

Notes on Mathematical Methods

1060-710: Mathematical and Statistical Methods for Astrophysics*

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1 Differential Equations

See Arfken & Weber, Chapter 9

1.1 General Properties; Superposition

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

$$\mathcal{L}\psi(\vec{r}) = 0 \quad (\text{homogeneous PDE}) \quad (1.1)$$

or

$$\mathcal{L}\psi(\vec{r}) = \rho(\vec{r}) \quad (\text{inhomogeneous PDE}) \quad (1.2)$$

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 (1.1), so is $c_1\psi_1 + c_2\psi_2$:

$$\mathcal{L}(c_1\psi_1 + c_2\psi_2) = c_1\mathcal{L}\psi_1 + c_2\mathcal{L}\psi_2 = 0. \quad (1.3)$$

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

$$\psi = \sum_n c_n \psi_n \quad (1.4)$$

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

$$\nabla^2\psi = 0 \quad (1.5)$$

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

$$\nabla^2\psi = 4\pi\rho \quad (1.6)$$

3. the Helmholtz equation

$$(\nabla^2 + k^2)\psi = 0 \quad (1.7)$$

4. the diffusion equation

$$\left(\nabla^2 - \frac{1}{a^2} \frac{\partial}{\partial t}\right)\psi = 0 \quad (1.8)$$

5. the wave equation

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right)\psi = 0 \quad (1.9)$$

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 $k = \omega/c$.) Let's look a bit into typical partial differential equations involving the Laplacian in some common coördinate systems.

1.2 The Laplacian; Separation of Variables

Recall from vector calculus that the Laplacian has the following forms in Cartesian coordinates $\{x, y, z\}$, cylindrical coordinates¹ $\{s, \phi, z\}$, and spherical coordinates $\{r, \theta, \phi\}$:

$$\begin{aligned}\nabla^2 &= \vec{\nabla} \cdot \vec{\nabla} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \\ &= \frac{1}{s} \frac{\partial}{\partial s} s \frac{\partial}{\partial s} + \frac{1}{s^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}\end{aligned}\tag{1.10}$$

Note that

- Every term in (1.10) has units of one over length squared.
- It's important to think of both the multiplication and the differentiation as operators, so for example

$$\left(\frac{1}{s} \frac{\partial}{\partial s} s \frac{\partial}{\partial s}\right) \psi = \frac{1}{s} \frac{\partial}{\partial s} \left(s \frac{\partial \psi}{\partial s}\right) = \frac{1}{s} \left(\frac{\partial \psi}{\partial s} + s \frac{\partial^2 \psi}{\partial s^2}\right) = \frac{\partial^2 \psi}{\partial s^2} + \frac{1}{s} \frac{\partial \psi}{\partial s} = \left(\frac{\partial^2}{\partial s^2} + \frac{1}{s} \frac{\partial}{\partial s}\right) \psi\tag{1.11}$$

This can mean there are equivalent ways of writing the Laplacian in a particular coordinate system, which look different. **Exercise:** work out a similar explicit form for the r and θ derivatives appearing in the spherical coordinate form of the Laplacian.

1.2.1 Useful Digression: Form of the Laplacian

The cylindrical and spherical coordinate expressions in (1.10) can be worked out in a number of ways, but there's a relatively simple way to remember them. It turns out (we won't prove it here) that the Laplacian can be written in any coordinate system as

$$\nabla^2 = \frac{1}{\sqrt{|g|}} \partial_i \left(\sqrt{|g|} g^{ij} \partial_j \right)\tag{1.12}$$

To decode this, we need to define a few bits of notation.

First of all, (1.12) is written using the Einstein summation convention, i.e., the indices i and j are each summed from 1 to 3.

Next, we need to explain what g^{ij} and g are. They're both defined in terms of the metric tensor, which has components $\{g_{ij}\}$. (Note that g_{ij} , with indices downstairs, is not the same as g^{ij} , with indices upstairs.) This tells the distance $d\ell$ between points with slightly different values of the coordinates. In Cartesian coordinates, the displacement vector is

$$\vec{d\ell} = \hat{x} dx + \hat{y} dy + \hat{z} dz\tag{1.13}$$

¹What to call the cylindrical radial coordinate $\sqrt{x^2 + y^2}$ 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 coordinates. 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 .

and so the infinitesimal distance follows the Pythagorean formula

$$(d\ell)^2 = (dx)^2 + (dy)^2 + (dz)^2 \quad (1.14)$$

In general, the metric for a coordinate system² $\{x^1, x^2, x^3\}$ is³

$$(d\ell)^2 = g_{ij}dx^i dx^j = g_{11}(dx^1)^2 + 2g_{12}dx^1 dx^2 + 2g_{13}dx^1 dx^3 + g_{22}(dx^2)^2 + 2g_{23}dx^2 dx^3 + g_{33}(dx^3)^2 \quad (1.15)$$

from which we can read off

$$g_{xx} = g_{yy} = g_{zz} = 1; \quad g_{xy} = g_{xz} = g_{yz} = 0 \quad (1.16)$$

The metric in spherical and cylindrical coordinates can be deduced from the distance formulas:

$$(d\ell)^2 = (dr)^2 + r^2(d\theta)^2 + r^2 \sin^2 \theta (d\phi)^2 = (ds)^2 + s^2(d\phi)^2 + (dz)^2 \quad (1.17)$$

so that the non-zero metric components in those coordinate systems are

$$g_{rr} = 1; \quad g_{\theta\theta} = r^2; \quad g_{\phi\phi} = r^2 \sin^2 \theta \quad (1.18)$$

and

$$g_{ss} = 1; \quad g_{\phi\phi} = s^2; \quad g_{zz} = 1 \quad (1.19)$$

Now we can define g appearing in (1.12): it is just the determinant of the matrix $\{g_{ij}\}$:

$$g = \det\{g_{ij}\} \quad (1.20)$$

In each of these coordinate systems, the metric is diagonal, so the determinant is just the product of those diagonal components:

$$g = g_{xx}g_{yy}g_{zz} = 1 \quad (\text{Cartesian coordinates}) \quad (1.21a)$$

$$g = g_{rr}g_{\theta\theta}g_{\phi\phi} = r^4 \sin^2 \theta \quad (\text{Spherical coordinates}) \quad (1.21b)$$

$$g = g_{ss}g_{\phi\phi}g_{zz} = s^2 \quad (\text{Cylindrical coordinates}) \quad (1.21c)$$

One thing to watch out for is that g , despite being written without any indices, is *not* a scalar, i.e., it does not take on the same value in every coordinate system. Instead, you have to transform from one coordinate system to another using the Jacobian determinant, which makes sense when you consider that $\sqrt{|g|}$ is the factor appearing in the volume element

$$d^3V = \sqrt{|g|} dx^1 dx^2 dx^3 = dx dy dz = r^2 \sin^2 \theta dr d\theta d\phi = s ds d\phi dz \quad (1.22)$$

Incidentally, an object which picks up factors of the Jacobian determinant when you transfer between coordinate systems is called a *density*, although this geometrical usage is slightly different from what we usually mean by density in a physical context. For example, the total mass in a mass distribution is

$$M = \iiint \rho(x^1, x^2, x^3) d^3V = \iiint \rho(x^1, x^2, x^3) \sqrt{|g|} dx^1 dx^2 dx^3 \quad (1.23)$$

²It's conventional in differential geometry to label coordinates with superscripts rather than subscripts

³The metric tensor is defined to be symmetric, i.e., $g_{ij} = g_{ji}$. Given the way it appears in (1.15), an antisymmetric component would be unmeasurable.

and it's the combination $\rho\sqrt{|g|}$ which transforms like a density.

Finally, the $\{g^{ij}\}$ are the elements of the matrix inverse of the metric $\{g_{ij}\}$. Since the metric is diagonal in each of the coördinate systems we considered, the inverse is relatively simple:

$$g^{xx} = \frac{1}{g_{xx}} = 1; \quad g^{yy} = \frac{1}{g_{yy}} = 1; \quad g^{zz} = \frac{1}{g_{zz}} = 1 \quad (1.24a)$$

$$g^{rr} = \frac{1}{g_{rr}} = 1; \quad g^{\theta\theta} = \frac{1}{g_{\theta\theta}} = \frac{1}{r^2}; \quad g^{\phi\phi} = \frac{1}{g_{\phi\phi}} = \frac{1}{r^2 \sin^2 \theta} \quad (1.24b)$$

$$g^{ss} = \frac{1}{g_{ss}} = 1; \quad g^{\phi\phi} = \frac{1}{g_{\phi\phi}} = \frac{1}{s^2}; \quad g^{zz} = \frac{1}{g_{zz}} = 1 \quad (1.24c)$$

where all of the off-diagonal elements of $\{g^{ij}\}$ are zero.

So that gives us all of the pieces, and we can write down, for example, in spherical coördinates,

$$\begin{aligned} \nabla^2 &= \frac{1}{\sqrt{|g|}} \partial_i \left(\sqrt{|g|} g^{ij} \partial_j \right) \\ &= \frac{1}{r^2 \sin \theta} \left[\partial_r \cdot 1 \cdot (r^2 \sin \theta \partial_r) + \partial_\theta \left(r^2 \sin \theta \frac{1}{r^2} \partial_\theta \right) + \partial_\phi \left(r^2 \sin \theta \frac{1}{r^2 \sin^2 \theta} \partial_\phi \right) \right] \\ &= \frac{1}{r^2} \partial_r r^2 \partial_r + \frac{1}{r^2 \sin \theta} \partial_\theta \sin \theta \partial_\theta + \frac{1}{r^2 \sin^2 \theta} \partial_\phi^2 \end{aligned} \quad (1.25)$$

1.2.2 Cartesian Coördinates

For concreteness, we'll consider the Helmholtz equation

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + k^2 \right) \psi(x, y, z) = 0. \quad (1.26)$$

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

$$\psi(x, y, z) = X(x)Y(y)Z(z). \quad (1.27)$$

(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 (1.27) into (1.26) and dividing by ψ gives us

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} + k^2 = 0 \quad (1.28)$$

Since the first term depends only on x , 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:

$$\underbrace{\frac{X''(x)}{X(x)}}_{=-k_x^2} + \underbrace{\frac{Y''(y)}{Y(y)}}_{=-k_y^2} + \underbrace{\frac{Z''(z)}{Z(z)}}_{=-k_z^2} + k^2 = 0 \quad (1.29)$$

so we can solve the original PDE if X , Y , and Z satisfy⁴

$$X''(x) + k_x^2 X(x) = 0 \quad (1.30a)$$

$$Y''(y) + k_y^2 Y(y) = 0 \quad (1.30b)$$

$$Z''(z) + k_z^2 Z(z) = 0 . \quad (1.30c)$$

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

Each of these, (1.30a) 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

$$X(x) \equiv \left\{ \begin{array}{l} e^{ik_x x} \\ e^{-ik_x x} \end{array} \right\} \text{ or equivalently } \left\{ \begin{array}{l} \sin k_x x \\ \cos k_x x \end{array} \right\} \quad (1.31)$$

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.

1.2.3 Cylindrical Coördinates

Now the PDE is

$$\left(\frac{1}{s} \frac{\partial}{\partial s} s \frac{\partial}{\partial s} + \frac{1}{s^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} + k^2 \right) \psi(s, \phi, z) = 0 \quad (1.32)$$

and guessing a separable solution

$$\psi(s, \phi, z) = S(s)\Phi(\phi)Z(z) \quad (1.33)$$

gives the equations

$$\frac{1}{s} \frac{[s S'(s)]'}{S(s)} + \frac{1}{s^2} \frac{\Phi''(\phi)}{\Phi(\phi)} + \frac{Z''(z)}{Z(z)} + k^2 = 0 \quad (1.34)$$

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

$$\frac{Z''(z)}{Z(z)} = -k_z^2 . \quad (1.35)$$

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

$$s^2 \frac{S''(s)}{S(s)} + s \frac{S'(s)}{S(s)} + (k^2 - k_z^2) s^2 + \frac{\Phi''(\phi)}{\Phi(\phi)} = 0 . \quad (1.36)$$

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

$$\Phi''(\phi) + m^2 \Phi(\phi) = 0 \quad (1.37)$$

has the solution

$$\Phi(\phi) = e^{im\phi} . \quad (1.38)$$

⁴We'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 coordinate with a period of 2π , so if the solution to the PDE is to be single-valued, we have to enforce

$$\Phi(\phi + 2\pi) = \Phi(\phi) . \quad (1.39)$$

This means we know the conditions on m :

m must be an integer

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

$$s^2 S''(s) + s S'(s) + [(k^2 - k_z^2) s^2 - m^2] S(s) = 0 . \quad (1.40)$$

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,

$$s \frac{d}{ds} = x \frac{d}{dx} \quad (1.41)$$

and the differential equation becomes

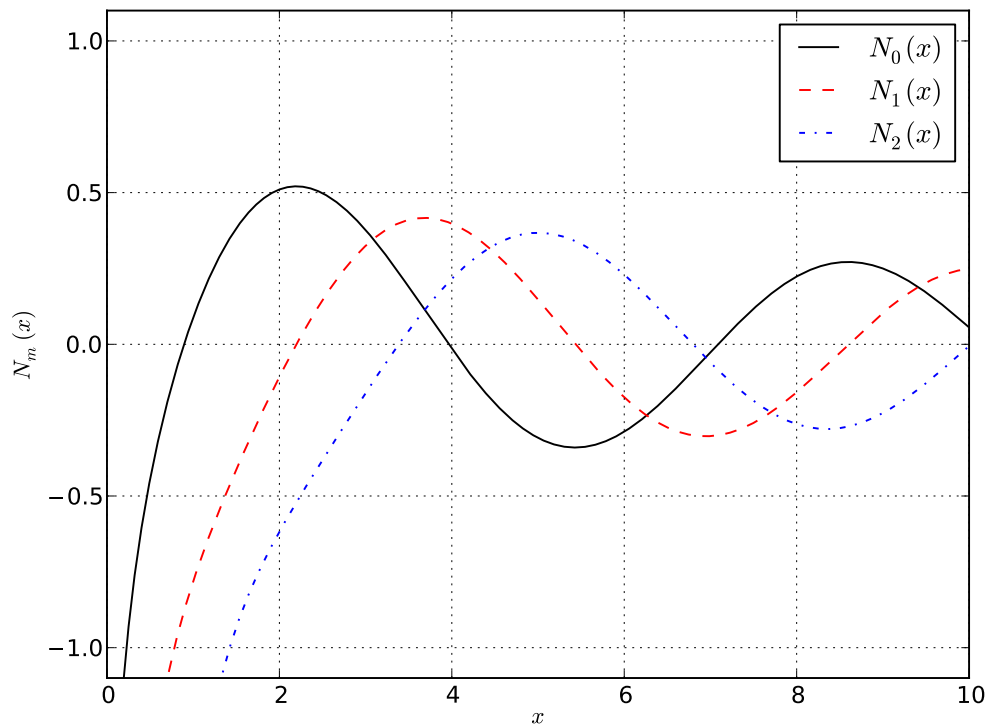
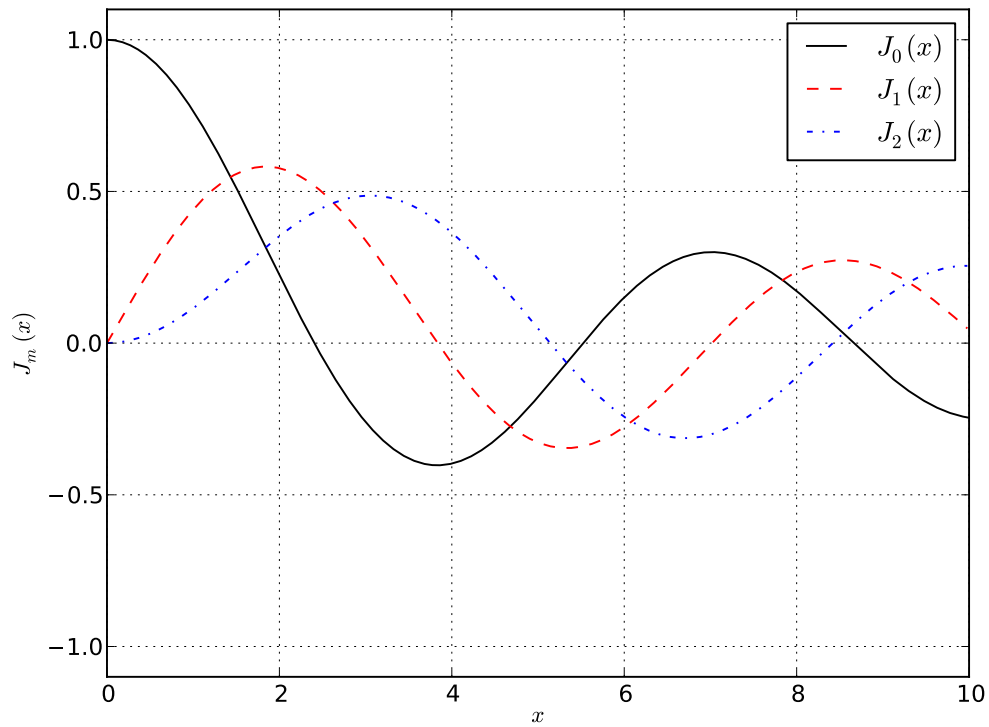
$$x^2 y''(x) + x y'(x) + [x^2 - m^2] y(x) = 0 . \quad (1.42)$$

This is Bessel's equation, and the two independent solutions to it are called Bessel functions $J_m(x)$ and $N_m(x)$. We can get a quick look at them with matplotlib:

```
> ipython -pylab
from scipy.special import *
x=linspace(0.0001,10,1000)
figure()
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('$J_m(x)$')
axis([0,10,-1.1,1.1])
grid(True)
savefig('besselJ.eps',bbox_inches='tight')
figure()
plot(x,yn(0,x),'k-',label='$N_0(x)$')
plot(x,yn(1,x),'r--',label='$N_1(x)$')
plot(x,yn(2,x),'b-.',label='$N_2(x)$')
legend()
```



```
xlabel('$x$')
ylabel('$N_m(x)$')
axis([0,10,-1.1,1.1])
grid(True)
savefig('neumann.eps',bbox_inches='tight')
```



1.2.4 Spherical Coördinates

In spherical coördinates, the PDE is

$$\left(\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + k^2 \right) \psi(r, \theta, \phi) = 0 \quad (1.43)$$

and the search for a separated solution

$$\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi) \quad (1.44)$$

gives us

$$\frac{1}{r^2} \frac{[r^2 R'(r)]'}{R(r)} + \frac{1}{r^2 \sin \theta} \frac{[\sin \theta \Theta'(\theta)]'}{\Theta(\theta)} + \frac{1}{r^2 \sin^2 \theta} \frac{\Phi''(\phi)}{\Phi(\phi)} + k^2 = 0 \quad (1.45)$$

As before, the ϕ dependence is

$$\Phi(\phi) = e^{im\phi} \quad m \in \mathbb{Z} \quad (1.46)$$

so multiplying by r^2 gives us

$$\underbrace{\frac{[r^2 R'(r)]'}{R(r)}}_{\ell(\ell+1)} + k^2 r^2 + \underbrace{\frac{1}{\sin \theta} \frac{[\sin \theta \Theta'(\theta)]'}{\Theta(\theta)}}_{-\ell(\ell+1)} - \frac{m^2}{\sin^2 \theta} = 0 \quad (1.47)$$

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

$$\Theta''(\theta) + \frac{\cos \theta}{\sin \theta} \Theta'(\theta) + \left(\ell(\ell+1) - \frac{m^2}{\sin^2 \theta} \right) \Theta(\theta) = 0 \quad (1.48)$$

turns out to have geometrically sensible solutions only when

$$|m| \leq \ell \in \mathbb{Z} \quad (1.49)$$

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 you'll investigate on the homework.

We could continue as before with the radial equation, and end up with the differential equation satisfied by *spherical Bessel functions*.

Thursday, September 9, 2010

1.3 Satisfying Boundary Conditions

Given one or more solutions to a homogeneous differential equation of the form

$$\mathcal{L}\psi = 0 \quad (1.50)$$

we can generate more solutions by using superposition. We find out which coefficients to use to solve the problem of interest by applying boundary conditions and/or initial conditions.

For example, consider the wave equation in 2+1 dimensions, written in terms of the polar coordinates (r, ϕ) and of time. (We could do this in cylindrical coordinates [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

$$\nabla^2 \psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} = \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \psi = 0 \quad (1.51)$$

has solutions (choose one from each column)

$$\begin{Bmatrix} J_m(kr) \\ N_m(kr) \end{Bmatrix} \begin{Bmatrix} \cos m\phi \\ \sin m\phi \end{Bmatrix} \begin{Bmatrix} \cos kct \\ \sin kct \end{Bmatrix} \quad (1.52)$$

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

To figure out what coefficients 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 $r = a$

$$\psi(a, \phi, t) = 0 \quad (1.53)$$

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

$$J_m(kr) \begin{Bmatrix} \cos m\phi \\ \sin m\phi \end{Bmatrix} \begin{Bmatrix} \cos kct \\ \sin kct \end{Bmatrix} \quad (1.54)$$

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.,

$$J_m(\gamma_{mn}) = 0 ; \quad (1.55)$$

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

$$J_m \left(\frac{\gamma_{mn}}{a} r \right) \begin{Bmatrix} \cos m\phi \\ \sin m\phi \end{Bmatrix} \begin{Bmatrix} \cos \frac{\gamma_{mn}}{a} ct \\ \sin \frac{\gamma_{mn}}{a} ct \end{Bmatrix} \quad n = 1, 2, \dots; \quad m = 0, 1, 2, \dots \quad (1.56)$$

To nail down all the coefficients, 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

$$\psi(r, \phi, 0) = f(r, \phi) \quad (1.57)$$

$$\dot{\psi}(r, \phi, 0) = 0 \quad (1.58)$$

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

$$J_m \left(\frac{\gamma_{mn}}{a} r \right) \begin{cases} \cos m\phi \\ \sin m\phi \end{cases} \cos \frac{\gamma_{mn}}{a} ct \quad n = 1, 2, \dots; \quad m = 0, 1, 2, \dots \quad (1.59)$$

and we can write the solution explicitly as

$$\psi(r, \phi, t) = \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} J_m \left(\frac{\gamma_{mn}}{a} r \right) (A_{mn} \cos m\phi + B_{mn} \sin m\phi) \cos \frac{\gamma_{mn}}{a} ct \quad (1.60)$$

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

$$f(r, \phi) = \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} J_m \left(\frac{\gamma_{mn}}{a} r \right) (A_{mn} \cos m\phi + B_{mn} \sin m\phi) \quad (1.61)$$

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

$$\int_0^{2\pi} \sin m_1 \phi \sin m_2 \phi d\phi = \begin{cases} \pi & m_1 = m_2 \neq 0 \\ 0 & m_1 \neq m_2 \end{cases} . \quad (1.62)$$

The Bessel part turns out to be handled with the identity

$$\int_0^a J_m \left(\frac{\gamma_{mn_1}}{a} r \right) J_m \left(\frac{\gamma_{mn_2}}{a} r \right) r dr = 0 \quad \text{if } n_1 \neq n_2 \quad (1.63)$$

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

$$0 = \left[r^2 \frac{d^2}{dr^2} + r \frac{d}{dr} + (k^2 r^2 - m^2) \right] J_m(kr) = r \left[\frac{d}{dr} \left(r \frac{dJ_m(kr)}{dr} \right) + \left(k^2 r - \frac{m}{r} \right) J_m(kr) \right] \quad (1.64)$$

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

$$0 = J_m(k_2 r) \frac{d}{dr} \left(r \frac{dJ_m(k_1 r)}{dr} \right) + \left(k_1^2 r - \frac{m}{r} \right) J_m(k_2 r) J_m(k_1 r) \quad (1.65)$$

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

$$0 = \left[J_m(k_2 r) r \left(\frac{dJ_m(k_1 r)}{dr} \right) \right]_0^a - \int_0^a \left(\frac{dJ_m(k_2 r)}{dr} \right) r \left(\frac{dJ_m(k_1 r)}{dr} \right) dr + \int_0^a \left(k_1^2 r - \frac{m}{r} \right) J_m(k_2 r) J_m(k_1 r) dr, \quad (1.66)$$

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

$$0 = \left[r J_m(k_2 r) \left(\frac{dJ_m(k_1 r)}{dr} \right) \right]_0^a - \left[r J_m(k_1 r) \left(\frac{dJ_m(k_2 r)}{dr} \right) \right]_0^a + (k_1^2 - k_2^2) \int_0^a J_m(k_1 r) J_m(k_2 r) r dr \quad (1.67)$$

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

$$0 = \frac{\gamma_{mn_1}^2 - \gamma_{mn_2}^2}{a^2} \int_0^a J_m\left(\frac{\gamma_{mn_1}}{a}r\right) J_m\left(\frac{\gamma_{mn_2}}{a}r\right) r dr \quad (1.68)$$

and so we see that indeed

$$\int_0^a J_m\left(\frac{\gamma_{mn_1}}{a}r\right) J_m\left(\frac{\gamma_{mn_2}}{a}r\right) r dr = 0 \quad \text{if } k_1 \neq k_2 \quad (1.69)$$

1.4 Sturm-Liouville Theory

See Arfken & Weber, Chapter 10

Just now we showed that

$$\int_0^a J_m(k_1r) J_m(k_2r) r dr = 0 \quad \text{if } k_1 \neq k_2 \text{ \& } J_m(k_1a) = 0 = J_m(k_2a) \quad (1.70)$$

by manipulating the differential equation

$$\left[\frac{1}{r} \frac{d}{dr} \left(r \frac{d}{dr} \right) - \frac{m^2}{r^2} + k^2 \right] J_m(kr) = 0 . \quad (1.71)$$

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

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

$$\mathbf{A}\mathbf{u} = \lambda\mathbf{u} . \quad (1.72)$$

First, recall the inner product

$$\langle \mathbf{u}, \mathbf{v} \rangle = \mathbf{u}^\dagger \mathbf{v} \quad (1.73)$$

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

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}^\dagger = (u_1^* \quad u_2^* \quad u_3^* \quad u_4^*) . \quad (1.74)$$

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

$$\langle \mathbf{u}, \mathbf{A}^\dagger \mathbf{v} \rangle = \mathbf{u}^\dagger \mathbf{A}^\dagger \mathbf{v} = (\mathbf{A}\mathbf{u})^\dagger \mathbf{v} = \langle \mathbf{A}\mathbf{u}, \mathbf{v} \rangle \quad (1.75)$$

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

$$\langle u, v \rangle = \int_a^b u^*(x) v(x) w(x) dx \quad (1.76)$$

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)

$$\langle u, \mathcal{L}v \rangle = \int_a^b u^*(x) [\mathcal{L}v(x)] w(x) dx \quad (1.77)$$

and

$$\langle u, \mathcal{L}^\dagger v \rangle = \int_a^b [\mathcal{L}u(x)]^* v(x) w(x) dx . \quad (1.78)$$

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

$$\mathbf{A}\mathbf{u}_1 = \lambda_1\mathbf{u}_1 \quad (1.79a)$$

$$\mathbf{A}\mathbf{u}_2 = \lambda_2\mathbf{u}_2 \quad (1.79b)$$

then

$$\langle \mathbf{u}_1, \mathbf{u}_2 \rangle = 0 \quad \text{if } \lambda_1 \neq \lambda_2 ; \quad (1.80)$$

The same thing is true of the eigenfunctions of a self-adjoint linear operator.

The demonstration is identical to the demonstration from linear algebra, but let’s go through it to jog our memory, starting with $\mathcal{L}u_1 = \lambda_1 u_1$ and $\mathcal{L}u_2 = \lambda_2 u_2$, with $\lambda_1 \neq \lambda_2$, for a self-adjoint operator $\mathcal{L} = \mathcal{L}^\dagger$. Consider

$$\langle u_1, \mathcal{L}u_2 \rangle = \langle \mathcal{L}^\dagger u_1, u_2 \rangle = \langle \mathcal{L}u_1, u_2 \rangle \quad (1.81)$$

where the first equality holds by the definition of the adjoint and the second holds because \mathcal{L} is a Hermitian (self-adjoint) operator. But if we apply the eigenvalue equation, we get

$$0 = \langle u_1, \mathcal{L}u_2 \rangle - \langle \mathcal{L}u_1, u_2 \rangle = \langle u_1, \lambda_2 u_2 \rangle - \langle \lambda_1 u_1, u_2 \rangle = (\lambda_2 - \lambda_1^*) \langle u_1, u_2 \rangle \quad (1.82)$$

We’ve been careful and written λ_1^* , but actually it’s another property of Hermitian operators that they have real eigenvalues⁵ and so we can write

$$0 = (\lambda_2 - \lambda_1) \langle u_1, u_2 \rangle \quad (1.83)$$

which means that if $\lambda_1 = \lambda_2$, the inner product $\langle u_1, u_2 \rangle$ has to vanish.

⁵You can show this by applying (1.82) with u_1 in place of u_2 to get $(\lambda_1 - \lambda_1^*) \langle u_1, u_1 \rangle$, and since the norm $\langle u_1, u_1 \rangle$ is non-zero for anything but the zero vector, $\lambda_1 = \lambda_1^*$.

So in the case of Bessel functions,

$$\mathcal{L} = \frac{1}{r} \frac{d}{dr} \left(r \frac{d}{dr} \right) - \frac{m^2}{r^2}, \quad (1.84)$$

$w(r) = r$,⁶ and the eigenvalue equation is

$$\mathcal{L}J_m(ks) = -k^2 J_m(ks). \quad (1.85)$$

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

$$\int_a^b u(s) \mathcal{L}v(s) s ds = \int_a^b [\mathcal{L}u(s)] v(s) s ds \quad (1.86)$$

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

$$u(0) \text{ is regular} \quad (1.87a)$$

$$u(a) = 0 \quad (1.87b)$$

The demonstration is similar to what we did above, and involves integrating by parts twice.

Tuesday, September 14, 2010

2 Fourier Analysis

See Arfken & Weber, Chapters 14-15, Numerical Recipes, Chapters 12-13, or Gregory, Appendix B

2.1 Fourier Series

Consider functions defined on an interval

$$-\frac{T}{2} \leq t \leq \frac{T}{2} \quad (2.1)$$

The differential equation

$$\frac{d^2}{dt^2} h(t) = -\omega^2 h(t) \quad (2.2)$$

has solutions, when $\omega \neq 0$, of⁷ $\cos \omega t$ and $\sin \omega t$. Or, equivalently, since

$$e^{i\omega t} = \cos \omega t + i \sin \omega t \quad (2.3)$$

one can also write the two solutions as $e^{i\omega t}$ and $e^{-i\omega t}$. From Sturm-Liouville theory, we recognize

$$\frac{d^2}{dt^2} \quad (2.4)$$

⁶The weighting function will typically be what's physically appropriate for the problem. In this case, $w(r) = r$ makes sense because of the area element $d^2A = r dr d\phi$.

⁷If $\omega = 0$, the independent solutions are 1 and t .

as a self-adjoint operator under the inner product

$$\langle h_1, h_2 \rangle = \int_{-T/2}^{T/2} h_1^*(t) h_2(t) dt \quad (2.5)$$

so its eigenfunctions should form an orthogonal basis. Note that $\cos \omega t$ and $\sin \omega t$ both have the eigenvalue $-\omega^2$, but symmetry properties ensure that

$$\int_{-T/2}^{T/2} \cos \omega_1 t \sin \omega_2 t dt = 0 . \quad (2.6)$$

It's actually easier to work with the complex versions, though, and we note that

$$i \frac{d}{dt} \quad (2.7)$$

is also a self-adjoint operator, and $e^{i\omega t}$ and $e^{-i\omega t}$ are eigenfunctions of that operator with different eigenvalues.

We can check orthogonality by writing

$$\langle e^{i\omega_1 t}, e^{i\omega_2 t} \rangle = \int_{-T/2}^{T/2} e^{i(\omega_2 - \omega_1)t} dt ; \quad (2.8)$$

For $\omega_1 = \omega_2$ this is T , while for $\omega_1 \neq \omega_2$ it is

$$\left. \frac{e^{i(\omega_2 - \omega_1)t}}{i(\omega_2 - \omega_1)} \right|_{-T/2}^{T/2} = \frac{e^{i(\omega_2 - \omega_1)T/2} - e^{-i(\omega_2 - \omega_1)T/2}}{i(\omega_2 - \omega_1)} = \frac{2}{(\omega_2 - \omega_1)} \sin \frac{(\omega_2 - \omega_1)T}{2} \quad (2.9)$$

so in general

$$\langle e^{i\omega_1 t}, e^{i\omega_2 t} \rangle = \begin{cases} T & \text{if } \omega_1 = \omega_2 \\ \frac{2}{(\omega_2 - \omega_1)} \sin \frac{(\omega_2 - \omega_1)T}{2} & \text{if } \omega_1 \neq \omega_2 \end{cases} \quad (2.10)$$

We didn't get zero in the $\omega_1 \neq \omega_2$ case, but we haven't yet imposed the boundary conditions on the eigenfunctions, which restrict the possible choices of ω . One choice of boundary conditions which makes the differential operators self-adjoint is to require periodicity, i.e.,

$$e^{i\omega T/2} = e^{i\omega(-T/2)} \quad (2.11)$$

which means that

$$\sin \frac{\omega T}{2} = 0 \quad (2.12)$$

and limit us to

$$\frac{\omega T}{2} = n\pi \quad (2.13)$$

so that

$$\omega_n = \frac{2\pi n}{T} \quad (2.14)$$

and we do get orthogonality because

$$\langle e^{i2\pi n_1 t/T}, e^{i2\pi n_2 t/T} \rangle = \begin{cases} T & \text{if } n_1 = n_2 \\ \frac{T}{\pi(n_2 - n_1)} \sin[(n_2 - n_1)\pi] = 0 & \text{if } n_1 \neq n_2 \end{cases} \quad (2.15)$$

or, written more compactly,

$$\int_{-T/2}^{T/2} (e^{i2\pi n_1 t})^* (e^{i2\pi n_2 t}) dt = T\delta_{n_1 n_2} \quad (2.16)$$

where δ_{mn} is the usual Kronecker delta.

Since we can expand any function in the eigenfunctions of $\frac{d^2}{dt^2}$ (or in this case of $i\frac{d}{dt}$), we can write

$$h(t) = \sum_{n=-\infty}^{\infty} c_n \exp\left(\frac{i2\pi n t}{T}\right) \quad (2.17)$$

We can use the orthogonality to find the coefficients:

$$\int_{-T/2}^{T/2} e^{-\frac{i2\pi m t}{T}} h(t) dt = \sum_{m=-\infty}^{\infty} c_m T \delta_{mn} = T c_n \quad (2.18)$$

i.e.,

$$c_n = \frac{1}{T} \int_{-T/2}^{T/2} h(t) \exp\left(-\frac{i2\pi n t}{T}\right) dt \quad (2.19)$$

2.2 Continuous Fourier Transform

Note that if we write

$$f_n = \frac{n}{T} = n \delta f \quad (2.20)$$

so that

$$h(t) = \sum_{n=-\infty}^{\infty} c_n e^{i2\pi f_n t} \quad (2.21)$$

the frequencies are spaced closer together for larger T . If we write

$$h(t) = \sum_{n=-\infty}^{\infty} \underbrace{T c_n}_{\tilde{h}(f_n)} e^{i2\pi f_n t} \delta f \quad (2.22)$$

and take the limit as $T \rightarrow \infty$ so that the sum becomes an integral, we get

$$h(t) = \int_{-\infty}^{\infty} \tilde{h}(f) e^{i2\pi f t} df \quad (2.23)$$

and the inverse

$$\tilde{h}(f_n) = T c_n = \int_{-T/2}^{T/2} h(t) e^{-i2\pi f_n t} dt \quad (2.24)$$

becomes

$$\tilde{h}(f) = \int_{-\infty}^{\infty} h(t) e^{-i2\pi ft} dt \quad (2.25)$$

Note that the orthogonality relation

$$\int_{-T/2}^{T/2} e^{i2\pi(f_2-f_1)t} dt = T \delta_{n_1 n_2} \quad (2.26)$$

becomes, in the limit of infinite T ,

$$\int_{-\infty}^{\infty} e^{i2\pi(f_2-f_1)t} dt = \delta(f_2 - f_1) \quad (2.27)$$

where $\delta(f_2 - f_1)$ is the Dirac delta function defined by

$$\int_{-\infty}^{\infty} \delta(f_2 - f_1) H(f_1) df_1 = H(f_2) ; \quad (2.28)$$

we can check that we got the normalization right by noting

$$\sum_{n_1=-\infty}^{\infty} T \delta_{n_1 n_2} \delta f = \sum_{n_1=-\infty}^{\infty} \delta_{n_1 n_2} = 1 \quad (2.29)$$

2.2.1 Convolution

A common physical situation is for one quantity, as a function of time, to be linearly related to another quantity, which we can write as:

$$g(t) = \int_{-\infty}^{\infty} A(t, t') h(t') dt' . \quad (2.30)$$

If the mapping of $h(t)$ onto $g(t)$ is *stationary*, e.g., doesn't depend on any time-dependent external factors, it can be written even more simply:

$$g(t) = \int_{-\infty}^{\infty} A(t - t') h(t') dt' . \quad (2.31)$$

This relationship is known as a *convolution* and is sometimes written $g = A * h$. It can be written even more simply if we substitute in the form of $A(t - t')$ and $h(t')$ in terms of their Fourier transforms:

$$h(t') = \int_{-\infty}^{\infty} \tilde{h}(f) e^{i2\pi f t'} df \quad (2.32)$$

$$A(t - t') = \int_{-\infty}^{\infty} \tilde{A}(f') e^{i2\pi f' (t-t')} df' \quad (2.33)$$

(where we have used different names for the two frequency integration variables so we don't mix them up) to get

$$\begin{aligned}
g(t) &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{A}(f') \tilde{h}(f) e^{i2\pi[f'(t-t')+ft']} df df' dt' \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{A}(f') \tilde{h}(f) e^{i2\pi f' t} \int_{-\infty}^{\infty} e^{i2\pi(f-f')t'} dt' df' df \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{A}(f') \tilde{h}(f) e^{i2\pi f' t} \delta(f-f') df' df \\
&= \int_{-\infty}^{\infty} \tilde{A}(f) \tilde{h}(f) e^{i2\pi f t} df
\end{aligned} \tag{2.34}$$

which means that

$$\tilde{g}(f) = \tilde{A}(f) \tilde{h}(f) , \tag{2.35}$$

i.e., convolution in the time domain is equivalent to multiplication in the frequency domain.

2.2.2 Properties of the Fourier Transform

There are a number of important and useful properties obeyed by Fourier transforms, and handy Fourier transforms of specific function.

- If $h(t)$ is real, then $\tilde{h}(-f) = \tilde{h}^*(f)$.
- If $h(t) = h_0$, a constant, then

$$\tilde{h}(f) = \int_{-\infty}^{\infty} h_0 e^{-i2\pi f t} dt = h_0 \delta(f) \tag{2.36}$$

- If $h(t) = h_0 \delta(t - t_0)$, then $\tilde{h}(f) = h_0 e^{-i2\pi f t_0}$
- If $h(t)$ is a square wave

$$h(t) = \begin{cases} h_0 & -\frac{\tau}{2} < t < \frac{\tau}{2} \\ 0 & |t| > \frac{\tau}{2} \end{cases} \tag{2.37}$$

then

$$\tilde{h}(f) = h_0 \frac{2\pi f \tau}{\pi f} = 2h_0 \tau \text{sinc } 2f\tau \tag{2.38}$$

where

$$\text{sinc } x = \frac{\sin \pi x}{\pi x} \tag{2.39}$$

is the normalized sinc function.

- If $h(t)$ is a Gaussian

$$h(t) = \frac{1}{\sigma\sqrt{2\pi}} e^{-t^2/2\sigma^2} \tag{2.40}$$

then its Fourier transform is also a Gaussian:

$$\tilde{h}(f) = e^{-(2\pi f)^2/2\sigma^{-2}} \quad (2.41)$$

Note that the narrower the Gaussian is in the time domain, the wider the corresponding Gaussian is in the frequency domain. This is related to the Heisenberg uncertainty principle.

- Dimensionally, the units of $\tilde{h}(f)$ are the units of $h(t)$ times time (or divided by frequency). We'll usually say, e.g., if $h(t)$ has units of "gertrudes", $\tilde{h}(f)$ has units of "gertrudes per hertz".

•

$$\int_{-\infty}^{\infty} h^*(t) g(t) dt = \int_{-\infty}^{\infty} \tilde{h}^*(f) \tilde{g}(f) df \quad (2.42)$$

It's a useful exercise, and not too hard, to demonstrate each of these.

Thursday, September 16, 2010

2.3 Discrete Fourier Transform

Recall that an ordinary Fourier series could be written in the form (2.22) relating a finite-duration $h(t)$ to its Fourier components $\tilde{h}(f_n)$, with inverse relationship (2.24). The time variable t is continuously-defined with finite duration, while the frequency f_n takes on only a discrete set of values, but ranges from $-\infty$ to ∞ . This situation is summarized as follows:

	Resolution	Extent
t	continuous	duration T
f	discrete, $\delta f = \frac{1}{T}$	infinite

When we took the limit as $T \rightarrow \infty$ to define the inverse Fourier transform (2.23) and the Fourier transform (2.25) we ended up with both frequency and time being continuously defined from $-\infty$ to ∞ :

	Resolution	Extent
t	continuous	infinite
f	continuous	infinite

In an experimental situation, on the other hand, not only is the duration finite, but the time is also discretely sampled. Consider the simplest case of N samples separated by a fixed sampling time of δt so that the total duration is $T = N \delta t$:

$$h_j = h(t_j) = h(t_0 + j \delta t) \quad j = 0, 1, \dots, N - 1 \quad (2.43)$$

we'd like to define the Fourier transform

$$\tilde{h}(f_k) = \int_{t_0}^{t_0+T} h(t) e^{-i2\pi f_k(t-t_0)} dt \quad (2.44)$$

but we don't have access to the full function $h(t)$, only the discrete samples $\{h_j\}$. The best we can do, then, is approximate the integral by a sum and see what we get:

$$\sum_{j=0}^{N-1} h_j e^{-i2\pi f_k(t_j-t_0)} \delta t = \sum_{j=0}^{N-1} h_j e^{-i2\pi(k \delta f)(j \delta t)} \delta t = \sum_{j=0}^{N-1} h_j e^{-i2\pi jk/N} \delta t \quad (2.45)$$

where in the last step we've used the fact that

$$\delta f \delta t = \frac{\delta t}{T} = \frac{1}{N} \quad (2.46)$$

Now, (2.45) is the discrete approximation to the Fourier transform, so we could call it something like \tilde{h}_k . But if you're a computer manipulating a set of numbers $\{h_j\}$, you don't really need to know the physical sampling rate, except for the factor of δt in (2.45). So the standard definition of the discrete Fourier transform leaves this out:

$$\hat{h}_k = \sum_{j=0}^{N-1} h_j e^{-i2\pi jk/N} \quad (2.47)$$

In principle (2.47) can be used to define the discrete Fourier transform for any integer k . However, we can see that not all of the \hat{h}_k are independent; in particular,

$$\hat{h}_{k+N} = \sum_{j=0}^{N-1} h_j e^{-i2\pi jk/N} e^{-i2\pi j} = \sum_{j=0}^{N-1} h_j e^{-i2\pi jk/N} = \hat{h}_k \quad (2.48)$$

where we have used the fact that

$$e^{-i2\pi j} = \cos 2\pi j - i \sin 2\pi j = 1 \quad (2.49)$$

since j is an integer. This means there are only N independent \hat{h}_k values, which is not surprising, since we started with N samples $\{h_j\}$. One choice is to let k go from 0 to $N-1$, and we can use that to calculate the inverse transform by starting with

$$\sum_{k=0}^{N-1} \hat{h}_k e^{i2\pi jk/N} = \sum_{k=0}^{N-1} \sum_{\ell=0}^{N-1} h_\ell e^{i2\pi(j-\ell)k/N} \quad (2.50)$$

If we recall that

$$1 - a^N = (1 - a)(1 + a + a^2 + \dots + a^{N-1}) \quad (2.51)$$

we can see that

$$\sum_{k=0}^{N-1} e^{i2\pi(j-\ell)k/N} = \sum_{k=0}^{N-1} (e^{i2\pi(j-\ell)/N})^k = \begin{cases} N & \text{if } j = \ell \pmod{N} \\ \frac{1 - e^{i2\pi(j-\ell)}}{1 - e^{i2\pi(j-\ell)/N}} = 0 & \text{if } j \neq \ell \pmod{N} \end{cases} \quad (2.52)$$

i.e.,

$$\sum_{k=0}^{N-1} e^{i2\pi(j-\ell)k/N} = N \delta_{j,\ell \pmod{N}} \quad (2.53)$$

so

$$\sum_{k=0}^{N-1} \widehat{h}_k e^{i2\pi jk/N} = \sum_{\ell=0}^{N-1} h_\ell N \delta_{j,\ell \bmod N} = Nh_j \quad (2.54)$$

and the inverse transform is

$$h_j = \frac{1}{N} \sum_{k=0}^{N-1} \widehat{h}_k e^{i2\pi jk/N} \quad (2.55)$$

Note that the asymmetry between the forward and reverse transform arose because we left out the factor of δt from (2.47); if we write

$$(\widehat{h}_k \delta t) = \sum_{j=0}^{N-1} h_j e^{-i2\pi jk/N} \delta t \quad (2.56)$$

then the inverse transform is

$$h_j = \sum_{k=0}^{N-1} (\widehat{h}_k \delta t) e^{i2\pi jk/N} \frac{1}{N \delta t} = \sum_{k=0}^{N-1} (\widehat{h}_k \delta t) e^{i2\pi jk/N} \delta f \quad (2.57)$$

which restores the notational symmetry of the continuous Fourier transform.

2.3.1 Nyquist Frequency and Aliasing

In this discussion we'll assume the number of samples N is even; the generalization to odd N is straightforward.

We saw above that if you take the discrete Fourier transform of N data points $\{h_j\}$, the periodicity $\widehat{h}_{k+N} = \widehat{h}_k$ means that only N of the Fourier components are independent. We implicitly considered those to be $\{\widehat{h}_k | k = 0, 1, \dots, N-1\}$, which is certainly convenient if you're a computer, but it doesn't really make the most physical sense.

For example, consider the behavior of the discrete Fourier transform if the original time series is real, so that $h_j^* = h_j$.

$$\text{if } h_j^* = h_j, \quad \widehat{h}_k^* = \left(\sum_{j=0}^{N-1} h_j e^{-i2\pi jk/N} \right)^* = \sum_{j=0}^{N-1} h_j e^{i2\pi jk/N} = \widehat{h}_{-k} = \widehat{h}_{N-k} \quad (2.58)$$

If we confine our attention to $0 \leq k \leq N-1$, the appropriate symmetry relation is $\widehat{h}_{N-k} = \widehat{h}_k^*$, which means the second half of the list of Fourier components is determined by the first. But this seems a little bit removed from the corresponding symmetry property $\widehat{h}(-f) = \widehat{h}^*(f)$ from the continuous Fourier transform.

To better keep positive and negative frequencies together, we'd like to consider the physically interesting set of N Fourier components to be

$$\left\{ \widehat{h}_k \mid k = -\frac{N}{2}, \dots, \frac{N}{2} - 1 \right\} . \quad (2.59)$$

It's a matter of convention that we include $-N/2$ rather than $N/2$ in the list. It makes things more convenient for `fftshift()` functions in SciPy, matlab, etc., which move the Fourier components $\{\widehat{h}_{N/2}, \dots, \widehat{h}_{N-1}\}$ to the front of a vector so they can represent $\{\widehat{h}_{-N/2}, \dots, \widehat{h}_{-1}\}$.

Note now that the reality condition becomes

$$\text{if } h_j^* = h_j, \quad \widehat{h}_k^* = \widehat{h}_{-k} \quad (2.60)$$

which means that all of the negative components $\{\widehat{h}_{-N/2+1}, \dots, \widehat{h}_{-1}\}$ of the DFT of a real series are just the complex conjugates of the corresponding positive components. The reality condition also enforces

$$\widehat{h}_0 = \widehat{h}_0^* \in \mathbb{R} \quad (2.61a)$$

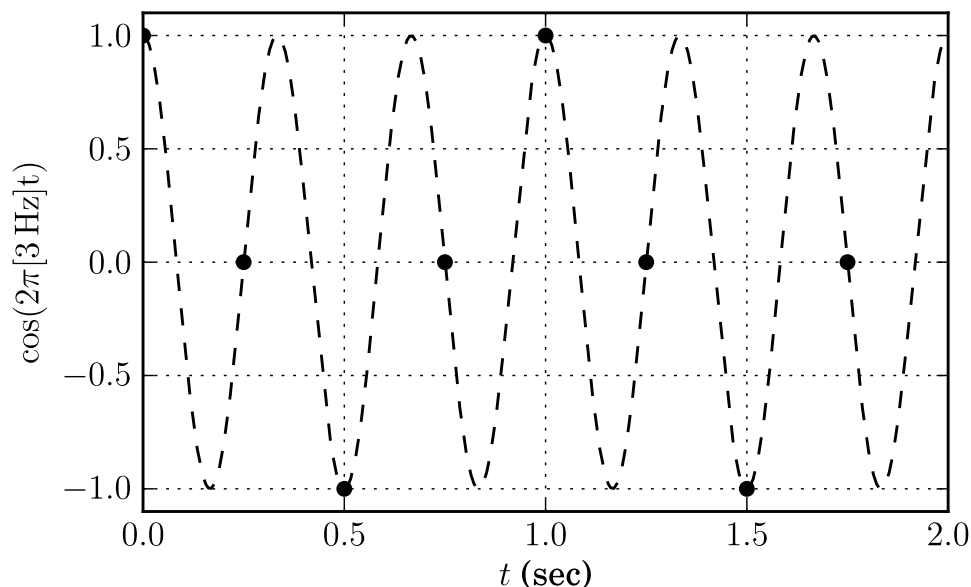
$$\widehat{h}_{-N/2} = \widehat{h}_{N/2}^* = \widehat{h}_{-N/2}^* \in \mathbb{R} \quad (2.61b)$$

So from N real samples $\{h_j | j = 0, \dots, N-1\}$ we get a discrete Fourier transform completely described by 2 real components \widehat{h}_0 and $\widehat{h}_{-N/2} = \widehat{h}_{N/2}$ and $\frac{N}{2} - 1$ complex components $\{\widehat{h}_k | k = 1, \dots, \frac{N}{2} - 1\}$.

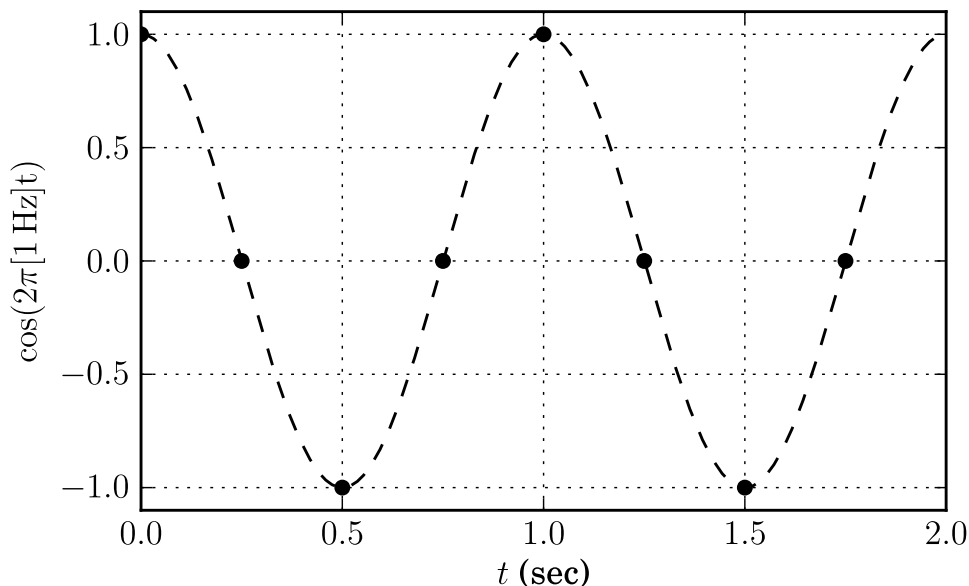
The frequency corresponding to the last Fourier component,

$$|f_{-N/2}| = |f_{N/2}| = \frac{N}{2} \delta f = \frac{1}{2 \delta t} \quad (2.62)$$

is half of the sampling frequency $1/\delta t$, and is known as the *Nyquist frequency*. It is the highest frequency which can be resolved in the discrete Fourier transform of a series sampled with a sampling time δt . Of course, as we've seen, frequencies above the Nyquist frequency, which correspond to Fourier components with $k > N/2$, aren't invisible, they just show up in the same place as lower frequencies. For example, consider a cosine wave with a frequency of 3 Hz, sampled with a time step of $\delta t = 0.25$ sec:



If we just look at the dots, they don't look like a 3 Hz cosine wave, but rather like one with a frequency of 1 Hz. And indeed, we'd get the exact same samples if we sampled a 1 Hz at the same rate:



This is because $f = 3\text{ Hz}$ is above the Nyquist frequency at this sampling rate, which is $f_{\text{Ny}} = 2\text{ Hz}$. The higher-frequency cosine wave has been *aliased* down to a frequency of $f_{\text{Ny}} - f = -1\text{ Hz}$.

Note, in closing, that the range of independent frequencies, from $-f_{\text{Ny}}$ to $+f_{\text{Ny}}$, is $2|f_{\text{Ny}}| = \frac{1}{\delta t}$ so we can fill in the table for time-frequency resolution and extent:

	Resolution	Extent
t	discrete, δt	duration T
f	discrete, $\delta f = \frac{1}{T}$	finite, $2 f_{\text{Ny}} = \frac{1}{\delta t}$

Tuesday, September 21, 2010

3 Numerical Methods (guest lectures by Joshua Faber)

3.1 Orthogonal functions

As shown in previous classes, sets of orthogonal functions play an important role in the solution of differential equations. A particularly useful choice is Chebyshev polynomials, as they combine several of the benefits of Fourier methods with the simplicity of closed-form polynomial expansions. Chebyshev polynomials have the distinction of being defined using trigonometric functions, which might seem at first glance like a contradiction in terms, with the n th Chebyshev polynomial (beginning from $n = 0$) defined as

$$T_n(x) = \cos(n \arccos x) \tag{3.1}$$

on the domain $[-1, 1]$. From the definition, it is clear that the range of the polynomials is also $[-1, 1]$, except for $T_0(x) = 1$. Less clear is that these are polynomials at all. To demonstrate this, we begin from the first two expressions $T_0(x) = 1$ and $T_1(x) = x$, and then note that

$$\begin{aligned}
2xT_n(x) - T_{n-1}(x) &= 2 \cos(\arccos x) \cos(n \arccos x) - \cos([n-1] \arccos x) \\
&= 2 \cos(\arccos x) \cos(n \arccos x) \\
&\quad - [\cos(\arccos x) \cos(n \arccos x) + \sin(\arccos x) \sin(n \arccos x)] \quad (3.2) \\
&= \cos(\arccos x) \cos(n \arccos x) - \sin(\arccos x) \sin(n \arccos x) \\
&= \cos([n+1] \arccos x) \equiv T_{n+1}(x)
\end{aligned}$$

and thus we can build up each new polynomial from the previous two using the recurrence relation.

Chebyshev polynomials satisfy a weighted continuous orthogonality relation with weight $(1-x^2)^{-1/2}$ given by

$$\int_{-1}^1 T_n(x)T_m(x) \frac{dx}{\sqrt{1-x^2}} = \begin{cases} 0 & n \neq m \\ \pi & n = m = 0 \\ \pi/2 & n = m \neq 0 \end{cases} \quad (3.3)$$

To prove this, we may use the trigonometric substitution $x = \cos \theta \rightarrow dx = -\sin \theta d\theta = -\sqrt{1-x^2}d\theta$, and note that

$$T_n(x) = T_n(\cos \theta) = \cos(n \arccos[\cos \theta]) = \cos(n\theta) \quad (3.4)$$

finding that

$$\int_{-1}^1 T_n(x)T_m(x) \frac{dx}{\sqrt{1-x^2}} = \int_{\pi}^0 \cos(n\theta) \cos(m\theta)(-d\theta) = \int_0^{\pi} \cos(n\theta) \cos(m\theta)d\theta \quad (3.5)$$

The proof of orthogonality is actually a nice exercise

$$\begin{aligned}
\int_0^{\pi} \cos(n\theta) \cos(m\theta)d\theta &= \frac{1}{2} \int_0^{\pi} [\cos([m+n]\theta) + \cos([m-n]\theta)] d\theta \\
&= \frac{1}{2(m+n)} \sin([m+n]\theta)\Big|_0^{\pi} + \frac{1}{2(m-n)} \sin([m-n]\theta)\Big|_0^{\pi} \quad (3.6)
\end{aligned}$$

If $m \neq n$, we get zero for both terms, if $m = n \neq 0$, the difference term yields $\pi/2$, and if $m = n = 0$, each term yields $\pi/2$ for a total of π .

The Chebyshev polynomials are even and odd depending on the index, and their endpoint values follow directly from the definition above. We find:

$$T_n(1) = 1 \quad T_n(-1) = (-1)^n \quad (3.7a)$$

$$T'_n(1) = n \quad T'_n(-1) = (-1)^{n+1}n \quad (3.7b)$$

From a practical standpoint, we often want to use a Chebyshev polynomial expansion to approximate a function. Instead of performing a series of integrals over a set of complicated functions, we can instead make use of the discrete orthogonality principle. Let

$$x_k = \cos\left(\frac{\pi(k + 1/2)}{n}\right); \quad 0 \leq k \leq n - 1 \quad (3.8)$$

be the n zeroes of $T_n(x)$, known as the Gauss-Lobatto points in the language of orthogonal functions. The Chebyshev polynomials satisfy the discrete orthogonality relation

$$\sum_{k=0}^{n-1} T_i(x_k) T_j(x_k) = \begin{cases} 0 & i \neq j \\ n & i = j = 0 \\ n/2 & i = j \neq 0 \end{cases} \quad (3.9)$$

which again may be derived from the properties of Fourier (cosine) modes.

To approximate a function using Chebyshev polynomials, we can use the discrete orthogonality relation to our advantage. Assume that we have an expansion

$$f(x) \approx \sum_{j=0}^{n-1} c_j T_j(x) \quad (3.10)$$

we find that

$$\sum_{k=0}^{n-1} f(x_k) T_j(x_k) = \sum_{k=0}^{n-1} c_i T_i(x_k) T_j(x_k) = \begin{cases} 0 & i \neq j \\ nc_0 & i = j = 0 \\ nc_i/2 & i = j \neq 0 \end{cases} \quad (3.11)$$

or inverting this result

$$c_0 = \frac{1}{n} \sum_{k=0}^{n-1} f(x_k) \quad (3.12a)$$

$$c_i = \frac{2}{n} \sum_{k=0}^{n-1} f(x_k) T_i(x_k) \quad (3.12b)$$

3.1.1 Runge's phenomenon and Minimax polynomials

Consider the curve $f(x) = \frac{1}{1+25x^2}$, which looks like a slightly less-curved Gaussian, and is smooth (infinitely differentiable) everywhere. It is not, however a polynomial. If we were to approximate it using a series of polynomials, our first attempt might be to try the Taylor series at $x = 0$. Unfortunately, the radius of convergence is $1/5$, so that doesn't get us very far... Next, we might choose $N + 1$ evenly spaced points and try to fit a polynomial through them. You will find that this works very well for the center, but terribly at the edges. In fact, the errors near the edges grow in magnitude, without bound, as we increase the number of points and the order of the polynomials with which we fit the function.

This is known as *Runge's Phenomenon*, after the mathematician perhaps better known for co-developing a fourth-order differential equation evolution system. It turns out that better sets of points for reducing the errors to zero is to choose them so that they are concentrated near the edges of the distribution. The optimal set of points would be to choose the points to be zeros of a cosine function. Unfortunately, working out each of the polynomial coefficients based on these N points would typically very slow. If we fit using Chebyshev polynomials, on the other hand, it is rather simple. As a result, Chebyshev interpolants $f_{\text{cheb}}(x)$ are known to be the best simple approximant to the *minimax polynomial* of smooth functions $f(x)$, where the minimax polynomial minimizes the quantity

$$\max |f(x) - f_{\text{cheb}}(x)| \quad (3.13)$$

over the set of all n th order polynomials.

3.2 Differentiation and Chebyshev encounters of the second kind

One of the convenient things about expanding functions in terms of Chebyshev polynomials is the fact we can solve differential equations, at least approximately, by converting continuous systems to discrete linear algebra systems. To do so, we need to be able to take derivatives of Chebyshev polynomials. Using the trig definition, we find that

$$T'_n(x) = \frac{n \sin(n \arccos x)}{\sqrt{1-x^2}} = n \frac{\sin(n \arccos x)}{\sin(\arccos x)} \equiv nU_{n-1}(x) \quad (3.14)$$

where we may define the functions $U_n(x)$, the so-called Chebyshev polynomials of the second kind, through the relation

$$U_n(x) \equiv \frac{\sin([n+1] \arccos x)}{\sin(\arccos x)} \quad (3.15)$$

As with the Chebyshev polynomials of the first kind, it is not immediately obvious that these are polynomials at all under the definition, though the differentiation identity above would seem to imply it. We note the following recurrence relation works as well. By inspection, $U_0(x) = 1$ and $U_1 = 2 \cos(\arccos x) = 2x$, and then we note that

$$\begin{aligned} U_n(x) &= \frac{\sin([n+1] \arccos x)}{\sin(\arccos x)} \\ &= \frac{1}{\sin(\arccos x)} [\sin(n \arccos x) \cos(\arccos x) + \cos(n \arccos x) \sin(\arccos x)] \\ &= xU_{n-1}(x) + T_n(x) \end{aligned} \quad (3.16)$$

It is important to note that unlike Chebyshev polynomials of the first kind, the second kind are not bounded between -1 and 1 . Indeed, one can check that $U_n(1) = n$ and by symmetry, $U_n(-1) = (-1)^n n$. There are countless additional recurrence relations linking the two types of Chebyshev polynomials, but we are most concerned here with this one:

$$T_n(x) = \cos(n \arccos x) \frac{\sin(\arccos x)}{\sin(\arccos x)} = \frac{\sin([n+1] \arccos x) - \sin([n-1] \arccos x)}{2 \sin(\arccos x)} = \frac{U_n - U_{n-2}}{2} \quad (3.17)$$

This allows us to establish the following identity about derivatives, after rewriting the previous equation as $U_n(x) = 2T_n(x) + U_{n-2}(x)$:

$$\begin{aligned} \frac{d}{dx}T_n(x) &= nU_{n-1}(x) = 2nT_{n-1}(x) + nU_{n-3}(x) \\ &= 2nT_{n-1}(x) + 2nT_{n-3}(x) + nU_{n-5}(x) \\ &= 2nT_{n-1}(x) + 2nT_{n-3}(x) + 2nT_{n-5}(x) + nU_{n-7}(x) \end{aligned} \quad (3.18)$$

and so on down the line until we reach either T_1 or T_0 , terminating the sequence. It is worth noting that we can prove this relation using the complex exponential definition of trig functions as well. Define $\Theta = \arccos x$, and we find

$$\begin{aligned} U_n(x) &= \frac{\sin([n+1]\Theta)}{\sin \Theta} = \frac{(e^{i(n+1)\Theta} - e^{-i(n+1)\Theta})/2i}{(e^{i\Theta} - e^{-i\Theta})/2i} \\ &= e^{in\Theta} + e^{i(n-2)\Theta} + e^{-(n-4)\Theta} + \dots + e^{-i(n-2)\Theta} + e^{-in\Theta} \\ &= 2[\cos(n\Theta) + \cos([n-2]\Theta) + \cos([n-4]\Theta) + \dots] \\ &= 2[T_n(x) + T_{n-2}(x) + T_{n-4}(x) + \dots] \end{aligned} \quad (3.19)$$

Going back to the idea of a polynomial expansion, we see that if we have a function being approximated as a sum of polynomials,

$$f(x) \approx \sum_{i=0}^n c_i T_i(x) \quad (3.20)$$

its derivative will involve a set of descending series:

$$\begin{aligned} \frac{df}{dx} &= 2nc_n(T_{n-1} + T_{n-3} + T_{n-5} + \dots) \\ &\quad + 2(n-1)c_{n-1}(T_{n-2} + T_{n-4} + \dots) \\ &\quad + 2(n-2)c_{n-2}(T_{n-3} + T_{n-5} + \dots) \\ &\quad + \dots = \sum_{i=0}^{n-1} d_i T_i(x) \end{aligned} \quad (3.21)$$

Looking carefully, we see that the only difference between the coefficient of the term T_{n-1} and T_{n-3} is generated by the coefficient c_{n-2} , so that in general, if

$$d_i = d_{i+2} + 2(i+1)c_{i+1} \quad (3.22)$$

This result can also be derived using *Clenshaw's algorithm*, which describes how to evaluate combinations of polynomials defined by a recurrence relation. Similarly, for integration, we can essentially read the identity above backwards, finding that if $\int f(x)dx \approx \sum b_i T_i(x)$, then

$$b_i = \frac{c_{i-1} - c_{i+1}}{2i} \quad (3.23)$$

3.3 Gauss’s phenomenon

Chebyshev interpolation is *spectrally accurate* for smooth (infinitely differentiable) functions: if we approximate a given function on $[-1, 1]$ using n polynomial coefficients, any error estimate you like including the \mathcal{L}_1 , \mathcal{L}_2 and \mathcal{L}_∞ error will scale like k^n , or in other words, exponentially. If the function we wish to interpolate is not smooth, this is no longer true. The error instead will decrease like n^{d+2} , where the function can be differentiated d times. Luckily, there is a simple solution to deal with these case. Consider a function we wish to interpolate that is smooth on the interval $[a, b]$. If we define a rescaled variable X through the relation $x = (a + b)/2 + (a - b)X/2$, so that the smooth interval satisfies $-1 < X < x$, then $T_n(X)$ will satisfy the exponential convergence property. If the function to be interpolated is piecewise smooth, we may interpolate each segment using a different set of scaled Chebyshev polynomials, to yield the required accuracy.

Thursday, September 23, 2010

3.4 Elliptic and Hyperbolic equations: an overview

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

$$\sum_{m=0}^k \sum_{n=0}^k A_{mn} \frac{\partial}{\partial x^m} \left(\frac{\partial f}{\partial x^n} \right) + \sum_{p=0}^k B_p \frac{\partial f}{\partial x^p} = F(f) \quad (3.24)$$

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:

$$\nabla^2 \Phi = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Phi = 4\pi G \rho \quad (3.25)$$

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:

$$\frac{\partial^2 f}{\partial t^2} - v^2 \frac{\partial^2 f}{\partial x^2} = 0 \quad (3.26)$$

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.

3.5 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.

3.5.1 Convolution

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

$$[\nabla^2 \Phi](\vec{r}) = 4\pi G \rho(\vec{r}) \Rightarrow \Phi(\vec{r}) = \iiint \frac{G \rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d^3V' \quad (3.27)$$

The key thing to notice is that we have one term involving a function of the variable we are integrating over (\vec{r}'), and one that depends on a difference between a fixed point in the integral (\vec{r}) and the integration variable (\vec{r}'). 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

$$\mathcal{F}\{\Phi(x)\} = G \int_{-\infty}^{\infty} dx e^{2\pi i k x} \int_{-\infty}^{\infty} dx' \rho(x') |x - x'|^{-1} \quad (3.28)$$

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

$$\begin{aligned} \mathcal{F}\{\Phi(x)\} &= G \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dy dx' e^{2\pi i k(x'+y)} \rho(x') |y|^{-1} \\ &= G \left(\int_{-\infty}^{\infty} dx' e^{2\pi i k x'} \rho(x') \right) \left(\int_{-\infty}^{\infty} dy e^{2\pi i k y} |y|^{-1} \right) \end{aligned} \quad (3.29a)$$

$$\begin{aligned} &= \mathcal{F}\{\rho(x)\} \cdot \mathcal{F}\{|x|^{-1}\} \\ \Phi(x) &= \mathcal{F}^{-1} \{ \mathcal{F}\{\rho(x)\} \cdot \mathcal{F}\{|x|^{-1}\} \} \end{aligned} \quad (3.29b)$$

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.

3.5.2 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

$$\rho_{\ell m}(r) \equiv \iint \rho(r, \theta, \phi) Y_{\ell m}^*(\theta, \phi) d^2\Omega \quad (3.30)$$

and noting that $\iint Y_{\ell' m'} Y_{\ell m}^* d^2\Omega = \delta_{\ell\ell'} \delta_{mm'}$ we may split the source term into a set of orthogonal moments, such that

$$\rho(r, \theta, \phi) = \sum_{\ell, m} \rho_{\ell m}(r) Y_{\ell m}(\theta, \phi) \quad (3.31)$$

Each term $\rho_{\ell m}$ generates a term in the solution $\Phi_{\ell m}$.

There is one issue with solving the general Poisson equation. For each mode, we need to solve the second order equation

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R_{\ell m}(r)}{\partial r} \right) - \frac{\ell(\ell+1)}{r^2} R_{\ell m}(r) = 4\pi G \rho_{\ell m}(r) \quad (3.32)$$

Which, being linear, will have a particular solution $R_{p;\ell m}(r)$ and two homogeneous solutions. For spherical harmonics, these are easily found to be

$$R_{\ell m}(r) = R_{p;\ell m}(r) + Cr^\ell + Dr^{-(\ell+1)} \quad (3.33)$$

but we have difficulty if we want the solution to remain finite at either $r = 0$ or $r \rightarrow \infty$. In practice, if we have a compact matter distribution, we use the trick to split the domain into two, radially. In the innermost domain, we set $D = 0$ so that the solution doesn't blow up at the origin, whereas in the outer one, we set $C = 0$ to avoid divergence at spatial infinity. We have two undetermined coefficients, but these may be fixed by requiring that $R(r)$ is continuous and differentiable at the interface, as would be expected for a second-order differential equation. Note that this implies that if a matter distribution has a spherical harmonic term $\rho_{\ell m}$, the resulting field falls off like $r^{-\ell-1}$.

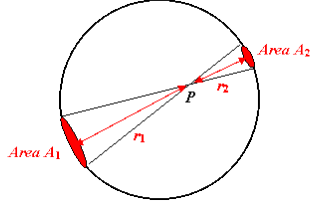
3.5.3 The Iron sphere theorem

The easiest mode to calculate of the mass distribution is the Y_{00} mode, which is given by the integral

$$\rho_{00} = \iiint \rho(\vec{r}) d^3V = M \quad (3.34)$$

yielding a potential $\Phi_{00} = -GM/r$. In practical terms, this implies the *Iron Sphere Theorem*: From the outside, one can tell the mass of a spherically symmetric mass distribution, but not its internal structure. From the inside of a spherical shell, there is no force at all. The proof, which reflects a 2-d integral over angles, says that since the area of a patch on opposite

sides of the sphere scales like r^2 , but the force falls off like r^{-2} , the force pulling in opposite directions cancels out completely.



3.5.4 Cartesian 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 $r^k Y_{\ell m}$ that satisfy the Laplacian equation with no source:

$$\frac{1}{r^2} \left[\frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \nabla_A^2 \right] r^k Y_{\ell m} = 0 \quad (3.35)$$

$$k(k+1)r^{k-2}Y_{\ell m} = \ell(\ell+1)r^{k-2}Y_{\ell m} \quad (3.36)$$

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:

$$Y_{00} = 1 \quad (3.37a)$$

$$rY_{10} = z \quad (3.37b)$$

$$\text{Re}(rY_{11}) = x \quad (3.37c)$$

$$\text{Im}(rY_{11}) = y \quad (3.37d)$$

$$r^2Y_{20} = 2z^2 - x^2 - y^2 \quad (3.37e)$$

$$\text{Re}(r^2Y_{21}) = xz \quad (3.37f)$$

$$\text{Im}(r^2Y_{21}) = yz \quad (3.37g)$$

$$\text{Re}(r^2Y_{22}) = x^2 - y^2 \quad (3.37h)$$

$$\text{Im}(r^2Y_{22}) = xy \quad (3.37i)$$

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, $Y_{20} = (-1, -1, 2)$, and $\text{Re} Y_{22} = (1, -1, 0)$. 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 $\ell = 2$ spherical harmonic representation of this quantity, since it is a radial factor multiplied by Y_{00} .

3.5.5 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 $r \rightarrow \infty$, our vacuum solution involves the terms in the form $r^{-(\ell+1)}Y_{\ell m}$. The general solution may be written

$$\Phi = G \left[\frac{M}{r} + \sum_i \frac{p_i \hat{x}^i}{r^2} + \frac{1}{2} \sum_{i,j} \frac{Q_{ij} \hat{x}^i \hat{x}^j}{r^3} + \dots \right] \quad (3.38)$$

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, $M = \iiint \rho d^3V$, the dipole term collects the $\ell = 1$ $Y_{\ell m}$ terms:

$$p_i \equiv \iiint \rho x^i d^3V \quad (3.39)$$

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

$$Q_{ij} \equiv \iiint \left(x^i x^j - \frac{1}{3} \delta^{ij} r^2 \right) \rho(\vec{r}) d^3V \quad (3.40)$$

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.

Tuesday, September 28, 2010

4 Spectral Analysis of Random Data

4.1 Amplitude Spectrum

Given a real time series $h(t)$ we know how to construct its Fourier transform

$$\tilde{h}(f) = \int_{-\infty}^{\infty} h(t) e^{-i2\pi ft} dt \quad (4.1)$$

or the equivalent discrete Fourier transform from a set of samples $\{h_j | j = 0, \dots, N-1\}$:

$$\hat{h}_k = \sum_{j=0}^{N-1} h_j e^{-i2\pi jk/N} \quad (4.2)$$

where $\hat{h}_k \delta t \sim \tilde{h}(f_k)$.

Think about the physical meaning of $\tilde{h}(f)$, by breaking this complex number up into an amplitude and phase

$$\tilde{h}(f) = A(f) e^{i\phi(f)} . \quad (4.3)$$

If $h(t)$ is real, the condition $\tilde{h}(-f) = \tilde{h}^*(f) = A(f)e^{-i\phi(f)}$ means $A(-f) = A(f)$ and $\phi(-f) = -\phi(f)$. Thus we can write the inverse Fourier transform as

$$\begin{aligned} h(t) &= \int_{-\infty}^0 A(f) e^{i[2\pi ft + \phi(f)]} df + \int_0^{\infty} A(f) e^{i[2\pi ft + \phi(f)]} df \\ &= \int_0^{\infty} A(f) (e^{i[2\pi ft + \phi(f)]} + e^{-i[2\pi ft + \phi(f)]}) df \\ &= \int_0^{\infty} 2 A(f) \cos(2\pi ft + \phi(f)) \end{aligned} \quad (4.4)$$

So $A(f)$ is a measure of the amplitude at frequency f and $\phi(f)$ is the phase.

Note also that

$$\int_{-\infty}^{\infty} [h(t)]^2 dt = \int_{-\infty}^{\infty} |\tilde{h}(f)|^2 df \quad (4.5)$$

This works pretty well if the properties of $h(t)$ are deterministic. But suppose $h(t)$ is modelled as random, i.e., it depends on a lot of factors we don't know about, and all we can really do is make statistical statements. What is a sensible description of the spectral content of h ?

4.2 Random Variables

Consider a *random variable* x . Its value is not known, but we can talk about statistical expectations as to its value. We will have a lot more to say about this soon, but for now imagine we have a lot of chances to measure x in an ensemble of identically-prepared systems. The hypothetical average of all of those imagined measurements is called the *expectation value* and we write it as $\langle x \rangle$. (Another notation is $E[x]$.) We can also take some known function f and talk about the expectation value $\langle f(x) \rangle$ corresponding to a large number of hypothetical measurements of $f(x)$.

The expectation value of x itself is the *mean*, sometimes abbreviated as μ . (This name is taken by analogy to the mean of an actual finite ensemble.) Since x is random, though, x won't always have the value $\langle x \rangle$. We can talk about how far off x typically is from its average value $\langle x \rangle$. Note however that

$$\langle x - \mu \rangle = \langle x \rangle - \langle \mu \rangle = \langle x \rangle - \mu = 0 \quad (4.6)$$

since the expectation value is a linear operation (being the analogue of an average), and the expectation value of a non-random quantity is just the quantity itself. So instead of the mean deviation from the mean, we need to consider the mean square deviation from the mean

$$\langle (x - \langle x \rangle)^2 \rangle \quad (4.7)$$

This is called the variance, and is sometimes written σ^2 . Its square root, the root mean square (RMS) deviation from the mean, is the standard deviation.

4.2.1 Random Sequences

Now imagine we have a bunch of random variables $\{x_j\}$; in principle each can have its own mean $\mu_j = \langle x_j \rangle$ and variance $\sigma_j^2 = \langle (x_j - \mu_j)^2 \rangle$. But we can also think about possible correlations $\sigma_{j\ell}^2 = \langle (x_j - \mu_j)(x_\ell - \mu_\ell) \rangle$; if the variables are uncorrelated $\sigma_{j\ell}^2 = \delta_{j\ell} \sigma_j^2$, but that need not be the case.

Think specifically about a series of N samples which are all uncorrelated random variables with zero mean and the same variance:

$$\langle x_j \rangle = 0; \quad \langle x_j x_\ell \rangle = \delta_{j\ell} \sigma^2; \quad (4.8)$$

what are the characteristics of the discrete Fourier transform of this sequence?

$$\hat{x}_k = \sum_{j=0}^{N-1} x_j e^{-i2\pi jk/N} \quad (4.9)$$

Well,

$$\langle \hat{x}_k \rangle = \sum_{j=0}^{N-1} \langle x_j \rangle e^{-i2\pi jk/N} = 0 \quad (4.10)$$

and

$$\langle \hat{x}_k \hat{x}_\ell^* \rangle = \sum_{j=0}^{N-1} \sum_{n=0}^{N-1} \langle x_j x_n \rangle e^{-i2\pi(jk-n\ell)/N} = \sum_{j=0}^{N-1} \sigma^2 e^{-i2\pi j(k-\ell)/N} = N\sigma^2 \delta_{k,\ell \bmod N} \quad (4.11)$$

so the Fourier components are also uncorrelated random variables with variance

$$\langle |\hat{x}_k|^2 \rangle = N\sigma^2 \quad (4.12)$$

Note this is independent of k , which is maybe a bit surprising. After all, it's natural to think all times are alike, but all frequencies need not be. Random data like this, which is the same at all frequencies, is called "white noise". To gain some more insight into white and colored noise, it helps to think about the same thing in the idealization of the continuous Fourier transform.

4.3 Continuous Random Data

Think about the continuous-time analog to the random sequence considered in section 4.2.1. This is a time series $x(t)$ which is characterized by statistical expectations. In particular we could talk about its expectation value

$$\langle x(t) \rangle = \mu(t) \quad (4.13)$$

and the expectation value of the product of samples taken at possibly different times

$$\langle x(t)x(t') \rangle = K_x(t, t') \quad (4.14)$$

(it's conventional not to subtract out $\mu(t)$ here). Note that $\langle x(t) \rangle$ is *not* the time-average of a particular instantiation of $x(t)$, although the latter may sometimes be used to estimate the former.

4.3.1 White Noise

Now, for white noise we need the continuous-time equivalent of (4.8), in which the data is uncorrelated with itself except at the very same time. In the case of continuous time, the sensible thing is the Dirac delta function, so white noise is characterized by

$$\langle x(t)x(t') \rangle = K_0 \delta(t - t') \quad (4.15)$$

where K_0 is a measure of how “loud” the noise is. In the frequency domain, this means

$$\begin{aligned} \langle \tilde{x}(f)\tilde{x}^*(f') \rangle &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \langle x(t)x(t') \rangle e^{-i2\pi(ft-f't')} dt dt' = K_0 \int_{-\infty}^{\infty} e^{-i2\pi(f-f')t} dt \\ &= K_0 \delta(f - f') . \end{aligned} \quad (4.16)$$

4.3.2 Colored Noise

A lot of times, the quantity measured in an experiment is related to some starting quantity by a linear convolution, so even if we start out with white noise, we could end up dealing with something that has different properties. If we consider some random variable $h(t)$ which is produced by convolving white noise with a deterministic response function $R(t - t')$, so that

$$h(t) = \int_{-\infty}^{\infty} R(t - t') x(t') dt' \quad (4.17)$$

and in the frequency domain

$$\tilde{h}(f) = \tilde{R}(f)\tilde{x}(f) \quad (4.18)$$

we have

$$\langle \tilde{h}(f)\tilde{h}^*(f') \rangle = K_0 \left| \tilde{R}(f) \right|^2 \delta(f - f') . \quad (4.19)$$

Note that even in this case, $\langle |h(f)|^2 \rangle$ blows up, so simply looking at the magnitudes of Fourier components is not the most useful thing to do. However, the quantity $K_0 \left| \tilde{R}(f) \right|^2$ which multiplies the delta function can be well-behaved, and gives a useful spectrum. We’ll see that this is the power spectral density $S_h(f)$, which we’ll define more carefully in a bit.

We can also go back into the time domain in this example, and calculate the autocorrelation

$$\begin{aligned} K_h(t, t') &= \langle h(t)h(t') \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} R(t - t_1) R(t' - t_1) \langle x(t_1)x(t'_1) \rangle dt_1 dt'_1 \\ &= \int_{-\infty}^{\infty} K_0 R(t - t_1) R(t' - t_1) dt_1 \end{aligned} \quad (4.20)$$

which is basically the convolution of the response function with itself, time reversed; unlike in the case of white noise, where $K_x(t, t')$ was a delta function, this will in general be finite.

Note that in this example, the autocorrelation $K_h(t, t')$ is unchanged by shifting both of its arguments:

$$\begin{aligned} K_h(t + \tau, t' + \tau) &= K_0 \int_{-\infty}^{\infty} R(t - [t_1 - \tau]) R(t' - [t_1 - \tau]) dt_1 \\ &= K_0 \int_{-\infty}^{\infty} R(t - t_2) R(t' - t_2) dt_2 = K_h(t, t') \end{aligned} \quad (4.21)$$

where we make the change of integration variables from t_1 to $t_2 = t_1 - \tau$. This means that in this colored noise case the autocorrelation is a function only of $t - t'$.

Thursday, September 30, 2010

4.4 Wide-Sense Stationary Data

We now turn to a general formalism which incorporates our observations about colored noise. A random time series $h(t)$ is called *wide-sense stationary* if it obeys

$$\langle h(t) \rangle = \mu = \text{constant} \quad (4.22)$$

and

$$\langle h(t)h(t') \rangle = K_h(t - t') . \quad (4.23)$$

Clearly, both our white noise and colored noise examples were wide-sense stationary. The appearance of a convolution in the time-domain (4.20) a product in the frequency domain (4.19) suggests to us that the Fourier transform of the auto-correlation function $K_h(t - t')$ is a useful quantity. We thus define the *power spectral density* as

$$S_h(f) = \int_{-\infty}^{\infty} K_h(\tau) e^{-i2\pi f\tau} d\tau . \quad (4.24)$$

Note that by the construction (4.23) the autocorrelation is even in its argument [$K_h(\tau) = K_h(-\tau)$] so the PSD of real data will be real and even in f .

We can then show that for a general wide-sense stationary process,

$$\begin{aligned} \langle \tilde{h}(f)\tilde{h}^*(f') \rangle &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \langle h(t)h(t') \rangle e^{-i2\pi(ft-f't')} dt dt' \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} K_h(\tau) e^{-i2\pi f\tau} e^{-i2\pi(f-f')t'} d\tau dt' = \delta(f - f') S_h(f) , \end{aligned} \quad (4.25)$$

where we make the change of variables from t to $\tau = t - t'$.

4.4.1 Symmetry Properties of the Auto-Correlation and the PSD

We can see from the definition (4.23) and the result (4.25) that, for real data, both $K_h(\tau)$ and $S_h(f)$ are real and even, and in particular that $S_h(f) = S_h(-f)$. (Of course the fact that $K_h(\tau)$ and $S_h(f)$ are Fourier transforms of each other means that once we know the symmetry properties of one, we can deduce the symmetry properties of the other.) Because it's defined at both positive and negative frequencies, the power spectral density $S_h(f)$ that we've been using is called the *two-sided PSD*. Since the distinction between positive and negative frequencies depends on things like the sign convention for the Fourier transform, it is sometimes considered more natural to define a *one-sided PSD* which is defined only at non-negative frequencies, and contains all of the power at the corresponding positive and negative frequencies:

$$S_h^{1\text{-sided}}(f) = \begin{cases} S_h(0) & f = 0 \\ S_h(-f) + S_h(f) & f > 0 \end{cases} \quad (4.26)$$

Apparently, for real data, $S_h^{1\text{-sided}}(f) = 2S_h(f)$ when $f > 0$.

If the original time series is not actually real, there is a straightforward generalization of the definition of the auto-correlation function:

$$\langle h(t)h^*(t') \rangle = K_h(t - t') \quad (4.27)$$

The PSD is then defined as the Fourier transform of this, and (4.25) holds as before. Examination of (4.27) and (4.25) shows that, for complex data, the symmetry properties which remain are

- $K_h(-\tau) = K_h^*(\tau)$
- $S_h(f)$ is real.

4.5 Power Spectrum Estimation

Suppose we have a stretch of data, duration T , sampled at intervals of δt , from a wide-sense stationary data stream,

$$h_j = h(t_0 + j \delta t) \quad (4.28)$$

where the autocorrelation

$$K_h(t - t') = \langle h(t)h(t') \rangle \quad (4.29)$$

and its Fourier transform the PSD

$$S_h(f) = \int_{-\infty}^{\infty} K_h(\tau) e^{-i2\pi f\tau} d\tau \quad (4.30)$$

are unknown. How do we estimate $S_h(f)$? One idea, keeping in mind that

$$\langle \tilde{h}(f)\tilde{h}^*(f') \rangle = \delta(f - f') S_h(f) , \quad (4.31)$$

is to use the discrete Fourier components to construct

$$\left| \hat{h}_k \right|^2 \quad (4.32)$$

this is, up to normalization, the *periodogram*. Now, we're going to have to be a little careful about just using the identification

$$\hat{h}_k \delta t \sim \tilde{h}(f_k) \quad (4.33)$$

where

$$f_k = k \delta f = \frac{k}{T} ; \quad (4.34)$$

after all, taking that literally would mean setting f and f' both to f_k and evaluating the delta function at zero argument. So we need to be a little more careful about the approximation that relates the discrete and continuous Fourier transforms.

4.5.1 The Discretization Kernel $\Delta_N(x)$

If we substitute the continuous inverse Fourier transform into the discrete forward Fourier transform, we find

$$\begin{aligned}\widehat{h}_k &= \sum_{j=0}^{N-1} h(t_0 + j \delta t) e^{-i2\pi j k/N} = \sum_{j=0}^{N-1} \int_{-\infty}^{\infty} \widetilde{h}(f) e^{-i2\pi j k/N} e^{i2\pi f j \delta t} df \\ &= \int_{-\infty}^{\infty} \left(\sum_{j=0}^{N-1} e^{-i2\pi j (f_k - f) \delta t} \right) \widetilde{h}(f) df = \int_{-\infty}^{\infty} \Delta_N([f_k - f] \delta t) \widetilde{h}(f) df\end{aligned}\tag{4.35}$$

where we have defined⁸

$$\Delta_N(x) = \sum_{j=0}^{N-1} e^{-i2\pi j x} .\tag{4.36}$$

Let's look at some of the properties of this $\Delta_N(x)$. First, if x is an integer,

$$\Delta_N(x) = \sum_{j=0}^{N-1} e^{-i2\pi j x} = \sum_{j=0}^{N-1} 1 = N \quad (x \in \mathbb{Z})\tag{4.37}$$

Next, note that $\Delta_N(x)$ is periodic in x with period 1, since

$$\Delta_N(x+1) = \sum_{j=0}^{N-1} e^{-i2\pi j(x+1)} = \sum_{j=0}^{N-1} e^{-i2\pi j x} e^{-i2\pi j} = \sum_{j=0}^{N-1} e^{-i2\pi j x} = \Delta_N(x) .\tag{4.38}$$

Note that this is not surprising for something that relates a discrete to a continuous Fourier transform; incrementing $[f_k - f] \delta t$ by 1 is the same as decrementing f by $1/\delta t$, which is twice the Nyquist frequency. This is just the usual phenomenon of aliasing, where many continuous frequency components, separated at intervals of $1/\delta t$, are mapped onto the same discrete component.

Note also that

$$\Delta_N(\ell/N) = \sum_{j=0}^{N-1} e^{-i2\pi j \ell/N} = 0 \quad \ell \in \mathbb{Z} \text{ and } \ell \neq 0 \pmod N\tag{4.39}$$

of course, it's sort of cheating to quote that result from before, since we got it by actually evaluating the sum, so let's do that again. Since

$$(1 - a^N) = (1 - a) \sum_{j=0}^{N-1} a^j ,\tag{4.40}$$

if we set $a = e^{-i2\pi x}$, we get, for $x \notin \mathbb{Z}$ (which means $a \neq 1$),

$$\Delta_N(x) = \frac{1 - e^{-i2\pi N x}}{1 - e^{-i2\pi x}} = \frac{e^{-i\pi N x} e^{i\pi N x} - e^{-i\pi N x}}{e^{-i\pi x} e^{i2\pi x} - e^{-i2\pi x}} = e^{-i\pi(N-1)x} \frac{\sin \pi N x}{\sin \pi x}\tag{4.41}$$

⁸This is closely related to the *Dirichlet kernel* $\sum_{k=-n}^n e^{-ikx} = \sin([2n+1]\frac{x}{2}) / \sin(\frac{x}{2})$.

so, to summarize,

$$\Delta_N(x) = \begin{cases} N, & x \in \mathbb{Z} \\ e^{-i\pi(N-1)x} \left(\frac{\sin \pi N x}{\sin \pi x} \right), & x \notin \mathbb{Z} \end{cases} \quad (4.42)$$

4.5.2 Derivation of the Periodogram

Now that we have a more precise relationship between \widehat{h}_k and $\widetilde{h}(f)$, we can think about $|\widehat{h}_k|^2$, and in particular its expectation value:

$$\begin{aligned} \left\langle |\widehat{h}_k|^2 \right\rangle &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Delta_N([f_k - f]\delta t) \Delta_N^*([f_k - f']\delta t) \left\langle \widetilde{h}(f) \widetilde{h}^*(f') \right\rangle df df' \\ &= \int_{-\infty}^{\infty} |\Delta_N([f_k - f]\delta t)|^2 S_h(f) df \end{aligned} \quad (4.43)$$

Let's get a handle on

$$|\Delta_N(x)|^2 = \left(\frac{\sin \pi N x}{\sin \pi x} \right)^2 \quad (4.44)$$

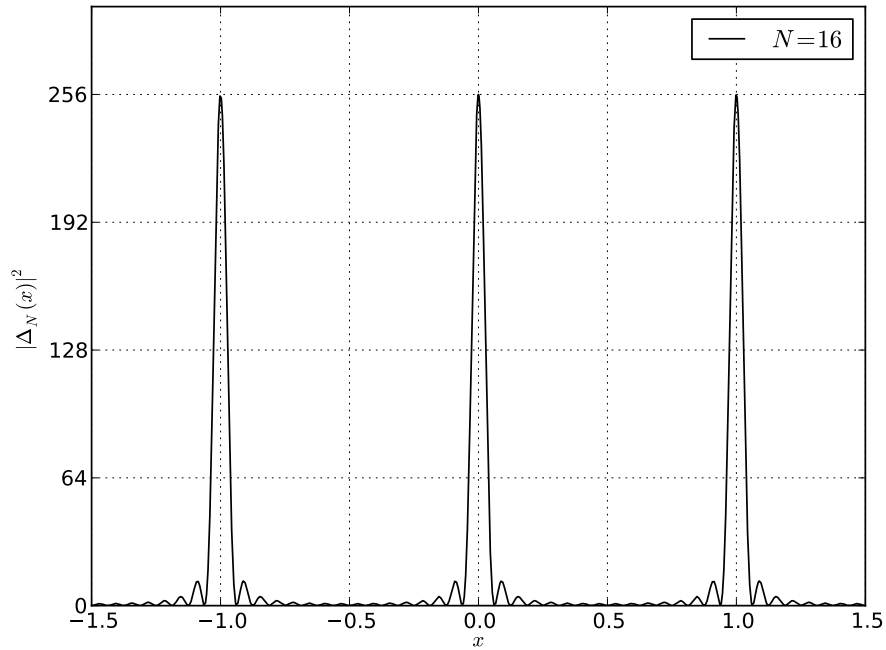
by looking at some plots of it in NumPy/matplotlib:

```
> ipython -pylab
x=linspace(-1.5,1.5,5e3)
D16 = (sin(16*pi*x)/sin(pi*x))**2
figure()
plot(x,D16,'k-',label=r'$N=16$')
legend()
xlabel(r'$x$')
ylabel(r'$|\Delta_N(x)|^2$')
yticks(arange(5)*64)
ylim([0,300])
grid(1)
savefig('Delta16.eps')
D64 = (sin(64*pi*x)/sin(pi*x))**2
figure()
plot(x,D16,'k-',label=r'$N=16$')
plot(x,D64,'b--',label=r'$N=64$')
legend()
xlabel(r'$x$')
ylabel(r'$|\Delta_N(x)|^2$')
yticks(arange(5)*1024)
ylim([0,4200])
xlim([-1./8,1./8.])
grid(1)
tickvals=arange(-3,4)/32.
ticklabs = [(r'%d/32$' % x) for x in range(-3,4)]
```

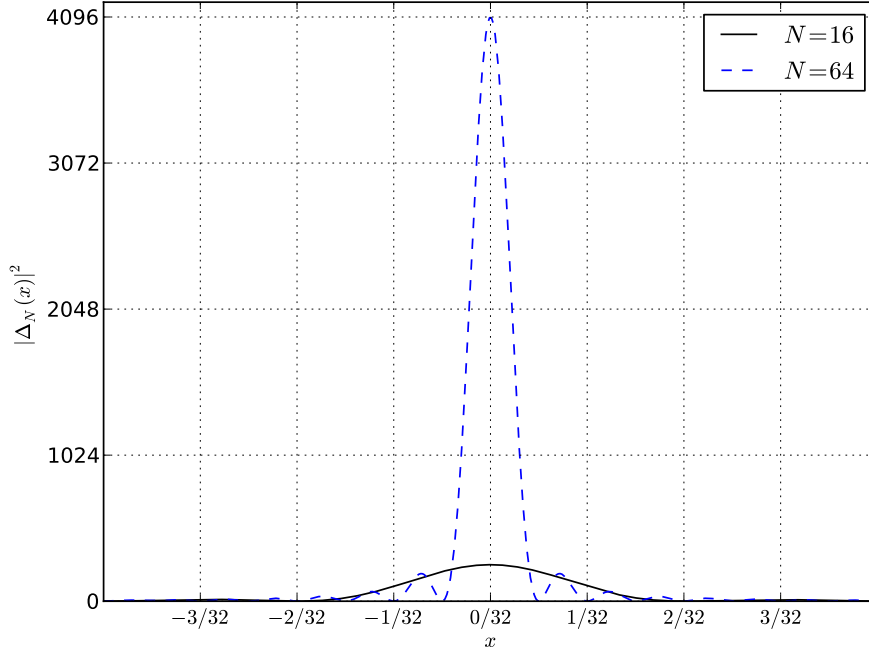


```
xticks(tickvals,ticklabs)
savefig('Delta64.eps')
```

If we look for $N = 16$, we see that $|\Delta_N(x)|^2$ is indeed periodic, with period 1, and has the value $N^2 = 16^2 = 256$ for integer x :



It's also pretty sharply peaked at integer values; we can zoom in and compare it to $|\Delta_N(x)|^2$ for $N = 64$:



We see now that the peak at $x = 0$ is at $N^2 = 64^2 = 4096$. Note we can also see the zeros at non-zero integer multiples of $1/N$ for both functions. And the function is getting more sharply peaked as N gets larger.

We can see, then, that $|\Delta_N(x)|^2$ is acting as an approximation to a sum of Dirac delta functions (one peaked at each integer value of x), and this approximation is better for higher N . We can write this situation as

$$|\Delta_N(x)|^2 \approx \mathcal{N}_N \sum_{s=-\infty}^{\infty} \delta(x + s) \quad (4.45)$$

To get the overall normalization constant \mathcal{N}_N , we have to integrate both sides of (4.45), using the fact that

$$\int_{-\infty}^{\infty} \delta(x) dx = 1 \quad (4.46)$$

Of course, we don't actually want to integrate $|\Delta_N(x)|^2$ from $-\infty$ to ∞ , because it's periodic, and we're bound to get something infinite when we add up the contributions from the infinite number of peaks. And likewise, the right-hand side contains an infinite number of delta functions. So we should just integrate over one cycle, using

$$\int_{-1/2}^{1/2} \delta(x) dx = 1 \quad (4.47)$$

and choose \mathcal{N}_N so that

$$\int_{-1/2}^{1/2} |\Delta_N(x)|^2 dx = \mathcal{N}_N \sum_{s=-\infty}^{\infty} \int_{-1/2}^{1/2} \delta(x + s) dx = \mathcal{N}_N \quad (4.48)$$

We could explicitly evaluate (or look up) the integral of $|\Delta_N(x)|^2 = \left(\frac{\sin \pi N x}{\sin \pi x}\right)^2$, but it turns out to be easier to evaluate it as

$$\mathcal{N}_N = \int_{-1/2}^{1/2} \Delta_N(x) [\Delta_N(x)]^* dx = \int_{-1/2}^{1/2} \sum_{j=0}^{N-1} e^{-i2\pi j x} \sum_{\ell=0}^{N-1} e^{i2\pi \ell x} dx = \sum_{j=0}^{N-1} \sum_{\ell=0}^{N-1} \int_{-1/2}^{1/2} e^{-i2\pi(j-\ell)x} dx. \quad (4.49)$$

But the integral is straightforward:

$$\int_{-1/2}^{1/2} e^{-i2\pi(j-\ell)x} dx = \begin{cases} 1 & j = \ell \\ \frac{\sin(\pi[j-\ell])}{\pi(j-\ell)} & j \neq \ell \end{cases} = \delta_{j\ell} \quad (4.50)$$

so

$$\int_{-1/2}^{1/2} e^{-i2\pi(j-\ell)x} dx = \delta_{j\ell} \quad j, \ell \in \mathbb{Z} \quad (4.51)$$

and the normalization constant is

$$\mathcal{N}_N = \sum_{j=0}^{N-1} \sum_{\ell=0}^{N-1} \delta_{j\ell} = N \quad (4.52)$$

and

$$|\Delta_N(x)|^2 \approx N \sum_{s=-\infty}^{\infty} \delta(x-s) \quad (4.53)$$

We can now substitute this back into (4.43) and find

$$\begin{aligned} \langle |\widehat{h}_k|^2 \rangle &= \int_{-\infty}^{\infty} |\Delta_N([f_k - f]\delta t)|^2 S_h(f) df \approx N \sum_{s=-\infty}^{\infty} \int_{-\infty}^{\infty} \delta([f_k - f]\delta t - s) S_h(f) df \\ &= \frac{N}{\delta t} \sum_{s=-\infty}^{\infty} \int_{-\infty}^{\infty} \delta(f - [f_k - s/\delta t]) S_h(f) df = \frac{N}{\delta t} \sum_{s=-\infty}^{\infty} S_h(f_k - s/\delta t). \end{aligned} \quad (4.54)$$

That means that the correct definition of the *periodogram* is

$$P_k := \frac{\delta t}{N} |\widehat{h}_k|^2. \quad (4.55)$$

Its expectation value is

$$\langle P_k \rangle = \int_{-\infty}^{\infty} \frac{\delta t}{N} |\Delta_N([f_k - f]\delta t)|^2 S_h(f) df \approx \sum_{s=-\infty}^{\infty} S_h(f_k - s/\delta t) \quad (4.56)$$

4.5.3 Shortcomings of the Periodogram

There are a few ways in which the periodogram is not quite an ideal estimate of the underlying PSD $S_h(f)$:

1. As noted above, it's not actually an approximation to the PSD at f_k , but to that, plus the PSD at $f_k + 1/\delta t$ plus the PSD at $f_k + 2/\delta t$ etc. This is the usual aliasing phenomenon; since $1/\delta t$ is twice the Nyquist frequency, we can avoid it by doing some sort of analog processing of our original time series so that $S_h(f) = 0$ if $|f|$ is above the Nyquist frequency, and then confining attention to k between $-N/2$ and $N/2 - 1$ so that f_k is between minus Nyquist and Nyquist. We'll assume we've done that.
2. The function $|\Delta_N([f_k - f]\delta t)|^2$ is not actually the greatest approximation to the Dirac delta function, because of the "ringing" in the side lobes outside of the main peak. This means the periodogram estimate at a given frequency will be "contaminated" with data from nearby frequencies to a greater degree than necessary. This phenomenon is called *spectral leakage*. The source of this problem is that by sampling $h(t)$ only from t_0 to $t_0 + T$, we've effectively multiplied it by a rectangular window in the time domain

$$W_r(t) = \begin{cases} 0 & t < t_0 \\ 1 & t_0 \leq t < T \\ 0 & t \geq T \end{cases} \quad (4.57)$$

which means the Fourier transform is the convolution of $\widetilde{W}(f)$ with $\widetilde{h}(f)$. We know that the Fourier transform of a rectangle is not the nicest thing in the world, so we're better off multiplying the data by a window which more smoothly rises from 0 to 1 and then goes back down again, since its Fourier transform will stretch out less in frequencies. We won't elaborate on that further right now, but see, e.g., Section 13.4 of *Numerical Recipes* for more.

3. While P_k has the right expected mean (4.56), its expected variance

$$\langle (P_k - \langle P_k \rangle)^2 \rangle = \langle P_k^2 \rangle - \langle P_k \rangle^2, \quad (4.58)$$

which is a measure of the square of the typical error associated with the estimate, is larger than we'd like. We can look at

$$\langle P_k^2 \rangle = \left(\frac{\delta t}{N} \right)^2 \langle \widehat{h}_k \widehat{h}_k^* \widehat{h}_k \widehat{h}_k^* \rangle; \quad (4.59)$$

now, we can't actually evaluate this without saying more about the properties of $h(t)$ than we've specified. We've talked about the expectation value and the autocorrelation, but not the full distribution of probabilities of possible values. We'll soon develop the machinery to consider such things, but for now, we'll just state that for some choices of that underlying distribution

$$\langle \widehat{h}_k \widehat{h}_k^* \widehat{h}_k \widehat{h}_k^* \rangle \sim 2 \langle \widehat{h}_k \widehat{h}_k^* \rangle \langle \widehat{h}_k \widehat{h}_k^* \rangle \quad (4.60)$$

and if that's the case

$$\langle P_k^2 \rangle \sim 2 \left(\frac{\delta t}{N} |\widehat{h}_k| \right)^2 = 2 \langle P_k \rangle^2 \quad (4.61)$$

but that means the expected mean square error is the square of the expectation value itself:

$$\langle (P_k - \langle P_k \rangle)^2 \rangle \sim \langle P_k \rangle^2 \approx [S_h(f_k)]^2 \quad (4.62)$$

so we have an estimate of the power whose typical error is the same size as the estimate itself!

Note that this is independent of T , which means you don't get any better of an estimate of the PSD of a wide-sense stationary process by including more data in the periodogram. This is perhaps not so surprising if we recall that the discrete Fourier transform was developed in the context of deterministic data. Having a longer stretch of data produces higher resolution in the frequency domain, because $\delta f = \frac{1}{T}$. So that means if you construct a periodogram from 50 seconds of data, you get not-very-accurate PSD estimates at frequencies separated by 0.02 Hz. If you use 200 seconds, you get PSD estimates at more frequencies, just 0.005 Hz apart, but they're not any more accurate; they still have RMS expected errors equal to their expectation values. However, if the underlying PSD $S_h(f)$ doesn't vary much as a function of frequency, then $S_h(43.000 \text{ Hz})$, $S_h(43.005 \text{ Hz})$, $S_h(43.010 \text{ Hz})$ etc may be more or less the same, and so the corresponding periodograms will be estimates of roughly the same quantity. So you'd want to average those together to get a more accurate estimate. I.e., you want to lower the frequency resolution.

You can get a lower frequency resolution by doing your Fourier transforms over a shorter time, i.e., by breaking up the time T into \mathcal{N}_c chunks, each of duration T/\mathcal{N}_c , then doing discrete Fourier transforms over the $N = \frac{T}{\mathcal{N}_c \delta t}$ samples in each chunk. The periodogram from the α th chunk is then

$$P_{\alpha k} = \frac{\delta t}{N} \left| \hat{h}_k \right|^2 ; \quad (4.63)$$

its frequency resolution is

$$\delta f = \frac{1}{N \delta t} = \frac{\mathcal{N}_c}{T} . \quad (4.64)$$

Each periodogram has expected mean

$$\langle P_{\alpha k} \rangle \approx P(f_k) = P(k\delta f) \quad (4.65)$$

and variance

$$\langle P_{\alpha k}^2 \rangle - \langle P_{\alpha k} \rangle^2 \approx [P(f_k)]^2 \quad (4.66)$$

as before. But we can take the average of all \mathcal{N}_c periodograms

$$\bar{P}_k = \frac{1}{\mathcal{N}_c} \sum_{\alpha=0}^{\mathcal{N}_c-1} P_{\alpha k} \quad (4.67)$$

and since averaging independent random variables lowers the resulting variance,

$$\langle \bar{P}_k \rangle = P(f_k) \quad (4.68)$$

and variance

$$\langle \overline{P}_k^2 \rangle - \langle \overline{P}_k \rangle^2 \approx \frac{[P(f_k)]^2}{\mathcal{N}_c} . \quad (4.69)$$

So the error in the PSD estimation shrinks like $1/\sqrt{\mathcal{N}_c}$. We can get a more accurate estimate of the PSD by breaking the time up into chunks and averaging, but at the expense of a coarser frequency resolution. The appropriate tradeoff depends on the sharpness of the features that we want to resolve in the spectrum.