\nu}(x) = \sqrt{\frac{2}{\pi x}} \mathcal{J}_{\nu}(x) \tag{3.39}$$

and then Bessel's equation (3.1) is equivalent (after applying the product rule and some algebra)

$$\mathcal{J}_{\nu}'' + \left(1 - \frac{\nu^2 - 1/4}{x^2}\right) \mathcal{J}_{\nu} = 0$$
(3.40)

So, for $\nu = 1/2$ this tells us that \mathcal{J}_{ν} can be a sine or cosine of x, which we've just found explicitly. But for large x we also get

$$\mathcal{J}_{\nu}''(x) + \mathcal{J}_{\nu} \stackrel{x \to \infty}{\longrightarrow} 0 .$$
 (3.41)

It turns out that the phase of the trig function in the asymptotic form is given by

$$J_{\nu} \xrightarrow{x \to \infty} \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{(2\nu + 1)\pi}{4}\right) \tag{3.42}$$

but the tools needed to show that are beyond what we can delve into in a timely fashion.

3.5 Hankel Functions

Using the asymptotic form of $J_{\nu}(x)$ and the definition of $N_{\nu}(x)$ you can show that the Neumann function has asymptotic form

$$N_{\nu}(x) \xrightarrow{x \to \infty} \sqrt{\frac{2}{\pi x}} \sin\left(x - \frac{(2\nu+1)\pi}{4}\right)$$
 (3.43)

Far from the origin, then, these look like trig functions with decaying amplitudes. But just as it's convenient sometimes to work with e^{ikx} and e^{-ikx} rather than $\cos x$ and $\sin x$, we might find a complex combination of the Bessel and Neumann functions useful. These are the Hankel functions

$$H_{\nu}^{(1)}(x) = J_{\nu}(x) + iN_{\nu}(x) \tag{3.44a}$$

$$H_{\nu}^{(2)}(x) = J_{\nu}(x) - iN_{\nu}(x) ; \qquad (3.44b)$$

evidently they have the asymptotic forms

$$H_{\nu}^{(1)}(x) \stackrel{x \to \infty}{\longrightarrow} \sqrt{\frac{2}{\pi x}} \exp\left(i\left[x - \frac{(2\nu+1)\pi}{4}\right]\right)$$
(3.45a)

$$H_{\nu}^{(2)}(x) \stackrel{x \to \infty}{\longrightarrow} \sqrt{\frac{2}{\pi x}} \exp\left(-i\left[x - \frac{(2\nu+1)\pi}{4}\right]\right) . \tag{3.45b}$$

3.6 Spherical Bessel Functions

The trick of multiplying a solution to Bessel's equation by a power of x to get a solution to a slightly differential equation can be used to define the *Spherical Bessel Functions*

$$j_{\ell}(x) = \sqrt{\frac{2}{\pi x}} J_{\ell+1/2}(x)$$
(3.46a)

$$n_{\ell}(x) = \sqrt{\frac{2}{\pi x}} N_{\ell+1/2}(x)$$
(3.46b)

$$h_{\ell}^{(1)}(x) = \sqrt{\frac{2}{\pi x}} H_{\ell+1/2}^{(1)}(x)$$
(3.46c)

$$h_{\ell}^{(2)}(x) = \sqrt{\frac{2}{\pi x}} H_{\ell+1/2}^{(2)}(x)$$
(3.46d)

These are *not* solutions to Bessel's equation, but rather to the equation

$$x^{2}y''(x) + 2xy'(x) + \left[x^{2} - \ell(\ell+1)\right]y(x) = 0$$
(3.47)

which we saw arises in the context of separating the Helmholtz equation in spherical coördinates. Note that from the known forms of $J_{1/2}(x)$ and $N_{1/2}(x)$, we can write

$$j_0(x) = \frac{\sin x}{x} \tag{3.48a}$$

$$n_0(x) = -\frac{\cos x}{x} \tag{3.48b}$$

The higher orders are not quite so simple, but they still can be writen as finite sums of trig functions and powers:

$$j_{\ell}(x) = (-x)^{\ell} \left(\frac{1}{x} \frac{d}{dx}\right)^{\ell} \left(\frac{\sin x}{x}\right)$$
(3.49a)

$$n_{\ell}(x) = (-x)^{\ell} \left(\frac{1}{x} \frac{d}{dx}\right)^{\ell} \left(-\frac{\cos x}{x}\right)$$
(3.49b)

Thursday, September 17, 2009

4 Sturm-Liouville Theory

Last time we showed that

$$\int_0^a J_m(k_1 s) J_m(k_2 s) s \, ds = 0 \qquad \text{if } k_1 \neq k_2 \, \& \, J_m(k_1 a) = 0 = J_m(k_2 a) \tag{4.1}$$

by manipulating the differential equation

$$\left[\frac{1}{s}\frac{d}{ds}\left(s\frac{d}{ds}\right) - \frac{m^2}{s^2} + k^2\right]J_m(ks) = 0.$$
(4.2)

This was not just a bit of isolated magic. You can do things like this in general, as an application of *Sturm-Liouville theory*. It can be understood by analogy to the eigenvalue problem in linear algebra:

Linear Algebra	Vector u	Square Matrix A	
Functional Analysis	Function $u(x)$	Linear operator \mathcal{L}	

Let's recall a few results about the eigenvalue problem in linear algebra

$$\mathbf{A}\mathbf{u} = \lambda \mathbf{u} \ . \tag{4.3}$$

First, recall the inner product

$$\langle \mathbf{u}, \mathbf{v} \rangle = \mathbf{u}^{\dagger} \mathbf{v} \tag{4.4}$$

where \mathbf{u}^{\dagger} is the adjoint of \mathbf{u} , i.e., the complex conjugate of its transpose, so in four dimensions

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}^{\dagger} = \begin{pmatrix} u_1^* & u_2^* & u_3^* & u_4^* \end{pmatrix} .$$
 (4.5)

The adjoint \mathbf{A}^{\dagger} of a square matrix \mathbf{A} has a handy property:

$$\langle \mathbf{u}, \mathbf{A}^{\dagger} \mathbf{v} \rangle = \mathbf{u}^{\dagger} \mathbf{A}^{\dagger} \mathbf{v} = (\mathbf{A} \mathbf{u})^{\dagger} \mathbf{v} = \langle \mathbf{A} \mathbf{u}, \mathbf{v} \rangle$$
 (4.6)

In the context of linear algebra, this is a simple identity, but in more abstract vector spaces (e.g., infinite-dimensional ones) this can act as the definition of the adjoint of an operator.

In a function space, where the "vectors" are sufficiently well-behaved functions on the interval $x \in [a, b]$, one inner product that can be defined is

$$\langle u, v \rangle = \int_{a}^{b} u^{*}(x) v(x) w(x) dx \qquad (4.7)$$

where we have allowed a real weighting function w(x) to be included in the measure w(x) dx. Now, if \mathcal{L} is a linear operator (e.g., a differential operator)

$$\langle u, \mathcal{L}v \rangle = \int_{a}^{b} u^{*}(x) \mathcal{L}v(x) w(x) dx$$
 (4.8)

and

$$\langle u, \mathcal{L}^{\dagger} v \rangle = \int_{a}^{b} [\mathcal{L} u^{*}(x)] v(x) w(x) dx . \qquad (4.9)$$

If we recall that in linear algebra, a self-adjoint (also known as Hermitian) matrix, for which $\mathbf{A}^{\dagger} = \mathbf{A}$ has the nice property that eigenvectors corresponding to different eigenfunctions are orthogonal, i.e., if

$$\mathbf{A}\mathbf{u}_1 = \lambda_1 \mathbf{u}_1 \tag{4.10a}$$

$$\mathbf{A}\mathbf{u}_2 = \lambda_2 \mathbf{u}_2 \tag{4.10b}$$

then

$$\langle \mathbf{u}_1, \mathbf{u}_2 \rangle = 0 \quad \text{if } \lambda_1 \neq \lambda_2 ;$$

$$(4.11)$$

The same thing is true of the eigenfunctions of a self-adjoint linear operator. (The demonstration is identical to the demonstration from linear algebra.)

So in the case of Bessel functions,

$$\mathcal{L} = \frac{1}{s} \frac{d}{ds} \left(s \frac{d}{ds} \right) - \frac{m^2}{s^2} , \qquad (4.12)$$

w(s) = s, and the eigenvalue equation is

$$\mathcal{L}J_m(ks) = -k^2 J_m(ks) . \tag{4.13}$$

The demonstration that \mathcal{L} is Hermitian is that

$$\int_{a}^{b} u(s) \mathcal{L}v(s) \, s \, ds = \int_{a}^{b} [\mathcal{L}u(s)] \, v(s) \, s \, ds \tag{4.14}$$

where u(s) and v(s) are real functions that satisfy the boundary conditions

$$u(0)$$
 is regular (4.15a)

$$u(a) = 0 \tag{4.15b}$$

The demonstration is similar to what we did in class last time, and involves integrating by parts twice.

Tue & Thu, September 22 & 24, 2009 (guest lectures by Joshua Faber)

5 Elliptic and Hyperbolic equations: an overview

Consider a second order differential equation in a k-dimensional space:

$$\sum_{m=0}^{k} \sum_{n=0}^{k} A_{mn} \frac{\partial}{\partial x^m} \left(\frac{\partial f}{\partial x^n} \right) + \sum_{p=0}^{N} B_p \frac{\partial f}{\partial x^p} = F(x)$$
(5.1)

If the matrix A is positive definite everywhere, we call the equation "elliptic".

Positive definite implies all eigenvalues of the matrix are positive. Rather than focus on the matrix aspects, we can concentrate on the physical examples. The most famous elliptic equation is the Poisson equation, which describes, among other things, Newtonian gravitational and electric fields:

$$\nabla^2 \Phi = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \Phi = 4\pi G\rho \tag{5.2}$$

You've already seen that the left hand side takes different forms in different coordinate systems, but all are elliptic.

Hyperbolic equations look much the same if the sign of one of the terms is negative, as we find in the wave equation:

$$\frac{\partial^2 f}{\partial t^2} - v^2 \frac{\partial^2 f}{\partial x^2} = 0 \tag{5.3}$$

From the standpoint of working with the equations, they could hardly be more different. Hyperbolic equations evolve forward in time (or whatever you name the variable with the opposite signature in the second derivative, and require the specification of initial data (values of the function f and its first derivative), and possibly boundary conditions depending on the particular equation, solution, domain, and numerical scheme. These are generally referred to as "Initial Value Problems". On the boundary of our domain, we need to impose some form of boundary condition, which typically comes in one of three types:

- 1. Dirichlet: f(x) is a specified function on the boundary
- 2. Von Neumann: $\nabla_N f(x)$ is specified on the boundary, where the gradient is taken normal to the boundary
- 3. Robin: $H[f(x), \nabla_N f(x)]$, some function of the value of the function and its normal gradient, is specified on the boundary

The boundary can be any surface, including one located at spatial infinity.

5.1 Elliptic Equations

There are two typical general ways to solve elliptic equation in the numerical sense. One is to deal with the values at a set of convenient points in space, and the other is to break the solution into a basis set of independent functions, typically orthogonal polynomials, and to work out what the coefficients must be. When dealing with points, the natural configuration to consider is a grid, ideally one adapted to the computational domain appropriate to the problem. For instance, if we have a circular domain in 2 dimensions, the natural grid is given in terms of s and ϕ . Under this mapping the grid becomes rectangular.

To begin our numerical investigation, the easiest grid configuration is a set of evenly spaced points. We need to determine how to express differential operators in a useful form. Since derivatives fundamentally involve the variation of functions over space, we know that the points will be linked. Moreover, since differential operator are linear, we would be wise to consider a matrix-based approach. Let us assume that

$$D\left[\frac{\partial^2}{\partial x^2}, \frac{\partial}{\partial x}\right]f = u \tag{5.4}$$

where D is a differential operator that includes first and/or second derivatives and u is the RHS. The problem can be written $D_{ij}[f^i] = u^j$, where u is a vector of length N containing the RHS expressions evaluated at the N points, and D_{ij} is an $N \times N$ matrix containing the as-yet undetermined coefficients. To evaluate a first derivative, we can make use of the fact that we know

$$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x-h)}{2h}$$
(5.5)

Obviously, when solving a problem numerically, limits never go to zero, so we instead evaluate

$$\frac{df}{dx} = \frac{f(x+a) - f(x-a)}{2a}$$
(5.6)

where a is the grid spacing. In the limit that $a \to 0$, this reproduces the first derivative exactly. For finite values of a, it represents an approximation. In terms of our matrix operator, we find $D_{k+1,k} = (2h)^{-1} = -D_{k-1,k}$.

This expression works well in the interior of the grid, but it can't be applied at either boundary, since we don't have points in both directions to evaluate. We could consider one sided derivatives, evaluating the following terms

$$x_1 \quad : \quad \frac{df}{dx} \approx \frac{f(x_2) - f(x_1)}{a} \tag{5.7a}$$

$$x_N$$
 : $\frac{df}{dx} \approx \frac{f(x_N) - f(x_{N-1})}{a}$ (5.7b)

but there is a problem. If we wanted to solve $\frac{df}{dx} = u$, we get the following matrix equation:

$$\frac{1}{2h} \begin{pmatrix} -2 & 2 & & \\ -1 & 0 & 1 & & \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ & & -1 & 0 & 1 \\ & & & -2 & 2 \end{pmatrix} \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{N-1}) \\ f(x_N) \end{pmatrix} = \begin{pmatrix} u(x_1) \\ u(x_2) \\ \vdots \\ u(x_{N-1}) \\ u(x_N) \end{pmatrix}$$
(5.8)

which has a solution $f = D^{-1}u$. It can be shown, though, that the matrix D_{ij} written like we did above is singular, i.e., it has determinant zero, and cannot be inverted. Indeed, if we label the rows of the metrix R_i , we find that

$$\sum_{i=2}^{N-1} (-1)^i R_i = 0.5(R_1 \pm R_N)$$
(5.9)

indicating that the rows are not linearly independent (the sign of the term for the last row is positive if we have an odd number of rows, and negative for even). This is not a surprise, since we have made no attempt whatsoever yet to impose boundary conditions. For this first-order equation, the only boundary condition we can impose is Dirichlet (the first-derivatives are explicitly given by the equation itself). We can impose such a condition at either boundary, but not both, since the condition at either boundary completely specifies the solution to the equation.

For second-order differential equations, we need to be able to express d^2f/dx^2 in terms of values at neighboring points. It can be shown that

$$\frac{d^2f}{dx^2} = \lim_{h \to 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$
(5.10)

so we may again approximate this by an expression where we assume the stepsize is finite:

$$\frac{d^2 f}{dx^2} \approx \frac{f(x+a) - 2f(x) + f(x-a)}{a^2}$$
(5.11)

which in matrix terms looks like the following:

$$\frac{\partial^2 f}{\partial x^2} = \frac{1}{2h} \begin{pmatrix} & \text{B.C.} & \\ 1 & -2 & 1 & \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ & 1 & -2 & 1 \\ & & \text{B.C.} & \end{pmatrix}$$
(5.12)

where "B.C." indicates that a boundary condition needs to be applied, rather than an expression representing a second derivative.

For practical applications, these stencils, as they are known, do not always work sufficiently well. In particular, they produce second-order accuracy: the overall magnitude of the error E between a numerical solution and the exact one will generally scale such that $E \propto h^2$. In order to cut your error by factor of 100, you need to use 10 times as many points, and thus invert a matrix which 100 times as many points, a process that takes 1000 times longer using even the best algorithms. In many cases, we'd like to do much better.

Let us write the first-derivative differencing stencil as $d_1(f,h) = [f(h) - f(-h)]/(2h)$. It is trivial to check that when applied to a constant function $F_0(x) = x^0 = 1$, $d_1(F_0,h) = 0$ for all possible choices of the stepsize h. When applied to a linear function, $F_1(x) = x$, we find $d_1(F_1,h) = 1$, which is good, since a first derivative had better correctly measure the slope of a linear function. Even better yet, when applied to a quadratic function, $F_2 = x^2$, we find $d_1(F_2,h) = 0$. This means that for any function whose Taylor series near a point can be expressed as $f(x) = c_0 + c_1 x + c_2 x^2$, we will measure the first derivative correctly using d_1 . Unfortunately, most functions do not have Taylor series that terminate, and it is easily checked that $d_1(F_3) = h^2$. Higher-order odd terms also make contributions. This is the source of the numerical error: a differencing stencil applied to a cubic function returns a slope even where the cubic has slope zero. The error scaling $E \propto h^2$ results from this term.

Such a flaw in our algorithm is not unavoidable, since we can include more points in order to correct the error in the cubic term. Letting a_{-2} , a_{-1} , a_0 , a_1 , and a_2 be the coefficients of the terms in the differencing operator, such that $d_k = \sum_k a_k f(kh)$. The second order expression above had $a_1 = 1/(2h)$, $a_0 = 0$, and $a_{-1} = -1/(2h)$. If we allow for five coefficients, we can fix five equations, so that $d_1(F_0) = d_1(F_2) = d_1(F_3) = d_1(F_4) = 0$ and $d_1(F_1) = 1$, as we would expect for a first derivative.

$$F_0 : a_{-2} + a_{-1} + a_0 + a_1 + a_2 = 0 (5.13a)$$

$$F_1 : -2ha_{-2} + -ha_{-1} + ha_1 + 2ha_2 = 1$$
(5.13b)

$$F_2 : 4h^2 a_{-2} + h^2 a_{-1} + h^2 a_1 + 4h^2 a_2 = 0$$
(5.13c)

$$F_3 : -8h^3a_{-2} - h^3a_{-1} + h^3a_1 + 8h^3a_2 = 0$$
(5.13d)

$$F_4 : 16h^4a_{-2} + h^4a_{-1} + h^4a_1 + 16h^4a_2 = 0$$
(5.13e)

The equations for F_0 , F_2 , and F_3 are sufficient to establish that $a_0 = 0$ and $a_{-i} = -a_i$. From the equation for F_3 , we see $a_2 = -a_1/8$, and finally from the equation for F_1 , we see that $a_1 = 2/(3h)$ and $a_2 = -1/(12h)$. The fourth-order centered first derivative operator is indeed

$$d_1^{(4)} = \frac{1}{12h} [f(-2h) - 8f(-h) + 8f(h) - f(2h)]$$
(5.14)

6 The Poisson equation

It is not difficult to find ways to solve the Poisson equation, which arises for both gravitational fields and electric fields in Newtonian physics. In some ways, the problem is choosing a method.

We can use:

- 1. Convolution
- 2. multipole moments (for the exterior)
- 3. Spectral methods

We will discuss the first two in turn.

6.1 Convolution

Mathematically speaking, convolution is the most elegant approach to the solution of the Poisson equation. We begin with a know integral form of the solution to the Poisson equation:

$$\nabla^2 \Phi = 4\pi G \rho(x) \Rightarrow \Phi = \int \frac{G \rho(x')}{|x - x'|} d^3 x'$$
(6.1)

The key thing to notice is that we have one term involving a function of the variable we are integrating over (x'), and one that depends on a difference between a fixed point in the integral (x) and the integration variable (x'). In general, there is a simple way to solve these problems using Fourier transforms, where we will make use of the fact that Fourier forward and reverse transforms are inverse operations.

Denoting the forward Fourier transform $\mathcal{F}\{g(x)\} = \int_{-\infty}^{\infty} e^{2\pi i k x} g(x) dx$, and considering the case of one-dimensional integrals, we find that

$$\mathcal{F}\{\Phi(x)\} = G \int_{-\infty}^{\infty} dx e^{2\pi i k x} \int_{-\infty}^{\infty} dx' \rho(x') |x - x'|^{-1}$$
(6.2)

Letting y = x - x', we find x = x' + y, and dx dx' = dx' dy and the integral becomes

$$\mathcal{F}\{\Phi(x)\} = G \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dy \, dx' \, e^{2\pi i k(x'+y)} \rho(x') \, |y|^{-1}$$
$$= G \left(\int_{-\infty}^{\infty} dx' \, e^{2\pi i kx'} \rho(x') \right) \left(\int_{-\infty}^{\infty} dy \, e^{2\pi i ky} \, |y|^{-1} \right)$$
$$= \mathcal{F}\{\rho(x)\} \cdot \mathcal{F}\{|x|^{-1}\}$$
(6.3)

 \mathbf{SO}

$$\Phi(x) = \mathcal{F}^{-1}\left\{\mathcal{F}\{\rho(x)\} \cdot \mathcal{F}\{|x|^{-1}\}\right\}$$
(6.4)

There is nothing special about the functions we convolve to find the potential, and this method, to Fourier transform both functions, multiply the transforms together pointwise, and then inverse transform, is the general technique for performing any convolution integral.

6.2 Mode expansion of the Poisson equation

By using spherical harmonics, we can break down the Poisson equation, which is linear, into independent multipole components. By defining

$$\rho_{\ell}^{m}(r) \equiv \int \rho(r,\theta,\phi) Y_{\ell}^{m*}(\theta,\phi) d\Omega$$
(6.5)

and noting that $\int Y_{\ell'}^{m'} Y_{\ell}^{m*} d\Omega = \delta_{ll'} \delta_{mm'}$ we may split the source term into a set of orthogonal moments, such that

$$\rho = \sum_{l,m} \rho_{\ell}^{m}(r) Y_{\ell}^{m}(\theta, \phi)$$
(6.6)

Each term ρ_{ℓ}^{m} generates a term in the solution Φ_{ℓ}^{m} , whose properties we will investigate after a digression into spherical harmonics.

6.3 Spherical Harmonics

Spherical harmonics are generally introduced as the eigenmodes of the angular Laplacian operator ∇_A^2 , but we can learn a great deal about them by looking at a particular expansion:

the solutions to the Laplacian equation that are regular at the origin. Noting that $\nabla_A^2 Y_\ell^m = -\ell(\ell+1)Y_\ell^m$, we can find solutions $r^s Y_\ell^m$ that satisfy the Laplacian equation with no source:

$$\frac{1}{r^2} \left[\frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \nabla_A^2 \right] r^s Y_\ell^m = 0$$
(6.7)

 \mathbf{SO}

$$s(s+1)r^{s-2}Y_{\ell}^{m} = \ell(\ell+1)r^{s-2}Y_{\ell}^{m}$$
(6.8)

The two radial solutions for a given value of ℓ are r^{ℓ} and $r^{-(\ell+1)}$, and we will look at the former, in particular combinations: $r^{\ell}(Y_{\ell}^m \pm Y_{\ell}^{-m})$, where we consider the real component, and $r^{\ell}(iY_{\ell}^m \pm iY_{\ell}^{-m})$, the imaginary component. We will ignore the scaling factors used to normalize spherical harmonics. We find the following expressions:

$$Y_0^0 = 1$$
 (6.9a)

$$rY_1^0 = z \tag{6.9b}$$

$$\operatorname{Re}(rY_1^1) = x \tag{6.9c}$$

$$\operatorname{Im}(rY_1^1) = y \tag{6.9d}$$

$$r^2 Y_2^0 = 2z^2 - x^2 - y^2 \tag{6.9e}$$

$$\operatorname{Re}(r^2 Y_2^1) = xz \tag{6.9f}$$

$$\operatorname{Im}(r^2 Y_2^1) = yz \tag{6.9g}$$

$$\operatorname{Re}(r^2 Y_2^2) = x^2 - y^2 \tag{6.9h}$$

$$\operatorname{Im}(r^2 Y_2^2) = xy \tag{6.9i}$$

For $\ell = 0$ and $\ell = 1$, we generate all of the polynomials of order ℓ that exist. For the case $\ell = 2$, there are six second-order polynomials– x^2 , y^2 , z^2 , xy, xz, yz, but only five spherical harmonics. The cross-terms appear in the spherical harmonic list, so we are obviously short one combination of the terms $\{x^2, y^2, z^2\}$. To figure out the term that is missing, express the two spherical harmonic terms as vectors, $Y_2^0 = (-1, -1, 2)$, and $\operatorname{Re} Y_2^2 = (1, -1, 0)$. The missing component is the cross product of these two, which works out to be (2, 2, 2). In other words, the vector proportional to $x^2 + y^2 + z^2$. There is no l = 2 spherical harmonic representation of this quantity, since it is a radial factor multiplied by Y_0^0 .

6.4 Multipole moments

If we have a compact density, i.e., one which is non-zero over a finite domain, , we can perform a multipole expansion of the solution. This involves breaking the source term into spherical harmonic modes, and solving each in turn. We have to remember that since the potential goes to a constant as $r \to \infty$, our vacuum solution involves the terms in the form $r^{-(\ell+1)}Y_{\ell}^m$. The general solution may be written

$$\Phi = G\left[\frac{M}{r} + \sum_{i} \frac{p_{i}\hat{x}^{i}}{r^{2}} + \frac{1}{2}\sum_{i,j} \frac{Q_{ij}\hat{x}^{i}\hat{x}^{j}}{r^{3}} + \dots\right]$$
(6.10)

where \hat{x}^i is the unit normal vector at a given point located at radius r. The monopole moment of the density distribution is given by the mass, $M = \int \rho dV$, the dipole term collects the Y_1^m terms:

$$p_i \equiv \int \rho x^i dV \tag{6.11}$$

and the Q_{ij} terms are the traceless quadrupole moments:

$$Q_{ij} \equiv \int \rho(x^i x^j - \frac{1}{3} \delta^{ij} r^2) dV$$
(6.12)

Why traceless? Based on previous discussion, the $\ell = 2$ spherical harmonics don't contain a term that represents a pure radial component r^2 , and thus such modes don't affect the gravitational potential outside of the matter distribution. This is commonly known as Newton's iron sphere theorem: a hollow sphere from the outside has the same gravitational potential as a solid one of the same mass. There are, of course, higher order moments as well, but the forms of each term get significantly more complicated as we progress.