Physical Mathematics 2012

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Abstract

These are the lecture notes to accompany the Physical Mathematics lecture course.

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Chapter 1

Introduction

1.1 Organisation

Online notes & tutorial sheets

`www.ph.ed.ac.uk/~paboyle/`

1.1.1 Books

There are many books covering the special functions material in this course. Good ones include:

- "Mathematical Methods for Physics and Engineering", K.F. Riley, M.P. Hobson and S.J. Bence (Cambridge University Press)
- "Mathematical Methods in the Physical Sciences", M.L. Boas (Wiley)
- "Mathematical Methods for Physicists", G. Arfken (Academic Press)

These, and plenty more besides, are available **for free** in the JCMB library.

1.1.2 On the web

There are some useful websites for quick reference, including:

- `http://mathworld.wolfram.com`,
- `http://en.wikipedia.org`,
- `http://planetmath.org`.
- Numerical Recipes: `http://apps.nrbook.com/c/index.html`.

1.1.3 Workshops

Workshops run from week 2 through week 11.
There are two sessions:

- Tuesday 11:10-12:00 (room 1206C JCMB)
- Tuesday 14:00-15:50 (room 3217 JCMB)

1.1.4 Feedback

In week 8, I will hand out a 60 minute mock exam, and example solutions.

Anyone who wishes to have their script marked for feedback can hand this in. **The mark will *not* contribute to your course mark, but serves as useful practice and diagnostic.**

1.1.5 Structure

This brief introduction is Chapter 1. The rest of the course is composed of two parts.

Chapter 2 covers techniques for the solution of the partial differential equations (PDE's) of physics.

Chapter 3 covers probability, statistics and the fitting of data.

The structure of the course is different compared to previous years, due to the reorganisation of MFP in the second year.

- We retain the material on special functions and PDEs in curvilinear coordinate systems.
- We add material on probability and statistics.

You will note however from past papers that previous years contained substantial emphasis on Fourier series and Fourier transforms, topics which it is now expected that you already know and are skilled in using.

Chapter 2

Special functions

2.1 PDE's and physics

Physics involves the description of behaviour of the universe with partial differential equations. The main PDEs in physics are:

Poisson equation (electrostatics)	Laplace equation
Wave equation	Schrödinger equation
Navier-Stokes equations	Maxwell's equations

Some common ones are summarised in the following table.

Name	Equation	Physical context
Poisson	$\nabla^2\phi(\boldsymbol{r}) = -\frac{\rho(\boldsymbol{r})}{\epsilon_0}$	Electrostatics: $\phi(\boldsymbol{r})$ = potential; $\rho(\boldsymbol{r})$ = charge density.
Wave	$\nabla^2 u(\boldsymbol{r},t) = \frac{1}{v^2}\frac{\partial^2}{\partial t^2}u(\boldsymbol{r},t)$	All areas: v = wave speed; $u(\boldsymbol{r},t)$ = 'displacement' from equilibrium.
Laplace	$\nabla^2\phi(\boldsymbol{r}) = 0$	Special cases of above.
Schrödinger	$\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r})\right)\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$	Quantum mechanics: $\psi(\boldsymbol{r})$ = wave function.

Solving these equations for two and three dimensional problems can be challenging, and the first half of this course addresses techniques for the solution of PDEs in common situations.

This general approach involves several concepts which we will cover in more detail later.

1. **Differential operators**
   Gradient, Divergence and Curl are the building blocks for three dimensional equations.

2. **Separation of variables**
   the problem can be simplified to independent one dimensional ODE's by seeking solutions of a particular form.

3. **Solution of the separated ODEs**
   Recognising solution (e.g. wave equation)
   Substitute a power series (Method of Froebenius)

4. **Reconstruct general solution**
   The *orthogonality* and *completeness* of the solutions of an ODE allow us to write any solution as a linear combination of the normal mode solutions.
   It is this property that allows us to represent general functions by Fourier series.

We shall see that the normal strategy for dealing with several dimensions in analytical calculation is to duck the issue, and reduce it to one dimensional problems. This works for symmetrical problems if we choose coordinate systems that possess the same symmetries.

For non-symmetrical situations, one often resorts to using numerical approaches. For example, computational fluid dynamics is used to optimise the shapes of complex objects like aeroplanes and cars.

2.2 The wave equation

We can describe the transverse displacement of a stretched string using a function $u(x,t)$ which tells us how far the infinitesimal element of string at (longitudinal) position x has been (transversely) displaced at time t. The function $u(x,t)$ satisfies a partial differential equation (PDE) known as the wave equation:

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\,\frac{\partial^2 u}{\partial t^2} \tag{2.1}$$

where c is a constant,and has units of length over time (i.e. of velocity) and is, in fact, the speed of propagation of travelling waves on the string.

In the absence of boundaries, the general solution can be seen by noting:

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} &= \left(\frac{\partial}{\partial x} - \frac{1}{c}\frac{\partial}{\partial t}\right)\left(\frac{\partial}{\partial x} + \frac{1}{c}\frac{\partial}{\partial t}\right) u \\ &= \left(\frac{\partial}{\partial x} + \frac{1}{c}\frac{\partial}{\partial t}\right)\left(\frac{\partial}{\partial x} - \frac{1}{c}\frac{\partial}{\partial t}\right) u\end{aligned}$$

This is solved by

$$u(x,t) = f(x-ct) + g(x+ct)$$

where f and g are arbitrary functions of a single variable. This represents the superposition of arbitrary left and right propagating waves.

2.2.1 Separation of variables

Our equation of motion in Eqn. (2.1) is perhaps the simplest second order partial differential equation (PDE) imaginable – it doesn't contain any mixed derivatives (e.g. $\frac{\partial^2 u}{\partial x \partial t}$). We call such a differential equation a *separable* one, or say that it is of *separable form.*

We can seek particular solutions in which variations with space and time are *independent.* Such *standing waves* are of the *seperable* form:

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

This really is a *restriction* of the class of possible solutions and there are certainly solutions to the wave equation that are *not* of separated form (e.g. travelling waves as above).

However, we shall see *all* solutions of the wave equation (separated form or not) can be written as a linear combination of solutions of separated form, so this restriction is not a problem.

Differentiating, we get

$$\begin{aligned}\frac{\partial u}{\partial x} &= \frac{dX}{dx}\,T \equiv X'T \qquad &\Rightarrow \qquad \frac{\partial^2 u}{\partial x^2} &= X''T \\ \frac{\partial u}{\partial t} &= X\,\frac{dT}{dt} \equiv X\dot{T} \qquad &\Rightarrow \qquad \frac{\partial^2 u}{\partial t^2} &= X\ddot{T}\end{aligned}$$

Substituting this into the PDE:

$$X''(x)T(t) = \frac{1}{c^2}X(x)\ddot{T}(t) \ ,$$

Thus,

$$\frac{X(x)''}{X(x)} = \frac{1}{c^2}\,\frac{\ddot{T}(t)}{T(t)}$$

Now

$$\frac{\partial}{\partial t}LHS = \frac{\partial}{\partial x}RHS = 0$$

Hence both LHS and RHS must be equal to the same constant and we may write

$$\frac{X''}{X} = \frac{1}{c^2}\,\frac{\ddot{T}}{T} = -k^2 \qquad \text{(say)},$$

where $-k^2$ is called the **separation constant**.

Now we have *separated* our PDE in two variables into two simple second order ordinary differential equations (ODEs) in one variable each:

$$\begin{aligned}\frac{d^2X}{dx^2} &= -\,k^2X(x)\\ \frac{d^2T}{dt^2} &= -\,\omega_k^2T(t)\end{aligned}$$

where the angular frequency $\omega_k = ck$. This is the interpretation of c for standing waves: it is the constant of proportionality that links the wavenumber k to the angular frequency ω_k.

Quantum mechanics terminology

These have the form of an *eigenvalue* problem, where $X(x)$ must be an *eigenfunction* of the *differential operator* $\frac{d^2}{dx^2}$ with *eigenvalue* $-k^2$. Similarly $T(t)$ must be an eigenfunction of $\frac{d^2}{dt^2}$ with eigenvalue $-\omega_k^2 = -c^2k^2$.

2.2.2 Solving the ODE's

We can now solve the two ODEs separately. The solutions to these are familiar from simple harmonic motion, and we can just write down the solutions:

$$\begin{aligned}X(x) =& A_k \sin kx + B_k \cos kx\\ T(t) =& C_k \sin \omega_k t + D_k \cos \omega_k t\\ \Rightarrow u(x,t) =& \left(A_k \sin kx + B_k \cos kx\right)\left(C_k \sin \omega_k t + D_k \cos \omega_k t\right)\end{aligned}$$

where A_k, B_k, C_k, and D_k are arbitrary constants. The subscript denotes that they can take different values for different values of k. At this stage there is no restriction on the values of k: each values provides a separate solution to the ODEs.

2.2.3 Boundary conditions

The details of a specific physical system may involve the boundary conditions (BCs) solutions must satisfy. For example, what happens at the ends of the string and what were the initial conditions.

- The string weight & tension on a guitar determine c.
- The length (& frets) of a guitar determine the boundary conditions.
- The plucking of the guitar determines the initial conditions.

Assume the string is stretched between $x = 0$ and $x = L$, then the BCs in this case are that

$$u(x = 0, t) = u(x = L, t) = 0$$

for all t. Because these BCs hold for all times at specific x, they affect $X(x)$ rather than $T(t)$. We find

$$\begin{aligned} u(0,t) = 0 \quad &\Rightarrow \quad B_k = 0 \,, \\ u(L,t) = 0 \quad &\Rightarrow \quad k_n = n\pi/L \,, \qquad n = 0, 1, 2 \ldots \end{aligned}$$

Here, BCs have restricted the allowed values of k and thus the allowed frequencies of oscillation. Different boundary conditions will have different allowed values. Restriction of eigenvalues by boundary conditions is a very general property in physics:

finite boundaries ⇒ discrete (quantised) eigenvalue spectrum ⇒ allowable separation constants.

Each n value corresponds to a *normal mode* of the string:

$$u(x,t) = A_n \sin k_n x \{C_n \sin \omega_n t + D_n \cos \omega_n t\}$$

A normal mode is an excitation of the string that obeys the BCs and oscillates with a single, normal mode frequency. We sometimes call these *eigenmodes* of the system, with associated *eigenfrequencies* $\omega_n = \omega_{k_n}$.

Completeness

Just like any vector can be represented as a linear combination of basis vectors, so the *general solution* to the wave equation is a linear superposition of (normal) eigenmode solutions:

$$\begin{aligned} u(x,t) &= \sum_{n=1}^{\infty} A_n \sin k_n x \{C_n \sin \omega_n t + D_n \cos \omega_n t\} \\ &\equiv \sum_{n=1}^{\infty} \sin k_n x \{E_n \sin \omega_n t + F_n \cos \omega_n t\} \end{aligned} \tag{2.2}$$

This normal mode decomposition *not* obvious and the proof is beyond the scope of this course. We will simply assume this to be true.

In fact, almost *any* function can be described by such a linear combination of normal modes.

Completeness of the normal modes is general and applies to all "Sturm Liouville" ODE's

As before $\omega_n = ck_n$. We sum only from $n = 1$ because $\sin k_0 x = 0$, and we do not need to include negative n because $\sin \frac{-n\pi x}{L} = -\sin \frac{n\pi x}{L}$. Constants A_n, C_n, D_n are all unknown, so we can merge them together to give $E_n = A_n C_n$ and $F_n = A_n D_n$.

We also see that the way we have ensured that $u(0,t) = 0$ is by making it an *odd function* in x: $u(-x,t) = -u(x,t) \Rightarrow u(0,t) = 0$.

2.2.4 Initial conditions

As we have a second order temporal ODE, we need two sets of initial conditions to solve the problem. Typically these are the the shape $f(x)$ and velocity profile $g(x)$ of the string at $t = 0$:

$$u(x,0) = f(x) = \sum_{n=1}^{\infty} F_n \sin k_n x$$
$$\dot{u}(x,0) = g(x) = \sum_{n=1}^{\infty} \omega_n E_n \sin k_n x$$

These conditions determine unique values for each of the E_n and F_n. Having got these, we can substitute them back into the general solution to obtain $u(x,t)$ and thus describing the motion for all times.

Consider the equation for F_n. Let's choose to calculate one, specific constant out of this set i.e. F_m for some specific m. To do this, multiply both sides by $\sin k_m x$ and integrate over the whole string (in this case $x = 0...L$) giving:

$$\int_0^L dx\ f(x) \sin k_m x = \sum_{n=1}^{\infty} F_n \int_0^L dx\ \sin k_n x\ \sin k_m x\ .$$

Now we note that the sine functions form an *orthogonal set*:

$$\begin{aligned}
\int_0^L dx\ \sin k_n x\ \sin k_m x &= \frac{1}{2}\int_0^L dx\ [\cos(k_n x - k_m x) - \cos(k_n x + k_m x)] \\
&= \frac{1}{2}\begin{cases} \left[\frac{\sin(k_n x - k_m x)}{k_n - k_m} - \frac{\sin(k_n x + k_m x)}{k_n + k_m}\right]_0^L & ;\quad n \neq m \\ \left[x - \frac{\sin(k_n x + k_m x)}{k_n + k_m}\right]_0^L & ;\quad n = m \end{cases} \\
&= \frac{L}{2}\delta_{mn}
\end{aligned}$$

where δ_{mn} is the Kronecker delta, giving zero for $m \neq n$

The *orthogonality* of normal modes is general and applies to all "Sturm Liouville" ODE's.

So:

$$\begin{aligned}\int_0^L dx\ f(x)\sin k_m x =& \sum_{n=1}^{\infty} F_n \int_0^L dx\ \sin k_n x\ \sin k_m x \\ =& \frac{L}{2}\sum_{n=1}^{\infty} F_n \delta_{mn} \\ =& \frac{L}{2} F_m\end{aligned}$$

using the sifting property. Therefore, after relabelling $m \to n$:

$$\begin{aligned}F_n =& \frac{2}{L}\int_0^L dx\ f(x)\sin k_n x \\ E_n =& \frac{2}{L\omega_n}\int_0^L dx\ g(x)\sin k_n x\ .\end{aligned} \tag{2.3}$$

We are given f and g, so as long as we can do the integrals on the RHS, we have determined all the unknown constants and therefore know the motion for all times.

The solution written as a sum of sine waves is an example of a Fourier series.

A quick example

Suppose the initial conditions are that the string is initially stretched into a sine wave $f(x) = a\sin(3\pi x/L)$ (for some a) and at rest, i.e. $g(x) = 0$.

The latter immediately gives $E_n = 0$ for all n. The former gives:

$$\begin{aligned}F_n =& \frac{2}{L}\int_0^L dx\ f(x)\sin k_n x \\ =& \frac{2a}{L}\int_0^L dx\ \sin\frac{3\pi x}{L}\sin\frac{n\pi x}{L} = \frac{2a}{L}\times\frac{L}{2}\delta_{n3}\end{aligned}$$

using the above relation. So all the F_n are zero except $F_3 = a$. So the motion is described by

$$u(x,t) = a\sin\frac{3\pi x}{L}\cos\frac{3\pi ct}{L}\ .$$

The answer is very simple. If the system starts as a pure *normal mode* of the system, it will remain as one.

2.3 Method of Froebenius

A general method that works for more complicated equations can be illustrated by pretending we do not know the solution to the wave equation.

2.3.1 Bill and Ted's excellent misadventure

Bill and Ted have brought Pythagoras to the future and lost him in a night club. We now live in a world without sin and cos. To rectify this we will use the method of Froebenius to rediscover these precious functions

1. Substitute the infinite series $y(x) = \sum_{n=0}^{\infty} C_n x^n$ to the differential equation

$$y'' + y = 0$$

We end up with two sums.

$$\sum_{n=0}^{\infty} c_n n(n-1)x^{n-2} + \sum_{n=0}^{\infty} c_n x^n = 0$$

2. Relabel the summation using $m = n - 2$ on the y'' term obtaining

$$\sum_{m=-2}^{\infty} c_{m+2}(m+2)(m+1)x^m + \sum_{n=0}^{\infty} c_n x^n = 0$$

3. Use a notation where $C_i = 0$ for $i < 0$ to sum the y term over the range $\sum_{n=-2}^{\infty}$

$$\sum_{m=-2}^{\infty} c_{m+2}(m+2)(m+1)x^m + \sum_{m=-2}^{\infty} c_m x^m = \sum_{m=-2}^{\infty} [c_{m+2}(m+2)(m+1) + c_m]x^m = 0$$

4. As this is true for all values of x, each Hence we obtain the *indicial equation*

$$C_{m+2}(m+1)(m+2) = -C_m$$

This relates every other coefficient in a *recurrence relation.*

5. Deduce that C_0 can be non-zero even though $C_{-2} = 0$, and that C_1 can be non-zero even though $C_{-1} = 0$ because

$$(m+2)(m+1) = 0$$

for $m = -1, -2$

We therefore have two independent series, and two free parameters C_0 and C_1 as should be the case for a 2nd order ODE.

6. We therefore find the series with

   (a) $C_0 = 1$, $C_1 = 0$

   $$\sum_{n=0}^{\infty}(-1)^{(n)}\frac{x^{2n}}{(2n)!} = 1 - \frac{x^2}{2.1} + \frac{x^4}{4.3.2.1}\ldots$$

   (b) $C_0 = 0$, $C_1 = 1$

   $$\sum_{n=0}^{\infty}(-1)^{(n)}\frac{x^{(2n+1)}}{(2n+1)!} = x - \frac{x^3}{3.2} + \frac{x^5}{5.4.3.2}\ldots$$

   Giving these two independent series their names we recognise

   $$\cos x \equiv 1 - \frac{x^2}{2!} + \frac{x^4}{4!}\ldots$$

   $$\sin x \equiv x - \frac{x^3}{3!} + \frac{x^5}{5!}\ldots$$

7. We can now make up the world's first table of sinusoids by summing the series to high order!

   Towards the end of the 1800's enormous effort was expended computing special functions by hand to high order in the Taylor expansion, and tabulating the values as a function of x.

   In fact, prior to scientific calculators it was common for laboriously computed Tables of Sines to be handed out in mathematics examinations, even in the 1980's.

2.4 Generalised Fourier Series

We often write a solution as a superposition of normal modes, and find that we can define an inner product so that these normal modes are orthogonal.

In some cases this inner product may need a weight function (e.g. a factor of r for Bessel functions). We have also used without proof the statement that the normal modes form a complete set of functions.

It turns out that these common themes are not coincidental, and *Sturm-Liouville theory* explains why not. Sturm-Liouville theory was originally developed to describe waves on a string of variable density, but it applies to a far wider class of physical problems.

Sturm-Liouville (S-L) theory makes predictions for a class of 1-dimensional Ordinary Differential Equations, and covers all of those we have so far obtained from separation of our Partial Differential Equations.

The beauty of S-L theory is that given properties of the differential equation it predicts properties of the normal modes (like orthogonality and completeness) *without even solving the equation!*

It also tells us exactly how to define our inner product (i.e. what weight function to include) in each case so we get the orthogonality relation needed to calculate coefficients in the normal mode expansion.

BCs & orthogonality of normal modes

Lets consider a simple case first.

Suppose X_1 and X_2 are eigenfunctions of $\frac{d^2}{dx^2}$, with eigenvalues $-\lambda_1$ and $-\lambda_2$, and satisfy some BCs at $x = a$ and $x = b$.

$$\ddot{X}_1 = -\lambda_1 X_1$$
$$\ddot{X}_2 = -\lambda_2 X_2$$

We define the *Wronskian* $W_{12}(x) = \dot{X}_1 X_2 - X_1 \dot{X}_2$, and observe that

$$\frac{d}{dx} W_{12}(x) = \frac{d}{dx}(\dot{X}_1 X_2 - X_1 \dot{X}_2) = \ddot{X}_1 X_2 - X_1 \ddot{X}_2$$

Thus,

$$\begin{aligned} \int_a^b \left(\ddot{X}_1 X_2 - X_1 \ddot{X}_2 \right) dx &= \left[\dot{X}_1 X_2 - X_1 \dot{X}_2 \right]_a^b \\ &= (\lambda_2 - \lambda_1) \int_a^b X_1 X_2 dx \end{aligned} \tag{4.1}$$

Now, for many standard boundary conditions $[W_{12}(x)]_a^b = \left[\dot{X}_1 X_2 - X_1 \dot{X}_2 \right]_a^b = 0$, for example:

Dirichlet $X_1(a) = X_1(b) = X_2(a) = X_2(b) = 0$

Neumann $\dot{X}_1(a) = \dot{X}_1(b) = \dot{X}_2(a) = \dot{X}_2(b) = 0$

Periodic $\dot{X}_1(a) = \dot{X}_1(b)\,; \dot{X}_2(a) = \dot{X}_2(b)\,; X_1(a) = X_1(b)\,; X_2(a) = X_2(b)$

Then we see

$$(\lambda_2 - \lambda_1) \int_a^b X_1 X_2 dx = 0$$

So, in these boundary conditions, eigenfunctions with distinct eigenvalues ($\lambda_2 \neq \lambda_1$) are *orthogonal* under the scalar (dot) product defined by:

$$X_1 \cdot X_2 = \int_a^b X_1 X_2 dx$$

If $\lambda_1 = \lambda_2$, then we are not guaranteed orthogonality, however, if X_1 and X_2 are genuinely different (linearly independent) then the Gramm-Schmidt procedure in section allows us to construct an orthonormal basis in any case.

2.4.1 Sturm Liouville problems

S-L theory applies to the class of differential equations that can be written in the form

$$\left[\frac{d}{dx}\left(P(x)\frac{d}{dx}\right) + Q(x)\right]\phi_i(x) = -\lambda_i\, \rho(x)\, \phi_i(x) \tag{4.2}$$

where $\phi_i(x)$ is the i-th normal mode solution with separation constant (eigenvalue) λ_i. The functions $P(x)$, $Q(x)$ and *weight* function $\rho(x)$ are "given" functions specific to the differential equation.

In this course they are defined by our curvilinear coordinate functions, and from the potential in quantum mechanics. For example:

Special function	$P(x)$	$Q(x)$	$\rho(x)$
Sinusoid	1	0	1
Bessel	x	$-\frac{n^2}{r}$	x
Legendre	$\sin\theta$	0	$\sin\theta$
Radial Schrodinger	r^2	$-[l(l+1) + r^2\frac{2m}{\hbar}V(r)$	r^2

S-L theory addresses problems defined over a region $[a, b]$ for which the following conditions are met.

1. $\rho(x)$, $P(x)$ and $Q(x)$ should be real functions
2. Neither $\rho(x)$ nor $P(x)$ should change sign in the interval $a \leq x \leq b$
3. The Boundary Conditions at $x = a$ and $x = b$ ensure

$$[W_{ij}(x)]_a^b = \left[P(x)\left(\phi_i^* \frac{d\phi_j}{dx} - \phi_j \frac{d\phi_i^*}{dx}\right)\right]_a^b = 0 \tag{4.3}$$

(i.e. [...] evaluated at $x = b$ minus [...] evaluated at $x = a$) for all combinations of i and j. This term is called the Wronskian for archaic reasons.)

If these conditions are satisfied, S-L theory predicts:

1. The eigenvalues λ_i are real (and there are an infinite number)
2. The eigenfunctions $\{ \phi_i(x) \}$ are orthogonal: $\phi_i \cdot \phi_j \propto \delta_{ij}$
3. The inner product should be defined as $f \cdot g \equiv \int_a^b dx\ \rho(x)\ f(x)^*\ g(x)$
4. The eigenfunctions form a complete set.
   So we can expand a general function $f(x)$ in the interval $a \leq x \leq b$:

$$f(x) = \sum_i a_i\ \phi_i(x) \qquad \Rightarrow \qquad a_i = \frac{\phi_i \cdot f}{\phi_i \cdot \phi_i}$$

2.4.2 Boundary condition choices

Our choice of spatial BCs is dictated by the physics of the problem that we are studying, but in most cases they are one of the following set. In each case, these BCs are sufficient to satisfy Eqn. (4.3) and allow us to make use of the powerful predictions from S-L theory.

1. Fixed BCs (a.k.a. Dirichlet BCs):
   $\phi_i(x = a) = \phi_i(x = b) = 0$ for all modes labelled by different i.
   e.g. a drumskin fixed at its edge
2. Open BCs (a.k.a. Neumann BCs):
   $\left.\frac{d\phi_i}{dx}\right|_{x=a} = \left.\frac{d\phi_i}{dx}\right|_{x=b} = 0$
   e.g. no ink flows out of the edge of a water tank i.e. no concentration gradient.
3. Mixed BCs:
   $\left.\left(\phi_i + c\frac{d\phi_i}{dx}\right)\right|_{x=a} = \left.\left(\phi_i + c\frac{d\phi_i}{dx}\right)\right|_{x=b} = 0$
   For some real value of c. Not so common.
4. Periodic BCs:
   $\phi_i(x = b) = \phi_i(x = a)$, $\left.\frac{d\phi_i}{dx}\right|_{x=b} = \left.\frac{d\phi_i}{dx}\right|_{x=a}$ and $P(x = a) = P(x = b)$.
   e.g. where x is an angular variable and $a = 0$, $b = 2\pi$.

N.B. For cases (1)-(3), we can make different choices of BCs et each end and still satisfy the S-L condition. So we might talk about Fixed-Open or Dirichlet-Neumann BCs, for instance.

The remainder of this section is more mathematical, and proves some of the properties that we have quoted above. Still, these proofs are a favourite examination question, so you should make sure you know how to do it.

2.4.3 Orthogonality

We consider two eigenfunctions ϕ_i and ϕ_j of the S-L operator. The S-L equation can be rearranged into

$$\left[\frac{d}{dx}\left(P(x)\frac{d}{dx}\right)\right]\phi_i(x) = [-Q(x) - \lambda_i\,\rho(x)\,]\,\phi_i(x) \tag{4.4}$$
$$\left[\frac{d}{dx}\left(P(x)\frac{d}{dx}\right)\right]\phi_j(x) = [-Q(x) - \lambda_j\,\rho(x)\,]\,\phi_j(x)$$

Consider the term

$$W_{ij}(x) = P(x)\left(\phi_i^*(x)\frac{d\phi_j(x)}{dx} - \phi_j(x)\frac{d\phi_i^*(x)}{dx}\right)$$

We take the derivative

$$\begin{aligned}\frac{d}{dx}W_{ij}(x) &= \phi_i^*(x)\frac{d}{dx}[P(x)\frac{d\phi_j(x)}{dx}] - \phi_j(x)\frac{d}{dx}[P(x)\frac{d\phi_i^*(x)}{dx}] \\ &+ \frac{d\phi_i^*(x)}{dx}P(x)\frac{d\phi_j(x)}{dx} - \frac{d\phi_j(x)}{dx}P(x)\frac{d\phi_i^*(x)}{dx} \\ &= \phi_i^*(x)\frac{d}{dx}[P(x)\frac{d\phi_j(x)}{dx}] - \phi_j(x)\frac{d}{dx}[P(x)\frac{d\phi_i^*(x)}{dx}]\end{aligned}$$

Here we can use Eq 4.4 to replace the fragment $\frac{d}{dx}[P(x)\frac{d\phi_i^*(x)}{dx}]$ with $[-Q(x) - \lambda_i^*\rho(x)]\phi_i^*(x)$. Thus,

$$\begin{aligned}\frac{d}{dx}W_{ij}(x) &= \phi_i^*(x)[-Q(x) - \lambda_j\rho(x)]\phi_j(x) - \phi_j(x)[-Q(x) - \lambda_i^*\rho(x)]\phi_i^*(x) \\ &= (\lambda_i^* - \lambda_j)\phi_j(x)\phi_i^*(x)\rho(x)\end{aligned}$$

This derivative is easy to integrate:

$$\int_a^b \frac{d}{dx}W_{ij}(x)dx = [W_{ij}(x)]_a^b = 0,$$

and this is zero due to the boundary conditions. We can now determine that

$$0 = \int_a^b \frac{d}{dx}W_{ij}(x)dx = (\lambda_i^* - \lambda_j)\int_a^b \rho(x)\phi_j(x)\phi_i^*(x)\rho(x)dx$$

Two cases are useful

1. If $i = j$ then $\int_a^b \rho(x)\phi_i(x)\phi_i^*(x)\rho(x)dx > 0$, and so $(\lambda_i^* - \lambda_i) = 0$.
   In other words, λ_i is real

2. If $\lambda_i \neq \lambda_j$ then $\int_a^b \rho(x)\phi_j(x)\phi_i^*(x)\rho(x)dx = 0$.
   In other words distinct eigenvectors are orthogonal.[1]
   The inner product involves the integral using the weight function $\rho(x)$.

[1]More precisely non degenerate eigenvectors are orthogonal and degenerate eigenvectors may be orthogonalised

2.4.4 Completeness of normal modes

Proof of completeness is beyond the scope of this course. However, we can state two theorems regarding different *meanings* of "completeness":

Uniform convergence:

if a function f has continuous first and second derivatives on $[a, b]$ and f satisfies the boundary conditions then f can be exactly represented by a sum of eigenmodes: it will match at *every* point.

That is the *maximum* deviation between $f(x)$ and the sum $S(x) = \sum_n a_n X_n$ of eigenmodes becomes zero as the number of modes included tends to ∞.

$$\max_{x \in a,b} |f(x) - S(x)|^2; \to 0 \tag{4.5}$$

Any continuous and differentiable function is faithfully reproduced everywhere by a sum of eigenmodes.

L_2 convergence:

If the function $f(x)$ has $\int_a^b |f(x)|^2 dx$ finite it can be approximated by a sum $S(x) = \sum_n a_n X_n$ of eigenmodes in the weaker sense

$$\int_a^b |f(x) - S(x)|^2 dx \to 0 \tag{4.6}$$

(4.6) means that the sum $S(x)$ can deviate from $f(x)$ at certain points, and the maximum error can remain non-zero. However, not for anything other than an *infinitessimal* distance (otherwise it would contribute something to the integral).

Thus the basis is complete it can describe and only differs infinitessimally close to discontinuities and violations of the boundary conditions.

Every bounded function on $[a, b]$ is faithfully reproduced by a sum of modes away from discontinuities & boundaries

2.5 First look at Bessel functions

We will take a first serious look at a Sturm Louiville problem with a coordinate dependent weight function. Sturm Louiville problems were first studied in this context.

2.5.1 Dangling ropes

We will show that Bessel functions are already familiar to you!

Consider a dangling rope with lower end at $y = 0$ and anchored at $y = H$. The rope is free to oscillate in the x-direction with displacement $x = u(y, t)$, and has a fixed mass density per unit length ρ.

The tension at a height y is $T(y) = \rho g y$.

By considering the forces on an infinitesimal segment of width Δy we can show that the wave equation for the rope is

$$\frac{\partial}{\partial y}\left(T(y)\frac{\partial}{\partial y}\right)u(y,t) = \rho\frac{\partial^2}{\partial t^2}u(y,t),$$

where $u(y)$ is the horizontal displacement of the rope from the vertical.

If we seek separable solutions of the form

$$u(y,t) = Y(y)F(t),$$

we can reduce this to two ODEs for y and t

$$\frac{\partial}{\partial y}\left(T(y)\frac{\partial}{\partial y}\right)Y(y)F(t) = \rho\frac{\partial^2}{\partial t^2}Y(y)F(t)$$

and dividing by $Y(y)F(t)$ we have

$$\frac{1}{\rho Y(y)}\frac{\partial}{\partial y}\left(T(y)\frac{\partial}{\partial y}\right)Y(y) = \frac{1}{F(t)}\frac{\partial^2}{\partial t^2}F(t) = -\omega^2$$

We solve this t-equation easily:

$$F(t) = A\cos\omega t + B\sin\omega t$$

and we make a change of variables

$$z = \sqrt{y}; y = z^2$$

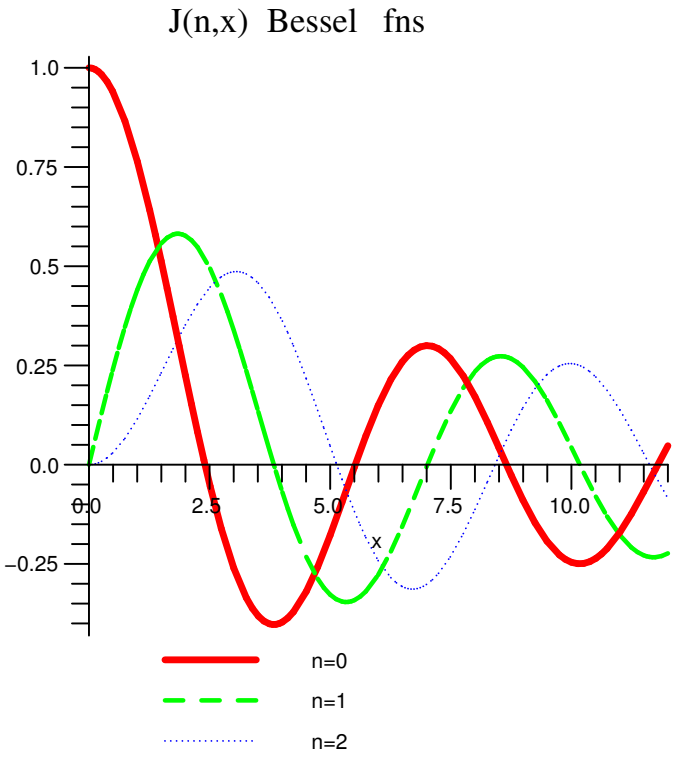


Figure 5.1: The first three Bessel functions of integral order.

$$dz = \frac{1}{2\sqrt{y}} dy$$

$$\frac{d}{dy} = \frac{dz}{dy}\frac{d}{dz} = \frac{1}{2\sqrt{y}}\frac{d}{dz} = \frac{1}{2z}\frac{d}{dz}$$

and this reduces the Y-equation to

$$\frac{1}{2z}\frac{d}{dz}\left(\tilde{T}(z)\frac{1}{2z}\frac{d}{dz}\right)\tilde{Y}(z) = -\omega^2\rho\tilde{Y}(z)$$

where we define $\tilde{Y}(z) = Y(y)$ and $\tilde{T}(z) = T(y) = \rho g z^2$, and we see that

$$z^2\tilde{Y}''(z) + z\tilde{Y}'(z) + k^2 z^2\tilde{Y}(z) = 0,$$

where

$$k^2 = 4\frac{\omega^2}{g}$$

This differential equation is in fact known as Bessels equation (of zeroth order), and the solution to this equation is the Bessel function $J_0(kz)$. We shall see that the same Bessel functions arise in circular coordinates

For now we see: a dangling rope swings in the shape of of a Bessel function

2.5.2 Boundary condition

The Bessel function (we shall see later) is oscillatory, but *without a fixed period* The first few J_n functions are plotted in Fig. 5.1.

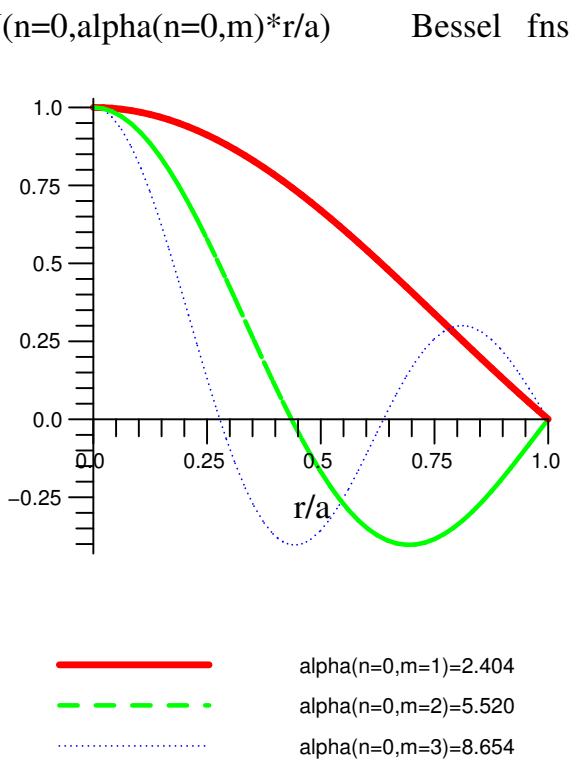


Figure 5.2: Rescaling the J_0 Bessel functions so that one of the nodes lies at the anchor

As the anchor is held fixed, this quantizes the allowable k_i to ensure $J_0(k_i\sqrt{H}) = 0$

The points where $J_0(kz) = 0$ or in other words the zeroes or roots $kz = \alpha_{0i}$ of the Bessel function are particularly important.

We find the i-th normal mode has $k_i = \frac{\alpha_{0i}}{\sqrt{H}}$

Thus the normal mode frequencies are

$$\omega_i = \frac{\sqrt{g}}{2\sqrt{H}}\alpha_{0i},$$

and these rescale the Bessel function argument to align the i-th zero with the fixed anchor (figure 5.2).

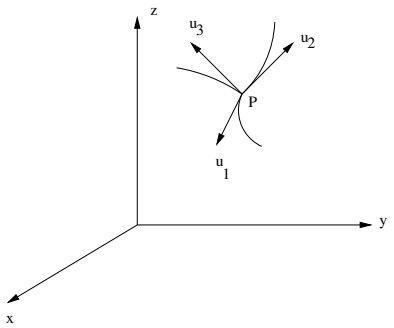


Figure 6.1: Orthogonal curvilinear coordinates in three dimensions.

2.6 Curvilinear coordinate systems

We now consider vector calculus in alternate coordinates systems which use some combination angles and distances.

Specifically we consider orthogonal curvilinear coordinate systems (fig. 6.1). Such coordinate systems can be particularly useful when the functions we are considering have symmetries, such as cylindrical or spherical symmetry.

In plain English these are orthogonal curvilinear coordinate systems systems that have perpendicular directions $\boldsymbol{e}_i$, but which rotate in some position dependent way, which we choose to track some symmetry of the physics.

The directions at each point are selected by the infinitessimal change in $\boldsymbol{x}$ generated by an infinitessimal change in each of the *curvilinear coordinates*.

We must be able to translate the differential equations of physics appropriately. If we label the curvilinear coordinates (ξ_1, ξ_2, ξ_3) the local axes are given by

$$\frac{\partial \boldsymbol{x}}{\partial \xi_i} = h_i \boldsymbol{e}_i$$

Here, $h_i = \left| \frac{\partial \boldsymbol{x}}{\partial \xi_i} \right|$ is a scale factor with that ensures $\boldsymbol{e_i}$ is a unit vector.

It is useful to consider a *locally* defined cartesian coordinate system

$$\tilde{\boldsymbol{x}}_i = \boldsymbol{x} \cdot \boldsymbol{e}_i$$

2.6.1 Circular (or plane) polar coordinates

Plane polar coordinates (r, ϕ) are defined by:

$$x = r\cos\phi\ , \qquad y = r\sin\phi\ , \tag{6.1}$$

The radial coordinate r (sometimes written as r) can range from 0 to ∞. The angular coordinate ϕ (sometimes written as θ) ranges from 0 to 2π.

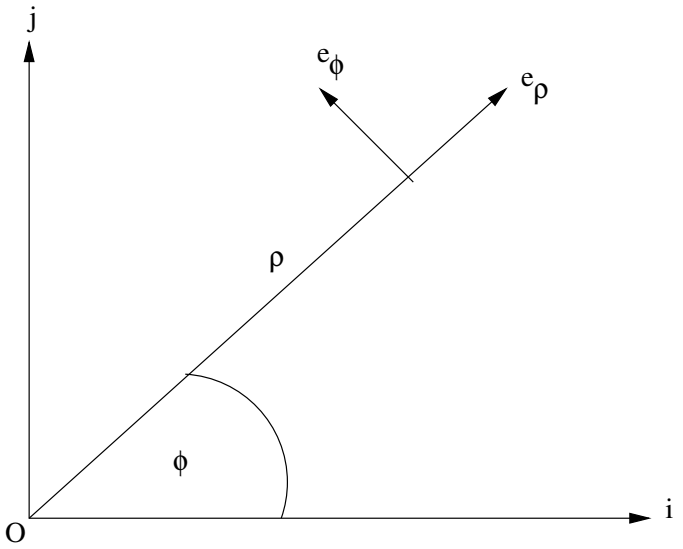


Figure 6.2: Plane polar coordinates.

The *local* orthonormal basis generated by polar coordinates is:

$$\begin{aligned}
\frac{\partial \boldsymbol{x}}{\partial r} &= (\cos\phi, \sin\phi) \\
\frac{\partial \boldsymbol{x}}{\partial \phi} &= r(-\sin\phi, \cos\phi) \\
h_r &= 1 \\
h_\phi &= r \\
e_r &= (\cos\phi, \sin\phi) \\
e_\phi &= (-\sin\phi, \cos\phi)
\end{aligned} \tag{6.2}$$

Exercise Show that this system is *orthogonal* by verifying that $(\frac{\partial \boldsymbol{x}}{\partial r}) \cdot (\frac{\partial \boldsymbol{x}}{\partial \phi}) = 0$

Area integrals

When we change coordinates in an integral, we have to include a scale factor in the integration variable.

As we increase each coordinate by an infinitesimal amount, we sweep out a small area which we call $d\mathcal{A}$. Now, as we chose *orthogonal* curvilinear coordinates we know $\boldsymbol{e}_r$ and $\boldsymbol{e}_\phi$ are perpendicular, and the area is

$$\begin{aligned}
d\mathcal{A} &= d\tilde{x}_r d\tilde{x}_\phi \\
&= h_r dr h_\phi d\phi \\
&= r dr d\phi
\end{aligned} \tag{6.3}$$

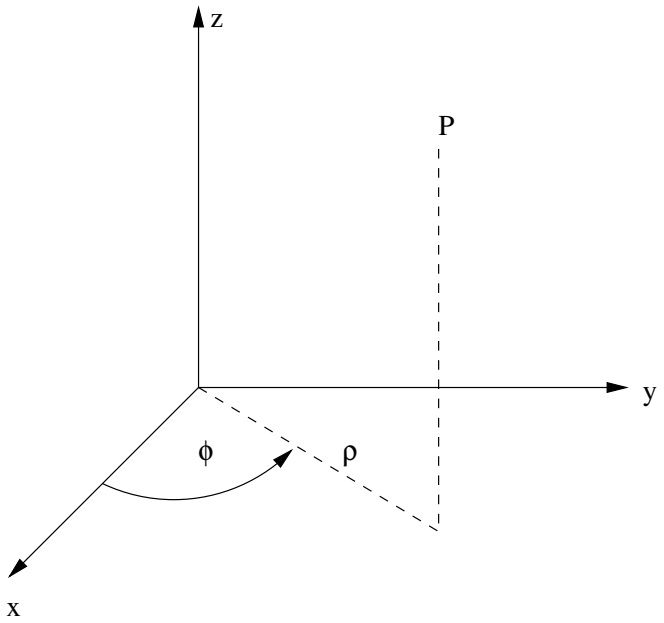


Figure 6.3: Cylindrical polar coordinates.

Example: area of circle Consider

$$\int_0^R dr \int_0^{2\pi} r d\phi = 2\pi \int_0^R r dr = \pi R^2$$

2.6.2 Cylindrical polar coordinates

An simple extension of plane polar coordinates into the third dimension: see Fig. 6.3.

$$x = r\cos\phi\,, \qquad y = r\sin\phi\,, \qquad z = z \tag{6.4}$$

- radius $r \in [0, \infty]$, angle $\phi \in [0, 2\pi]$, and z coordinate $z \in [-\infty, \infty]$.
- Scale factors: $h_r = 1$, $h_\phi = r$, $h_z = 1$.

Example: volume of a cylinder Consider

$$\int_0^L dz \int_0^R dr \int_0^{2\pi} r d\phi = 2\pi L \int_0^R r dr = \pi R^2 L$$

2.6.3 Spherical polar coordinates

Useful when there is spherical symmetry: see Figure 6.4.

$$x = r\sin\theta\cos\phi, \qquad y = r\sin\theta\sin\phi, \qquad z = r\cos\theta \tag{6.5}$$

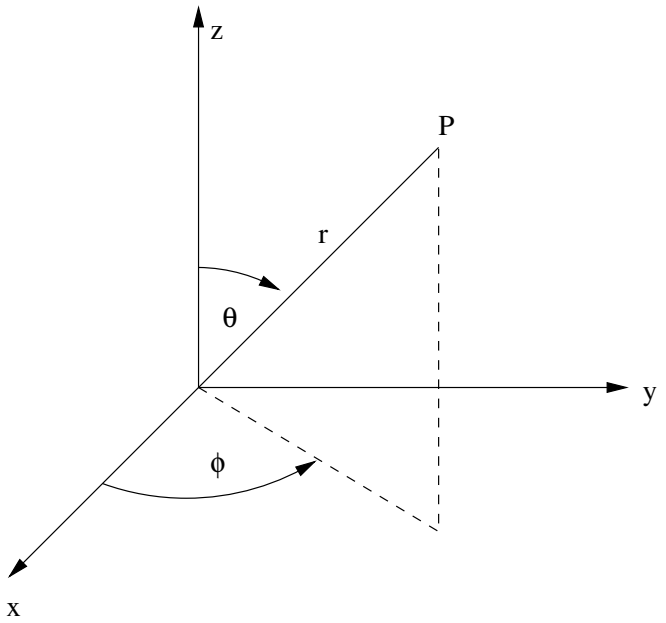


Figure 6.4: Spherical polar coordinates.

- radius $r \in [0, \infty]$, angle $\theta \in [0, \pi]$, angle $\phi \in [0, 2\pi]$.

$$\begin{aligned}
\frac{\partial \boldsymbol{x}}{\partial r} &= (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \\
\frac{\partial \boldsymbol{x}}{\partial \theta} &= r(\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta) \\
\frac{\partial \boldsymbol{x}}{\partial \phi} &= r(-\sin\theta\sin\phi, \sin\theta\cos\phi, 0) \\
h_r &= 1 \\
h_\theta &= r \\
h_\phi &= r\sin\theta
\end{aligned} \tag{6.6}$$

Example : volume of sphere

$$\begin{aligned}
\int_0^R dr \int_0^\pi r d\theta \int_0^{2\pi} r\sin\theta d\phi &= 2\pi \int_0^R r^2 dr \int_0^\pi \sin\theta d\theta \\
&= 2\pi \left[\frac{r^3}{3}\right]_0^R [-\cos\theta]_0^\pi \\
&= \frac{4}{3}\pi R^3
\end{aligned} \tag{6.7}$$

Example : area of sphere

$$\begin{aligned}
\int_0^\pi R d\theta \int_0^{2\pi} R\sin\theta d\phi &= 2\pi R^2 \int_0^\pi \sin\theta d\theta \\
&= 2\pi R^2 [-\cos\theta]_0^\pi \\
&= 4\pi R^2
\end{aligned} \tag{6.8}$$

2.6.4 Gradient

In the *local* coordinate system the gradient operator is

$$\sum_i \frac{\partial}{\partial \tilde{x}_i} \boldsymbol{e}_i = \sum_i \frac{1}{h_i} \frac{\partial}{\partial \tilde{\xi}_i} \boldsymbol{e}_i$$

Circular polars

$$\begin{aligned} \boldsymbol{\nabla} f &= \frac{\partial f}{\partial \tilde{x}_r} \boldsymbol{e}_r + \frac{\partial f}{\partial \tilde{x}_\phi} \boldsymbol{e}_\phi \\ &= \frac{\partial f}{h_r \partial r} \boldsymbol{e}_r + \frac{\partial f}{h_\phi \partial \phi} \boldsymbol{e}_\phi \\ &= \frac{\partial f}{\partial r} \boldsymbol{e}_r + \frac{1}{r} \frac{\partial f}{\partial \phi} \boldsymbol{e}_\phi \end{aligned} \tag{6.9}$$

Cylindrical polars

$$\boldsymbol{\nabla} = \frac{\partial f}{\partial r} \boldsymbol{e}_r + \frac{1}{r} \frac{\partial f}{\partial \phi} \boldsymbol{e}_\phi + \frac{\partial f}{\partial z} \hat{z}$$

Spherical polars

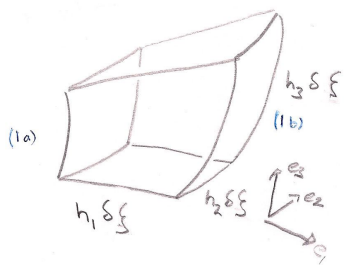
$$\boldsymbol{\nabla} = \frac{\partial f}{\partial r} \boldsymbol{e}_r + \frac{1}{r} \frac{\partial f}{\partial \theta} \boldsymbol{e}_\theta + \frac{1}{r \sin\theta} \frac{\partial f}{\partial \phi} \boldsymbol{e}_\phi$$

2.6.5 Divergence

For the divergence we must be a little bit more careful. The coordinate dependence of the scale factors themselves must be taken into account.

$$\boldsymbol{\nabla} \cdot \boldsymbol{v} = \lim_{V \to 0} \frac{\int_{\mathcal{A}} \boldsymbol{v} \cdot \hat{\boldsymbol{n}} d\mathcal{A}}{V}$$

Consider the infinitessimal cube



Flux through (1a) is $F_1 = v_1\ h_2\ d\xi_2\ h_3\ d\xi_3$.

Net flux difference between (1a) and (1b) is $\frac{\partial F_1}{\partial \xi_1} \delta \xi_1$.

Thus, summing over all pairs of faces

$$\begin{aligned}\boldsymbol{\nabla}\cdot\boldsymbol{v} &= \frac{1}{h_1h_2h_3\delta\xi_1\delta\xi_2\delta\xi_3}\left[\frac{\partial F_1}{\partial\xi_1}\delta\xi_1+\frac{\partial F_2}{\partial\xi_2}\delta\xi_2+\frac{\partial F_3}{\partial\xi_3}\delta\xi_3\right]\\ &= \frac{1}{h_1h_2h_3}\left[\frac{\partial h_2h_3v_1}{\partial\xi_1}+\frac{\partial h_3h_1v_2}{\partial\xi_2}+\frac{\partial h_1h_2v_3}{\partial\xi_3}\right]\end{aligned} \tag{6.10}$$

Circular polars

$$\boldsymbol{\nabla}\cdot\boldsymbol{v}=\frac{1}{r}\frac{\partial}{\partial r}(rv_r)+\frac{1}{r}\frac{\partial}{\partial\phi}v_\phi$$

Cylindrical polars

$$\boldsymbol{\nabla}\cdot\boldsymbol{v}=\frac{1}{r}\frac{\partial}{\partial r}(rv_r)+\frac{1}{r}\frac{\partial}{\partial\phi}v_\phi+\frac{\partial}{\partial z}v_z$$

Spherical polars

$$\boldsymbol{\nabla}\cdot\boldsymbol{v}=\frac{1}{r^2}\frac{\partial}{\partial r}(r^2v_r)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta v_\theta)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}v_\phi$$

2.6.6 Laplacian

We can now form the Laplacian as simply the divergence of the gradient, combining the results of the previous two subsections:

$$\boldsymbol{\nabla}^2f=\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}f$$

leading to:

Circular polars

$$\nabla^2f=\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial f}{\partial r})+\frac{1}{r^2}\frac{\partial^2f}{\partial\phi^2}$$

Cylindrical polars

$$\nabla^2f=\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial f}{\partial r})+\frac{1}{r^2}\frac{\partial^2f}{\partial\phi^2}+\frac{\partial^2f}{\partial z^2}$$

Spherical polars

$$\nabla^2f=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial f}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2f}{\partial\phi^2}. \tag{6.11}$$

Note, that there are no mixed second order derivatives and that these equations are seperable.

2.6.7 Curl

Take i, j, k a cyclic permutation, and we consider an infinitessimal surface aligned with curvilinear coordinate axes, and generated by parameter changes $\delta\xi_i$ and $\delta\xi_j$

We consider Stoke's theorem to obtain the k component of curl which is perpendicular to this surface. The curl is then the line integral of a vector field v around the perimeter divided by the area.

$$\begin{aligned}(\nabla \times v)_k &\sim \frac{1}{h_i h_j \delta\xi_i \delta\xi_j} \begin{pmatrix} h_i \delta\xi_i v_i(A) + h_j \delta\xi_j v_j(A + \delta\xi_i) \\ -h_i \delta\xi_i v_i(A + \delta\xi_j + \delta\xi_i) - h_j \delta\xi_j v_j(A + \delta\xi_j) \end{pmatrix} \\ &\to \frac{1}{h_i h_j} \left(\frac{\partial}{\partial_i} h_j v_j - \frac{\partial}{\partial_j} h_i v_i \right) \end{aligned} \tag{6.12}$$

Circular polars

$$\nabla \times A = \hat{z} \frac{1}{r} \left(\frac{\partial}{\partial r} r A_\phi - \frac{\partial}{\partial \phi} A_r \right) \tag{6.13}$$

Cylindrical polars

$$\begin{aligned}\nabla \times A &= \hat{z} \frac{1}{r} \left(\frac{\partial}{\partial r} r A_\phi - \frac{\partial}{\partial \phi} A_r \right) && (6.14) \\ &\quad + \hat{r} \left(\frac{1}{r} \frac{\partial}{\partial \phi} A_z - \frac{\partial}{\partial z} A_\phi \right) && (6.15) \\ &\quad + \hat{\phi} \left(\frac{\partial}{\partial z} A_r - \frac{\partial}{\partial r} A_z \right) && (6.16) \end{aligned}$$

Spherical polars

$$\begin{aligned}\nabla \times A &= \hat{r} \frac{1}{r \sin\theta} \left[\frac{\partial}{\partial \theta} (A_\phi \sin\theta) - \frac{\partial}{\partial \phi} (A_\theta) \right] \\ &\quad + \hat{\theta} \frac{1}{r} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \phi} A_r - \frac{\partial}{\partial r} (r A_\phi) \right] \\ &\quad + \hat{\phi} \frac{1}{r} \left[\frac{\partial}{\partial r} (r A_\theta) - \frac{\partial}{\partial \theta} A_r \right] \end{aligned}$$

2.7 Wave equation in circular polars

Equivalently, solving the wave equation for a circular drum

$$\nabla^2 u = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} \ .$$

In this section we shall use r for the radial coordinate. As before, we consider solutions of separated form: $u(r,\phi,z,t) = R(r)\Phi(\phi)T(t)$. Substitute into wave equation and divide across by $u = R\Phi T$.

$$\frac{1}{R}\frac{\partial^2 R}{\partial r^2} + \frac{1}{rR}\frac{\partial R}{\partial r} + \frac{1}{r^2\Phi}\frac{\partial^2 \Phi}{\partial \phi^2} = \frac{1}{c^2 T}\frac{\partial^2 T}{\partial t^2} \ .$$

First separation: time equation: $\mathrm{LHS}(r,\phi,z) = \mathrm{RHS}(t) = \text{constant}$

$$\frac{1}{c^2}\frac{1}{T}\frac{d^2 T}{dt^2} = -k^2.$$

The solutions to this are of the form $T(t) = G_k \cos\omega_k t + H_k \sin\omega_k t$ with $\omega_k \equiv ck$.

Second separation: Multiply through by r^2 and separate again:

$$\mathrm{LHS}(r) = \mathrm{RHS}(\phi) = \text{a constant}.$$

For the angular dependence:

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -n^2;$$

The solution is $\Phi = C\cos n\phi + D\sin n\phi$.

We want the solution to the wave equation to be *single valued*, so $\Phi(\phi + 2\pi) = \Phi(\phi)$, forcing n to be integer-valued: $n = 0, \pm 1, \pm 2 \ldots$

The equation describing the radial dependence is the only difficult one to solve:

$$\frac{d^2 R}{dr^2} + \frac{1}{r}\frac{dR}{dr} - \frac{n^2}{r^2}R + k^2 R = 0 \ .$$

Multiply across by r^2 and rewrite

$$r^2 R'' + rR' + (k^2 r^2 - n^2)R = 0 \ . \tag{7.17}$$

This is known as *Bessel's equation of order n.* The solutions are known as Bessel functions. Being a quadratic ODE, there are two independent solutions called $J_n(kr)$ and $Y_n(kr)$. Note we have labelled the solutions with integer n.

Method of Froebenius

We can solve Bessel's equation by substituting a general *Laurent series* as a trial solution. A Laurent series is a generalisation of a Taylor series to possibly include negative power terms (called poles).

We try a solution

$$R(r) = \sum_{i=0}^{\infty} C_i r^{i+m}$$

where c_i and m are unknowns. m represents the lowest power of r that occurs in the solution, and where it arises $c_i = 0$ for $i < 0$ because otherwise m would *not* represent the lowest power of r.

Differentiating we get

$$R'(r) = \sum_{i=0}^{\infty}(i+m)C_i r^{i+m-1}$$

$$rR'(r) = \sum_{i=0}^{\infty}(i+m)C_i r^{i+m}$$

$$r^2R''(r) = \sum_{i=0}^{\infty}(i+m)(i+m-1)C_i r^{i+m}$$

Bessel's equation becomes a relation between coefficients:

$$\sum_{i=0}^{\infty}(i+m)C_i r^{i+m} + (i+m)(i+m-1)C_i r^{i+m} - n^2 C_i r^{i+m} + k^2 C_{i-2} r^{i+m}$$

Since this must be true for all r, then we have the *indicial equation*

$$\left[(i+m) + (i+m)(i+m-1) - n^2\right] C_i + k^2 C_{i-2} = 0$$

The series *switches on* when $C_{-2} = 0$ and $C_0 \neq 0$. Then,

$$m^2 = n^2.$$

We are interested in the case where $m \geq 0$ so that the solutions are finite at $r = 0$.

Next, we are interested in forming a recurrence relation between coefficients. The above indicial equation suggests

$$C_i = \frac{k^2}{n^2 - (i+m)^2} C_{i-2}$$

If we consider the Bessel function $J_0(r)$, we take $n = m = 0$ and have (up to normalisation)

$$\begin{aligned} C_0 &= 1 \\ C_2 &= -\frac{k^2}{4} \\ C_4 &= +\frac{k^4}{4.16} \\ C_6 &= -\frac{k^6}{4.16.36} \\ &\ldots \end{aligned} \tag{7.18}$$

The series is

$$1 - \frac{(kr)^2}{4} + \frac{(kr)^4}{4.16} - \frac{(kr)^6}{4.16.36}\ldots$$

and is purely a function of (kr). As the sign oscillates we have many turning points.

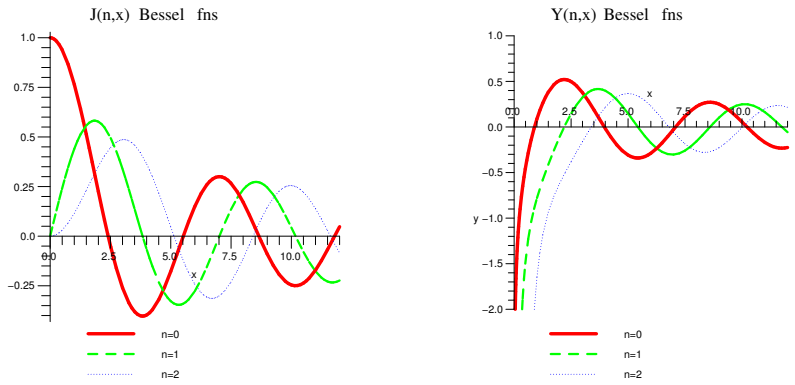


Figure 7.5: The first three Bessel functions of integral order.

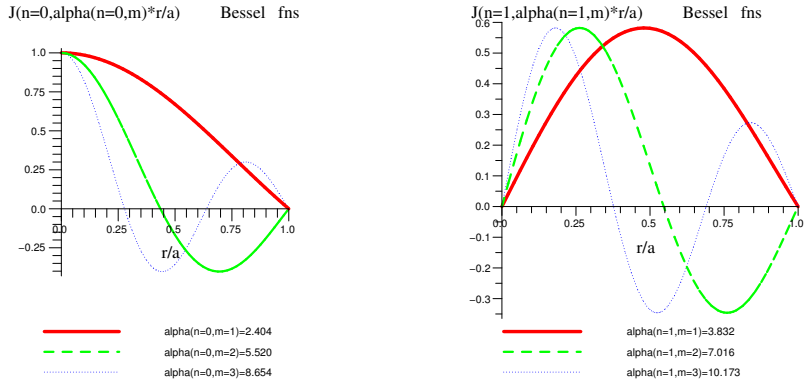


Figure 7.6: Rescaling the J_0 and J_1 Bessel functions so that one of the nodes lies at $r = a$

Roots of Bessel functions

The first few J_n and Y_n functions are plotted in Fig. 7.5. The Y_n functions diverge at the origin and so are not suitable for describing oscillations of a drumskin.

The Bessel functions $J_n(x)$ have a series of zeros ("nodes" or "roots") which we label α_{n1}, α_{n2}, α_{n3}.

For the function $\sin nx$, the nodes occur at $x = \alpha_{nm} = m\pi$ are equally spaced. For Bessel functions, however, they are not. The nodes must be found numerically, in practice either looked up in tables or calculated using packages such as Maple.

Spatial BCs and normal modes

Our solution can be written as

$$u(r, \phi, t) = J_n(kr)\ (C \cos n\phi + D \sin n\phi)\ (G \cos \omega_k t + H \sin \omega_k t)$$

with $\omega_k = ck$ and currently no restriction on k.

We now apply spatial boundary conditions. Recall periodicity in ϕ quantised n. In the radial direction we require that the drumskin does not move at the rim:

$$u(r = a, \phi, t) = 0 \text{ for all } \phi \text{ and } t.$$

We therefore want the edge of the drum to coincide with one of the nodes of the Bessel function. The m^{th} node of the Bessel function of order n occurs when the argument of the Bessel function takes value α_{nm}, and we rescale the Bessel function so that one of these zeros coincides with $r = a$.

It doesn't matter which node we choose to lie at $r = a$, so we have different normal mode solutions depending on which m we choose. The allowed values of k are therefore

$$k_{nm}a = \alpha_{nm}.$$

Quantising k also quantises ω_k. This is like we fond for the harmonics, but the normal mode frequencies are here not equally spaced (because the α_{nm} are not evenly spaced). This proves why the drum is not as harmonious as the guitar.

Some examples of rescaling for $n = 0$ and $n = 1$ are shown in Fig. 7.6.

Our normal mode solutions are therefore

$$u(r, \phi, t) = J_n\left(\alpha_{nm}\frac{r}{a}\right)\ (C_{nm}\cos n\phi + D_{nm}\sin n\phi)\ (G_{nm}\cos\omega_{nm}t + H_{nm}\sin\omega_{nm}t)\ .$$

Each normal mode is labelled by n and m and will have different constants so we label them appropriately. k depends on n and m via α_{nm}, so we also change the label on ω.

Zeros and nodal lines

Only J_0 is zero at the origin (e.g. Fig. 7.5) so $u = 0$ at $r = 0$ for all t if $n > 0$.

Nodal lines are other points on the drumskin that remain stationary for this normal mode:

- We find $(m-1)$ nodal lines in r: they occur at $\alpha_{nm}r/a = \alpha_{nm'} \implies r = a\alpha_{nm'}/\alpha_{nm}$ for $m' = 1, 2 \ldots (m-1)$. (See Fig. 7.6.)
- $2n$ nodal lines in ϕ: occur at intervals $\delta\phi = \pi/n$ for $n \neq 0$. N.B. do not need to start at $\phi = 0$.

Some low-lying modes are shown in Fig. 7.7. Note that the wave equation had rotational symmetry. This does not mean that the solutions have to have rotational symmetry ($n = 1, 2 \ldots$ do not). It means that if we take normal mode solution and then rotate it, it is still a solution of the wave equation.

The general solution

The general solution is a linear superposition of all allowed modes:

$$u(r, \phi, t) = \sum_{n=0}^{\infty}\sum_{m=1}^{\infty} J_n\left(\alpha_{nm}\frac{r}{a}\right)\ (C_{nm}\cos n\phi + D_{nm}\sin n\phi)\ (G_{nm}\cos\omega_{nm}t + H_{nm}\sin\omega_{nm}t) \tag{7.19}$$

Each (n, m) term contains *two* normal modes ($\cos n\phi$ and $\sin n\phi$), and there are four unknown constants. Two unknowns per mode is what we expect for a second order differential equation.

We will use initial conditions to fix the unknowns, but before that we need to learn a bit more about the properties of Bessel functions. In particular we need an orthogonality relation.

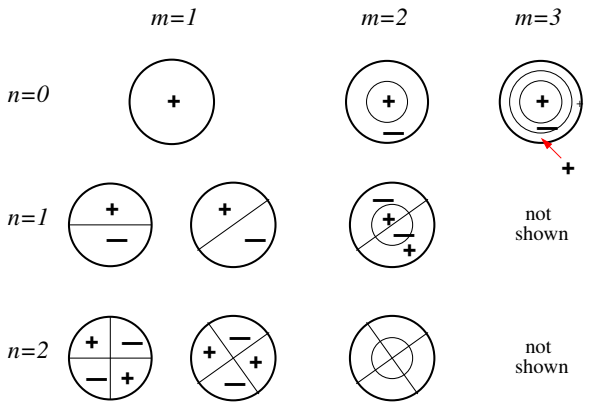


Figure 7.7: Some normal modes for a round drum.

Orthogonality and completeness

We state one orthogonality relation without proof. For given, fixed n

$$\int_0^a dr\ J_n\left(\alpha_{nm}\frac{r}{a}\right) J_n\left(\alpha_{nl}\frac{r}{a}\right) r = \frac{a^2}{2}[J_{n+1}(\alpha_{nm})]^2\delta_{m,l}\ , \tag{7.20}$$

where $J_n(\alpha_{nm}) = 0$, i.e. α_{nm} is the m^{th} root of the Bessel function of integral order n.

The extra factor of r compared with Fourier orthogonality arises *mathematically* because Bessel's equation contained first order derivatives in r.

The extra factor of r compared with Fourier orthogonality arises *physically* because Bessel's equation arose in the radial direction of two dimensional wave equation. It is a *vestigial circumference* factor $2\pi r$, turning a line integral into an area integral that is appropriate for a 2D orthogonality relation.

The set of Bessel functions $\{J_n(\alpha_{nm}x)\ ;\ m = 1\ldots\infty\}$ for fixed n form a complete set, so any function can be expanded in the interval $0 \le r \le a$ as a *Bessel* (or Fourier-Bessel) *series*:

$$f(r) = \sum_{m=1}^{\infty} A_{nm} J_n\left(\alpha_{nm}\frac{r}{a}\right), \tag{7.21}$$

The coefficients are determined using the orthogonality condition in the usual way, as we shall now see.

Initial conditions for the drumskin

The general solution for the displacement of a circular drumskin of radius a was given in Eqn. (7.19). Combining constants we have:

$$f(r,\phi,t) = \sum_{n=0}^{\infty}\sum_{m=1}^{\infty} J_n\left(\frac{\alpha_{nm}r}{a}\right)(A_{nm}\cos n\phi + B_{nm}\sin n\phi)\cos(\omega_{nm}t + \varepsilon_{nm})$$

Typical initial conditions are that the drumskin is initially at rest (implying $\varepsilon_{nm} = 0$) and described by given function $p(r, \phi)$:

$$f(r, \phi, t = 0) \equiv \sum_{n=0}^{\infty} \sum_{m=1}^{\infty} A_{nm} J_n \left(\frac{\alpha_{nm} r}{a} \right) \cos n\phi + B_{nm} J_n \left(\frac{\alpha_{nm} r}{a} \right) \sin n\phi = p(r, \phi) \ . \quad (7.22)$$

Given initial conditions $p(r, \phi)$ we can find the coefficients A_{nm} and B_{nm} via our orthogonality relations. We rewrite the initial condition equation as

$$\sum_{n=0}^{\infty} \sum_{m=1}^{\infty} (A_{nm} \Psi_{nm}(r, \phi) + B_{nm} \Phi_{nm}(r, \phi)) = p(r, \phi) \ . \quad (7.23)$$

where we have basis functions

$$\Psi_{nm}(r, \phi) = J_n \left(\frac{\alpha_{nm} r}{a} \right) \cos n\phi \ , \qquad \Phi_{nm}(r, \phi) = J_n \left(\frac{\alpha_{nm} r}{a} \right) \sin n\phi \ . \quad (7.24)$$

Define the inner product of two of these basis functions as

$$S \cdot T \equiv \int dA \ S \ T = \int dr \ \int d\phi \ r \ S(r, \phi) \ T(r, \phi) \ ,$$

and we find that $\{\Psi_{nm}, \Phi_{nm}\}$ form an orthogonal set:

$$\begin{aligned} \Psi_{uv} \cdot \Psi_{nm} &= \frac{a^2 \pi}{2} (1 + \delta_{u0}) [J_u(\alpha_{uv})]^2 \ \delta_{un} \ \delta_{vm} \\ \Psi_{uv} \cdot \Phi_{nm} &= 0 \\ \Phi_{uv} \cdot \Phi_{nm} &= \frac{a^2 \pi}{2} [J_u(\alpha_{uv})]^2 \ \delta_{un} \ \delta_{vm} \end{aligned}$$

We might term such functions the (unnormalised) *Circular Harmonics*. They are orthogonal, but not orthonormal. Note that the extra r is just what we get when we transform an area integral from Cartesian to circular polar coordinates. Note also that the angular orthogonality ensures we only compare Bessel functions of the same order (which is all Eqn. (7.20) covered).

We can use this orthogonality to obtain the coefficients from Eqn. (7.22). Applying $(\Psi_{uv} \cdot)$ or $(\Phi_{uv} \cdot)$ to both sides we get

$$\begin{aligned} A_{uv} &= \frac{2}{a^2 \pi (1 + \delta_{u0}) [J_u(\alpha_{uv})]^2} \times \int_0^a dr \ \int_0^{2\pi} d\phi \ r \ \Psi_{uv}(r, \phi) \ p(r, \phi) \\ B_{uv} &= \frac{2}{a^2 \pi [J_u(\alpha_{uv})]^2} \times \int_0^a dr \ \int_0^{2\pi} d\phi \ r \ \Phi_{uv}(r, \phi) \ p(r, \phi) \end{aligned}$$

We probably have to do these integrals numerically.

2.8 Wave equation in spherical polar coordinates

We now look at solving problems involving the Laplacian in spherical polar coordinates. The angular dependence of the solutions will be described by *spherical harmonics*.

We take the wave equation as a special case:

$$\nabla^2 u = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}$$

The Laplacian given by Eqn. (6.11) can be rewritten as:

$$\nabla^2 u = \underbrace{\frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r}}_{\text{radial part}} + \underbrace{\frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 u}{\partial\phi^2}}_{\text{angular part}} . \tag{8.1}$$

2.8.1 Separating the variables

We consider solutions of separated form

$$u(r,\theta,\phi,t) = R(r)\,\Theta(\theta)\,\Phi(\phi)\,T(t) .$$

Substitute this into the wave equation and divide across by $u = R\Theta\Phi T$:

$$\frac{1}{R}\frac{d^2R}{dr^2} + \frac{2}{rR}\frac{dR}{dr} + \frac{1}{r^2}\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = \frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2}.$$

First separation: r, θ, ϕ versus t

$$\text{LHS}(r,\theta,\phi) = \text{RHS}(t) = \text{constant} = -k^2.$$

This gives the T equation:

$$\frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2} = -k^2 \tag{8.2}$$

which is easy to solve.

Second separation: θ, ϕ versus r

Multiply LHS equation by r^2 and rearrange:

$$-\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) - \frac{1}{\sin^2\theta}\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = \frac{r^2}{R}\frac{d^2R}{dr^2} + \frac{2r}{R}\frac{dR}{dr} + k^2r^2 . \tag{8.3}$$

$$\text{LHS}(\theta,\phi) = \text{RHS}(r) = \text{constant} = \lambda$$

We choose the separation constant to be λ. For later convenience, it will turn out that $\lambda = l(l+1)$ where l has to be integer.

Multiplying the RHS equation by R/r^2 gives the R equation:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left[k^2 - \frac{\lambda}{r^2}\right]R = 0. \tag{8.4}$$

This can be turned into Bessel's equation; we'll do this later.

Third separation: θ versus ϕ

Multiply LHS of Eqn. (8.3) by $\sin^2\theta$ and rearrange:

$$\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\lambda\sin^2\theta=-\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=m^2$$

$$\text{LHS}(\theta)=\text{RHS}(\phi)=\text{constant}=-m^2\ .$$

The RHS equation gives the Φ equation without rearrangement:

$$\frac{d^2\Phi}{d\phi^2}=-m^2\Phi\ . \tag{8.5}$$

Multiply the LHS by $\Theta/\sin^2\theta$ to get the Θ equation:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left[\lambda-\frac{m^2}{\sin^2\theta}\right]\Theta=0\ . \tag{8.6}$$

2.8.2 Solving the separated equations

Now we need to solve the ODEs that we got from the original PDE by separating variables.

Solving the T equation

Eqn. (8.2) is of simple harmonic form and solved as before, giving sinusoids as solutions:

$$\frac{d^2T}{dt^2}=-c^2k^2T\equiv-\omega_k^2T\ ,$$

with $\omega_k=ck$.

Solving the Φ equation

Eqn. (8.5) is easily solved. Rather than using cos and sin, it is more convenient to use complex exponentials:

$$\Phi(\phi)=e^{\pm im\phi}$$

Note that we have to include both positive and negative values of m.

As ϕ is an angular coordinate, we expect our solutions to be *single-valued*, i.e. unchanged as we go right round the circle $\phi\to\phi+2\pi$:

$$\Phi(\phi+2\pi)=\Phi(\phi)\qquad\Rightarrow\qquad e^{i2\pi m}=1\qquad\Rightarrow\qquad m=\text{integer.}$$

This is another example of a BC (periodic in this case) quantising a separation constant.

In principle m can take any integer value between $-\infty$ and ∞.

It turns out in Quantum Mechanics that

$$\boxed{m\text{ is the integer magnetic quantum number and }-l\le m\le l}$$

for the z-component of angular momentum. In that context we will see that it is restricted to the range $-l\le m\le l$.

Solving the Θ equation

Starting from Eqn. (8.6), make a change of variables $w = \cos\theta$:

$$\frac{d}{dw} = \frac{d\theta}{dw}\,\frac{d}{d\theta} = \left(\frac{dw}{d\theta}\right)^{-1}\frac{d}{d\theta} = -\frac{1}{\sin\theta}\,\frac{d}{d\theta}\,,$$
$$(1-w^2)\frac{d}{dw} = -\frac{1-\cos^2\theta}{\sin\theta}\,\frac{d}{d\theta} = -\frac{\sin^2\theta}{\sin\theta}\,\frac{d}{d\theta} = -\sin\theta\,\frac{d}{d\theta}\,,$$
$$\frac{d}{dw}(1-w^2)\frac{d}{dw} = -\frac{1}{\sin\theta}\,\frac{d}{d\theta}\left[-\sin\theta\,\frac{d}{d\theta}\right] = \frac{1}{\sin\theta}\,\frac{d}{d\theta}\left[\sin\theta\,\frac{d}{d\theta}\right]\,.$$

Eqn. (8.6) becomes

$$\left(\frac{d}{dw}(1-w^2)\frac{d}{dw} + \lambda - \frac{m^2}{1-w^2}\right)\Theta(w) = 0\,.$$

which is known as the *Associated Legendre Equation*. Solutions of the Associated Legendre Equation are the Associated Legendre Polynomials. Note that the equation depends on m^2 and the equation and solutions are the same for $+m$ and $-m$.

It will turn out that there are smart ways to generate solutions for $m \neq 0$ from the solutions for $m = 0$ using angular momentum ladder operators (see quantum mechanics of hydrogen atom). So it would be unnecessarily "heroic" to directly solve this equation for $m \neq 0$.

In this course we will only solve this equation for $m = 0$.

Solving the Legendre equation

For $m = 0$ we can write the special case as the *Legendre Equation*:

$$\left((1-w^2)\frac{d^2}{dw^2} - 2w\frac{d}{dw} + \lambda\right)\Theta(w) = 0\,.$$

We apply the method of Froebenius by taking

$$\Theta(w) = \sum_{i=0}^{\infty} c_i w^i$$

Then

$$\sum_{i=0}^{\infty} c_i i(i-1)(w^{i-2} - w^i) - 2c_i i w^i + \lambda c_i w^i = 0$$

and rearranging the series to always refer the power w^i,

$$\sum_{i=0}^{\infty} \left[c_{i+2}(i+2)(i+1) + c_i(\lambda - i(i-1) - 2i\right] w^i = 0$$

Since this is true for all w, it is true term by term, and the indicial equation is

$c_{i+2}\left((i+2)(i+1)\right) = c_i\left(i(i+1) - \lambda\right)$

Start The series "switches on" when $c_0 \times 0 = 0$ admits $c_0 \neq 0$ and $c_{-2} = 0$
Also when $c_1 \times 0 = 0$ admits $c_1 \neq 0$ and $c_{-1} = 0$.

Termination Note, however $c_{i+2} \simeq c_i$ for large i. This gives an ill convergent series and for finite solutions the series must terminate at some value of i, which we call l. Thus,

$$\lambda = l(l+1)$$

for some (quantised) integer value l.

It will turn out in quantum mechanics that l is the orbital angular momentum quantum number.

Legendre polynomials

We denote the solutions the Legendre polynomials

$$P_l(w) \equiv P_l(\cos\theta)$$

For example: P_0 starts, and terminates with a single term C_0.
P_1 starts, and terminates with a single term C_1.
P_2 starts, with C_0 and terminates on C_2.
etc...

The first few are

$$\begin{aligned} P_0(w) &= 1 \\ P_1(w) &= w \\ P_2(w) &= \frac{1}{2}(3w^2 - 1) \\ P_3(w) &= \frac{1}{2}(5w^3 - 3w) \end{aligned}$$

Exercise: use the recurrence relation

$$c_{i+2}\left((i+2)(i+1)\right) = c_i\left(i(i+1) - l(l+1)\right)$$

to verify that these are our series solutions of Legendre's equation.

Orgthogonality

The orthogonality relation is

$$\int_{-1}^{1} P_m(w)P_n(w)dw = \int_0^{\pi} P_m(\cos\theta)P_n(\cos\theta)\sin\theta d\theta = N_m\delta_{mn}$$

where N_m is a normalisation factor that we do not need here.

In quantum mechanics this is already sufficient to cover S, P , D and F orbitals.

Associated Legendre polynomials

As mentioned the associated Legendre polynomials can be produced from Legendre polynomials in quantum mechanics using angular momentum ladder operators. Firstly,

$$P_l^0(w) = P_l(w)$$

Without proof, we can note that it can be shown that if $P_l(w)$ satisfies Legendre's equation, then

$$P_l^{|m|}(w) = (1-w^2)^{|m|/2}\frac{d^{|m|}}{dw^{|m|}}P_l(w)$$

will satisfy the associated Legendre polynomial for magnetic quantum number m.

As P_l is a polynomial of order l, then the above m-th derivative vanishes for $|m| > l$ and thus $m = -l, -l+1, \ldots, 0, \ldots l-1, l$.

General angular solution

Putting aside the radial part for the moment, the rest of the general solution is:

$$\Theta(\theta)\Phi(\phi)T(t) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} P_l^m(\cos\theta)\, e^{im\phi}\ (E_{ml}\cos\omega_k t + F_{ml}\sin\omega_k t)$$

The angular dependence is given by the combination:

$$P_l^m(\cos\theta)\, e^{im\phi} \propto Y_m^l(\theta,\phi)$$

These are known as the *spherical harmonics* (once we include a normalisation constant). We'll discuss these more in Sec. 2.8.3. What we have not yet established is the link between the value of k (and hence ω_k) and the values of m and l. To do this, we would need to solve the radial equation for various special cases.

2.8.3 The spherical harmonics

Spherical harmonics $\{Y_l^m(\theta,\phi)\}$ provide a complete, orthonormal basis for expanding the angular dependence of a function. They crop up a lot in physics because they are the normal mode solutions to the angular part of the Laplacian. They are defined as:

$$Y_l^m(\theta,\phi) = \frac{(-1)^m}{\sqrt{2\pi}}\sqrt{\frac{2l+1}{2}\cdot\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\phi}\ .$$

The extra factor of $(-1)^m$ introduced is just a convention and does not affect the orthonormality of the functions.

The spherical harmonics satisfy an orthogonality relation:

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta\ \sin\theta\ \left[Y_{l_1}^{m_1}(\theta,\phi)\right]^* Y_{l_2}^{m_2}(\theta,\phi) = \delta_{l_1,l_2}\delta_{m_1,m_2}\ .$$

Note that they are orthonormal, not just orthogonal, as the constant multiplying the product of Kronecker deltas is unity.

Completeness and the Laplace expansion

The completeness property means that any function $f(\theta, \phi)$ evaluated over the surface of the unit sphere can be expanded in the double series known as the *Laplace series*:

$$f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_{lm} Y_l^m(\theta, \phi) \ ,$$

$$\Rightarrow \qquad a_{lm} = \int_0^{\pi} d\theta \int_{-\pi}^{\pi} d\phi \ \sin\theta \ [Y_l^m(\theta, \phi)]^* f(\theta, \phi) \ .$$

Note that the sum over m only runs from $-l$ to l, because the associated Laplace polynomials P_l^m are zero outside this range.

2.8.4 Time independent Schroedinger equation in central potential

Consider

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{x})+\tilde{V}(r)\psi(\boldsymbol{x})=\tilde{E}\psi(\boldsymbol{x}).$$

We consider solutions of separated form: $\psi(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)$. Substitute into Schroedinger equation and divide across by $\psi=R\Theta\Phi$.

$$\frac{2m}{\hbar^2}\left(V(r)-E\right)-\frac{1}{R}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R=\frac{1}{\Theta}\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\Theta+\frac{1}{\Phi}\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Phi$$

Multiplying through by r^2

$$r^2\frac{2m}{\hbar^2}\left(V(r)-E\right)-\frac{1}{R}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R=\frac{1}{\Theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\Theta+\frac{1}{\Phi}\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Phi$$

First separation: radial & angular dependence

$$\mathrm{LHS}(r)=\mathrm{RHS}(\theta,\phi)=\text{constant}=-l(l+1).$$

Radial equation

$$\left[-\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+l(l+1)+r^2\frac{2m}{\hbar^2}(V(r)-E)\right]R=0$$

The differential equation is simplified by a substitution,

$$\begin{aligned}u(r)&=rR(r)\\u'(r)&=R(r)+rR'(r)\\u''(r)&=2R'(r)+rR''(r)=\frac{1}{r}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R\end{aligned}$$

and so

$$\left[-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+\frac{2m}{\hbar^2}(V(r)-E)\right]u(r)=0$$

We take a Coulomb potential and will be considering bound states, with $E<0$. It is convenient to rewrite in terms of the modulus $|E|$ and introduce explicit negative sign. We also change variables to $\rho=\frac{\sqrt{8m|E|}}{\hbar}r$

$$V(r)=\frac{-e^2}{4\pi\epsilon_0 r}=\frac{-e^2\sqrt{8m|E|}}{4\pi\epsilon_0\hbar\rho},$$

and so multiplying by $\frac{1}{r}$ and expressing in terms of u

$$\left\{\frac{8m|E|}{\hbar^2}\left[-\frac{d^2}{d\rho^2}+\frac{l(l+1)}{\rho^2}\right]+\frac{2m}{\hbar^2}\left[|E|-\frac{e^2}{4\pi\epsilon_0\rho}\sqrt{\frac{8m|E|}{\hbar^2}}\right]\right\}u(\rho)=0$$

We define $\lambda=\frac{e^2}{4\pi\epsilon_0\hbar}\sqrt{\frac{m}{2|E|}}=\alpha\sqrt{\frac{mc^2}{2|E|}}$, where $\alpha=\frac{e^2}{4\pi\epsilon_0\hbar c}\simeq\frac{1}{137}$ is the fine structure constant. This gives us

$$\left[\frac{d^2}{d\rho^2}-\frac{1}{4}-\frac{l(l+1)}{\rho^2}+\frac{\lambda}{\rho}\right]u(\rho)=0$$

Solution by method of Froebenius

We are now (almost!) ready to apply the method of Froebenius. In principle it could immediately be applied and we would get a an infinite Taylor series that indeed solves the equation.

However, a closed form solution can be obtained with one extra transformation that removes an over all exponential dependence on ρ. Observe that this equation for large ρ tends to

$$\to \left[\frac{d^2}{d\rho^2} - \frac{1}{4}\right] u(\rho)$$

which has as a normalisable solution $u(\rho) \to e^{-\frac{\rho}{2}}$ (and in addition a non-normalisable solution $u(\rho) \to e^{+\frac{\rho}{2}}$ which we ignore).

We can do rather better by taking a trial solution:

$$u(\rho) = e^{-\frac{\rho}{2}} f(\rho).$$

Then,

$$u' = e^{-\frac{\rho}{2}} \left[f'(\rho) - \frac{1}{2} f(\rho)\right].$$

$$u'' = e^{-\frac{\rho}{2}} \left[f''(\rho) - f'(\rho) + \frac{1}{4} f(\rho)\right].$$

Now,

$$\left[\frac{d^2}{d\rho^2} - \frac{d}{d\rho} + \cancel{\frac{1}{4}} \cancel{- \frac{1}{4}} - \frac{l(l+1)}{\rho^2} + \frac{\lambda}{\rho}\right] f(\rho) = 0$$

We now apply the method of Froebenius for a series substituting $f(\rho) = \sum_{i=0}^{\infty} c_i \rho^i$,

$$\sum_{i=0}^{\infty} c_i(i)(i-1)\rho^{i-2} - c_i(i)\rho^{i-1} - l(l+1)c_i\rho^{i-2} + \lambda c_i \rho^{i-1}$$

Thus, reexpressing so that all terms are of equal power ρ^{i-1}

$$\sum_{i=-1}^{\infty} c_{i+1}(i+1)(i)\rho^{i-1} - c_i(i)\rho^{i-1} - l(l+1)c_{i+1}\rho^{i-1} + \lambda c_i \rho^{i-1}$$

and we have the indicial equation,

$$\boxed{c_{i+1}\left[i(i+1) - l(l+1)\right] = c_i\left[i - \lambda\right]}$$

Series start: The series "switches on" for $c_k \equiv c_{i+1}$ when $i(i+1) = (k-1)k = l(l+1)$.

The first term c_k has $k = l + 1$.

Series termination: If the series does not terminate, then $c_{i+1} \to \frac{c_i}{i}$, and $f \to \sum \frac{\rho^i}{i!}$. This looks like the other solution that is a non-normalisable exponential $u(\rho) \simeq e^{+\frac{\rho}{2}}$ which we do not seek.

Only if $\lambda = i = n$ then the series "switches off" after $n - l$ terms.

$$c_{i+1} = c_i \frac{i - \lambda}{i(i+1) - l(l+1)}$$

We call n the principal quantum number. Note that for any given l, then $n \geq l + 1$ as the series commences at $k = l + 1$. The energy is

$$\alpha \sqrt{\frac{mc^2}{2|E|}} = n$$

Thus

$$|E| = \frac{\alpha^2 mc^2}{2n^2}$$

This energy is consistent with the Hydrogen spectrum (Lymann, Balmer series etc...).

Wavefunctions

We denote the radial solution for $L = l$, and principle quantum number $n \geq l + 1$ as R_{nl}.

Using our recurrence relation

$$c_{i+1} = c_i \frac{i - n}{i(i+1) - l(l+1)}$$

we have

	$n = 1, l = 0$	$n = 2, l = 0$	$n = 2, l = 1$
c_0	0	0	0
c_1	1	1	0
c_2	0	$-\frac{1}{2}$	1
c_3	0	0	0

The above energy relation gives us that for each n

$$\rho = \frac{\sqrt{8m|E|}}{\hbar} r \tag{8.7}$$

$$= \frac{2}{n} \frac{\alpha mc}{\hbar} r \tag{8.8}$$

$$= \frac{2}{n} \frac{r}{a_0} \tag{8.9}$$

where $a_0 = \frac{\hbar}{\alpha mc}$ is the usual Bohr radius.

The solutions are then

$$
\begin{aligned}
R_{1S} &\propto \frac{1}{\rho} e^{-\frac{\rho}{2}} \rho && (8.10)\\
&= e^{-\frac{\rho}{2}} && (8.11)\\
&= e^{-\frac{r}{a_0}} && (8.12)\\
R_{2S} &\propto \frac{1}{\rho} e^{-\frac{\rho}{2}} \left(\rho - \frac{1}{2}\rho^2\right) && (8.13)\\
&= e^{-\frac{\rho}{2}} \left(1 - \frac{1}{2}\rho\right) && (8.14)\\
&= e^{-\frac{r}{2a_0}} \left(1 - \frac{1}{2}\frac{r}{a_0}\right) && (8.15)\\
R_{2P} &\propto \frac{1}{\rho} e^{-\frac{\rho}{2}} \rho^2 && (8.16)\\
&= e^{-\frac{\rho}{2}} \rho && (8.17)\\
&= e^{-\frac{r}{2a_0}} \frac{r}{a_0} && (8.18)
\end{aligned}
$$

Note, we have not carefully normalised these radial wavefunctions. For each l the different wavefunctions for the various $n > l$ are orthogonal to each other. The orthogonality relation contains a residual r^2 factor corresponding to a vestige of the required orthogonality of wavefunctions under the 3d volume integral.

$$\int_0^\infty R_{nl}(r) R_{ml}(r) r^2 dr = N_n N_m \delta_{nm}$$

A complete orthonormal set can of course be formed as usual but is beyond the scope of the course.

2.9 Ladder operators

There is a general theory behind *factorising* Sturm-Liouville equations that gives rise to ladder operators that allow to relate solutions of different eigenvalues.

For simplicity, we will just consider some specific examples to illustrate the approach (for more detail see e.g. Chapter 9 of "Mathematical methods in science and engineering", S. Bayin).

Consider Bessel's equation

$$[\frac{d^2}{dx^2} + \frac{1}{x}\frac{d}{dx} + 1 - \frac{n^2}{x^2}]J(x) = \mathcal{B}_n J(x) = 0$$

We can introduce *ladder* operators (by *operator* I mean a term, or fragment of an equation, containg derivatives)

$$L_+^n = \left(\frac{d}{dx} - \frac{n}{x}\right)$$
$$L_-^n = \left(\frac{d}{dx} + \frac{n}{x}\right)$$

these allow to factorise $\mathcal{B}_n$ because

$$\begin{aligned}
\mathcal{B}_n &= \frac{d^2}{dx^2} + \frac{1}{x}\frac{d}{dx} + 1 - \frac{n^2}{x^2} \\
&= \left(\frac{d}{dx} + \frac{n+1}{x}\right)\left(\frac{d}{dx} - \frac{n}{x}\right) + 1 \\
&= L_-^{n+1} L_+^n + 1 \\
&= \left(\frac{d}{dx} - \frac{n-1}{x}\right)\left(\frac{d}{dx} + \frac{n}{x}\right) + 1 \\
&= L_+^{n-1} L_-^n + 1
\end{aligned}$$

Now, suppose we have a solution $J_n(x)$, such that $\mathcal{B}_n J_n(x) = 0$.

Consider

$$F(x) = L_+^n J_n(x)$$

Then,

$$\begin{aligned}
\mathcal{B}_{n+1} F(x) &= \left(L_+^n L_-^{n+1} + 1\right) L_+^n J_n(x) \\
&= L_+^n \left(L_-^{n+1} L_+^n + 1\right) J_n(x) \\
&= L_+^n B_n J_n(x) \\
&= 0
\end{aligned}$$

Thus, $F(x)$ is a solution of Bessels equation for a different value of n, and

$$J_{n+1}(x) = L_+^n J_n(x)$$

.

Similarly

$$J_{n-1}(x) = L_-^n J_n(x)$$

.

and given $J_0(x)$, which we already found, we can find all other J_n by applying L_+^n the appropriate number of times.

$$J_n(x) = L_+^{n-1} \dots L_+^0 J_0(x)$$

Similar ladder operators can be found to raise and lower

- Solutions to the harmonic oscillator
- the m quantum number in spherical harmonics
- the l quantum number in spherical harmonics
- the n quantum number in the radial hydrogen atom

The first two of these are very well known.

These can be thought of as applying differential operators that turn a normal mode solution for one separation constant (eigenvalue of S-L problem), into a different normal with a modified separation constant.

See tutorial question on Hermite Polynomials

Chapter 3

Statistical analysis and fitting data

3.1 Probability distributions

In this part of the course we will consider the analysis and fitting of data. This requires a foundation in the study of probability and statistics. We shall see that Gaussian distributions play a particular role in this study.

3.1.1 Random variables

A *random variable* X is a measurent or process that gives you a different result each time. The results are distributed randomly according to a *probability density* P_X.

$$P_X(x)dx$$

is the probability that any measurement of variable X will have a value between x and $x+dx$.

As all measurements return a value between $-\infty$ and ∞ we have

$$\int_{-\infty}^{\infty} P_X(x)dx = 1$$

The average, or mean, value is the first moment of this distribution

$$\bar{X} = \int_{-\infty}^{\infty} xP_X(x)dx$$

The variance is the mean squared deviation from the mean

$$\mathrm{Var}(X) = \int_{-\infty}^{\infty} (x-\bar{X})^2 P_X(x)dx$$

3.1.2 Zero mean, unit variance

Any random variable X can be brought into convenient zero mean, unit variance form by considering in its place the scaled and shifted variable

$$X' = b(X-a)$$

where $a = \bar{X}$, and $b = \frac{1}{\sqrt{\mathrm{Var}X}}$. Then X' has zero mean, and unit variance.

3.1.3 Independent random variables

Two random variables are *independent* if the value obtained from one does not affect the value obtained from another.

For example, when tossing coins, *even if you have already obtained five heads in a row.* you are equally likely to obtain heads or tails on the sixth try. If you collect statistics on the number of heads, each attempt is independent.

In contrast, if you are drawing cards from a single deck these are not independent as once the Ace of Spades is drawn, all players are very unlikely to receive another (unless you are in an establishment of particularly ill-repute).

3.1.4 Adding random variables

We consider adding two independent random variables X and Y together. This is a key to understanding the process of averaging results. Because the variables (measurements) are independent, we can consider measuring one first without affecting the distribution of the other. The probability distribution of the sum s_{xy} is just the *convolution* of the two probability distributions.

$$P_{X+Y}(s_{xy}) = \int_{-\infty}^{\infty} P_X(x)P_Y(s_{xy} - x)dx$$

This can be seen by noting that the probability for variable X to give a result in band $x \to x + dx$ is $P_X(x)dx$. The probability density in the sum $s_{xy} = x + y$ that variable Y then gives a value between value $y = s_{xy} - x$ and $y = s_{xy} - x + ds$ is $P_Y(s_{xy} - x)$.

This can be repeated, adding a third random variable gives

$$P_{X+Y+Z}(s_{xyz}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P_X(x)P_Y(s_{xy} - x)P_Z(s_{xyz} - s_{xy})dxds_{xy}$$

and so on.

3.1.5 Scaling random variables

If we scale the random variable by a constant C, the probability of having a result between $u = Cx$ and $u + du = Cx + Cdx$ must equal the orginal probability between x and $x + dx$. Thus

$$P_{CX}(u)du = P_{CX}(Cx)Cdx = P_X(x)dx$$

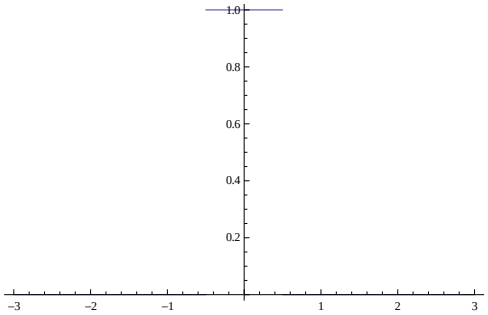
so that

$$P_{CX}(u) = \frac{1}{C}P_X(\frac{u}{c}).$$

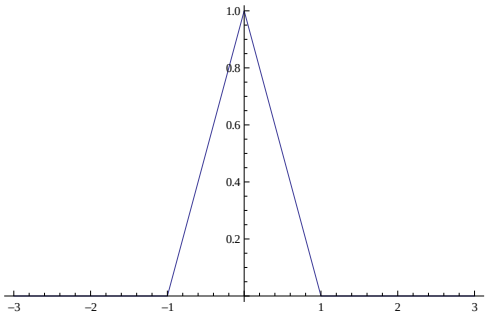
3.1.6 Some examples

Now let's add something simple like the top function to itself a number of times. It is well known, and easy to show that performing this operation once produces a triangular function. Beyond this gets tricky due to the piecewise bounds on integrations. However, we can continue to make progress using Mathematica to illustrate our point:

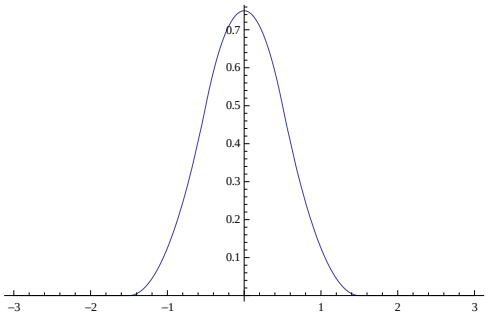
```
h[x] = PieceWise[ {0,x < -0.5}, {1, -0.5<=x<=0.5}, {0,x>0.5}]
Plot[ h[x] , {x,-3,3}]
```



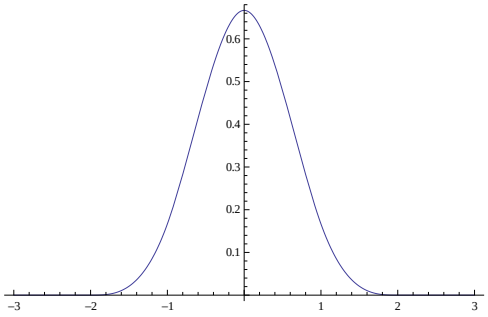

```
Plot[ Convolve[ h[y],h[y],y,x]], {x,-3,3}]
```




```
Plot[ Convolve[Convolve[ h[y],h[y],y,z],h[z],z,x]], {x,-3,3}]
```




```
Plot[ Convolve[Convolve[Convolve[ h[y],h[y],y,z],h[z],z,w],h[w],w,x], {x,-3,3}]
```



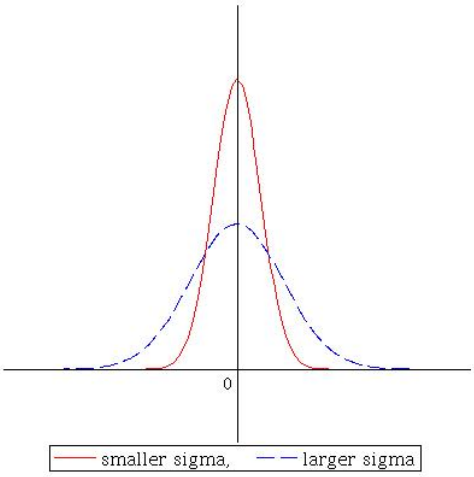
A curious thing happens to the distribution of the average. It is looking more and more bell shaped!

3.2 Gaussian distributions

A particularly common form of distribution is the Gaussian, or normal distribution $\mathcal{N}$

$$P_{\mathcal{N}}(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{x^2}{2\sigma^2}}$$

The Gaussian curve is also known as the bell-shaped or normal curve.



Sketch of normalised Gaussians. The intercepts are $P_{\mathcal{N}}(0) = \frac{1}{\sqrt{2\pi\sigma^2}}$.

In order to check this probability is indeed normalised we must evaluate a Gaussian integral. Under a change of variables to $\tilde{x} = \frac{x}{\sqrt{2}\sigma}$ the integrated probability becomes.

$$\int_{-\infty}^{\infty} P_{\mathcal{N}}(x)dx = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\tilde{x}^2} d\tilde{x}$$

3.2.1 Gaussian integral

Gaussian integrals occur regularly in physics. We are interested in

$$I = \int_{-\infty}^{\infty} \exp -x^2 dx$$

This can be solved via a trick in polar coordinates: observe

$$\begin{aligned} I^2 &= \int_{-\infty}^{\infty} \exp -x^2 dx \int_{-\infty}^{\infty} \exp -y^2 dy \\ &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \exp -(x^2+y^2) \\ &= \int_0^{\infty} dr 2\pi r \exp -r^2 \\ &= \pi \int_0^{\infty} du \exp -u \\ &= \pi \left[-\exp -u \right]_0^{\infty} \\ &= \pi \end{aligned}$$

Thus,

$$I = \int_{-\infty}^{\infty} \exp -x^2 dx = \sqrt{\pi}$$

Thus, we see

$$\int_{-\infty}^{\infty} P_{\mathcal{N}}(x) dx = 1$$

3.2.2 Cumulative distribution, and the error function

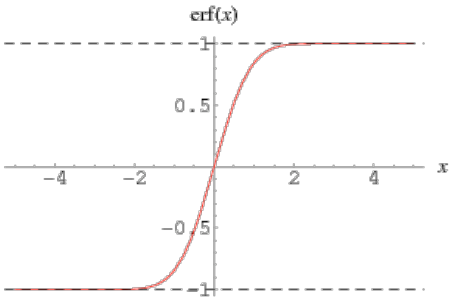
We are often interested in the probability of having a result deviating from its mean by some amount. The question of "what was the chance of that" is measured by the cumulative probability to have a result deviating by an amount measured in standard deviations $a = \frac{x}{\sigma}$ from its mean and is given by the error function

$$\begin{aligned} \mathrm{erf}(\frac{a}{\sqrt{2}}) &= \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} e^{\frac{-x^2}{2}} dx \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\frac{a}{\sqrt{2}}}^{\frac{a}{\sqrt{2}}} e^{-\tilde{x}^2} d\tilde{x} \end{aligned}$$

where $\tilde{x} = \frac{x}{\sqrt{2}}$. We generally have to look up this function in tables, or use numerical software to evaluate.

You will notice, unfortunately, there is a $\frac{1}{\sqrt{2}}$ factor between the argument of $\mathrm{erf}(\frac{a}{\sqrt{2}})$ and the deviation from the mean a measured in standard deviations. Thus, the probability of deviating by less than 1σ is $\mathrm{erf}(0.707) \sim 68\%$.

Deviation less than		Percent
1σ	$\mathrm{erf}(0.707)$	68%
2σ	$\mathrm{erf}(1.414)$	95%
3σ	$\mathrm{erf}(2.12)$	99.7%
4σ	$\mathrm{erf}(2.83)$	99.992%
5σ	$\mathrm{erf}(2.12)$	99.99993%



The process of integrating a probability distribution function (PDF), such as the Gaussian, to find the total probability of having a deviation below the observed deviation is common and useful to estimate the likelihood of our having observed something.

This integrated version of the probability, as a function of this threshold, is known as the cumulative distribution function (CDF).

- erf(x) is the CDF corresponding to the Gaussian PDF.
- $1, 2, 3\sigma$ correspond to 68%, 95%, 99.7%
  - Enshrined/rote learned as the "68-95-99.7" rule in statistics
- *Warning:* conventions vary w.r.t. the CDF being integrated from $[-a, a]$ or from $[-\infty, a]$.

Life and death safety margins (3σ)

Under EU law, rock climbing carabiners are tested to ensure they can withstand a load of around $21KN$ (around 2 tonnes) with a 3 sigma margin.

This means, worryingly that around 3 in every 1000 *cannot* withstand the 2 tonne rating, however the σ for the distribution is never disclosed to the climbers. Your lecturer very much hopes that a 5σ bound that includes even these weak ones is still more than fit for purpose!

Experimental discovery standards (5 σ)

Another example is that standards to which particle physics adheres for particle discovery. When new particles, such as the Higgs boson, are discovered, it no longer always possible to simply "spot it" as a particle track because they decay so quickly.

Rather the theoretical prediction for their contributions to decays must be compared to experimental observation, involving fitting mathematical expressions to data.

The significance of the contribution from a Higgs boson, compared to not having the Higgs boson is critically important. Particle Physicists hold themselves to a 5σ criterion, which means that there can only be a 0.00007% chance they were simply fooled by luck if or when they claim LHC has "discovered" the Higgs boson.

3.2.3 Fourier transform of gaussian

A function $f(x)$ and its Fourier transform $F(k)$ are related by:

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\ f(x)\ e^{ikx}\ , \tag{2.1}$$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\ F(k)\ e^{-ikx}\ . \tag{2.2}$$

The FT of the Gaussian is

$$\begin{aligned}
\tilde{P}_{\mathcal{N}}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx P_{\mathcal{N}}(x) e^{ikx} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\ \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{x^2}{2\sigma^2}\right)\ e^{ikx} \\
&= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{k^2\sigma^2}{2}\right)\ ,
\end{aligned}$$

i.e. the FT of a Gaussian is another Gaussian (this time as a function of k).

Deriving the FT For notational convenience, let's write $a = \frac{1}{2\sigma^2}$, so

$$\tilde{P}_{\mathcal{N}}(k) = \frac{1}{\sqrt{2\pi}\sigma} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\ \exp\left(-\left[ax^2 - ikx\right]\right)$$

Now we can complete the square inside $[\ldots]$:

$$-ax^2 + ikx = -\left(x\sqrt{a} - \frac{ik}{2\sqrt{a}}\right)^2 - \frac{k^2}{4a}$$

giving

$$\tilde{P}_{\mathcal{N}}(k) = \frac{1}{2\pi\sigma} e^{-k^2/4a} \int_{-\infty}^{\infty} dx\ \exp\left(-\left[x\sqrt{a} - \frac{ik}{2\sqrt{a}}\right]^2\right)\ .$$

We then make a change of variables:

$$u = x\sqrt{a} - \frac{ik}{2\sqrt{a}}\ .$$

This does not change the limits on the integral, and the scale factor is $dx = du/\sqrt{a}$, giving

$$\tilde{P}_{\mathcal{N}}(k) = \frac{1}{2\pi\sigma} \frac{1}{\sqrt{a}}\ e^{-k^2/4a} \int_{-\infty}^{\infty} du\ e^{-u^2} = \frac{1}{2\sqrt{\pi}\sigma} \frac{1}{\sqrt{a}} \cdot e^{-k^2/4a}\ . \tag{2.3}$$

Finally, we change back from a to σ.

3.2.4 Convolution of Gaussians

We can use the convolution theorem to convolve together two Gaussians $P_{\mathcal{N}_1}(x)$ and $P_{\mathcal{N}_2}(x)$ of width σ_1 and σ_2 to represent the distribution of the sum using the convolution theorem:

$$P_{\mathcal{N}_1}(x) * P_{\mathcal{N}_2}(x) = \sqrt{2\pi}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk \tilde{P}_{\mathcal{N}_1}(k)\tilde{P}_{\mathcal{N}_2}(k)e^{-ikx}\right)$$

$$\begin{aligned} P_{\mathcal{N}_1}(x) * P_{\mathcal{N}_2}(x) &= \sqrt{2\pi}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk e^{-ikx}\frac{1}{\sqrt{2\pi}}e^{-\frac{k^2\sigma_1^2}{2}}\frac{1}{\sqrt{2\pi}}e^{-\frac{k^2\sigma_2^2}{2}} \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk e^{-ikx}\frac{1}{\sqrt{2\pi}}e^{-\frac{k^2(\sigma_1^2+\sigma_2^2)}{2}} \end{aligned}$$

Which we can recognise from Eq. 2.3 as a normalised Gaussian of width $\sigma^2 = \sigma_1^2 + \sigma_2^2$.

- This is important - Gaussian distributed random variables remain Gaussian distributed under addition (also their widths add in quadrature).
- Further, we just saw in a handwaving sense that random variables of other distributions become more Gaussian-like after addition.

It appears that the Gaussian distribution "attracts" all other distributions under the avergaing process, and we shall see in the next section that this is indeed true.

3.3 Central limit theorem

The Central Limit Theorem (CLT) is of fundamental importance to almost all experimental science.

Take X as a zero mean, unit variance random variable with *any* distribution $P_X(x)$.

The random variable for the average of N of these random variables

$$S_N = \frac{1}{N}\left(X_1 + X_2 + \ldots X_N\right)$$

and in the limit of large N, this is distributed according to

$$\lim_{N\to\infty} P_{S_N}(x) \to \frac{\sqrt{N}}{\sqrt{2\pi}} e^{-\frac{Nx}{2}}$$

Proof

The key point is that the average of many measurements becomes increasingly dominated by the lowest frequencies in the probability distribution.

In other words, small wiggles in the probability distribution will cancel and not affect the average of many measurements; sometimes you get lucky, sometimes unlucky, but on average small wiggles disappear rapidly.

1. First we represent sum of N independent random variables drawn with probability $P_X(x)$ as a convolution.

$$P_{NX}(x') = \int_{-\infty}^{\infty} dx_1 \ldots \int_{-\infty}^{\infty} dx_{N-1} P_X(x_1) P_X(x_2 - x_1) P_X(x_3 - x_2) \ldots P_X(x' - x_{N-1})$$

2. We can apply the convolution theorem $N-1$ times obtaining

$$P_{NX}(x') = \frac{1}{\sqrt{2\pi}}(\sqrt{2\pi})^{N-1} \int_{-\infty}^{\infty} dk e^{-ikx'} \left(\tilde{P}_X(k)\right)^N dk$$

3. Taking the factor of $\frac{1}{N}$ for the average and applying our scaling rule Section 3.1.5 gives

$$\begin{aligned} P_{S_N}(u) &= N\frac{1}{\sqrt{2\pi}}(\sqrt{2\pi})^{N-1} \int_{-\infty}^{\infty} dk e^{-ikNu} \left(\tilde{P}_X(k)\right)^N dk \\ &= \frac{1}{\sqrt{2\pi}}(\sqrt{2\pi})^{N-1} \int_{-\infty}^{\infty} dk' e^{-ik'u} \left(\tilde{P}_X(\frac{k'}{N})\right)^N dk' \end{aligned}$$

4. In the limit of large N, the lowest frequency terms of $\tilde{P}_X(\frac{k'}{N})$ dominate, and these correspond to the lowest *moments* of the distribution.

We can Taylor expand

$$\begin{aligned}\tilde{P}_X(\frac{k'}{N}) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\frac{k'x}{N}} P_X(x)dx \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[1+\frac{ik'x}{N}-\frac{k^2x^2}{2N^2}+\ldots\right]P_X(x)dx \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}P_X(x)dx+\frac{ik'}{N}\int_{-\infty}^{\infty}xP_X(x)dx-\frac{k^2x^2}{2N^2}\int_{-\infty}^{\infty}x^2P_X(x)dx \\ &= \frac{1}{\sqrt{2\pi}}\left(1-\frac{k^2}{2N^2}+\ldots\right)\end{aligned}$$

where we have used the fact that $P_X(x)$ is normalised, zero mean, and unit variance.

5. Inserting this into the full expression for $P_{S_N}(u)$ we have

$$\begin{aligned}P_{S_N}(u) &= \frac{1}{\sqrt{2\pi}}(\sqrt{2\pi})^{N-1}(\frac{1}{\sqrt{2\pi}})^N\int_{-\infty}^{\infty}dk'e^{-ik'u}\left(1-\frac{k^2}{2N}\frac{1}{N}\right)^N dk' \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty}dk'e^{-ik'u}\left(1-\frac{k^2}{2N}\frac{1}{N}\right)^N dk'\end{aligned}$$

6. The final significant step is to note that with $b=-\frac{k^2}{2N}$

$$\begin{aligned}\left(1+\frac{b}{N}\right)^N &= \sum_{r=0}^{N}\frac{(N!)}{r!(N-r)!}b^r \\ &= \sum_{r=0}^{N}\frac{N(N-1)\ldots(N-r+1)}{N^r}\frac{b^r}{r!} \\ &\to \sum_{r=0}^{N}\frac{b^r}{r!} \\ &\to e^b\end{aligned}$$

Thus,

$$P_{S_N}(u)\to\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dk'e^{-ik'u}\frac{1}{\sqrt{2\pi}}e^{-\frac{k^2}{2N}}dk'$$

which we can recognise from Eq 2.3 as a normalised Gaussian of width $\sigma_S^2=\frac{1}{N}$

$$\begin{aligned}P_{S_N}(u) &= \frac{\sqrt{N}}{\sqrt{2\pi}}e^{-\frac{u^2N}{2}} \\ &= \frac{1}{\sqrt{2\pi}\sigma_S}e^{-\frac{u^2}{2\sigma_S^2}}\end{aligned}$$

Consequences

This theorem has very important consequences that permeate most of science!

- If we measure something many times, we can assume the average has a *Gaussian* distribution.
- If the original non-Gaussian distribution had unit variance, the variance of the average is $\frac{1}{\sqrt{N}}$.
- If original distribution was not unit variance, the variance of the mean is reduced by $\frac{1}{\sqrt{N}}$

3.4 Analysing data

We now consider how to analyse and/or fit experimental (or numerical) data. Each data point can be measured a number of times, and the mean and the error on the mean can be computed as follows.

If we take N-measurements $\{x_1, \ldots, x_N\}$, sampled randomly from a (non-Gaussian) probability distribution $P_X(x)$

The sample mean is

$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

This differs from the true mean

$$\bar{X} = \int_{-\infty}^{\infty} x P_X(x) dx$$

but will become equal in the limit of infinite N.

The sample mean is the best estimate of the mean of the non-Gaussian distribution P_X one can make given the finite number of measurements.

3.4.1 Variance

The variance of the sample is

$$\sigma^2 = \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \bar{x})^2$$

This is a best estimate of the variance of the non-Gaussian distribution P_X one can make given the finite number of measurements.

The $(N-1)$ arises from an adjustment to prevent underestimating the variance with a finite sample size. Practically, if the change from N to $(N-1)$ makes a worrying difference, your Lecturer recommends you get more data.

3.4.2 Standard deviation

An important question that arises is how incorrect is the sample mean *likely* to be. For a finite sample size, this question cannot be answered without knowing the details of the original distribution $P_X(x)$.

However, if we are prepared to assume that we have sufficiently many measurements that our finite sample yields a good estimate of variance of $P_X(x)$, and that the distributions of averages will approach its asymptotic Gaussian form we can proceed.

The variance of the Gaussian distributed mean will be $\frac{1}{\sqrt{N}}\sigma$.

For moderate N it is more conventional to take the standard error of the mean as

$$\text{std.err.} = \sqrt{\frac{1}{N(N-1)}\sum_{i=1}^{N}(x_i - \bar{x})^2}$$

3.5 χ^2/dof and the χ^2 distribution

If you roll a dice many times, you are bound to eventually get lucky or unlucky. If we make a million measurements we expect to see one in a million probability events.

So, when we make many measurements, we should ask how likely we were to have seen a certain set of deviations: me must ask if, on the balance of probability, is this *consistent* with the errors we have calculated for each data point.

- Suppose we take N-samples $\{x_i\}$ from normally distributed variables of unit variance, zero mean, each with probability $P_{\mathcal{N}}(x)$.

  We consider these N-samples as be a single sample from a N-dimensional space.

- The probability distribution for this quantity χ^2 is determined by the normal distributions of the individual variables.

  Since the variables are independent, they probability density for the N-samples is just the product of the individual variables probabilities:

$$P(x_1, \ldots, x_N)dx_1 \ldots dx_N = P_{\mathcal{N}}(x_1) \ldots P_{\mathcal{N}}(x_N)dx_1 \ldots dx_N$$

- It is simpler to reduce our measurement of the vector $\{x_1, \ldots x_N\}$ to a single number. To do this, we define the quantity χ^2 to be the sum of the deviations from zero:

$$\chi^2 = \sum_i x_i^2$$

- The expectation value of χ^2 is given by

$$\begin{aligned}
\langle\chi^2\rangle &= \int \chi^2 P_{\chi^2}(\chi^2)d(\chi^2) \\
&= \int (x_1^2 + \ldots + x_N^2) P_{\mathcal{N}}(x_1) \ldots P_{\mathcal{N}}(x_N)dx_1 \ldots dx_N \\
&= \int x_1^2 P_{\mathcal{N}}(x_1)dx_1 \int P_{\mathcal{N}}(x_2)dx_2 \ldots \int P_{\mathcal{N}}(x_N)dx_N \\
&+ \int P_{\mathcal{N}}(x_1)dx_1 \int x_2^2 P_{\mathcal{N}}(x_2)dx_2 \ldots \int P_{\mathcal{N}}(x_N)dx_N \\
&\ldots \\
&+ \int P_{\mathcal{N}}(x_1)dx_1 \int P_{\mathcal{N}}(x_2)dx_2 \ldots \int x_N^2 P_{\mathcal{N}}(x_N)dx_N \\
&= 1 + \ldots + 1 \\
&= N
\end{aligned}$$

where we have made use of the fact that the distribution $P_{\mathcal{N}}(x)$ had unit variance, and unit total probability.

- The average value for χ^2 is N, the number of datapoints.
  - A value of $\chi^2/N \gg 1$ will indicate non-Gaussian, or significantly underestimated errors.
  - A value of $\chi^2/N \ll 1$ will indicate significantly overestimated errors.
  - One does not expect to be either abnormally lucky, or unlucky and having results that appear so may indicate other problems in data or model.

3.5.1 Some detail on the distribution of χ^2

We wish to obtain the probability distribution $P^N_{\chi^2}(\chi^2)$ of χ^2 for N variables in more detail than simply its mean value.

We must use theta functions to evaluate the integral of probability to find χ^2 in the spherical shell corresponding to radius $r \equiv \sqrt{\chi^2}$ between $r = \sqrt{\chi^2}$ and $r + \delta r = \sqrt{\chi^2 + \delta(\chi^2)}$ in the N-dimensional space of deviations $\{x_i\}$.

We need to do this to identify the 68th percentile in the cumulative distribution of χ^2 for n independent variables (for example). This is critical to estimating the uncertainty in parameters after a fit.

$$\begin{aligned}
P^N_{\chi^2}(\chi^2)\delta(\chi^2) &= \frac{1}{(\sqrt{2\pi})^N}\int \theta(|X|^2-\chi^2)\theta(\chi^2+\delta(\chi^2)-|X|^2)e^{-\frac{x_1^2}{2}}\dots e^{-\frac{x_N^2}{2}}dx_1\dots dx_N \\
&= \frac{1}{(\sqrt{2\pi})^N}\int \theta(|X|^2-\chi^2)\theta(\chi^2+\delta(\chi^2)-|X|^2)e^{-\frac{\chi^2}{2}}dx_1\dots dx_N \\
&= \frac{1}{(\sqrt{2\pi})^N}e^{-\frac{r^2}{2}}S^N(r)\delta r
\end{aligned}$$

Here $S^N(r)$ is the surface area of an N-dimensional ball of radius r for general dimensions (without proof here), this is

$$S^N(r) = \frac{Nr^{N-1}\pi^{\frac{N}{2}}}{\Gamma(N/2+1)}$$

Recall, $\Gamma(x) = (x-1)\Gamma(x-1)$, $\Gamma(N) = (N-1)!$, and $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. It can be easily verified for two and three dimensions that this produces formulae we know and love!

$$\begin{aligned}
S_2(r) &= 2\pi r \\
S_3(r) &= 4\pi r^2 \\
S_4(r) &= 2\pi^2 r^3
\end{aligned}$$

Note that

$$\delta(\chi^2) = \delta(r^2) = 2r\delta r,$$

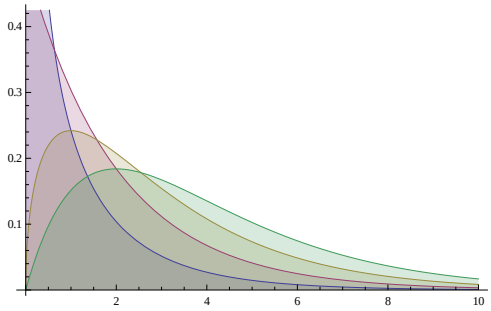
and so

$$\delta r = \frac{\delta\chi^2}{2r}$$

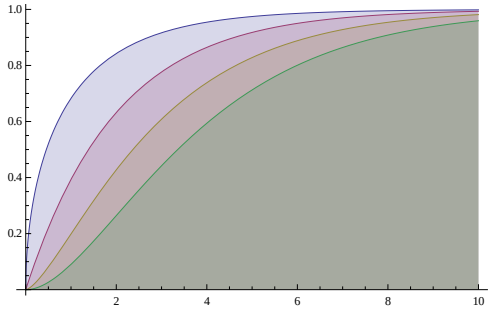
Thus,

$$P^N_{\chi^2}(\chi^2)\delta(\chi^2) = \frac{1}{(\sqrt{2})^N}\frac{\delta(\chi^2)}{2\sqrt{\chi^2}}e^{-\frac{\chi^2}{2}}\frac{N(\chi^2)^{\frac{N-1}{2}}}{\Gamma(N/2+1)}$$
$$= \frac{(\chi^2)^{\frac{N}{2}-1}}{2^{\frac{N}{2}}\Gamma(N/2)}e^{-\frac{\chi^2}{2}}\delta(\chi^2)$$

The prefactors are painful normalisation. However, the change in the power of χ^2 in front of the exponential as N is varied is much more important as these change the shape of the χ^2 distribution as a function of N.



The probability distribution function $P^N_{\chi^2}(\chi^2)$ for χ^2 as a function χ^2 for different numbers n of random Gaussian variables that are averaged ($n = 1, 2, 3, 4$).



The cumulative distribution function (CDF)

$$P^{\text{CDF}}_{\chi^2}(N, \chi^2) = \int_0^{\chi^2} P^N_{\chi^2}(Q)dQ$$

for χ^2 as a function χ^2 for different numbers n of random Gaussian variables that are averaged ($n = 1, 2, 3, 4$).

Here (this is *not* proven)

$$P^{\text{CDF}}_{\chi^2}(N, \chi^2) = \frac{1}{\Gamma\frac{N}{2}}\gamma(\frac{N}{2}, \frac{\chi^2}{2})$$

where γ is the lower imcomplete gamma function

$$\gamma(s, x) = \int_0^x t^{s-1}e^{-t}dt$$

As we expect from our discussion of the mean value of χ^2, the cumulative distribution grows roughly linearly in N.

We will be interested in the value of χ^2 that covers 68.3% of fluctuations (or in other words 1σ). This means the value of χ^2 for which the cumulative distrubution function has value 0.683. This value is dependent on the number of degrees of freedom.

n	68th percentile χ^2
1	1
2	2.3
3	3.5
4	4.7
5	5.9

We can now meaningfully ask how model parameters could be varied while staying within this bound on χ^2.

3.6 χ^2 minimisation

The definition of χ^2 can now be generalised to the case where the i-th variable has non-zero mean and non-unit variance in the obvious way.

$$\chi^2 = \sum_i \frac{(x_i - \bar{x}_i)^2}{\sigma_i^2}$$

All the earlier results remain applicable because the modified variables $\tilde{x} = \frac{x-\bar{x}}{\sigma}$ are normally distributed with zero mean and unit variance, and our generalised χ^2 is just

$$\chi^2 = \sum_i \frac{(x_i - \bar{x}_i)^2}{\sigma_i^2} = \sum_i \tilde{x}_i^2$$

In particular, we still expect that the average generalised χ^2 should still be the number variables N.

Thus far we assumed that there was some external, given probability distribution. In the real world, the true distribution will *not* be known.

3.6.1 Averaging *is* fitting to a constant

Suppose the data is distributed as a normal distribution around some unknown mean A, but all the data has the same width σ.

$$P_X(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-A)^2}{2\sigma^2}}$$

As we do not know A independent of the data, we must ask what is the *probability* for having obtained our set of N results x_i, for each possible value of A. This probability is just

$$P_X(x_1)P_X(x_2)\dots P_X(x_N) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^N e^{-\sum \frac{(x_i-A)^2}{2\sigma^2}}$$

Gaussian statistics tells us the probability of data having been produced from some "externally given" model. The maximum likelihood method involves the reasonable approach of turning this around: use the the Gaussian probability for the data having been produced for each possible parameter to *distinguish* which is the *right* parameter.

Thus, the most *likely* value for $A_{\min}$ is obtained by maximising this probability. This is achieved by minimising the term in the exponent $\frac{(x_i-A)^2}{2\sigma^2}$, and hence by minimising our χ^2.

The minimum of χ^2 is found by requiring the derivative wrt A be zero:

$$0 = \frac{d}{dA}\chi^2 = -\frac{1}{\sigma^2}\sum_i 2(x_i - A)$$

and so

$$A_{\min} = \frac{1}{N}\sum_i x_i$$

and unsurprisingly the most likely value for A is the average of the data.

Further, we can Taylor expand

$$\chi^2(A)$$

around the minimum,

$$\chi^2(A) = \chi^2_{\min} + \frac{1}{2}\left(\frac{d^2}{dA^2}\chi^2\right)(\delta A)^2$$

where $\delta A = A - A_{\min}$ is the difference of A from the value that minimises χ^2. The first derivative vanishes at the minimum and we may interpret the second derivative as creating a Gaussian distribution (with higher order corrections that vanish in the limit of small variance) because it is a quadratic term. We may therefore use this to interpret the likelihood as a Gaussian probability for A,

$$P(A) = Ne^{-\frac{1}{2}\frac{1}{2}\left(\frac{d^2}{dA^2}\chi^2\right)(\delta A)^2}.$$

where N is some normalisation that absorbs the $e^{-\chi^2_{\min}}$ term. Comparing to the standard Gaussian distribution

$$P_N(A) = \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{A^2}{2\sigma^2}}$$

we see that when $\delta A = \sigma_A$ the exponential is equal to $e^{-\frac{1}{2}}$.

That is

$$\frac{1}{2}\frac{1}{2}\left(\frac{d^2}{dA^2}\chi^2\right)\sigma_A^2 = \frac{1}{2}.$$

In this particular case,

$$\left(\frac{d^2}{dA^2}\chi^2\right) = \frac{2N}{\sigma^2}$$

and so the usual $\sqrt{N}$ scaling of statistical errors arises

$$\sigma_A^2 = \frac{\sigma^2}{N}$$

The importance of this very predictable result is that it points the way forward for more complicated situations.

The above argument is more easily remembered and encoded as a simple rule, known as the $\Delta\chi^2 = 1$ rule. The error for single parameter is the shift of the parameter from the minimum of χ^2 that raises χ^2 by one. This variation rule is simple to remember .

3.6.2 Weighted Averages

Suppose we have data distributed as a normal distribution around some unknown mean A, but where each measured data point has a different width σ_i.

$$P_{X_i}(x_i) = \frac{1}{\sqrt{2\pi}\sigma_i} e^{-\frac{(x_i - A)^2}{2\sigma_i^2}}$$

Now, varying A to maximising the probability of the distribution describing our data yields:

$$0 = \frac{d}{dA}\chi^2 = -2\sum_i \frac{x_i - A}{\sigma_i^2}$$

and so,

$$A = \frac{\sum_i \frac{x_i}{\sigma_i^2}}{\sum_j \frac{1}{\sigma_j^2}}$$

This is the (famous) weighted mean for averaging data points with errors.

At the minimum,

$$\frac{d^2\chi^2}{dA^2} = 2\sum_i \frac{1}{\sigma_i^2}$$

We take the variance of the weighted average as

$$\sigma_A^2 = \frac{1}{\sum_j \frac{1}{\sigma_j^2}}$$

If we vary A by an amount σ_A, then the change in χ^2 is

$$\Delta\chi^2 = \frac{1}{2} \cdot \frac{d^2\chi^2}{dA^2}\sigma_A^2 = 1$$

If all the σ_i are the same, this gives our familiar $\sqrt{N}$ reduction for the error on the mean.

PDG scale factors

When combining results in some way (either weighted average or by fitting) χ^2/dof is a key measure of the statistical self-consistency of the analysis.

χ^2/dof is much bigger than one there is likely a problem with the error estimates of at least one of the measurements, because obtaining a large χ^2 should have been unlikely.

It is common practice (e.g. the Particle Data Group, or PDG) to conservatively inflate the error after averaging or fitting by a scale factor

$$\sigma^{\text{scaled}} = \sqrt{\chi^2/N_{dof}}\sigma.$$

This corresponds to replacing up all input errors with increased errors that would yield a statistically believable $\chi^2/N_{dof} = 1$.

3.7 General curve fitting

Suppose we have some number N_x of experimental inputs (x-values, $\{x_i\}$) and experimental results (y-values, $\{y_i\}$), each of which has a random error, $\{\sigma_i\}$.

The random variables are now the co-ordinates y_i, and the x_i are precisely known ordinates. We seek to fit a model curve $y = f_{\{p\}}(x)$

These which can be plotted on a two dimensional plot, and we have some expected model function $f_{\{p\}}(x)$ depending on some set of N_p parameters $\{p_i\} = \{p_1, \ldots, p_{N_p}\}$.

We expect that, with the "true" parameters,

$$y = f_{\{p\}}(x)$$

will be a curve that well describes the data,

Our expected probability distribution depends on the parameters $\{p\}$

$$P_{Y_i}(y_i) = \frac{1}{\sqrt{2\pi}\sigma_i} e^{-\frac{(y_i - f_{\{p\}}(x_i))^2}{2\sigma_i^2}}$$

The definition of χ^2 becomes

$$\chi^2 = \sum_i \frac{(y_i - f_{\{p\}}(x_i))^2}{\sigma_i^2}$$

and we seek the parameters p that minimise χ^2.

We must find parameters $\{p\}$ such that for all j

$$0 = \frac{\partial \chi^2}{\partial p_j} = -2 \sum_n \frac{\partial f_{\{p\}}(x_n)}{\partial p_j} \frac{(y_n - f_{\{p\}}(x_n))}{\sigma_n^2}$$

For general functions this minimisation has to be performed numerically. This is normally perfromed using the Marquardt-Levenberg algorithm, which itself is an improvement on steepest descent.

3.7.1 Quality of fit

A fit has some number $N_{dof} = N_x - N_p$ of degrees of freedom. For example, if fitting 7 data points with a 2 parameter function we have dof $= 5 = 7 - 2$.

As discussed above, we expect $\chi^2 \sim N_{dof}$ for any fit after we have determined the most likely parameters.

For example, a line always fits two data points perfectly and gives zero χ^2 after fitting. It is only once we have three data points for a two parameter linear fit that we gain any measure of the statistical consistency of the data.

We are interested in the value of χ^2 after we have found those parameters that minimise χ^2. If this χ^2 is too high, we have not been successful in fitting the data with our model.

If χ^2/N_{dof} is too low, we have unbelievably good fit, and have likely overestimated the errors on the individual datapoints.

3.7.2 Confidence regions

We can ask how much the fitted parameters are likely to vary.

There is some set of parameters $\{p_{\min}\}$ that minimise χ^2. At this minimum

$$\frac{\partial}{\partial p_j}\chi^2(\{p_{\min}\}) = 0$$

We define a matrix M_{ij} as the second partial derivative

$$M_{ij} = \frac{\partial^2}{\partial p_i \partial p_j}\chi^2(\{p_{\min}\}) = \sum_n \frac{2}{\sigma_n^2}\left[\frac{\partial f_{\{p\}}(x_n)}{\partial p_i}\frac{\partial f_{\{p\}}(x_n)}{\partial p_j} - \frac{\partial^2 f_{\{p\}}(x_n)}{\partial p_i \partial p_j}(y_n - f_{\{p\}}(x_n))\right]$$

M_{ij} is symmetric, so for example, $M_{12} = M_{21}$. In the region of the minimum we define the parameter shifts

$$\{\tilde{p}\} = \{p\} - \{p_{\min}\}$$

we can Taylor expand χ^2 in the region of the minimum as

$$\chi^2(\tilde{p}) = \chi^2_{\min} + \frac{1}{2}\tilde{p}^T M \tilde{p}$$

The best definition for a region of confidence for our fitted parameters is to select the subset of possible parameters that represents the most likely 68% of the distribution (for example).

As the maximum likelihood interpretation of χ^2 is as a probability for the parameters, the boundary of such a confidence region is necessarily a curve, or contour of constant χ^2. We take the shift of this contour from the absolute minimum of χ^2 and the region is defined by

$$\chi^2_{\min} - \chi^2(\tilde{p}) = \frac{1}{2}\tilde{p}^T M \tilde{p} \leq \Delta\chi^2 \tag{7.4}$$

The correct approach is to take $\Delta\chi^2$ to cover the 68th percentile of the cumulative distribution

$$P^{\text{CDF}}_{\chi^2}(N_{\text{dof}}, \Delta_{\chi^2}) = 0.68$$

(see table in section 3.5.1).

It is also fairly common for the Δ_{χ^2} defining the allowed space to be simply taken as the approximate value $\frac{\Delta_{\chi^2}}{N_{\text{dof}}} = 1$ (i.e.$\Delta_{\chi^2} = N_{\text{dof}}$).

- With one parameter there is an allowed band

$$\frac{1}{2}\tilde{p}_1^2 M_{11} \leq \Delta_{\chi^2} = 1$$

- With two parameters there is an allowed ellipse [1]

$$\frac{1}{2}[\tilde{p}_1^2 M_{11} + 2\tilde{p}_1\tilde{p}_2 M_{12} + \tilde{p}_2^2 M_{22}] \leq \Delta_{\chi^2} = 2.3$$

General case

With N_p parameters we determine an ellipsoid region parameter space. M_{ij} is symmetric because $\frac{\partial^2}{\partial_i \partial_j} = \frac{\partial^2}{\partial_j \partial_i}$. Symmetric matrices are diagonalisable, and thus M_{ij} is diagonalisable with

$$M_{ij} = V^T \text{diag}(\lambda_1, \ldots, \lambda_N) V$$

where V is a unitary matrix representing a change of basis and whose rows contain the N_p eigenvectors e_k of M_{ij}, and these are orthogonal to each other.

Example

For example, for $N_p = 2$ parameters, V must have the form

$$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

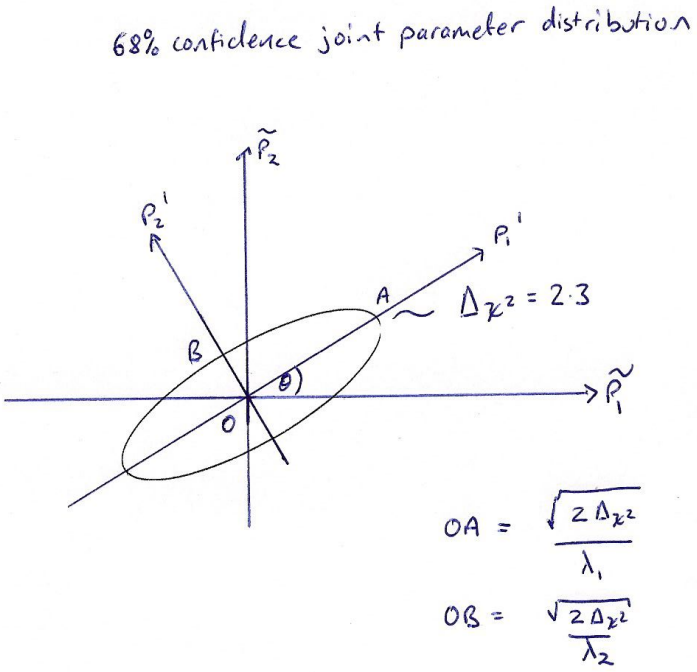
In other words, there are *rotated* parameters

$$p_1' = \cos\theta\tilde{p}_1 + \sin\theta\tilde{p}_2$$
$$p_2' = \cos\theta\tilde{p}_2 - \sin\theta\tilde{p}_1$$

for which the equation $\chi^2 = 2.3$ gives the simple ellipse

$$\lambda_1 p_1'^2 + \lambda_2 p_2'^2 = 2\Delta_{\chi^2}$$

[1] Recall, general ellipse is $ax^2 + by^2 + cxy = d$



The width of the ellipse (major and minor axes) in the p_1' and p_2' directions are $\sqrt{\frac{2\Delta_{\chi^2}}{\lambda_1}}$ and $\sqrt{\frac{2\Delta_{\chi^2}}{\lambda_2}}$ respectively.

We can expand out M

$$\begin{aligned} M &= \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \\ &= \begin{pmatrix} \cos^2\theta\lambda_1 + \lambda_2\sin^2\theta & \sin\theta\cos\theta(\lambda_1 - \lambda_2) \\ \sin\theta\cos\theta(\lambda_1 - \lambda_2) & \sin^2\theta\lambda_1 + \cos^2\theta\lambda_2 \end{pmatrix} \end{aligned}$$

and so,

$$\frac{2M_{12}}{M_{11} - M_{22}} = \frac{2\sin\theta\cos\theta}{\cos^2\theta - \sin^2\theta} = \tan 2\theta$$

Further,

$$\lambda_1 + \lambda_2 = M_{11} + M_{12}$$

and

$$\lambda_1 - \lambda_2 = \frac{M_{12}}{\sin\theta\cos\theta}$$

3.7.3 Single parameter errors

Independent standard deviations on *correlated* fit parameters are somewhat ambiguous as the parameters do not independently vary.

The rule is that we take the error on the j-th parameter as

$$\sigma_j^2 = 2(M^{-1})_{jj}$$

It is common to define a covariance matrix

$$C_{ij} = 2(M^{-1})_{ij}$$

and the error on the j-th parameter is given by

$$\sigma_j^2 = C_{jj}$$

Gnuplot will be introduced in the next section. For completeness, Gnuplot prints the correlation matrix

$$\mathrm{Corr}_{ij} = \frac{C_{ij}}{\sigma_i \sigma_j}$$

In principle this can be used to connect parameter errors σ_j to the ellipsoid region of the joint distribution as given above.

Your lecturer does not believe this is often done in practice because it is involved.

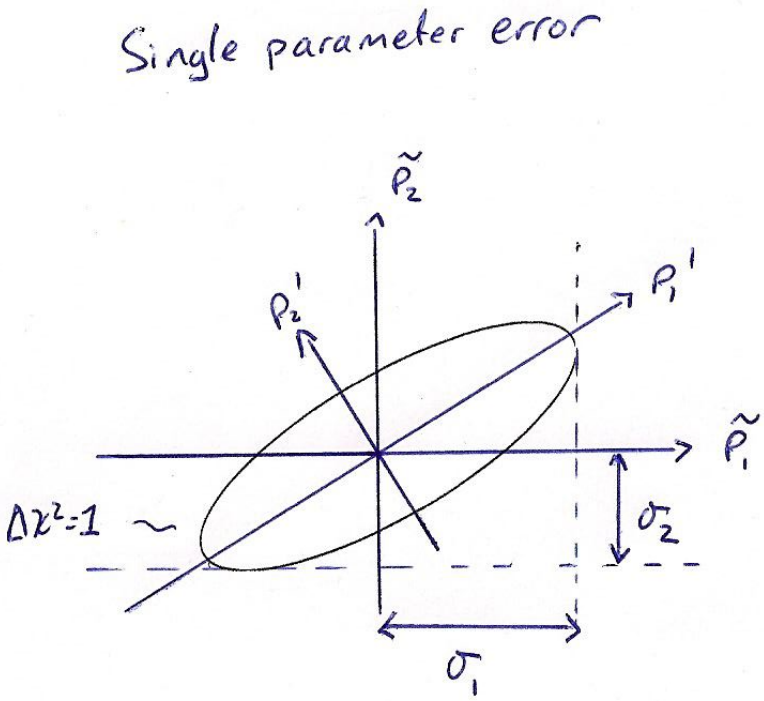
3.7.4 Detail on the single parameter error

We must displace one parameter ($\tilde{p}_1$ for example) at a time by an amount σ, while leaving the other parameters ($\tilde{p}_2 \ldots \tilde{p}_{N_p}$) free to take whatever minimises $\chi^2(\{\tilde{p}\}$.

The error is defined from the 68th percentile of this single degree of freedom χ^2 distribution[2]. That is we find the value of $\tilde{p}_1$ leading to $\delta\chi^2 = 1$ (subject to allowing the other parameters to float to a minimum of χ^2).

Pictorially this means we displace p_1 as far as we can while satisfying $\Delta_{\chi^2} = 1$, and select the vertical tangent to the $\Delta_{\chi^2} = 1$ contour

[2] Note that if we were to consider the parameter errors in the diagonalised basis p'_j fluctuations would combine in the usual way of a χ^2 distribution of two degrees of freedom so that single parameter error estimates with $\Delta\chi^2 = 1$ are consistent with joint two parameter fluctuations at $\Delta\chi^2 = 2.3$.



Mathematically, we must minimise

$$\chi^2(\tilde{p}) = \chi^2_{\min} + \frac{1}{2}\tilde{p}^T M \tilde{p}$$

Subject to the *constraint* that $\tilde{p}_1 = \sigma_1$.

Constrained minimisation: Lagrange multipliers

We introduce a general method for constrained minimisation called the method of Lagrange multipliers. This is generally useful, and not specific to this context.

To minimise $\chi^2(\tilde{p})$ over the surface of $\tilde{p}_1 = \sigma_1$ by varying $\tilde{p}_1 \ldots \tilde{p}_{N_p}$ we require that the components for $\nabla_p \chi^2(\tilde{p})$ parallel to the surface be zero (otherwise, we can reduce χ^2 by moving within the surface).

The normal to this surface is (in our case) $\hat{n} = (1, 0, \ldots, 0)$. [3]

This means that at the minimum $\nabla\chi^2$ must be parallel to the normal and so they are

[3] for a general surface $f(\vec{p}) = C$, the normal is parallel to ∇f

proportional with an unknown constant of proportionality λ

$$\nabla_p \chi^2(\tilde{p}) = M_{ij}\tilde{p}_j = \lambda\hat{n} = \begin{bmatrix} \lambda \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Where λ is an unknown constant called a Lagrange multiplier. Thus,

$$\tilde{p}_j = \lambda M^{-1}_{j1}$$

Now, we chose our surface to have $\tilde{p}_1 = \lambda M^{-1}_{11} = \sigma_1$, and so $\lambda = \frac{\sigma_1}{M^{-1}_{11}}$.

We will then define the value of σ_1 by requiring that χ^2 hold the value $\chi^2(\tilde{p}) = 1$, in order that we obtain the 68th percentile for a single variable χ^2 distribution. This means that

$$\begin{aligned} \Delta_{\chi^2} = 1 &= \frac{1}{2}\tilde{p}^T M \tilde{p} \\ &= \frac{1}{2}\frac{\sigma_1^2}{(M^{-1}_{11})^2} M^{-1}_{1j} M_{jk} M^{-1}_{k1} \\ &= \frac{1}{2M^{-1}_{11}}\sigma_1^2 \end{aligned}$$

and generalising to any parameter p_j

$$\sigma_j^2 = 2(M^{-1})_{jj}$$

3.8 gnuplot

The common Linux package gnuplot includes an implementation of the Marquardt-Levenberg algorithm and can plot and fit any function you care to type in.

This is quite useful to demonstrate the topics discussed in this chapter.

First we must prepare our experimental data in a form that gnuplot can read.

1. Use a text editor (emacs or similar) to prepare a file "experiment.dat" containing x, y σ_y columns

   ```
   # x y dy
   1 1.01 0.01
   2 3.98 0.02
   3 9.02 0.03
   ```

2. start gnuplot in the same directory as the file

   ```
   bash$ gnuplot
   ```

3. First simply plot the data file. For example:

```
gnuplot> plot 'experiment.dat' using 1:2:3 with yerrorbars
gnuplot> set xrange [0:4]
gnuplot> set yrange [0:10]
gnuplot> replot
```

4. We can define a fit function as follows

```
gnuplot> y(x) = A * x*x
gnuplot> A=0.5
gnuplot> replot y(x)
```

5. We can tell gnuplot to perform a fit as follows:

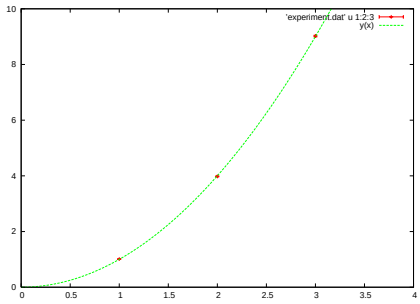
```
gnuplot> fit y(x) 'experiment.dat' using 1:2:3 via A
```

6. We can replot with the fit results

```
gnuplot> replot
```

7. We can save the fit to a postscript file with

```
gnuplot> set terminal postscript landscape color
gnuplot> set output 'experiment.ps'
gnuplot> replot
```



8. We can look at the fitted parameters. Gnuplot prints

```
After 4 iterations the fit converged.
final sum of squares of residuals : 2.37302
rel. change during last iteration : -1.13084e-11

degrees of freedom (ndf) : 2
rms of residuals      (stdfit) = sqrt(WSSR/ndf)      : 1.08927
variance of residuals (reduced chisquare) = WSSR/ndf : 1.18651

Final set of parameters            Asymptotic Standard Error
=======================            ==========================
```

```
A               = 1.00071          +/- 0.002911     (0.2909%)


correlation matrix of the fit parameters:

               A
A               1.000
```

This means it obtained $A = 1.00071$ with $\sigma_A = 0.0029$ (in otherwords $A = 1.001(3)$).

3.9 Multi-parameter fits

It is always a good idea to test statistical fitting code with fake data. Here is a simple C++ programme for generating fake data

```
#include <stdio.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <math.h>

using namespace std;

#define Np (2)

double f(double *params, double x);

double f(double *params, double x)
{
  double y = params[0]+x*params[1];
  return y;
}

int main(int argc,char **argv)
{

  double g ;

  gsl_rng * rng = gsl_rng_alloc(gsl_rng_taus);

  double param_sigma [Np] = {0.1,0.2};
  double param_mean  [Np] = {4, 6};

  double params[Np];

  for(int d=0;d<1000;d++){

    double x = d*0.1;
```

```
    for(int p=0;p<Np;p++) {
      params[p] = param_mean[p]+gsl_ran_gaussian( rng,param_sigma[p]);
    }

    double y=f(params,x);

    double sigmasq=0.0;
    double sigma;
    for(int p=0;p<Np;p++){
      double y0;
      double y1;
      for(int pp=0;pp<Np;pp++){
params[pp] = param_mean[p];
      }
      y0=f(params,x);

      params[p] = param_mean[p]+param_sigma[p];
      y1=f(params,x);
      sigmasq+=(y1-y0)*(y1-y0);
    }
    sigma=sqrt(sigmasq);

    printf("%le %le %le\n",x,y,sigma);
  }
}
```

This can be compiled and run to produce a data file 'fake.dat'

```
g++ fake_data.C -o fake_data -lgsl -lgslcblas
./fake_data > fake.dat
```

We can fit this in gnuplot as follows:

```
f(x)=a+b*x
fit f(x) 'fake.dat' u 1:2:3 via a , b
```

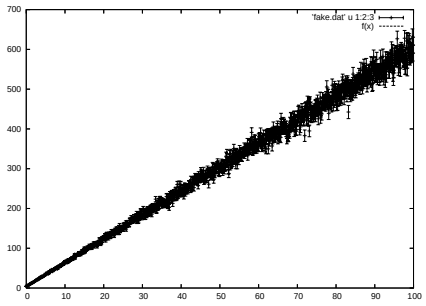
Gnuplot prints

```
Final set of parameters            Asymptotic Standard Error
=======================            ==========================

a               = 3.99426          +/- 0.03571      (0.894%)
b               = 5.99001          +/- 0.006545     (0.1093%)


correlation matrix of the fit parameters:
```

```
               a      b
a               1.000
b              -0.291  1.000
```

The fit can be plotted

```
plot 'fake.dat' u 1:2:3 w e, f(x)
```



and a postscript graph saved for inclusion in reports or lecture notes:

```
set terminal postscript landscape color
set output 'fake.ps'
replot
```

3.9.1 Correlation matrix

Recall, we previously defined the parameter covariance matrix

$$C_{ij} = 2(M^{-1})_{ij}$$

where

$$M_{ij} = \frac{\partial^2}{\partial p_i \partial p_j} \chi^2(\{p_{\min}\})$$

Gnuplot plots the corresponding correlation matrix:

$$\mathrm{Corr}_{ij} = \frac{C_{ij}}{\sqrt{C_{ii} C_{jj}}}$$

If the off diagonal elements of this become close to 1 or -1 we might worry that the parameter confidence region will have a complex shape.

3.9.2 How do I convince myself the error is right?

Well, there are 1000 data points.

Note that our fake data has an error (0.2)from the slope parameter that grows linearly in x. All datapoints except for the very small X datapoints do not particularly constrain the constant, but do constrain the slope.

This slope, with error of 0.2 is estimated roughly 1000 times with independent random selections from the distribution. The error on the mean should be $\frac{0.2}{\sqrt{1000}=0.00632}$ which is indeed close to the result from Gnuplot.

3.10 Defining fit functions

Gnuplot allows you to define your own functions as shown above.

These can be simple expressions, such as polynomials, or be built out of pre-existing Gnuplot functions.

The most useful of the pre-existing functions are:

Sinusoid) sin, cos, tan, asin, acos, atan

Exponential) exp, log

Bessel) besj0, besj1

Others) sqrt, erf, abs, gamma

3.11 Help in gnuplot

The command "help" is probably the most useful. Try:

- help plot
- help fit
- help set

Ranges for graphs, titles, axis labels, logarithmic axes etc. can all be set with the *set* command.

3.12 More information

Gnuplot is installed in the CP Lab, and can be run as **gnuplot44**

See:

`http://gnuplot.sourceforge.net/`

The following links within sourceforge are very useful

- Demos
- Documentation
- Tutorials, learning and help