Mathematical Methods of Physics

John Boccio

Why a mathematical methods Course? This Mathematical Methods in Physics course was designed for **one purpose only**, namely, to **supplement** standard mathematics courses normally taken by physics majors with an **extensive discussion of the theoretical and computational methods and techniques that are needed for studying advanced physics**.

Specifically, we decided to **forego extensive proofs** in favor of presenting the details of methods and techniques, presenting lots of examples and making some connections to physics and astronomy.

Often, a procedure will be defined or a method proposed **without any justification** (and certainly without any proof). This is being done **on purpose**. We simply do not have the **time** to do both the methods **and** the proofs. Often the **only justification** required for using a particular mathematical procedure or making a particular mathematical definition in physics or astronomy is that **it works**, that is, it gives results (solutions of equations) that **agree with experiments** in the real world.

Mathematicians are able to **create** (choose the relevant axioms or postulates) their own **worlds** and then proceed to investigate their properties.

Physicists **must derive** their axioms and postulates from the **real world systems** under investigation. This can only be done via **experimentation**. **Based on** the axioms and postulates so derived from experimenting with the real world, we then make definitions, design methods and techniques and invent theories.

For example, when studying partial differential equations (PDEs), the **mathematician** will spend most of the time understanding **existence and uniqueness** properties of solutions. The **physicist**, on the other hand, spends **almost no time** in these areas. We **know** the solutions exist because we can set up real systems in the laboratory and experiment on them. We **know** the solutions are unique because the experimental results are reproducible.

More **important** to the physicist are the **equations** representing the system, the solution **methods**, the **exact or approximate** particular solutions we can find when applying the solution methods to the equations and the **physical properties** of the solutions.

The question "**why we make certain choices**" is really not relevant. The answer will always be simply "**that is the way the real world seems to work**".

This is the **approach** I will take in lectures and **your questions**, etc, should also **take into account** this approach to the mathematics. In this way, we will have harmonious and efficient classroom lectures and discussions.

Inroduction Space of Physics

Scalar = a number (temperature, minutes after noon, ...)

Vector = set of 3 numbers (characterizes a point in the 3-dimensional world)

The vector representing the location of a point in 3-dimensional space relative to a given origin is called the **position vector.**

It is represented by the 3-tuple

$$\vec{r} = (x, y, z) = (x_1, x_2, x_3)$$

This is a shorthand notation for

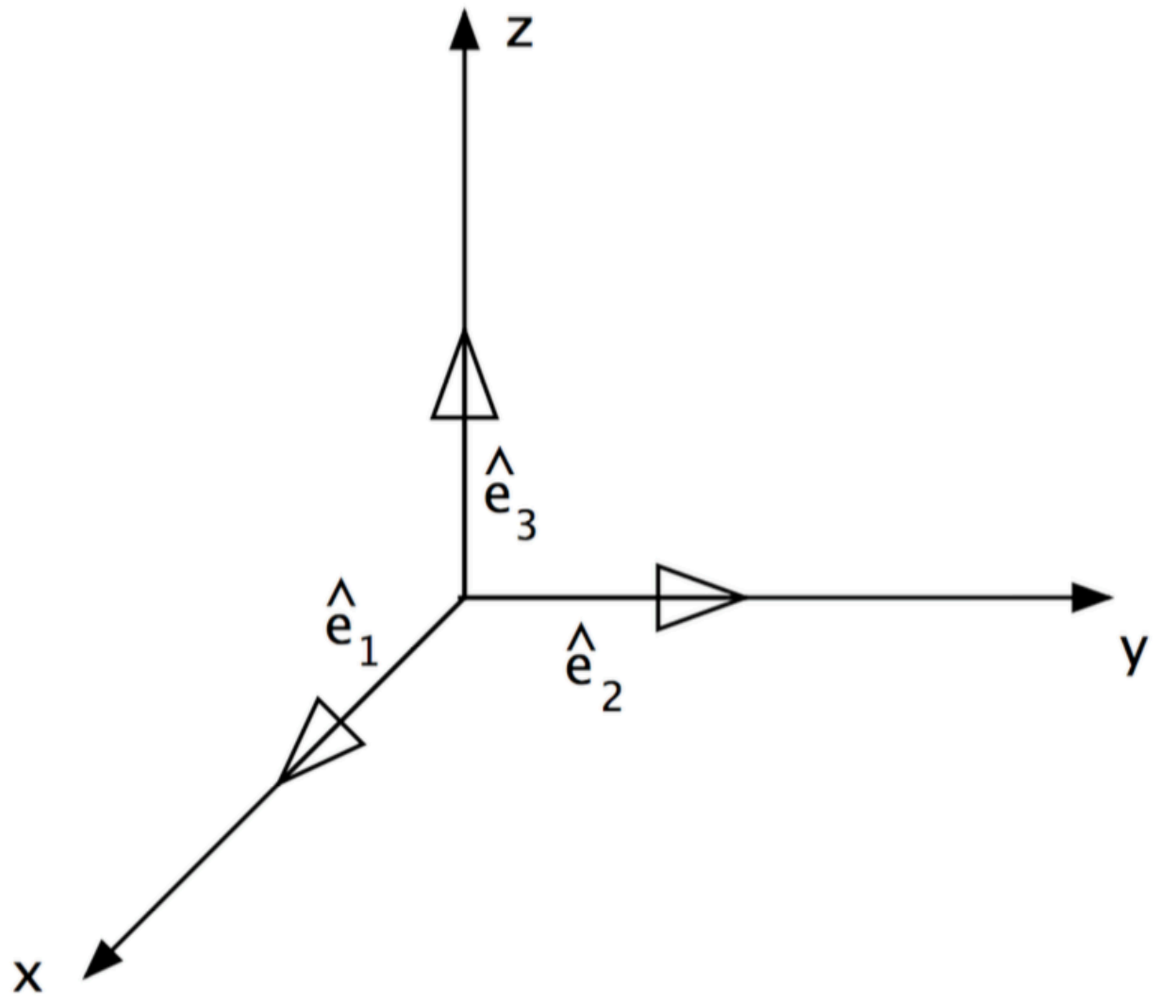
$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k} = x_1\hat{e}_1 + x_2\hat{e}_2 + x_3\hat{e}_3$$

which are equivalent representations of the position vector.

The three(for 3 dimensions) vectors

$$\hat{e}_1, \hat{e}_2, \hat{e}_3 \quad \text{or} \quad \hat{i}, \hat{j}, \hat{k}$$

are unit vectors (length = 1) defining a right-handed coordinate system as show below:



The numbers (x, y, z) are called the components of the vectors with respect to the chosen unit vectors.

The unit vectors are chosen to be orthogonal (perpendicular) for convenience as we shall see.

The length of the position vector is given (Pythagorean theorem) by

$$r = |\vec{r}| = \sqrt{x^2 + y^2 + z^2}$$

We define a **vector product operation** (symbol $= \cdot$) called the **scalar** or **dot** or **inner product** by the following relations among the unit vectors:

$$\hat{e}_i \cdot \hat{e}_j = \delta_{ij} = \text{ Kronecker delta} = \begin{cases} 1 & i = j \\ 0 & \text{otherwise} \end{cases}$$

In terms of the scalar product we have

$$r^2 = \vec{r} \cdot \vec{r} = \left(\sum_{i=1}^{3} x_i \hat{e}_i \right) \cdot \left(\sum_{j=1}^{3} x_j \hat{e}_j \right)$$

$$= \sum_{i,j=1}^{3} x_i x_j \hat{e}_i \cdot \hat{e}_j = \sum_{i,j=1}^{3} x_i x_j \delta_{ij} = \sum_{i,=1}^{3} x_i^2$$

We now define the Einstein summation convention, which assumes a summation anytime that a repeated index appears in the same term.

Using this convention the above derivation looks like

$$r^2 = \vec{r} \cdot \vec{r} = (x_i \hat{e}_i) \cdot (x_j \hat{e}_j) = x_i x_j \hat{e}_i \cdot \hat{e}_j = x_i x_j \delta_{ij} = x_i x_i$$

We define a unit vector in the direction of the position vector by

$$\hat{e}_r = \hat{e}(\vec{r}) = \hat{r} = \frac{\vec{r}}{r} = \frac{x_i \hat{e}_i}{r} \rightarrow \vec{r} = r\hat{e}_r$$

This rule generalizes to an arbitrary vector as follows:

$$\vec{A} = A_i \hat{e}_i = A\hat{e}(\vec{A})$$

Vector Algebra

$$\vec{C} = C_i \hat{e}_i$$

$$\vec{C} = \vec{A} + \vec{B} = (A_i + B_i)\hat{e}_i \rightarrow C_i = A_i + B_i$$

$$\vec{C} = \lambda\vec{A} = \lambda A_i \hat{e}_i \rightarrow C_i = \lambda A_i$$

$$\vec{0} = (0,0,0) = \text{ zero or null vector}$$

$$-\vec{A} = (-A_i)\hat{e}_i = -A\hat{e}(\vec{A})$$

$$(-\vec{A}) + \vec{A} = \vec{0}$$

$$\hat{(}e)(-\vec{A}) = -\hat{e}(\vec{A})$$

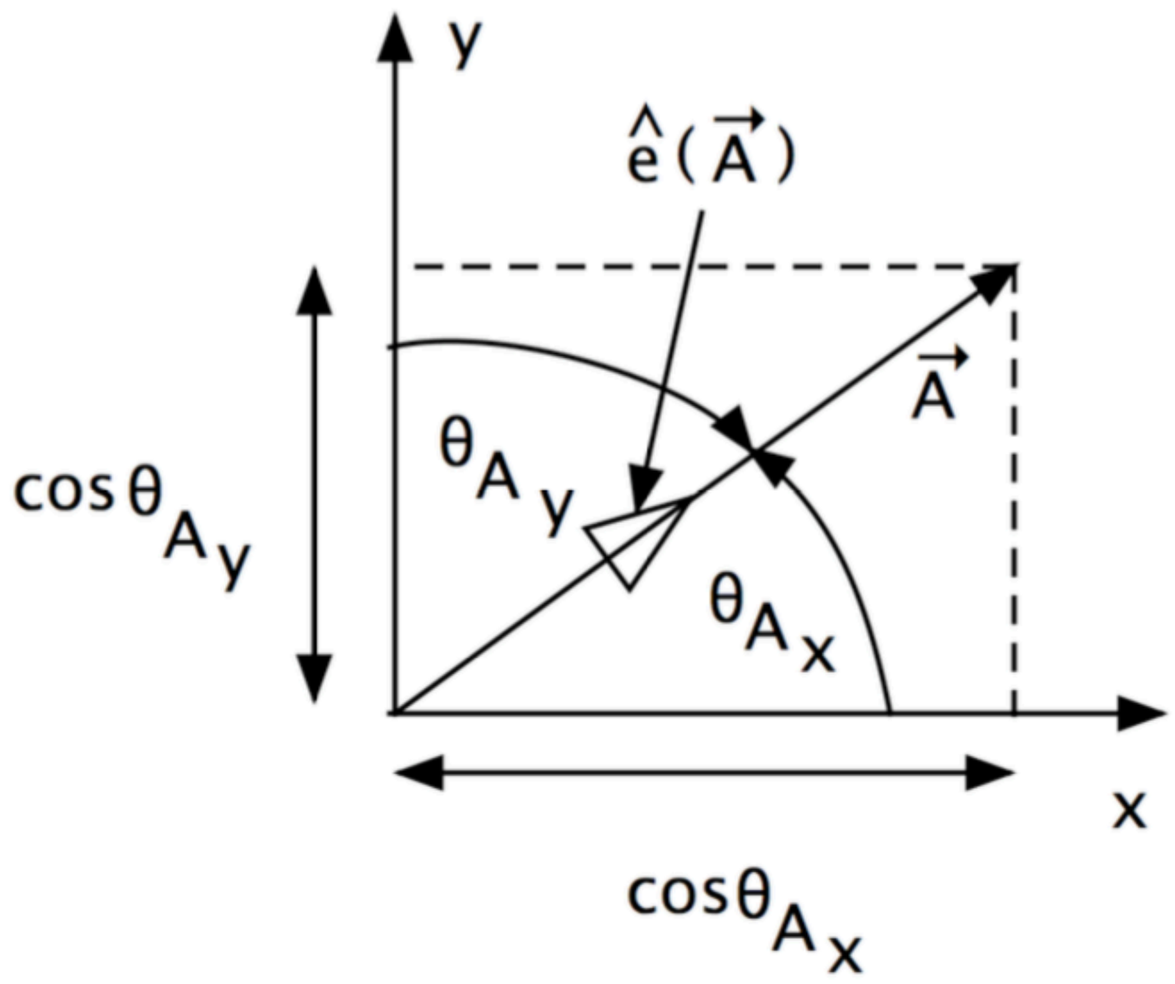
Geometry of Space

For general vectors $\vec{A}$ and $\vec{B}$, the scalar product gives

$$\vec{A} \cdot \vec{B} = A_i B_j \hat{e}_i \cdot \hat{e}_j = A_i B_j \delta_{ij} = A_i B_i$$

and the length squared of a vector is $\vec{A} \cdot \vec{A}$.

In 2-dimensions (completely general result because any two vectors form a single 2-dimensional plane) using the diagram below



we have

$$\hat{e}(\vec{A}) = \cos\theta_{A_x}\hat{e}_x + \sin\theta_{A_x}\hat{e}_y = \cos\theta_{A_x}\hat{e}_x + \cos\theta_{A_y}\hat{e}_y$$

These components are called **direction cosines**.

In general,

$$\hat{e}(\vec{A}) \cdot \hat{e}_x = \cos\theta_{A_x} \qquad \text{and so on.}$$

So, in general we have

$$\hat{e}(\vec{A}) = \cos\theta_{A_x}\hat{e}_x + \cos\theta_{A_y}\hat{e}_y + \cos\theta_{A_z}\hat{e}_z = (\hat{e}(\vec{A}) \cdot \hat{e}_i)\hat{e}_i$$

For a general vector

$$\vec{A} = A\hat{e}(\vec{A}) \rightarrow \vec{A} \cdot \hat{e}_i = i^{th} \text{ component } = A\hat{e}(\vec{A}) \cdot \hat{e}_i = A\cos\theta_{A_i}$$

This leads to the general rule

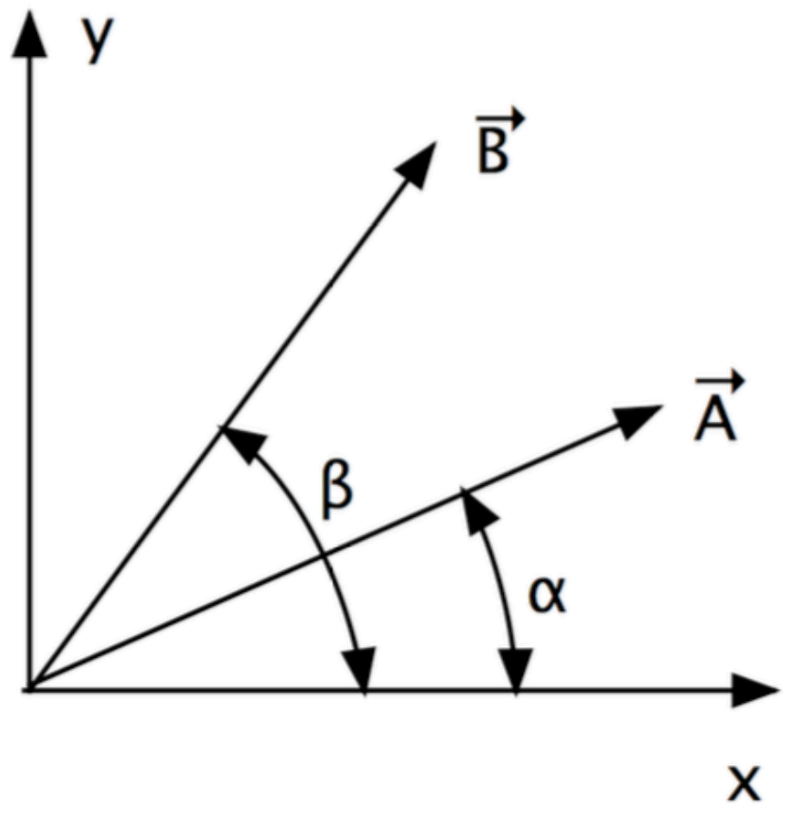
$$\vec{A} \cdot \vec{B} = AB\hat{e}(\vec{A}) \cdot \hat{e}(\vec{B}) = AB\cos\theta_{AB}$$

where

$$\theta_{AB} = \text{ angle between } \vec{A} \text{ and } \vec{B}$$

So if two vectors are perpendicular or orthogonal, then their scalar product is equal to zero.

Another way of writing relation this (using the diagram below)



gives

$$\vec{A}\cdot\vec{B} = AB\cos(\beta-\alpha) = A_xB_x+A_yB_y = AB(\cos\alpha\cos\beta-\sin\alpha\sin\beta)$$

This implies that

$$\cos(\beta-\alpha) = \cos\alpha\cos\beta - \sin\alpha\sin\beta$$

which we know to be correct!

Vector Product

We define the term *permutation* as a rearrangement of the elements of a set of numbers. The word *permutation* also refers to the act or process of changing the linear order of an ordered set; even/odd = even/odd number of moves in rearrangement.

Then, we define the vector product(symbol $= \times$) of two vectors in terms of the standard cartesian unit vectors as follows:

$$\hat{e}_i \times \hat{e}_j = \epsilon_{ijk} \hat{e}_k$$

where ϵ_{ijk} is the totally antisymmetric tensor (we will define all of it properties in detail later in the course) in 3-dimensions and is given by

$$\epsilon_{ijk} = \begin{cases} 1 & \text{if } ijk = \text{ even permutation of } 123 \\ -1 & \text{if } ijk = \text{ odd permutation of } 123 \\ 0 & \text{otherwise} \end{cases}$$

Let us work out some properties of vectors derivable from this vector(or cross) product definition involving ϵ_{ijk}.

For two arbitrary vectors we have

$$\vec{A} \times \vec{B} = (A_i \hat{e}_i) \times (B_j \hat{e}_j) = A_i B_j \hat{e}_i \times \hat{e}_j = \epsilon_{ijk} A_i B_j \hat{e}_k = \epsilon_{ijk} A_j B_k \hat{e}_i$$

In 2-dimensions(for simplicity) using the diagram above we have

$$\begin{aligned}
\vec{A} \times \vec{B} &= (A_1 \hat{e}_1 + A_2 \hat{e}_2) \times (B_1 \hat{e}_1 + B_2 \hat{e}_2) \\
&= A_1 B_1 \hat{e}_1 \times \hat{e}_1 + A_1 B_2 \hat{e}_1 \times \hat{e}_2 + A_2 B_1 \hat{e}_2 \times \hat{e}_1 + A_2 B_2 \hat{e}_2 \times \hat{e}_2 \\
&= (A_1 B_2 - A_2 B_1) \hat{e}_1 \times \hat{e}_2 = (A_1 B_2 - A_2 B_1) \hat{e}_3 \\
&= AB(\cos\alpha \sin\beta - \sin\alpha \cos\beta) \hat{e}_3 \\
&= AB \sin(\beta - \alpha) \hat{e}_3
\end{aligned}$$

So if two vectors are parallel, then their vector product is equal to zero.

The relation

$$\vec{A} \times \vec{B} = \epsilon_{ijk} A_j B_k \hat{e}_i \rightarrow (\vec{A} \times \vec{B})_i = \epsilon_{ijk} A_j B_k$$

Why should we introduce ϵ_{ijk}?

(1) It is the easiest way to do complicated vector algebra in 3-dimensions

(2) For higher dimensions ϵ_{ijk} it is the only way.

(3) It makes for a natural transition to other areas of mathematics (tensors) that are used in more advanced courses.

Properties

$$\epsilon_{mnk}\epsilon_{ijk} = \delta_{mi}\delta_{nj} - \delta_{ni}\delta_{mj}$$

$$\epsilon_{mjk}\epsilon_{ijk} = 2\delta_{mi}$$

$$\epsilon_{ijk}\epsilon_{ijk} = 6$$

Example of use in complex vector identity:

$$\begin{aligned}
\vec{A} \times (\vec{B} \times \vec{C}) &= \epsilon_{ijk} A_j (\vec{B} \times \vec{C})_k \hat{e}_i \\
&= \epsilon_{ijk} A_j (\epsilon_{kmn} B_m C_n) \hat{e}_i \\
&= \epsilon_{ijk} \epsilon_{mnk} A_j B_m C_n \hat{e}_i \\
&= (\delta_{im}\delta_{jn} - \delta_{in}\delta_{jm}) A_j B_m C_n \hat{e}_i \\
&= A_j B_i C_j \hat{e}_i - A_j C_i B_j \hat{e}_i \\
&= \vec{B}(\vec{A} \cdot \vec{C}) - \vec{C}(\vec{A} \cdot \vec{B})
\end{aligned}$$

The Rotation Matrix

We will designate a matrix (rectangular array of numbers) by the symbol

$$[M] = \begin{pmatrix} 1 & 7 & 0 \\ 3 & -4 & 5 \\ -2 & 0 & 9 \end{pmatrix}$$

The individual elements are written with subscripts, i.e.,

$$M_{12} = 7 = M_{row,column}$$

The matrix product of $[M]$ and $[N]$, where

$$[N] = \begin{pmatrix} -3 & 0 & 7 & 1 \\ 8 & 1 & 7 & 4 \\ -6 & 2 & -5 & -9 \end{pmatrix}$$

is written as $[M][N] = [P]$ where we must have the number of columns in $[M]$ must equal to the number of rows in $[N]$ and the number of rows in $[P]$ is equal to the number of rows in $[M]$ and the number of columns in $[P]$ is equal to the number of columns in $[N]$.

In the summation convention we write

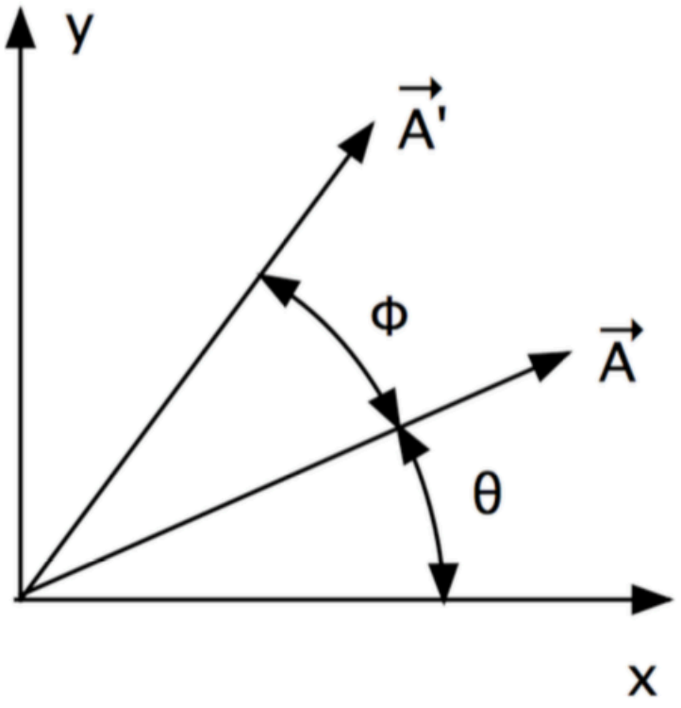
$$P_{ij} = M_{ik} N_{kj}$$

Vector Rotation

Consider a vector

$$\vec{A} = A_1\hat{e}_1 + A_2\hat{e}_2 = A\cos\theta\hat{e}_1 + A\sin\theta\hat{e}_2$$

Now rotate the vector through an angle ϕ as shown:



We then have

$$\vec{A}' = A_1'\hat{e}_1 + A_2'\hat{e}_2 = A\cos(\theta+\phi)\hat{e}_1 + A\sin(\theta+\phi)\hat{e}_2$$

Therefore we have that the components transform as

$$A_1' = A_1 \cos\phi - A_2 \sin\phi$$
$$A_2' = A_1 \sin\phi + A_2 \cos\phi$$

Using matrix notation we have

$$[A'] = [R(\phi)][A]$$
$$\begin{pmatrix} A_1' \\ A_2' \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix}$$

The matrix $[R(\phi)]$ is called the rotation matrix and is defined by (for a rotation about the z-axis 0r 3-axis) as

$$[R(\phi)] = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}$$

In summation notation we have

$$A_i' = R_{ij} A_j \rightarrow \vec{A}' = R_{ij} A_j \hat{e}_i$$

The rotation matrix is an orthogonal matrix since

$$[R(\phi)]^{\dagger}[R(\phi)] = \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos phi \end{pmatrix} \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = [I] = \text{ identity matrix}$$

This says that the length of the vector does not change under the rotation transformation, i.e.,

$$\vec{A'} \cdot \vec{A'} = (R_{ij} A_j \hat{e}_i) \cdot (R_{mn} A_n \hat{e}_m) = A_j A_n R_{ij} R_{mn} \hat{e}_i \cdot \hat{e}_m = A_j A_n R_{ij} R_{mn} \delta_{im}$$

$$= A_j A_n R_{ij} R_{in} = A_j A_n ([R^{\dagger}])_{ji} R_{in} = A_j A_n ([R^{\dagger} R])_{jn}$$

$$= A_j A_n \delta_{jn} = A_j A_j$$

$$= \vec{A} \cdot \vec{A}$$

Partial Fractions

It is very useful to be able to express a function that is the ratio of two polynomials

$$f(x) = \frac{g(x)}{h(x)}$$

in a form that easier to work with.

The critical behavior of $f(x)$ is determined by the location of the zeroes of its denominator, that is, where $h(x) = 0$.

Later, when we study complex variables we will call these points the poles (or singularities) of $f(x)$.

To make the behavior of $f(x)$ at the poles explicit we try to write $f(x)$ as a sum of terms of the form

$$\frac{A}{(x-\alpha)^n}$$

where α is one of the zeroes of $h(x)$, that is,$h(\alpha) = 0$ and A is a constant.

This expansion is called writing $f(x)$ in **partial fractions**.

Example: Consider the expression

$$f(x) = \frac{g(x)}{h(x)} = \frac{4x+2}{x^2+3x+2}$$

Rules:

(1) The number of distinct terms on the RHS is equal to the number of distinct roots of $h(x) = 0$.

(2) Each term having a different root α_i has a denominator $(x - \alpha_i)^{n_i}$

(3) If α_i is a multiple root, then the value assigned to $n_i =$ value of exponent when $h(x)$ is expressed in terms of its roots, that is, as

$$h(x) = (x - \alpha_1)^{n_1}(x - \alpha_2)^{n_2}.....$$

and $n_1 + n_2 + ... = n =$ highest power in $h(x)$.

If $n_i > 1$, then A must be replaced by and $n_i - 1$ degree polynomial.

Applying these rules to our example we have:

$h(x)$ has 2 roots $\rightarrow$ 2 terms in expansion.

Roots come from:

$h(x) = x^2 + 3x + 2 = (x + 1)(x + 2) = 0 \rightarrow \alpha_1 = -1,$

$\alpha_2 = -2, n_1 = 1, n_2 = 1$

$n_1 + n_2 = n = 2$

Thus, we write

$$f(x) = \frac{g(x)}{h(x)} = \frac{4x+2}{x^2+3x+2} = \frac{A_1}{x+1} + \frac{A_2}{x=2}$$

We determine A_1 and A_2 using algebra as follows:

$$\begin{aligned} 4x+2 &= A_1(x+2) + A_2(x+1) \\ 4 &= A_1 + A_2 \\ 2 &= 2A_1 + A_2 \\ A_1 &= -2, A_2 = 6 \end{aligned}$$

so that

$$f(x) = \frac{g(x)}{h(x)} = \frac{4x+2}{x^2+3x+2} = -\frac{2}{x+1} + \frac{6}{x=2}$$

Complex Numbers

The crucial quantity here is the number i.

It has the property

$$i^2 = -1, i^3 = -i, i^4 = +1, i^5 = i, ...$$

We represent a complex number z as a 2-component object in a cartesian basis as

$$z = (x, y) = x + iy = \mathrm{Real}(z) + i\mathrm{Imag}(z)$$

Alternatively, we can represent it with a plane-polar basis as

$$x = r\cos\theta \;\;,\;\; y = r\sin\theta \;\;,\;\; 0 \leq r \leq \infty \;\;,\;\; -\pi \leq \theta \leq \pi$$

$$r = (x^2 + y^2)^{1/2} \;\;,\;\; \theta = \tan^{-1}\frac{y}{x}$$

$$z = r(cos\theta + i\sin\theta)$$

Now using

$$\sin\theta = \theta - \frac{\theta^3}{3!} + ... \quad , \quad \cos\theta = 1 - \frac{\theta^2}{2!} + ...$$

we get

$$z = r(cos\theta + i\sin\theta) = r\left(1 + i\theta + \frac{(i\theta)^2}{2!} + \frac{(i\theta)^3}{3!}.....\right) = re^{i\theta}$$

This generalizes to let us write

$$\left(1 + im\theta + \frac{(im\theta)^2}{2!} + \frac{(im\theta)^3}{3!}.....\right) = e^{im\theta} = \cos m\theta + i\sin m\theta$$

We can also write

$$e^{im\theta} = \cos m\theta + i\sin m\theta = (e^{i\theta})^m = (cos\theta + i\sin\theta)^m$$

which can be used to get expressions for $\cos m\theta, \sin m\theta$, etc since

$$\cos 2\theta + i \sin 2\theta = (cos\theta + i \sin \theta)^2 = \cos^2 \theta - \sin^2 \theta + 2i \sin \theta \cos \theta$$

$$\rightarrow \cos 2\theta = \cos^2 \theta - \sin^2 \theta$$

$$\rightarrow \sin 2\theta = 2 \sin \theta \cos \theta$$

We define the complex conjugate of z by

$$z^* = x - iy = re^{-i\theta} = r(cos\theta - i \sin \theta)$$

$$zz^* - z^*z = r^2 = |z|^2$$

Note a few special results:

$$e^{2\pi ni} = 1, \rightarrow e^{i\theta} = e^{i(\theta+2n\pi)} \quad , \quad n = \text{ integer}$$

$$e^{i\pi} = -1 \ , \ e^{i\pi/2} = i$$

Using the standard definitions of some mathematical functions we get:

$$z^{1/2} = \sqrt{z} = (re^{i\theta})^{1/2} = \sqrt{r}e^{i\theta/2} = (re^{i(\theta+2n\pi)})^{1/2} = \sqrt{r}e^{i(\theta/2+n\pi)} \quad n = \text{ integer}$$

$$\log z = \log re^{i\theta} = \log r + i\theta = \log re^{i(\theta+2n\pi)} = \log r + i(\theta+2n\pi) \quad n = \text{ integer}$$

This means that these functions are **multi-valued**, that is, the square root has 2 values for each (r, θ) pair and the log has an infinite number of values for each (r, θ) pair.

The ambiguity is avoided by agreement.

We choose $n = 0$ as the principal value of multi-valued functions and restrict $-\pi \leq \theta \leq \pi$.

More Functions:

$$z_1 z_2 = r_1 r - 2e^{i(\theta_1+\theta_2)} \quad , \quad \frac{z_1}{z_2} = \frac{r_1}{r_2} e^{i(\theta_1-\theta_2)}$$

$$z^{1/n} = r^{1/n} e^{i\theta/n} = r^{1/n}(\cos(\theta/n) + i\sin(\theta/n))$$

$$\sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i} \quad , \quad \cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2}$$

This last expression also works for complex angles

$$\cos(iy) = \frac{e^{-y} + e^{y}}{2i} = i\sinh y \rightarrow \cos(i) = \frac{e^{-1} + e^{1}}{2} = 1.54$$

$$\sin(iy) = \frac{e^{-y} - e^{y}}{2} = \cosh y$$

Complex Roots and Powers:

$$a^b = e^{\ln a^b} = e^{b \ln a}$$

$$\rightarrow i^{-2i} = e^{-2i \ln i} = e^{-2i \ln e^{i(\pi/2 \pm 2n\pi)}} = e^{-2i(\ln 1 + i(\pi/2 \pm 2n\pi))} = e^{\pi \pm 4n\pi}$$
$$= e^{\pi \pm 4n\pi} = e^{5\pi}, e^{-3\pi}, e^{9\pi}, ... = 23.14, ...$$

Inverse functions:

$$z = \sinh^{-} 1\left(\frac{x}{a}\right) \rightarrow \frac{x}{a} = sinhz = \frac{e^{z} - e^{-z}}{2}$$

$$\text{Let } e^{z} = u \rightarrow \frac{2x}{a} = u - \frac{1}{u} \rightarrow au^{2} - 2xu - a = 0$$

$$u = e^{z} = \frac{x \pm \sqrt{x^{2} + a^{2}}}{a}$$

The above formula must be valid for all z.

Now for real z, $e^{z} > 0$ which means we must use the $+$ sign or

$$z = \ln\left(e^{z}\right) = x + \sqrt{x^{2} + a^{2}} - \ln\left(a\right)$$

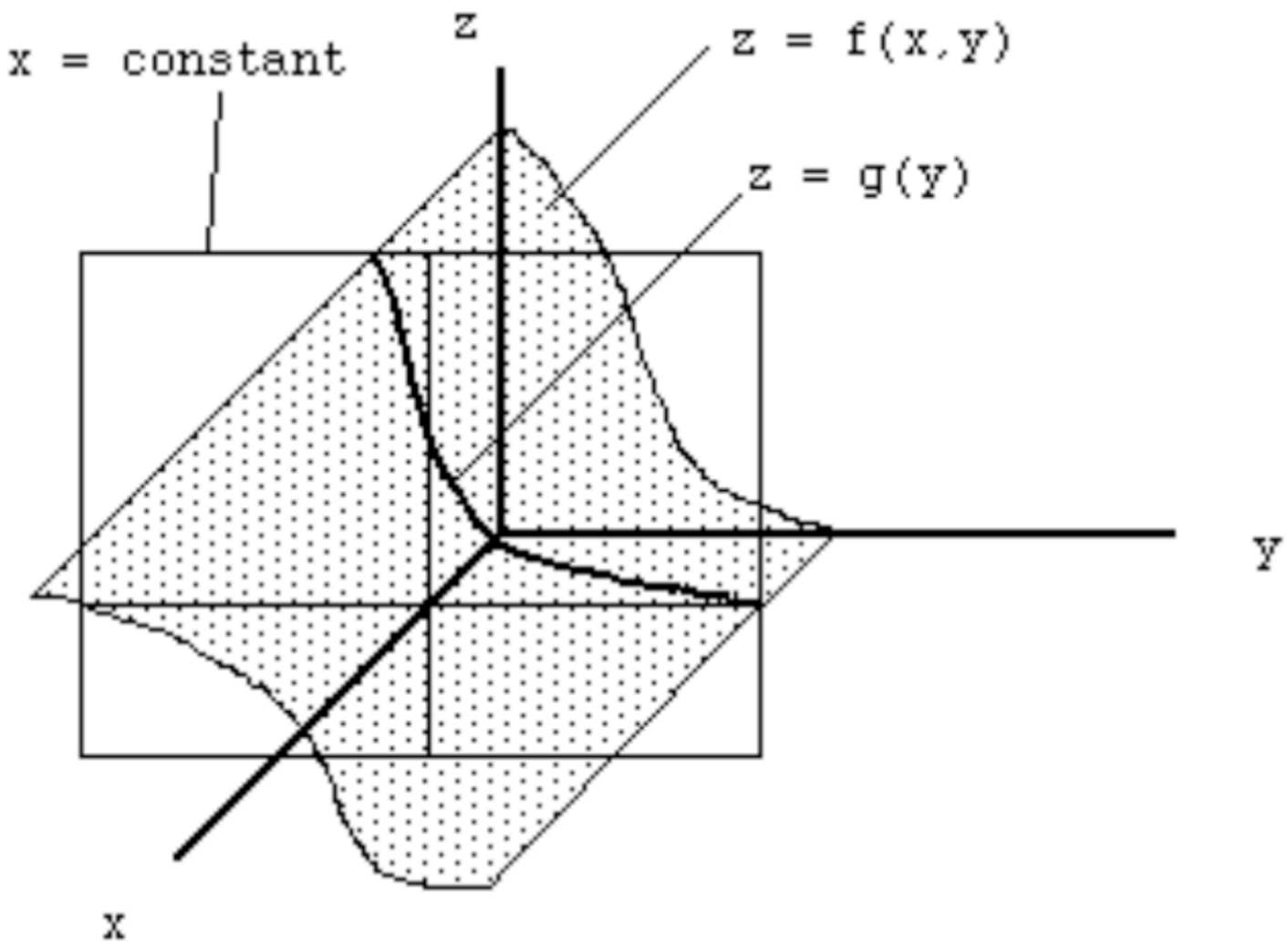
Partial Differentiation

Given the relationship $y = f(x)$, which represents a curve in 2-dimensions, then

$$\frac{dy}{dx} = \frac{df(x)}{dx} = \text{ slope of the curve } y = f(x) \text{ or the rate of change of } y \text{ wrt } x$$

Now, if instead, we are given the relationship $z = f(x, y)$, which represents a surface in 3-dimensions, then differentiation is a bit more complicated.

Suppose $x =$ constant, which is a plane intersecting the surface as shown:



The points satisfying $z = f(x, y)$ and $x =$ constant lie on a curve (as shown in the figure).

To learn about this curve, where $z = g(y)$, we might write dz/dy, but this does not indicate that z really is a function of 2 variables and we are temporarily holding one of the variables constant.

So, instead, we write

$$\frac{\partial z}{\partial y} = \text{ partial derivative of } z \text{ wrt } y$$

where

$$y = f(x) \rightarrow \frac{dy}{dx} = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

$$z = f(x, y) \rightarrow \left(\frac{\partial z}{\partial x}\right)_y = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x, y) - f(x, y)}{\Delta x}$$

If the subscript indicating which variable(s) are constant is left off, then it means that all other variables are constant.

It is important to understand that the notation means z has to be written as a function of x and y only and then differentiated wrt x holding y constant (last equation).

Notation

$$\frac{\partial}{\partial x}\frac{\partial z}{\partial x} \equiv \frac{\partial^2 z}{\partial x^2} \;\;,\;\; \frac{\partial}{\partial x}\frac{\partial z}{\partial y} \equiv \frac{\partial^2 z}{\partial x \partial y} \;\;,\;\; \frac{\partial}{\partial x}\frac{\partial^2 z}{\partial x \partial y} \equiv \frac{\partial^3 z}{\partial x^2 \partial y} \;\;,\;\; etc.....$$

Some examples:

(1)

$$z = x^2 - y^2$$

Using

$$x = r\cos\theta \;\;,\;\; y = r\sin\theta \;\;,\; x^2 + y^2 = r^2$$

we have

$$z = x^2 - y^2 = r^2\cos^2\theta - r^2\sin^2\theta \rightarrow \left(\frac{\partial z}{\partial r}\right)_\theta = 2r(\cos^2\theta - \sin^2\theta)$$

$$z = 2x^2 - r^2 \rightarrow \left(\frac{\partial z}{\partial r}\right)_x = -2r$$

$$z = r^2 - 2y^2 \rightarrow \left(\frac{\partial z}{\partial r}\right)_y = 2r$$

(2)

$$
\begin{aligned}
z = & f(x,y) = xy + x^2 \\
& \rightarrow \frac{\partial z}{\partial x} = y + 2x = \left(\frac{\partial z}{\partial x}\right)_y \\
& \rightarrow \frac{\partial z}{\partial y} = x = \left(\frac{\partial z}{\partial y}\right)_x
\end{aligned}
$$

Suppose that $g = xy$, then we have

$$z = f(x,y) = xy + x^2$$

$$z = h(x,g) = g + x^2$$

$$\left(\frac{\partial f}{\partial x}\right)_g = \left(\frac{\partial h}{\partial x}\right)_g = 2x$$

We now digress to look at **total differentials** and find some interesting facts.

$$\begin{aligned}\Delta f(x,y) &= f(x+\Delta x, y+\Delta y) - f(x,y) \\ &= f(x+\Delta x, y+\Delta y) - f(x+\Delta x, y) + f(x+\Delta x, y) - f(x,y)\end{aligned}$$

Taking the limit as

$$\Delta x \to 0 \quad \text{and} \quad \Delta y \to 0$$

we get

$$df(x,y) = \left(\frac{\partial f}{\partial x}\right)_y dx + \left(\frac{\partial f}{\partial y}\right)_x dy$$

This result easily generalizes to any number of cartesian coordinates.

Now for some function $g(x, y)$, pick dx, dy s.t. $g(x, y) = \text{constant}$ as $(x \to x + \Delta x, y \to y + \Delta y)$.

This implies that

$$g(x + \Delta x, y + \Delta y) = g(x, y)$$

which in turn implies that

$$\left.\frac{df}{dx}\right|_{dg=0} = \left(\frac{\partial f}{\partial x}\right)_y \left.\frac{dx}{dx}\right|_{dg=0} + \left(\frac{\partial f}{\partial y}\right)_x \left.\frac{dy}{dx}\right|_{dg=0}$$

$$\to \left(\frac{\partial f}{\partial x}\right)_g = \left(\frac{\partial f}{\partial x}\right)_y + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial x}\right)_g$$

Going back to our old example we have

$$f = xy + x^2 \quad , \quad g = xy$$

$$\left(\frac{\partial f}{\partial x}\right)_g = \left(\frac{\partial f}{\partial x}\right)_y + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial x}\right)_g$$

$$= (y + 2x) + (x)\left(\frac{\partial \left(\frac{g}{x}\right)}{\partial x}\right)_g$$

$$= (y + 2x) + (x)\left(-\frac{g}{x^2}\right)$$

$$= y + 2x - \frac{g}{x}$$

$$= y + 2x - y = 2x \quad \text{as before}$$

Chain Rule

Suppose we have a function $u(x(t), y(t))$.

For example,

$$u = xy \quad , \quad x(t) = t \quad , \quad y(t) = e^{\alpha t}$$

This implies that

$$\frac{du}{dt} = \frac{d}{dt}(te^{\alpha t}) = e^{\alpha t} + \alpha te^{\alpha t}$$

Nothing new arises if we use the chain rule

$$du(x, y) = \left(\frac{\partial u}{\partial x}\right)_y dx + \left(\frac{\partial u}{\partial y}\right)_x dy$$

$$\frac{du(x, y)}{dt} = \left(\frac{\partial u}{\partial x}\right)_y \frac{dx}{dt} + \left(\frac{\partial u}{\partial y}\right)_x \frac{dy}{dt} = y\frac{dx}{dt} + x\frac{dy}{dt} = e^{\alpha t} + \alpha te^{\alpha t}$$

But what if

$$u = xy \quad , \quad x(t) = t \quad , \quad e^{-y} - y = t$$

This is an implicit rather than explicit equation for $y(t)$.

Using the chain rule we now get

$$\frac{du(x,y)}{dt} = \left(\frac{\partial u}{\partial x}\right)_y \frac{dx}{dt} + \left(\frac{\partial u}{\partial y}\right)_x \frac{dy}{dt} = y\frac{dx}{dt} + x\frac{dy}{dt} = y + t\frac{dy}{dt}$$

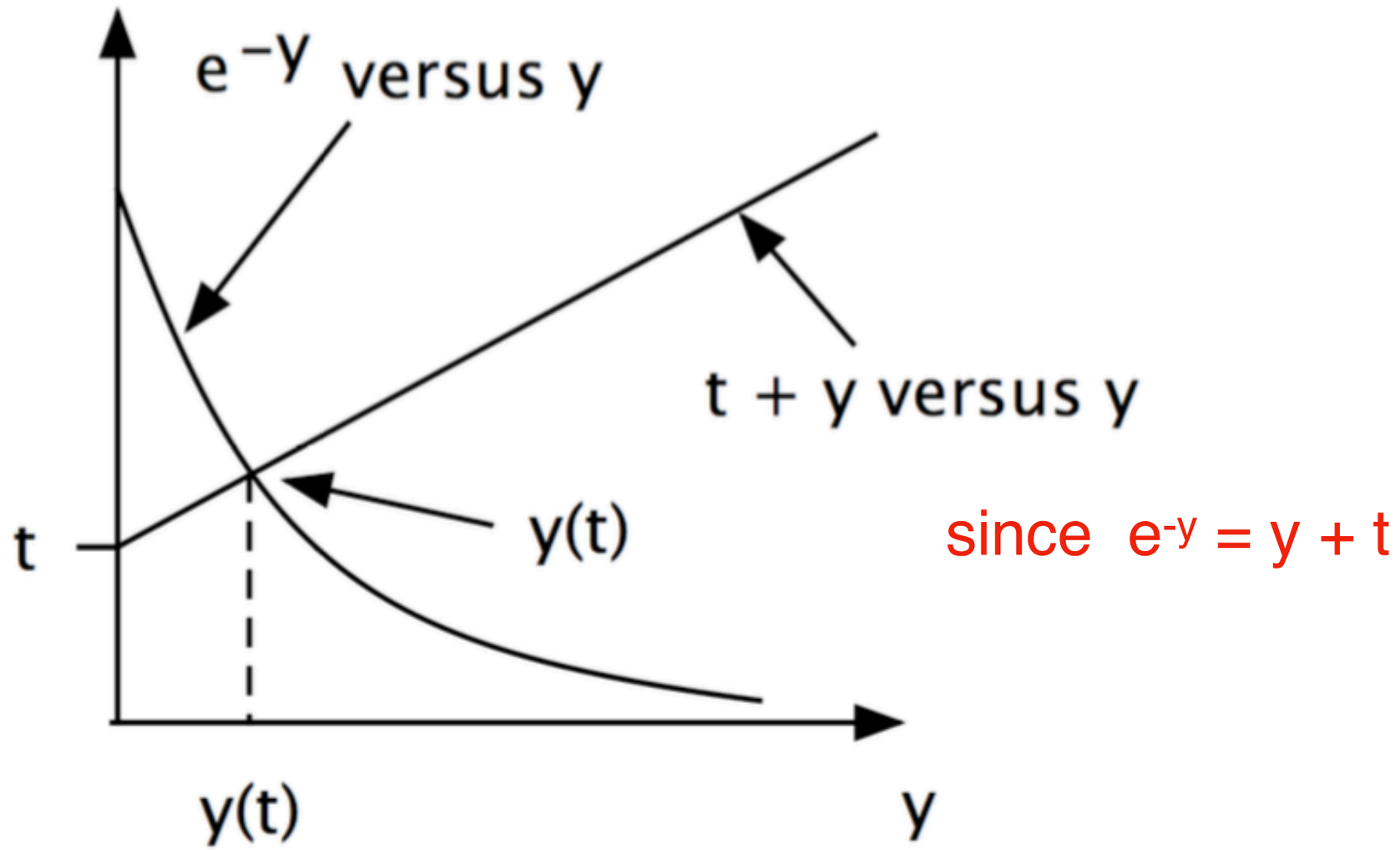
We have

$$dt = d(e^{-y} - y) = (-e^{-y} - 1)dy \rightarrow \frac{dy}{dt} = -\frac{1}{e^{-y} + 1}$$

and therefore

$$\frac{du}{dt} = y + t\frac{dy}{dt} = y - \frac{1}{e^{-y} + 1}$$

We now plot as shown below



since $e^{-y} = y + t$

which gives us $y(t)$ and we thus obtain

$$\frac{du}{dt} \quad \text{at} \quad t$$

General Chain Rule

Given $u(x, y)$, $x(s, t)$, $y(s, t)$ we have

$$du = \left(\frac{\partial u}{\partial x}\right)_y dx + \left(\frac{\partial u}{\partial y}\right)_x dy$$

$$dx = \left(\frac{\partial x}{\partial s}\right)_t ds + \left(\frac{\partial x}{\partial t}\right)_s dt$$

$$dy = \left(\frac{\partial y}{\partial s}\right)_t ds + \left(\frac{\partial y}{\partial t}\right)_s dt$$

which gives

$$
\begin{aligned}
du &= \left(\frac{\partial u}{\partial x}\right)_y \left(\left(\frac{\partial x}{\partial s}\right)_t ds + \left(\frac{\partial x}{\partial t}\right)_s dt\right) \\
&\quad + \left(\frac{\partial u}{\partial y}\right)_x \left(\left(\frac{\partial y}{\partial s}\right)_t ds + \left(\frac{\partial y}{\partial t}\right)_s dt\right) \\
&= \left(\left(\frac{\partial u}{\partial x}\right)_y \left(\frac{\partial x}{\partial s}\right)_t + \left(\frac{\partial u}{\partial y}\right)_x \left(\frac{\partial y}{\partial s}\right)_t\right) ds \\
&\quad + \left(\left(\frac{\partial u}{\partial x}\right)_y \left(\frac{\partial x}{\partial t}\right)_s + \left(\frac{\partial u}{\partial y}\right)_x \left(\frac{\partial y}{\partial t}\right)_s\right) dt
\end{aligned}
$$

Since we can also write

$$
du = \left(\frac{\partial u}{\partial s}\right)_t ds + \left(\frac{\partial u}{\partial t}\right)_s dt
$$

we have

$$\left(\frac{\partial u}{\partial s}\right)_t = \left(\frac{\partial u}{\partial x}\right)_y \left(\frac{\partial x}{\partial s}\right)_t + \left(\frac{\partial u}{\partial y}\right)_x \left(\frac{\partial y}{\partial s}\right)_t$$

$$\left(\frac{\partial u}{\partial t}\right)_s = \left(\frac{\partial u}{\partial x}\right)_y \left(\frac{\partial x}{\partial t}\right)_s + \left(\frac{\partial u}{\partial y}\right)_x \left(\frac{\partial y}{\partial t}\right)_s$$

Example:

$$u = x^2 + y \quad , \quad x = s + t \quad , \quad x - y = s^2$$

These give

$$x = \frac{s + t + s^2}{2} \quad , \quad y = \frac{s + t - s^2}{2}$$

and

$$\left(\frac{\partial x}{\partial s}\right)_t = \frac{1 + 2s}{2} \quad , \quad \left(\frac{\partial y}{\partial s}\right)_t = \frac{1 - 2s}{2}$$

$$\left(\frac{\partial u}{\partial s}\right)_t = (2x)\frac{1 + 2s}{2} + (1)\frac{1 - 2s}{2} = (s + t)(1 - 2s) + \frac{1}{2} - s$$

$$= \frac{1}{2} + t - 2ts - 2s^2$$

Taylor Series

If a function $f(x)$ in 1-dimension has a power series expansion

$$f(x) = \sum_{n=0}^{\infty} a_n x^n$$

we then find that

$$f(0) = a_0 \ , \ f'(0) = a_1 \ , \ \frac{1}{2!} f''(0) = a_2 \ , \ \ldots\ldots\ldots\ldots$$

or, in general,

$$\frac{1}{n!} f(n)(0) = a_n$$

and thus

$$f(x) = \sum_{n=0}^{\infty} \frac{f(n)(0)}{n!} x^n$$

This is also called the Taylor expansion for $f(x)$ about the origin $x = 0$.

A Taylor series, in general, means a power series in powers of $(x - a)$ where $a =$ some constant.

The derivation of the coefficients is identical to the last derivation except that we use $x = a$ instead of $x = 0$.

Let

$$f(x) = \sum_{n=0}^{\infty} a_n (x - a)^n$$

We then have

$$f(a) = a_0 \quad , \quad f'(a) = a_1 \quad , \quad \frac{1}{2!} f''(a) = a_2 \quad , \quad \ldots\ldots\ldots\ldots$$

or, in general,

$$\frac{1}{n!} f(n)(a) = a_n$$

and thus

$$f(x) = \sum_{n=0}^{\infty} \frac{f(n)(a)}{n!} (x - a)^n$$

Let us now determine $f(x+h)$ using a neat method.

Consider the following construction for an infinitesimal displacement

$$f(x+\delta x) = f(x) + \Delta x \frac{df}{dx} = \left(1 + \Delta x \frac{d}{dx}\right) f(x)$$

where we have used the definition of the derivative(exact only in the limit of course).

Now make another displacement

$$f(x+2\delta x) = \left(1 + \Delta x \frac{d}{dx}\right) f(x+\delta x) = \left(1 + \Delta x \frac{d}{dx}\right)^2 f(x)$$

Since a finite displacement h can always be constructed from an infinite number of consecutive infinitesimal displacements, we have

$$f(x+h) = \lim_{n\to\infty} \left(1 + \frac{h}{n}\frac{d}{dx}\right)^n f(x) = \exp\left(h\frac{d}{dx}\right) f(x)$$

where we have used the interesting result that

$$\lim_{n\to\infty}\left(1+\frac{h}{n}Q\right)^n = \exp\left(hQ\right)$$

The differential operator

$$\exp\left(h\frac{d}{dx}\right)$$

is called the displacement operator.

Since the exponential function has the power series representation

$$\exp\left(ax\right) = \sum_{k=0}^{\infty}\frac{(ax)^k}{k!}$$

we can write

$$f(x+h) = \exp\left(h\frac{d}{dx}\right)f(x) = \sum_{k=0}^{\infty}\frac{h^k}{k!}f^{(k)}(x)$$

Example:

$$\sin\omega(t+\tau) = \exp\left(\tau\frac{d}{dt}\right)\sin(\omega t)$$

$$= \left[1+\tau\frac{d}{dt}+\frac{1}{2!}\tau^2\frac{d^2}{dt^2}+\frac{1}{3!}\tau^3\frac{d^3}{dt^3}+\ldots\ldots\ldots\right]\sin(\omega t)$$

$$= \left[\sin(\omega t)+\omega\tau\cos(\omega t)-\frac{1}{2!}(\omega\tau)^2\sin(\omega t)\right.$$
$$\left.-\frac{1}{3!}(\omega\tau)^3\cos(\omega t)+\ldots\ldots\ldots\right]$$

$$= \sin(\omega t)\left[1-\frac{1}{2!}(\omega\tau)^2+\ldots\ldots\right]$$
$$+\cos(\omega t)\left[\omega\tau-\frac{1}{3!}(\omega\tau)^3+\ldots\ldots\right]$$

$$= \sin(\omega t)\cos(\omega\tau)+\cos(\omega t)\sin(\omega\tau)$$

which we know to be correct.

These results generalize easily to 3-dimensions as

$$f(\vec{r}+\vec{a}) = \sum_{n=0}^{\infty} \frac{1}{n!}(\vec{a}\cdot\nabla)f(\vec{r})$$

and also can be used for displacements in time

$$f(t+\tau) = \exp\left(\tau\frac{d}{dt}\right)f(t)\sum_{k=0}^{\infty}\frac{\tau^k}{k!}f^{(k)}(t)$$

Binomial Series

Consider the following function

$$f(x) = (1+x)^n$$

If we expand this out we get

$$f(x) = (1+x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \ldots.$$
$$= \sum_{m=0}^{\infty} \frac{n!}{m!(n-m)!}x^m = \sum_{m=0}^{\infty} \binom{n}{m} x^m$$

this is called the Binomial series and the symbol $\binom{n}{m}$ is the Binomial coefficient.

For $n =$ integer, the series terminates at $m = n$.

In a similar way we can write(for $n =$ integer),

$$(p+q)^n = \sum_{m=0}^{\infty} \frac{n!}{m!(n-m)!}p^m q^{n-m} = \sum_{m=0}^{\infty} \binom{n}{m} p^m q^{n-m}$$

This has an interesting interpretation in the following example.

Suppose we have n coins that we will flip onto a table and we count the number heads and tails.

Suppose the probability of getting a heads $= p$ and the probability of getting a tails is q.

Hence $p + q = 1$.

This means we have

$$(p+q)^n = (1)^n = 1 = \sum_{m=0}^{\infty} \binom{n}{m} p^m q^{n-m}$$

Now the probability of throwing m heads and $n - m$ tails is given by

$$p^m q^{n-m}$$

and the number of indistinguishable ways we can do this is

$$\frac{n!}{m!(n-m)!}$$

Therefore the total probability of throwing m heads and $n-m$ tails is given by

$$P(n,m) = \frac{n!}{m!(n-m)!} p^m q^{n-m} = C(n,m) p^m q^{n-m}$$

Since the probability of something happening is sum of all of these probabilities, the sum must $= 1$ as we have already seen above.

Does this really work? Consider $n = 3$, so we can actually do it.

For $n = 3$, the number of possible outcomes $= 2 \times 2 \times 2 = 8$ and we have

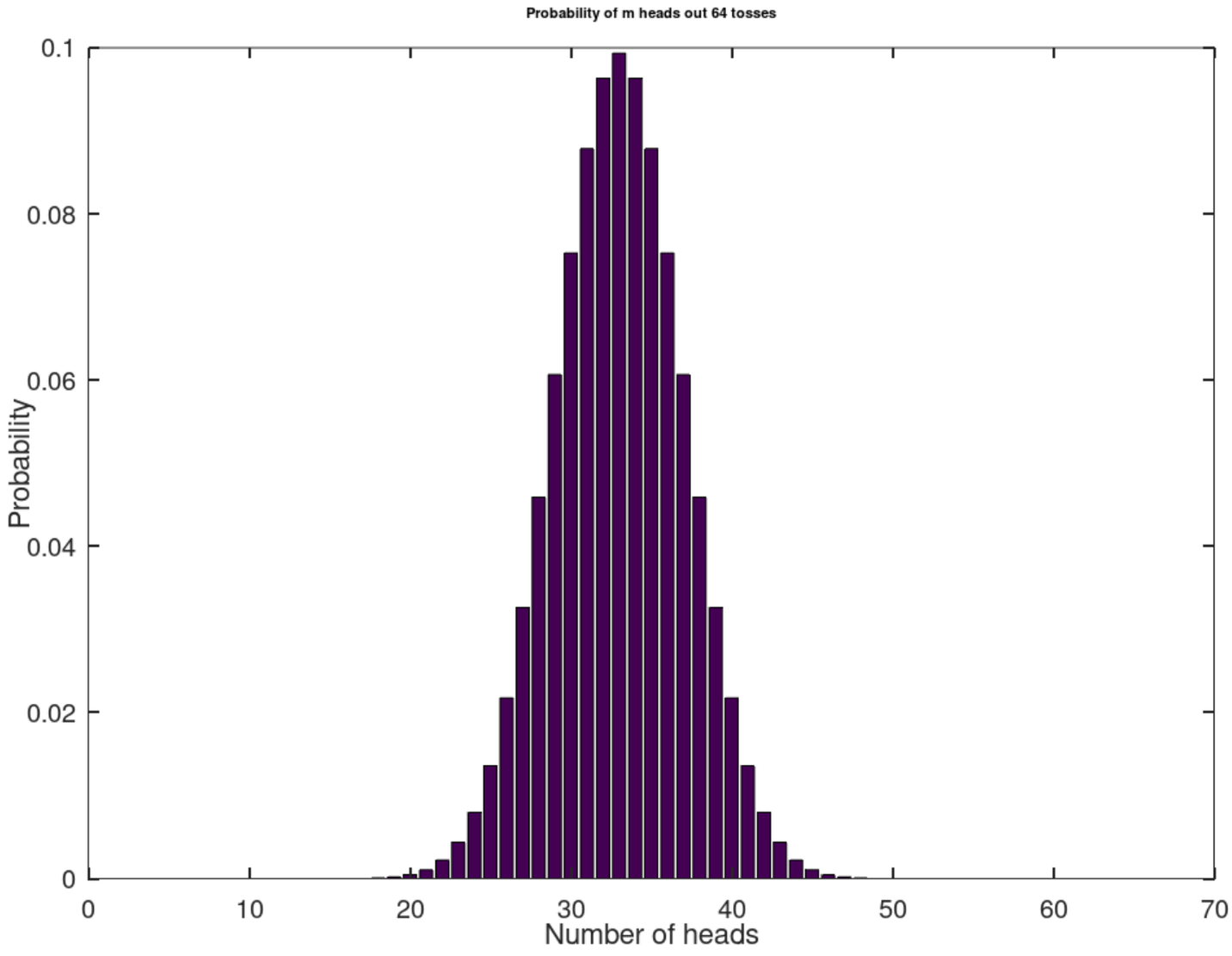
$$\begin{aligned}
ppp &= 1 = C(3,3) - P(3,3) = 1/8 \\
ppq, pqp, qpp &= 1 = C(3,3) - P(3,2) = 3/8 \\
qqp, qpq, pqq &= 1 = C(3,2) - P(3,1) = 3/8 \\
qqq &= 1 = C(3,0) - P(3,0) = 1/8
\end{aligned}$$

So it does work!

Octave Program for case $n = 64$

```
\% m-file coins1.m
\% 64 coins with p = q = 1/2
p=0.5; N=64; pn=[];
for m=-N:2:N
 pn=[pn,(prod(1:N)*(0.5)^N)/ ...
        (prod(1:((N+m)/2))*prod(1:((N-m)/2)))];
end
bar(pn)
title('Probability of m heads out 64 tosses');
xlabel('Number of heads');
ylabel('Probability')
```

See diagram below.



We note that the quantity $n!$ that we have been using is usually defined only for positive integers.

As we shall later in the course, there is a more general definition of this function, which reduces to the same values when $n =$ integer.

It is given by

$$s! = \int_0^\infty x^s e^{-x} dx = \Gamma(s+1)$$

for all s not equal to negative integer. It is the **gamma function**.

Taylor Expansion in more than 1 variable

We now generalize the Taylor expansion to more than 1 dimensions:

$$\begin{aligned}
f(x,y) =& f(a,b) + (x-a)f_x(a,b) + (y-b)f_y(a,b) \\
&+ \frac{1}{2!}(x-a)^2 f_{xx}(a,b) + \frac{2}{2!}(x-a)(y-b)f_{xy}(a,b) \\
&+ \frac{1}{2!}(y-b)^2 f_{yy}(a,b) + \frac{1}{3!}(x-a)^3 f_{xxx}(a,b) \\
&+ \frac{3}{3!}(x-a)^2(y-b)f_{xxy}(a,b) + \frac{3}{3!}(x-a)(y-b)^2 f_{xyy}(a,b) \\
&= \frac{1}{3!}(y-b)^3 f_{yyy}(a,b) + ...
\end{aligned}$$

and so on.

Curvilinear Coordinates

First we mention cartesian coordinate systems.

We have

$$\text{basis vectors } = \hat{e}_i \quad , \quad i = 1, 2, 3$$

These systems have intuitive appeal since they

(1) make use of straight lines

(2) make use of perpendicular(orthogonal) directions of flat space

(3) vector differential/integral operators take their simplest forms

However, many physical systems are not naturally rectangular, i.e., the surface of a sphere.

In this case the rectangular coordinates of a point on its surface are changing from point to point, but in spherical polar coordinates the surface is specified simply as a surface of constant radius r.

Thus, the choice of coordinate systems can be important in the description of a physical system.

A good choice may lead to greater simplification and insight in the description of the physical system.

There is, of course, a price to pay for this improvement.

Coordinate systems other than rectangular are less intuitive and harder to visualize.

Integral and differential operators have more complicated forms.

We now show that the task is quite tractable, perhaps even enjoyable, when approached from the right point of view.

It turns out to just be a matter of changing directions and changing scales as we shall now see.

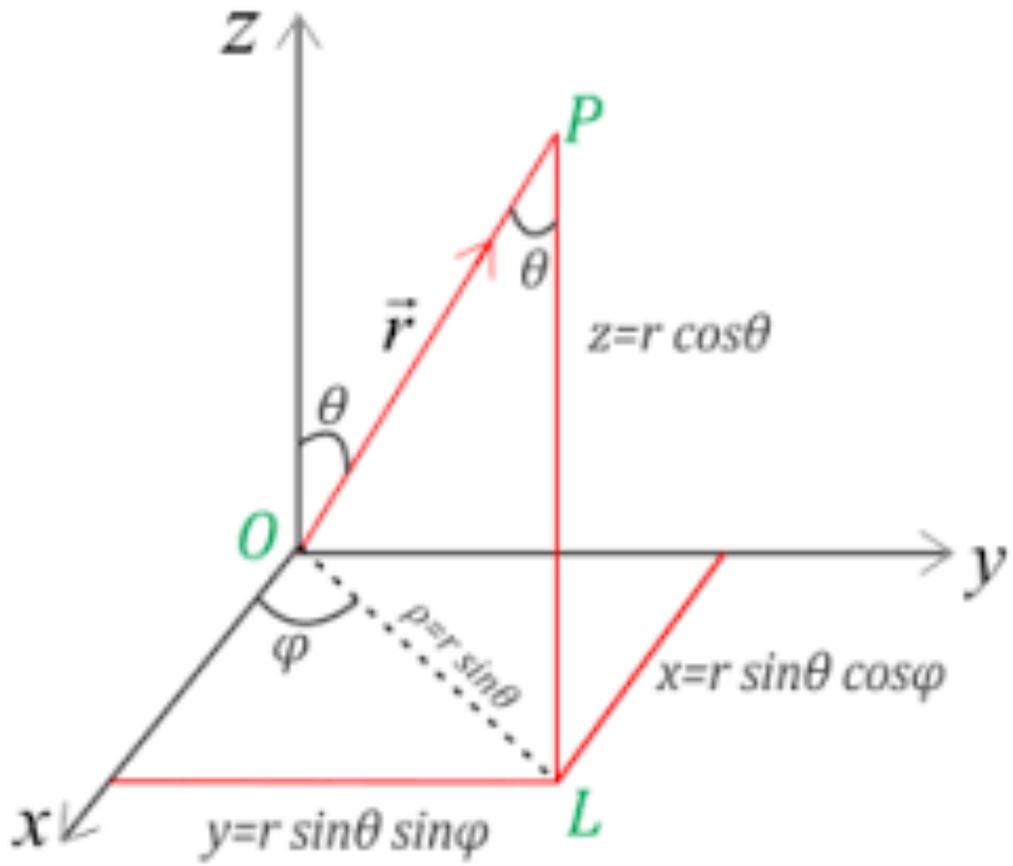
Generalized Coordinates

We begin by noting that any 3 independent variables (u_1, u_2, u_3) can be used to form a coordinate system if they uniquely specify the position of a point in space.

For convenience we start with the familiar rectangular coordinates $(x, y, z) = (x_1, x_2, x_3)$ and specify the new generalized coordinates by the relations $u_i = u_i(x, y, z)$.

For the transformation between these two coordinate systems to be **well-defined and unique**, it is necessary that the inverse relations $x_i = x_i(u_1, u_2, u_3)$ also exist, and that all of these relations are **single-valued functions**.

Example: spherical polar coordinates $r, \theta, \phi)$: See diagram below.



Here we have the relations

$$r = (x^2+y^2+z^2)^{1/2} \quad , \quad \theta = \tan^{-1}\left(\frac{(x^2+y^2)^{1/2}}{z}\right) \quad , \quad \phi = \tan^{-1}\left(\frac{y}{x}\right)$$

and the inverse relations

$$x = r\sin\theta\cos\phi \quad , \quad x = r\sin\theta\sin\phi \quad , \quad z = r\cos\theta$$

A **coordinate axis** now becomes a **coordinate curve** along which only one of the coordinates is changing (same as in the cartesian case). The coordinate curves in spherical polar coordinates are:

radii	(only r varies, $\theta, \phi =$ constant)
longitudes	(only θ varies, $r, \phi =$ constant)
latitudes	(only ϕ varies, $r, \theta =$ constant)

It is easy to find explicit algebraic expressions describing these coordinate curves because by definition only one of the coordinates changes along such a curve, while the others remain unchanged.

For example, if $\vec{r} = r\hat{e}_r = r\hat{e}(\vec{r})$ represents a coordinate curve, then **the equations**

$$\frac{\partial \vec{r}}{\partial r} = \hat{e}_r \quad , \quad \frac{\partial \vec{r}}{\partial \theta} = r\frac{\partial \hat{e}_r}{\partial \theta} \quad , \quad \frac{\partial \vec{r}}{\partial \phi} = r\frac{\partial \hat{e}_r}{\partial \phi}$$

describe the vectorial changes along this coordinate curve.

We state a rule:

Each of these derivatives is a vector in space; it has a length h_i and a direction $\hat{e}_i$, where $i = r, \theta$ or ϕ.

We can readily obtain their explicit forms with the help of rectangular coordinates, where the basis vectors are constants:

$$\frac{\partial \vec{r}}{\partial r} = \frac{\partial}{\partial r}(x\hat{e}_x + y\hat{e}_y + z\hat{e}_z)$$
$$= \sin\theta\cos\phi\hat{e}_x + \sin\theta\sin\phi\hat{e}_y + \cos\theta\hat{e}_z = h_r\hat{e}_r$$
$$\frac{\partial \vec{r}}{\partial \theta} = \frac{\partial}{\partial \theta}(x\hat{e}_x + y\hat{e}_y + z\hat{e}_z)$$
$$= r\cos\theta\cos\phi\hat{e}_x + r\cos\theta\sin\phi\hat{e}_y - r\sin\theta\hat{e}_z = h_\theta\hat{e}_\theta$$
$$\frac{\partial \vec{r}}{\partial \phi} = \frac{\partial}{\partial \phi}(x\hat{e}_x + y\hat{e}_y + z\hat{e}_z) = -r\sin\theta\sin\phi\hat{e}_x + r\sin\theta\cos\phi\hat{e}_y = h_\phi\hat{e}_\phi$$

We then have (taking scalar products)

$$h_r^2 = \sin^2\theta\cos^2\phi + \sin^2\theta\sin^2\phi + cos^2\theta = 1 \rightarrow h_r = 1$$
$$h_\theta^2 = r^2\cos^2\theta\cos^2\phi + r^2\cos^2\theta\sin^2\phi + -r^2\sin^2\theta = r^2 \rightarrow h_\theta = r$$
$$h_\phi^2 = r^2\sin^2\theta\sin^2\phi + r^2\sin^2\theta\cos^2\phi = r^2\sin^2\theta \rightarrow h_\phi = r\sin\theta$$

Now

$$\begin{aligned} d\vec{r} &= \frac{\partial \vec{r}}{\partial r} dr + \frac{\partial \vec{r}}{\partial \theta} d\theta + \frac{\partial \vec{r}}{\partial \phi} d\phi \\ &= h_r \hat{e}_r dr + h_\theta \hat{e}_\theta d\theta + h_\phi \hat{e}_\phi d\phi \\ &= dr\hat{e}_r + rd\theta\hat{e}_\theta + r\sin\theta d\phi\hat{e}_\phi \end{aligned}$$

which should look familiar from our earlier discussions.

In the general case (u_1, u_2, u_3) we have

$$d\vec{r} = \frac{\partial \vec{r}}{\partial u_1} du_1 + \frac{\partial \vec{r}}{\partial u_2} du_2 + \frac{\partial \vec{r}}{\partial u_3} du_3$$

where

$$\frac{\partial \vec{r}}{\partial u_i} = \frac{\partial}{\partial u_i}(x\hat{e}_x + y\hat{e}_y + z\hat{e}_z) = \frac{\partial x}{\partial u_i}x\hat{e}_x + \frac{\partial y}{\partial u_i}\hat{e}_y + \frac{\partial z}{\partial u_i}\hat{e}_z$$
$$= \text{vector (actually the tangent vector)}$$
$$= h_i(\vec{r})\hat{e}_i(\vec{r})$$

so that

$$h_i(\vec{r}) = \left[\left(\frac{\partial x}{\partial u_i}\right)^2 + \left(\frac{\partial y}{\partial u_i}\right)^2 + \left(\frac{\partial z}{\partial u_i}\right)^2\right]^{1/2}$$

and the **displacement vector** is

$$d\vec{r} = \sum_i h_i(\vec{r})\hat{e}_i(\vec{r})du_i = \hat{e}_i(\vec{r})ds_i \quad , \quad ds_i = h_i du_i$$

Thus, $\hat{e}_i(\vec{r})$ defines the coordinate curve since it gives the unit vector tangent to the curve at $\vec{r}$.

The infinitesimal scalar displacement $ds_i = h_i(\vec{r})du_i$ gives the displacement along this coordinate curve.

The function $h_i(\vec{r})$ is a scale factor.

It ensures that the displacement has the dimensions of length, independent of the dimensions of the u_i.

All other geometrical quantities can be calculated readily in terms of these scale factors and unit tangent vectors.

The infinitesimal scalar displacement ds along a path in space is

$$(ds)^2 = d\vec{r} \cdot d\vec{r} = \sum_{ij} (h_i \hat{e}_i du_i) \cdot (h_j \hat{e}_j du_j) = \sum_{ij} g_{ij} du_i du_j$$

where $g_{ij} = h_i h_j \hat{e}_i \cdot \hat{e}_j$ gives the so-called **metric coefficients** of the generalized coordinate system.

The differential elements of surface and volume can be written down as

$$\begin{aligned} d\vec{A}_{ij} = d\vec{\sigma}_{ij} &= \left(\frac{\partial \vec{r}}{\partial u_i} du_i\right) \times \left(\frac{\partial \vec{r}}{\partial u_j} du_j\right) \\ &= h_i h_j (\hat{e}_i \times \hat{e}_j) du_i du_j = (\hat{e}_i \times \hat{e}_j) ds_i ds_j \end{aligned}$$

(Think of the Cartesian case to understand this result. What does the direction mean?) and

$$d\tau = dV = ds_1 ds_2 ds_3 \hat{e}_1 \cdot (\hat{e}_2 \times \hat{e}_3)$$

where the last factor is the volume of a unit parallelpiped.

Orthonormal Curvilinear Coordinates

If at every point $\vec{r}$, the three unit tangents $\hat{e}_i(\vec{r})$ are orthogonal to one another(mutually orthogonal), that is, if

$$\hat{e}_i(\vec{r}) \cdot \hat{e}_j(\vec{r}) = \delta_{ij}$$

or equivalently, if

$$\frac{\partial \vec{r}}{\partial u_i} \cdot \frac{\partial \vec{r}}{\partial u_j} \propto \delta_{ij}$$

then the generalized coordinates u_i are said to form an **orthogonal curvilinear coordinate system**.

In this system, the unit tangents $\hat{e}_1(\vec{r}), \hat{e}_2(\vec{r}), \hat{e}_3(\vec{r})$ form a cartesian coordinate system at every point $\vec{r}$ (not the same one at different points).

The only complication is that their orientation changes from point to point (different than in the case of a cartesian system) in space.

In such orthogonal systems, the metric coefficients

$$g_{ij} = h_i^2 \delta_{ij} \rightarrow \text{ diagonal and } \quad h_i^2 = \left(\frac{\partial x}{\partial u_i}\right)^2 + \left(\frac{\partial y}{\partial u_i}\right)^2 + \left(\frac{\partial z}{\partial u_i}\right)^2$$

and the squared length

$$(ds)^2 = ds^2 = \sum_i h_i^2 (du_i)^2 = \sum_i (ds_i)^2$$

contains **NO CROSS TERMS** (so things can get worse!).

The differential surface/volume elements are

$$d\vec{\sigma}_{ij} = ds_i ds_j \sum_k \epsilon_{ijk} \hat{e}_k$$

$$d\tau = ds_1 ds_2 ds_3$$

Thus, the ds_i are very much like the rectangular coordinates dx_i.

However, the tangent directions change from point to point, except in the case of rectangular coordinates for which they are constant unit vectors.

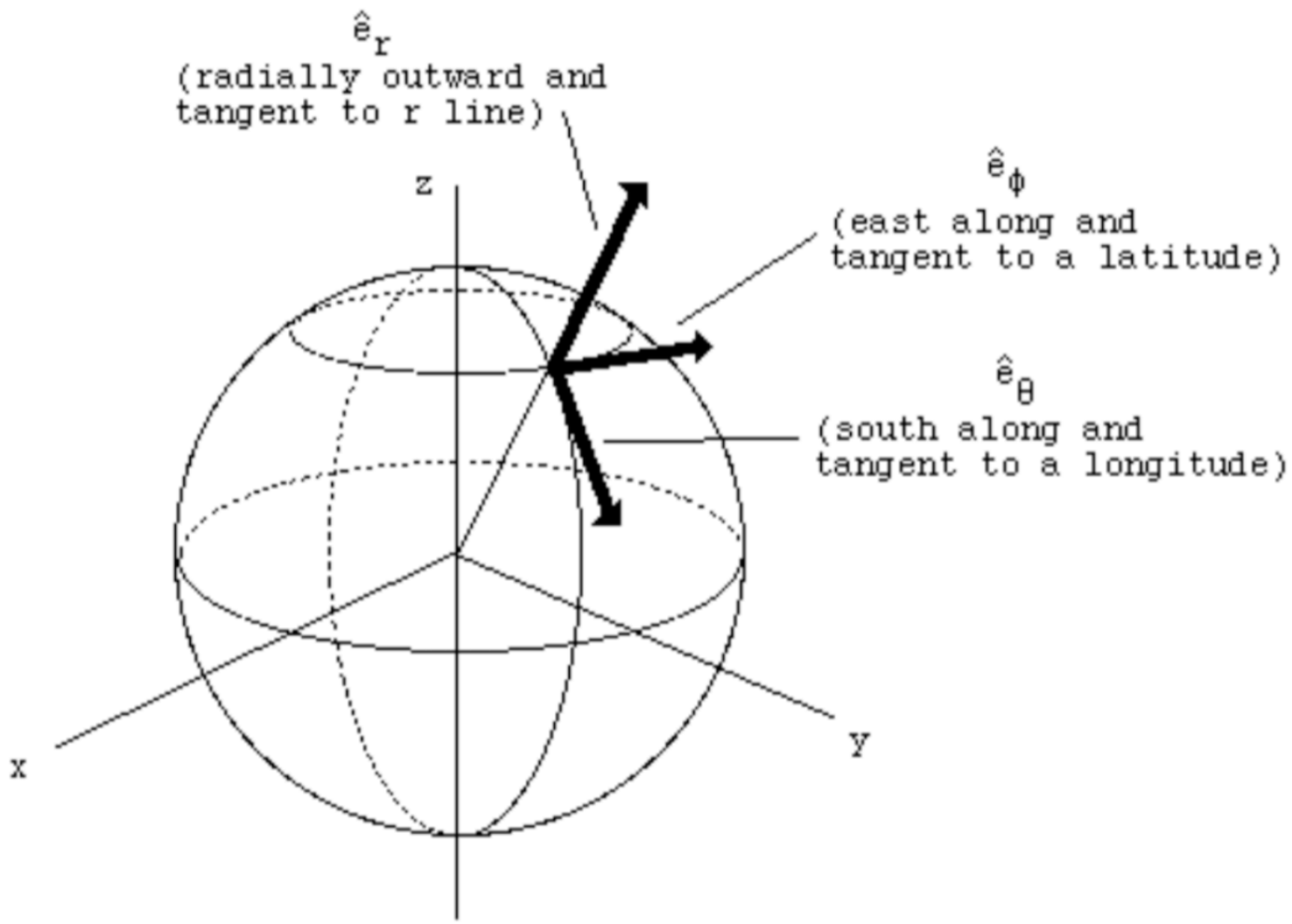
Examples:

Spherical polar coordinates (orthogonal)

$$h_r = 1 \ , \quad h_\theta = r \ , \quad h_\phi = r \sin\theta$$

$$\hat{e}_r = \frac{1}{h_r}\frac{\partial \vec{r}}{\partial r} \ , \quad \hat{e}_\theta = \frac{1}{h_\theta}\frac{\partial \vec{r}}{\partial \theta} \ , \quad \hat{e}_\phi = \frac{1}{h_\phi}\frac{\partial \vec{r}}{\partial \phi}$$

See figure below



Then

$$\sin\theta\cos\phi\hat{e}_x + \sin\theta\sin\phi\hat{e}_y + \cos\theta\hat{e}_z = \hat{e}_r$$
$$\cos\theta\cos\phi\hat{e}_x + \cos\theta\sin\phi\hat{e}_y - \sin\theta\hat{e}_z = \hat{e}_\theta$$
$$-\sin\phi\hat{e}_x + \cos\phi\hat{e}_y = \hat{e}_\phi$$

where

$$\hat{e}_r \cdot \hat{e}_\theta = \hat{e}_r \cdot \hat{e}_\phi = \hat{e}_\phi \cdot \hat{e}_\theta = 0 \quad , \quad \hat{e}_r \times \hat{e}_\theta = \hat{e}_\phi \quad , \quad \hat{e}_\phi \times \hat{e}_r = \hat{e}_\theta \quad , \quad \hat{e}_\theta \times \hat{e}_\phi = \hat{e}_r$$

In addition,

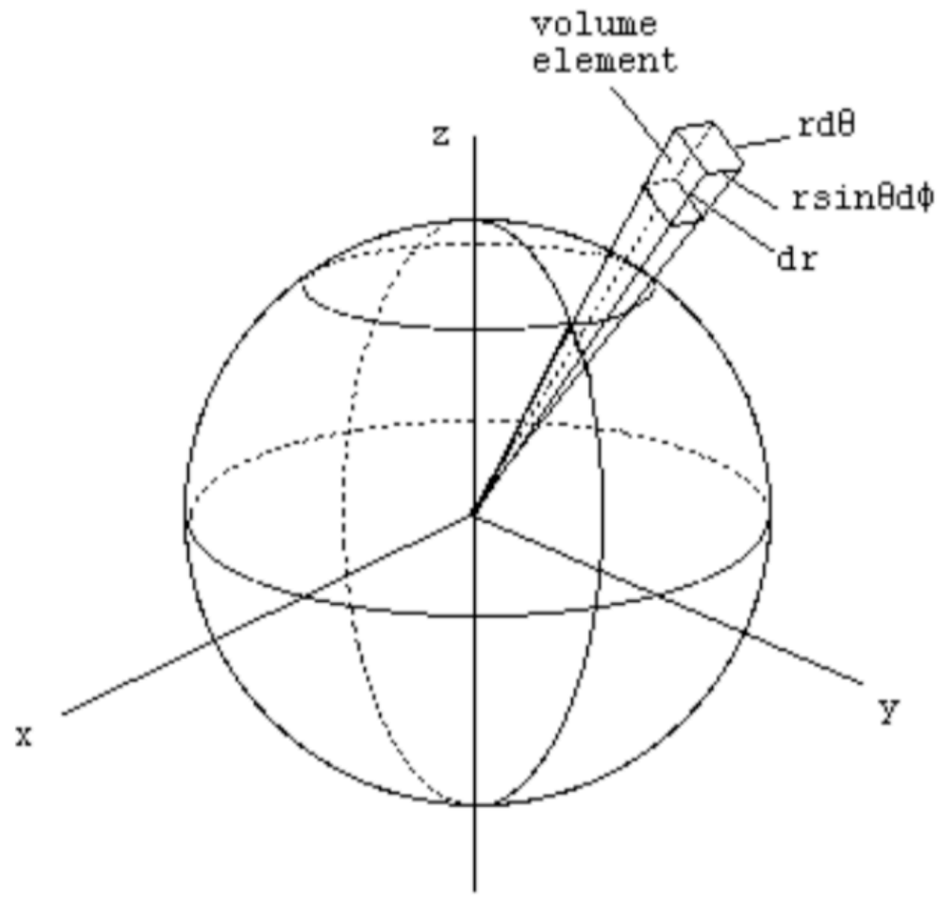
$$d\vec{r} = h_r dr \hat{e}_r + h_\theta d\theta \hat{e}_\theta + h_\phi d\phi \hat{e}_\phi$$
$$ds_r = dr \quad , \quad ds_\theta = r d\theta \quad , \quad ds_\phi = r \sin\theta d\phi$$
$$ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta d\phi^2$$

and

$$d\vec{\sigma}_{r\theta} = r dr d\theta \hat{e}_\phi = -d\vec{\sigma}_{\theta r}$$
$$d\vec{\sigma}_{\theta\phi} = r^2 \sin\theta d\theta d\phi \hat{e}_r = -d\vec{\sigma}_{\phi\theta}$$
$$d\vec{\sigma}_{\phi r} = r \sin\theta dr d\phi \hat{e}_\theta = -d\vec{\sigma}_{r\phi}$$

$$d\tau = ds_r ds_\theta ds_\phi = r^2 \sin\theta dr d\theta d\phi$$

The volume element looks like



Does it work for the cartesian coordinates (x, y, z)?

$$\frac{\partial \vec{r}}{\partial x} = \frac{\partial}{\partial x}(x\hat{e}_x + y\hat{e}_y + z\hat{e}_z) = \hat{e}_x \ , \ \frac{\partial \vec{r}}{\partial y} = \hat{e}_y \ , \ \frac{\partial \vec{r}}{\partial z} = \hat{e}_z$$

$$h_x = h_y = h_z = 1 \rightarrow d\vec{r} = dx\hat{e}_x + dy\hat{e}_y + dz\hat{e}_z = \frac{\partial \vec{r}}{\partial x}\hat{e}_x + \frac{\partial \vec{r}}{\partial y}\hat{e}_y + \frac{\partial \vec{r}}{\partial z}\hat{e}_z$$

$$ds_x = dx \;\;,\;\; ds_y = dy \;\;,\;\; ds_z = dz \rightarrow ds^2 = dx^2 + dy^2 + dz^2$$

$$d\vec{\sigma}_{xy} = dxdy\hat{e}_x \times \hat{e}_y = dxdy\hat{e}_z \;\;,\;\; d\vec{\sigma}_{yz} = dydz\hat{e}_x \;\;,\;\; d\vec{\sigma}_{zx} = dxdz\hat{e}_y$$

$$d\tau = dxdydz\hat{e}_x \cdot (\hat{e}_y \times \hat{e}_z) = dxdydz$$

Clearly it does!

Finally, remember that the coordinate $\vec{r}(t)$ of a physical event is a function of the time t.

It can be differentiated wrt t to give

$$\vec{v} = \frac{d\vec{r}}{dt} \quad \text{and} \quad \vec{a} = \frac{d\vec{v}}{dt} = \frac{d^2\vec{r}}{dt^2}$$

If cartesian coordinates are used, then their will only be contributions from the time derivatives of the components and not the unit vectors (since they are constant in time).

But for curvilinear coordinates we get contributions from both, i.e.,

$$\frac{d}{dt}(\text{components} + \frac{d}{dt}\text{unit vectors}$$

because the unit vectors are also changing in time.

Vector Differential Operators in Curvilinear Coordinates

If we define the differential operator symbol ∇ (called the "gradient" or "del") as

$$\nabla = \left(\frac{\partial}{\partial x}\hat{e}_x + \frac{\partial}{\partial y}\hat{e}_y + \frac{\partial}{\partial z}\hat{e}_z\right)$$

then we can ask, what do $\nabla\Phi$, $\nabla \cdot \vec{V}$, and $\nabla \times \vec{V}$ look like?

We have $\vec{r} = (u_1, u_2, u_3) =$ position in space and a scalar field $\phi(u_1, u_2, u_3)$ and a vector field $\vec{V}(u_1, u_2, u_3)$.

The quantity $\nabla\Phi(u_1, u_2, u_3)$ describes at every point $\vec{r}$, a vector that can be decomposed into components along the local unit tangents $\hat{e}_i(\vec{r})$, that is,

$$\nabla\Phi(\vec{r}) = \sum_i \hat{e}_i(\vec{r})(\nabla\Phi)_i = \sum_i \hat{e}_i(\vec{r})(\nabla\Phi \cdot \hat{e}_i(\vec{r}))$$

If we expand the gradient in rectangular coordinates(we can use any) then we get

$$(\nabla\Phi)_i = \left(\frac{\partial\Phi}{\partial x}\hat{e}_x + \frac{\partial\Phi}{\partial y}\hat{e}_y + \frac{\partial\Phi}{\partial z}\hat{e}_z\right) \cdot \hat{e}_i(\vec{r})$$

From earlier we have

$$d\vec{r} = \sum_i h_i(\vec{r})\hat{e}_i(\vec{r})du_i = \sum_i \hat{e}_i(\vec{r})ds_i$$

and then

$$\hat{e}_x \cdot \hat{e}_i = \hat{e}_x \cdot \frac{\partial \vec{r}}{\partial s_i} = \hat{e}_x \cdot \frac{\partial x \hat{e}_x + y \hat{e}_y + z \hat{e}_z}{\partial s_i} = \frac{\partial x}{\partial s_i}$$

Therefore,

$$(\nabla \Phi)_i = \left(\frac{\partial \Phi}{\partial x} \frac{\partial x}{\partial s_i} + \frac{\partial \Phi}{\partial y} \frac{\partial y}{\partial s_i} + \frac{\partial \Phi}{\partial z} \frac{\partial z}{\partial s_i} \right) = \frac{\partial \Phi}{\partial s_i}$$

or

$$\nabla \Phi(u_1, u_2, u_3) = \sum_i \hat{e}_i(\vec{r}) \frac{\partial \Phi}{\partial s_i} = \sum_i \hat{e}_i(\vec{r}) \frac{1}{h_i} \frac{\partial \Phi}{\partial u_i}$$

This implies that the u_i in $\nabla \Phi(u_1, u_2, u_3)$ can be treated as if they were rectangular coordinates if the **local tangents** $\hat{e}_i(\vec{r})$ are used together with **local displacements** $ds_i = h_i du_i$.

Example:

$$\nabla\Phi(r,\theta,\phi) = \left(\hat{e}_r\frac{\partial\Phi}{\partial r} + \hat{e}_\theta\frac{1}{r}\frac{\partial\Phi}{\partial\theta} + \hat{e}_\phi\frac{1}{r\sin\theta}\frac{\partial\Phi}{\partial\phi}\right)$$

In general,

$$\nabla u_j(\vec{r}) = \sum_i \hat{e}_i(\vec{r})\frac{\partial u_j}{\partial u_i} = \sum_i \hat{e}_i(\vec{r})\frac{1}{h_i}\delta_{ij} = \frac{\hat{e}_j(\vec{r})}{h_j}$$

which implies that a generalized coordinate curve has a **natural curliness** of

$$\nabla\times\hat{e}_j = -h_j\nabla\left(\frac{1}{h_j}\right)\times\hat{e}_j(\vec{r})$$

Summarizing, we get(algebra is nasty) for vector operators in orthogonal curvilinear coordinates $u_1, u_2, u_3,\ h_1, h_2, h_3$, with Φ a scalar field and $\vec{V}$ a vector field

$$\nabla \Phi = \sum_i \frac{1}{h_i} \frac{\partial \Phi}{\partial u_i} \hat{e}_i$$

$$\nabla \cdot \vec{V} = \sum_i \frac{1}{p_i} \frac{\partial}{\partial u_i} (p_i V_i)$$

where

$$p_i = \frac{h_1 h_2 h_3}{h_i}$$

$$\nabla \times \vec{V} = \frac{1}{h_1 h_2 h_3} \sum_{ijk} \epsilon_{ijk} \frac{\partial}{\partial u_i} (h_j V_j) h_k \hat{e}_k$$

$$\nabla^2 \Phi = \sum_i \frac{1}{p_i} \frac{\partial}{\partial u_i} \left(p_i \frac{\partial}{\partial u_i} \right) \Phi$$

Jacobians

For different coordinate systems we have

carteian	$dV = dxdydz$
cylindrical polar	$dV = rdrd\theta dz$
spherical polar	$dV = r^2 sin\theta drd\theta d\phi$

How do we convert between area and volume elements in different coordinate systems?

The rules are:

$$\text{if } (x, y) \to (q, t), \text{ then } dA = |J| dqdt$$
$$\text{if } (x, y, z) \to (q, t, w), \text{ then } dA = |J| dqdtdw$$

where J is a determinant of partial derivatives called the **Jacobian**.

$$J = J\left(\frac{(x,y)}{(q,t)}\right) = \begin{vmatrix} \frac{\partial x}{\partial q} & \frac{\partial x}{\partial t} \\ \frac{\partial y}{\partial q} & \frac{\partial y}{\partial t} \end{vmatrix} \quad \text{in 2-dimensions}$$

and

$$J = J\left(\frac{(x,y)}{(q,t)}\right) = \begin{vmatrix} \frac{\partial x}{\partial q} & \frac{\partial x}{\partial t} & \frac{\partial x}{\partial w} \\ \frac{\partial y}{\partial q} & \frac{\partial y}{\partial t} & \frac{\partial y}{\partial w} \\ \frac{\partial z}{\partial q} & \frac{\partial z}{\partial t} & \frac{\partial z}{\partial w} \end{vmatrix} \quad \text{in 3-dimensions}$$

Examples:

$$q = r \ , \ t = \theta$$

$$\rightarrow J = \begin{vmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{vmatrix} = r$$

$$\rightarrow dA = dxdy = rdrd\theta$$

$$q = r \ , \ t = \theta \ , \ w = \phi$$

$$\rightarrow J = \begin{vmatrix} \sin\theta\cos\phi & r\cos\theta\cos\phi & -r\sin\theta\sin\phi \\ \sin\theta\sin\phi & r\cos\theta\sin\phi & r\sin\theta\cos\phi \\ \cos\theta & -r\sin\theta & 0 \end{vmatrix} = r^2\sin\theta$$

$$\rightarrow dV = dxdydz = r^2\sin\theta drd\theta d\phi$$

Eigenvalues/Eigenvectors of Hermitian Matrices

Many matrices that appear in quantum theory are Hermitian matrices where

$$H^\dagger = H^{*T} = H$$

Some properties of Hermitian matrices are:

- all eigenvalues are real
- eigenvectors belonging to different eigenvectors are orthogonal
- eigenvectors belonging to **degenerate** eigenvalues ($\lambda_1 = \lambda_2$) can be made orthogonal using the Gram-Schmidt process

In quantum physics these matrices or operators representing observable quantities, so it is necessary that all the eigenvalues, which will correspond to the possible values of a measurement of the observable, are real.

The orthogonality properties mean that the eigenvectors of any Hermitian operator can be used to define a cartesian coordinate system(orthonormal) or **basis** in the space of the n-dimensional vectors.

This is very useful for doing calculations.

Let us see how some of these properties arise:

$$Hu_i = \lambda_i u_i$$

$$(u_i)^\dagger u_i = (\text{length})^2 \text{ of the vector } \geq 0$$

If $(u_i)^\dagger u_j = 0$, then u_i and u_j are orthogonal.

Now

$$(u_i)^\dagger H u_j = \lambda_j (u_i)^\dagger u_j$$

If we digress for a moment to derive a property of the transpose operation, we find

$$C = AB \rightarrow C^T = (AB)^T$$

$$(C^T)_{ij} = C_{ji} = (AB)_{ji} = \sum_k A_{jk} B_{ki} = \sum_k (B^T)_{ik} (A^T)_{kj}$$

$$(C^T)_{ij} = (B^T A^T)_{ij}$$

$$\rightarrow C^T = B^T A^T$$

that is, the order reverses!

This implies that

$$C^\dagger = B^\dagger A^\dagger$$

Using this result we have

$$\begin{aligned}((u_i)^\dagger H u_j)^{\dagger\dagger} &= (\lambda_j (u_i)^\dagger u_j)^{\dagger\dagger} = (\lambda_j^* (u_j)^\dagger u_i)^\dagger = \lambda_j (u_i)^\dagger u_j \\ &= ((u_j)^\dagger H^\dagger u_i)^\dagger = ((u_j)^\dagger H u_i)^\dagger = ((u_j)^\dagger \lambda_i u_i)^\dagger \\ &= \lambda_i^* ((u_j)^\dagger u_i)^\dagger\end{aligned}$$

Thus,

$$\lambda_j (u_i)^\dagger u_j = \lambda_i^* ((u_j)^\dagger u_i)^\dagger = \lambda_i^* (u_i)^\dagger u_j$$

or

$$(\lambda_j - \lambda_i^*)(u_i)^\dagger u_j = 0$$

If we set $i = j$, then since $(u_i)^\dagger u_j \neq 0$, we have

$$\lambda_i - \lambda_i^* = 0 \rightarrow \text{ the } \lambda_i \text{ are real}$$

In addition, we find that if $\lambda_i \neq \lambda_j$, then $(u_i)^\dagger u_j = 0$ or the corresponding eigenvectors are orthogonal.

Diagonalization of Matrices

$$U = \begin{pmatrix} (u_1)_1 & (u_2)_1 & \cdots & \cdots & (u_n)_1 \\ (u_1)_2 & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ (u_1)_n & \cdots & \cdots & \cdots & (u_n)_n \end{pmatrix}$$

where $(u_i)_j$ is the j^{th} component of the i^{th} eigenvector of the Hermitian matrix H, i.e., the columns are constructed from these orthonormal eigenvectors.

If we evaluate the matrix product

$$U^\dagger U =$$

$$\begin{pmatrix} (u_1)_1^* & (u_1)_2^* & \cdots & \cdots & (u_1)_n^* \\ (u_2)_1^* & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ (u_n)_1^* & \cdots & \cdots & \cdots & (u_n)_n^* \end{pmatrix} \begin{pmatrix} (u_1)_1 & (u_2)_1 & \cdots & \cdots & (u_n)_1 \\ (u_1)_2 & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ (u_1)_n & \cdots & \cdots & \cdots & (u_n)_n \end{pmatrix}$$

it is clear that

$$(U^\dagger U)_{ij} = (u_i)^\dagger u_j = \delta_{ij} \rightarrow U^\dagger U = I \rightarrow U \text{ is a unitary matrix}$$

Now consider

$$D = U^\dagger H U \rightarrow D_{ij} = (U^\dagger H U)_{ij} = \sum_{k,m} (U^\dagger)_{ik} H_{km} U_{mj} = (u_i)^\dagger H u_j$$

$$= \lambda_j (u_i)^\dagger U_j = \lambda_j \delta_{ij}$$

Note that this calculation involves the i^{th} row of $U^\dagger$ and the j^{th} column of U.

This means that D is a **diagonal matrix** containing the eigenvalues of H on the diagonal.

The matrix $U^\dagger HU$ is a **unitary transformation** of H that diagonalizes it.

We also see that

$$\begin{aligned}(H-\lambda_\alpha)u_\alpha = 0 = U^\dagger(H-\lambda_\alpha)u_\alpha &= U^\dagger(H-\lambda_\alpha)Iu_\alpha \\ &= U^\dagger(H-\lambda_\alpha)UU^\dagger u_\alpha = (U^\dagger HU-\lambda_\alpha U^\dagger U)U^\dagger u_\alpha \\ &= (D-\lambda_\alpha)U^\dagger u_\alpha = (D-\lambda_\alpha)u'_\alpha\end{aligned}$$

Since D in the above equation is diagonal, the new eigenvector $U^\dagger u_\alpha = u'_\alpha$ must be a unit vector along the coordinate axes, i.e.,

$$u'_j = \begin{pmatrix} 0 \\ \cdots \\ \cdots \\ 1 \\ \cdots \\ 0 \end{pmatrix} \quad \text{the 1 is in the } j^{th} \text{ component}$$

Example:

Consider

$$H = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

and let us diagonalize H, H^2, H^n, e^H.

The eigenvalue problem is:

$$Hu_i = \lambda_i u_i \quad , \quad u_i = \begin{pmatrix} a_i \\ b_i \end{pmatrix} \quad , \quad a_i^2 + b_i^2 = 1$$

The characteristic equation is

$$\begin{vmatrix} 1-\lambda & 1 \\ 1 & 1-\lambda \end{vmatrix} = 0 \rightarrow \lambda_{i1,2} = 0, 2$$

and

$$u_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad , \quad u_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

The unitary matrix

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \qquad U^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

which contains the eigenvectors as columns should diagonalize H.

$$U^\dagger H U = \frac{1}{2}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix} = \begin{pmatrix}0 & 0\\ 0 & 2\end{pmatrix} = \begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix} = D$$

We also have

$$U^\dagger u_1 = u_1' = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix} = \begin{pmatrix}1\\ 0\end{pmatrix}$$

as expected. Now

$$U^\dagger H^2 U = U^\dagger H U U^\dagger H U = D^2 = \begin{pmatrix}0 & 0\\ 0 & 4\end{pmatrix} = \begin{pmatrix}\lambda_1^2 & 0\\ 0 & \lambda_2^2\end{pmatrix}$$

and

$$U^\dagger H^n U = D^n = \begin{pmatrix}\lambda_1^n & 0\\ 0 & \lambda_2^n\end{pmatrix}$$

Now for the function of H, e^H, we get

$$U^\dagger e^H U = \sum_{n=0}^{\infty} \frac{1}{n!} U^\dagger H^n U = \sum_{n=0}^{\infty} \frac{1}{n!} D^n = e^D$$

Now since D is diagonal and since the product of diagonal matrices is also diagonal

$$(e^D)_{ii} = \sum_{n=0}^{\infty} \frac{D_{ii}^n}{n!] = e^{D_{ii}}} \rightarrow e^D = \begin{pmatrix} 1 & 0 \\ 0 & e^2 \end{pmatrix}$$

In general, for $n \times n$ matrices

$$U^\dagger E^{\alpha H} U = e^{\alpha D} = \begin{pmatrix} e^{\alpha\lambda_1} & 0 & 0 & 0 & \cdots & 0 \\ 0 & e^{\alpha\lambda_2} & 0 & 0 & \cdots & 0 \\ 0 & 0 & e^{\alpha\lambda_3} & 0 & \cdots & 0 \\ & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & \cdots & e^{\alpha\lambda_n} \end{pmatrix}$$

$$\det\left(U^\dagger e^{\alpha H} U\right) = \det\left(e^{\alpha H} U U^\dagger\right) = \det\left(e^{\alpha H}\right) = \det\left(e^{\alpha D}\right)$$
$$= e^{\alpha\lambda_1} e^{\alpha\lambda_2} e^{\alpha\lambda_3} \cdots e^{\alpha\lambda_n} = e^{\alpha(\lambda_1+\lambda_2+\lambda_3+\cdots+\lambda_n)} = e^{\alpha \mathrm{Tr} D}$$

and

$$\mathrm{Tr}(U^\dagger H U) = \mathrm{Tr}(H U U^\dagger) = \mathrm{Tr}(H) = \mathrm{Tr}(D) = \sum_i \lambda_i$$

Fourier Series Introduction

Many complicated functions can be represented by power series.

Another powerful way of representing such functions is using a sum of sine and cosine terms, which is called a Fourier series.

Unlike Taylor series, a Fourier series can describe functions that are not everywhere continuous and/or differentiable.

Derivation

The world is full of vibrations. The sound we hear is an acoustic wave, the things we see are electromagnetic waves and the surfers in Santa Cruz, CA ride on gravity waves of the ocean.

The simplest wave motion in 1-dimension is described by the 1-dimensional wave equation

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\right) u(x,t) = 0$$

Let us assume a solution (we will see why this is a solution later when we study partial differential equations))

$$u(x,t) = \chi(x)e^{i\omega t}$$

Substitution into the full wave equation gives an equation for the wave amplitude $\chi(x)$.

$$\left(\frac{d^2\chi(x)}{dx^2}+\frac{\omega^2}{v^2}\chi(x)\right)e^{i\omega t}=0\rightarrow\left(\frac{d^2}{dx^2}+k^2\right)\chi(x)=0\ \ ,\ \ \frac{\omega^2}{v^2}=k^2$$

This new equation(an ordinary differential equation) is easily solved(we will see why later) by the function

$$\chi(x)=a\cos kx+b\sin kx$$

which gives the shape (at fixed time t) of the vibrating system (say a string).

This is like taking a photograph of the vibrating string at one instant of time.

Let us choose a string of length π fixed at both ends.

We then have the **boundary conditions**:

$$\chi(0) = 0 = \chi(\pi)$$

which implies that

$$\chi(0) = a = 0 \quad \text{and} \quad \chi(\pi) = 0 = b \sin k\pi \rightarrow k = n = \text{ integer}$$

so that

$$\chi(x) = b \sin nx \quad , \quad n = 1, 2, 3, ...$$

which is called the n^{th} **normal mode** of the string (given by its shape).

Each such mode has a different frequency and shape.

Historically, the wave equation was first studied in the 1700s.

In 1742, Bernoulli showed that

vibrations of different modes (frequency) could coexist in the string

In 1753, D'Alembert, Euler and Bernoulli showed that

all possible shapes of a vibrating string, even when the ends were not fixed, were representable by the series

$$f(x) = \sum_{n=1}^{\infty} b_n \sin nx$$

There was great dispute about this result.... what about the cosine series, i.e., how does one represent even functions of x?

Even though $f(x)$ solves the wave equation, others disputed the claim that this was the most general solution.

In 1807, Fourier (in a paper on heat conduction) showed that

every function in the closed interval

$$[-\pi, \pi] \quad \text{or} \quad -\pi \leq x \leq \pi$$

could be represented in the form

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty}(a_n \cos nx + b_n \sin nx)$$

He re-derived integral formulas for the coefficients a_n, b_n had already been obtained by Euler in 1777.

Fourier, however, broke new ground by pointing out that these integral formulas were well-defined even for arbitrary functions and that the resulting coefficients were identical for different functions that agreed within the interval, but not outside it.

The paper by Fourier **was rejected** by Lagrange, Laplace and Legendre on behalf of the Academy of Sciences on the grounds that it lacked mathematical rigor.

A second version of the paper won the Academy's Grand prize in 1812.

This work has had a great impact on the development of mathematical physics in the 1800s and it is still influencing things now.

The Sine-Cosine Series

The general Fourier series expansion is sum of sine and cosine terms of the form

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos \omega_n t + \sum_{n=1}^{\infty} b_n \sin \omega_n t$$

where the frequencies

$$\omega_n = \frac{2\pi n}{T_0}$$

are integer multiples of a fundamental frequency

$$\omega_0 = \frac{2\pi}{T_0}$$

and T_0 is determined either by the natural periodicity of $f(t)$ or possibly by an enforced periodicity of some sort.

Different treatments of this subject can have definitions of T_0 which differ by various factors.

The results of all calculations are the same.

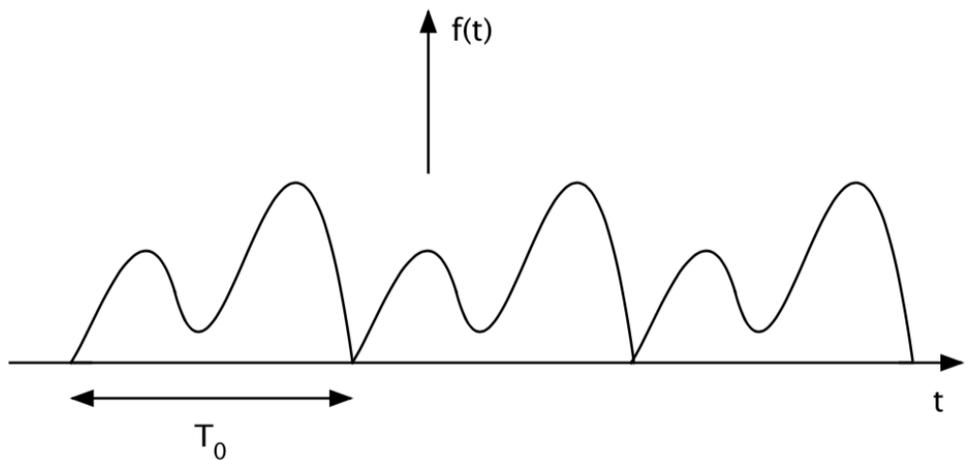
The assumed form guarantees that $f(t)$ has periodicity T_0, i.e.,

$$f(t) = f(t + T_0) \quad \text{for all} \quad t$$

In terms of the independent variable t, $f(t)$ has this periodicity for the entire interval

$$-\infty < t < \infty$$

as shown below



The typical Fourier series problem is such that we are given a function $g(t)$ and we then determine both T_0 and the a_n and b_n coefficients so that the series expansion is equal to $g(t)$ for all t.

This requires that

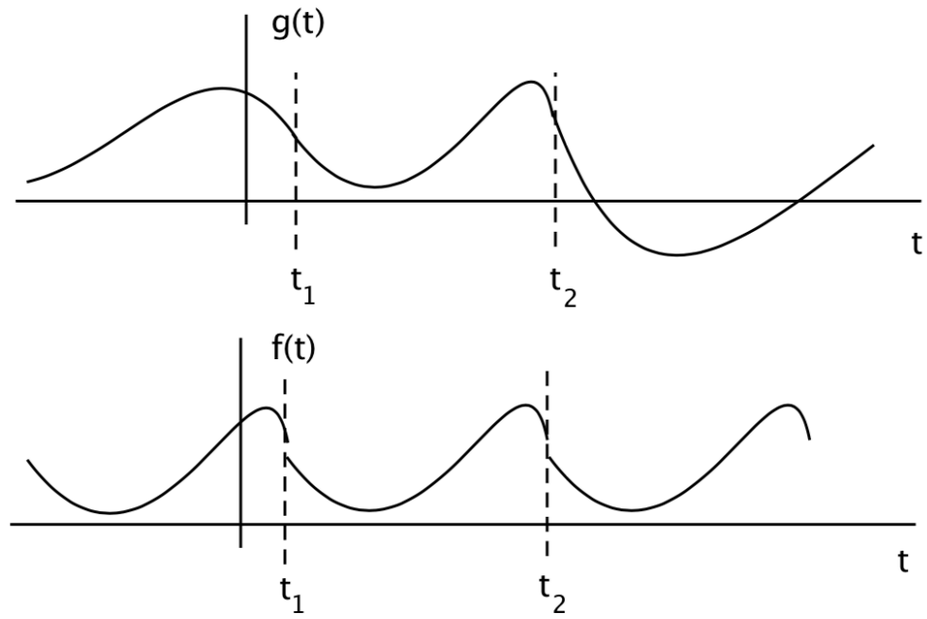
$$g(t) = g(t + T_0) \quad \text{for all} \quad t$$

The **smallest value** of T_0 that satisfies this equation is the **period** of $g(t)$.

What if $g(t)$ is not periodic?

In this case we cannot use a general Fourier series to represent $g(t)$ for **all** t.

On the other hand, we can make the series equal to $g(t)$ for some finite interval as shown below



Clearly, $g(t)$ above is not periodic.

Suppose however we define the basic period for the Fourier series to be $T_0 = t_2 - t_1$ where the interval $t_1 < t < t_2$ is as shown.

The Fourier series $f(t)$ can then be made identical to $g(t)$ in that interval.

Outside the interval, the Fourier series $f(t)$ is periodic and will not match $g(t)$ as shown.

Digression: The formal mathematical requirements that a function $f(x)$ must satisfy in order that it may be expanded in a Fourier series are known as the **Dirichlet conditions**, which are summarized as follows:

- the function must be periodic
- it must be single-valued and continuous, except possibly at a finite number of finite discontinuities
- it must have only a finite number of maxima and minima within one period
- the integral over one period of $|f(x)|$ must converge

The Orthogonality Conditions

We can determine the coefficients a_n and b_n using so-called **orthogonality conditions** (proved using calculus)

$$\int_{t_0}^{t_0+T_0} dt\, \sin\left(\frac{2\pi n}{T_0}t\right) \sin\left(\frac{2\pi m}{T_0}t\right) = \delta_{nm}\frac{T_0}{2}$$

$$\int_{t_0}^{t_0+T_0} dt\, \cos\left(\frac{2\pi n}{T_0}t\right) \cos\left(\frac{2\pi m}{T_0}t\right) = \delta_{nm}\frac{T_0}{2}$$

$$\int_{t_0}^{t_0+T_0} dt\, \sin\left(\frac{2\pi n}{T_0}t\right) \cos\left(\frac{2\pi m}{T_0}t\right) = 0$$

for **integer** values of m and n.

In addition we have

$$\int_{t_0}^{t_0+T_0} dt\, \sin\left(\frac{2\pi n}{T_0}t\right) = 0 \quad , \quad \int_{t_0}^{t_0+T_0} dt\, \cos\left(\frac{2\pi n}{T_0}t\right) = \delta_{n0}\, T_0$$

We can now evaluate the coefficients as follows.

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos \omega_n t + \sum_{n=1}^{\infty} b_n \sin \omega_n t$$

The integral operation

$$\int_{t_0}^{t_0+T_0} dt\, f(t) = \int_{t_0}^{t_0+T_0} dt\, \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \int_{t_0}^{t_0+T_0} dt\ \cos \omega_n t$$

$$+ \sum_{n=1}^{\infty} b_n \int_{t_0}^{t_0+T_0} dt\ \sin \omega_n t$$

$$= \int_{t_0}^{t_0+T_0} dt\, \frac{a_0}{2} = \frac{a_0 T_0}{2}$$

determines a_0, i.e.,

$$a_0 = \frac{2}{T_0} \int_{t_0}^{t_0+T_0} dt\, f(t)$$

The integral operation

$$\int_{t_0}^{t_0+T_0} dt\ \cos\omega_m t f(t) = \int_{t_0}^{t_0+T_0} dt\ \cos\omega_m t \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \int_{t_0}^{t_0+T_0} dt\ \cos\omega_m t \cos\omega_n t + \sum_{n=1}^{\infty} b_n \int_{t_0}^{t_0+T_0} dt\ \cos\omega_m t \sin\omega_n t$$

$$= \sum_{n=1}^{\infty} a_n \int_{t_0}^{t_0+T_0} dt\ \cos\omega_m t \cos\omega_n t$$

$$= \sum_{n=1}^{\infty} a_n \delta_{nm} \frac{T_0}{2} = a_m \frac{T_0}{2}$$

determines a_m, $m > 0$, i.e.,

$$a_m = \frac{2}{T_0} \int_{t_0}^{t_0+T_0} dt\ \cos\omega_m t f(t)$$

The integral operation

$$\int_{t_0}^{t_0+T_0} dt\ \sin\omega_m t f(t) = \int_{t_0}^{t_0+T_0} dt\ \sin\omega_m t \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \int_{t_0}^{t_0+T_0} dt\ \sin\omega_m t \cos\omega_n t + \sum_{n=1}^{\infty} b_n \int_{t_0}^{t_0+T_0} dt\ \sin\omega_m t \sin\omega_n t$$

$$= \sum_{n=1}^{\infty} b_n \int_{t_0}^{t_0+T_0} dt\ \sin\omega_m t \sin\omega_n t$$

$$= \sum_{n=1}^{\infty} b_n \delta_{\boldsymbol{nm}} \frac{T_0}{2} = b_m \frac{T_0}{2}$$

determines b_m, $m > 0$, i.e.,

$$b_m = \frac{2}{T_0} \int_{t_0}^{t_0+T_0} dt\ \sin\omega_m t f(t)$$

Several questions arise:

(1) Do these Fourier coefficients exist?

(2) Is the Fourier series convergent?

(3) Does it converge to the original function?

The answer is **YES for all physically realizable systems!!!!**

Examples:

(1) The function $f(t)$ is

$$f(t) = \sin(t)$$

This function is periodic with period $T_0 = 2\pi \rightarrow \omega_n = n$.

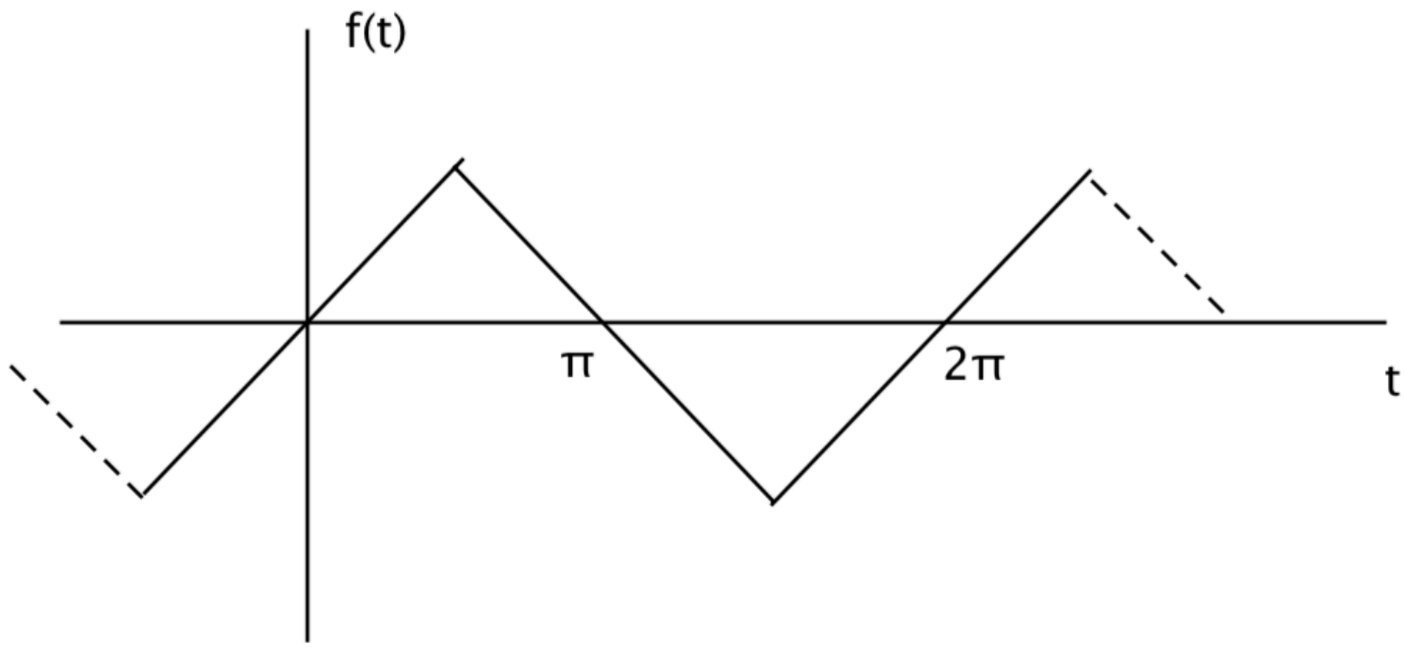
Therefore the Fourier series looks like

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \sin nt + \sum_{n=1}^{\infty} b_n \cos nt$$

This example requires no calculations. It is clear that

$$a_m = 0 \quad \text{for all} \quad m \quad , \quad b_m = 0 \quad \text{for all} \quad m \neq 1 \quad , \quad b_1 = 1$$

(2) The function $f(t)$ equals the periodic triangle wave shown above.



In the interval $-\pi/2 < t < 3\pi/2$ this has the functional form

$$f(t) = \begin{cases} \frac{2t}{\pi} & -\frac{\pi}{2} \leq t \leq \frac{\pi}{2} \\ 2 - \frac{2t}{\pi} & \frac{\pi}{2} \leq t \leq \frac{3\pi}{2} \end{cases}$$

Once again the basic period is $T_0 = 2\pi$ which again gives $\omega_n = n$.

We have

$$a_m = \frac{2}{T_0} \int_{-\pi/2}^{3\pi/2} dt \, \cos \omega_n t f(t) = 0 \quad \text{for all} \quad m$$

since the integrand is the **product of an odd and an even function**.

We also have

$$b_m = \frac{2}{T_0} \int_{-\pi/2}^{3\pi/2} dt \, \sin \omega_n t f(t) = \frac{8}{\pi^2 n^2} \sin \frac{n\pi}{2}$$

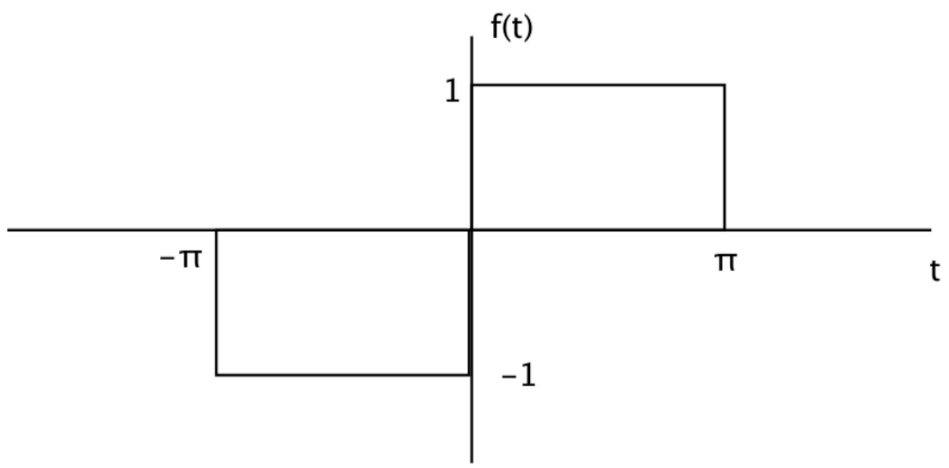
Therefore, we get

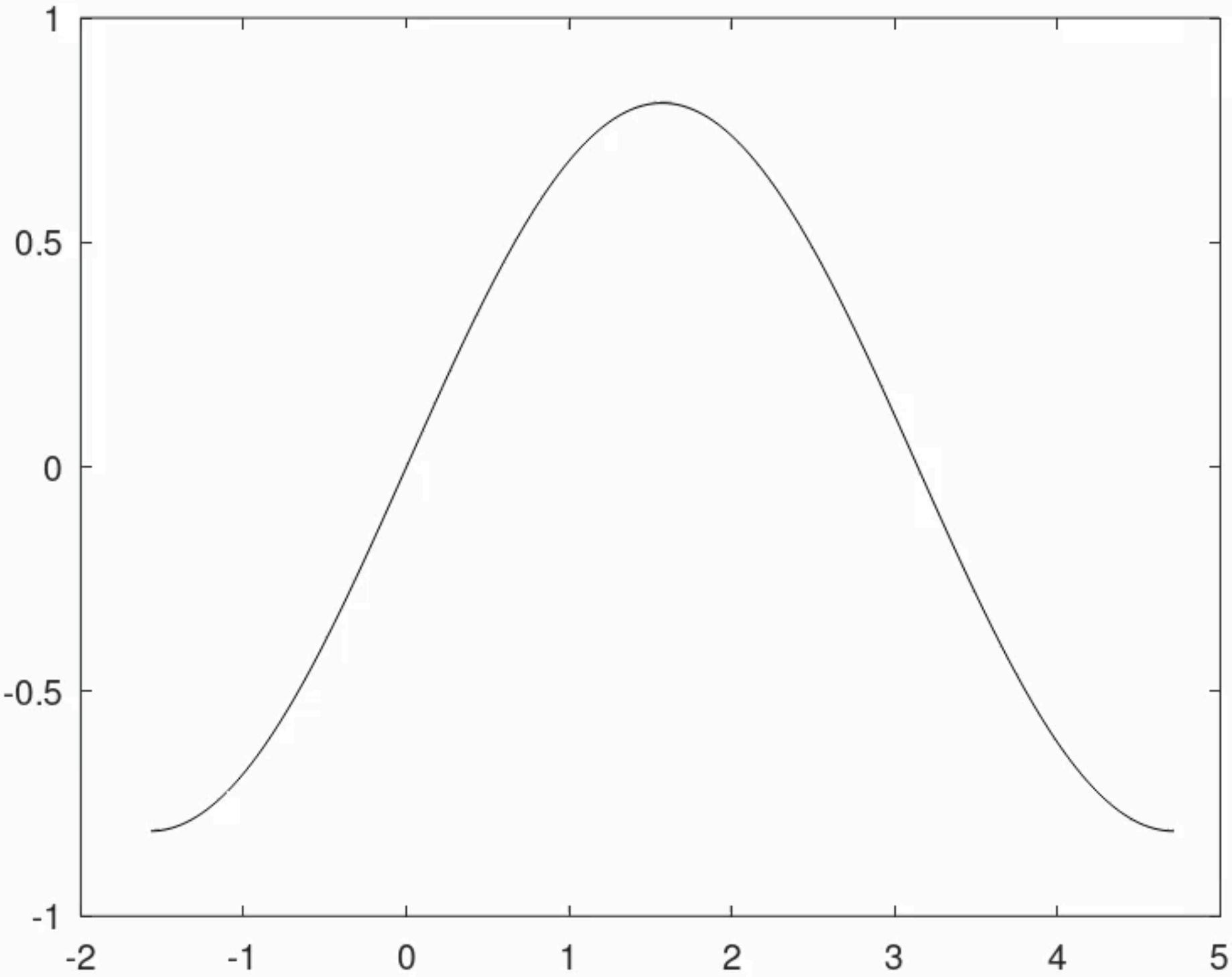
$$f(t) = \sum_{n=1,odd} \frac{8}{\pi^2 n^2} \sin \frac{n\pi}{2} \sin nx$$

Illustrate in class with Octave program:

```
% illustrate Fourier Series
% triangle wave
% gives sequence of images building
% up to final curve
x=-pi/2:pi/100:3*pi/2;
val = zeros(1,length(x));
figure(1);
for m=1:2:100
 f=8/(m*pi)^2*sin(m*pi/2)*sin(m*x);
 val=val+f; m
 clf;
 plot(x,val, '-k');
  axis([-pi/2 3*pi/2 -1.5 1.5]);
 hold on;
 pause(1);
end
```

(3) $f(t)$ is the square wave function

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1
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3
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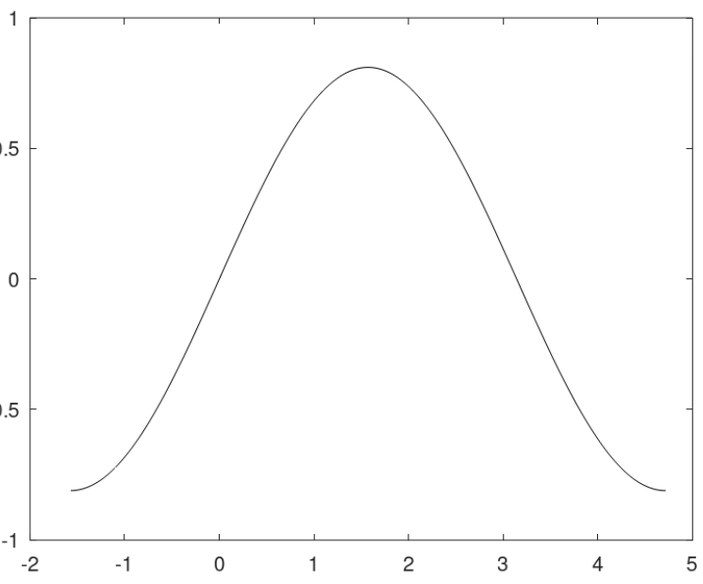
5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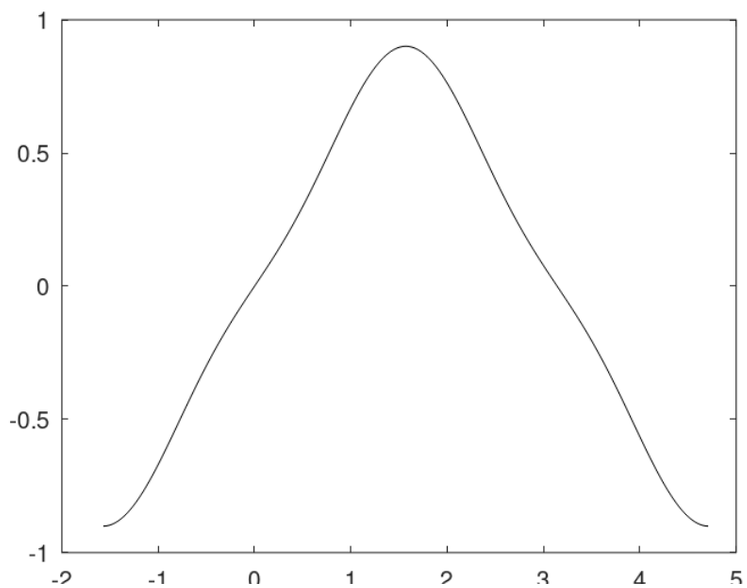
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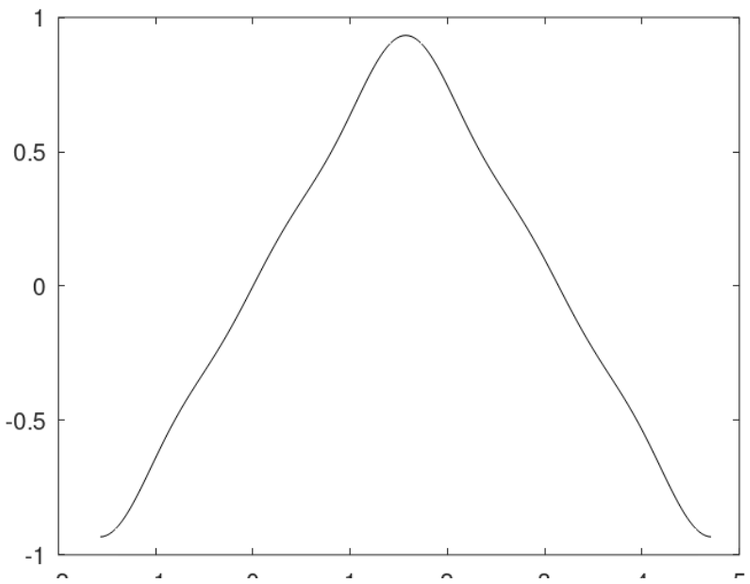
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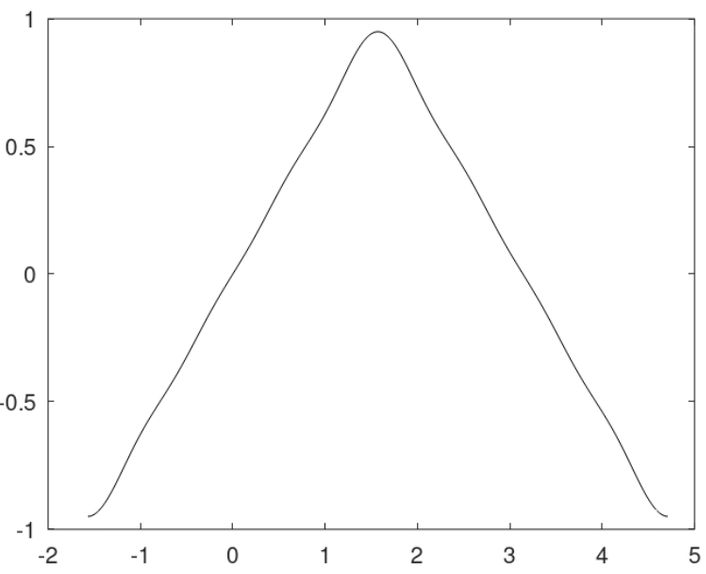
-1
5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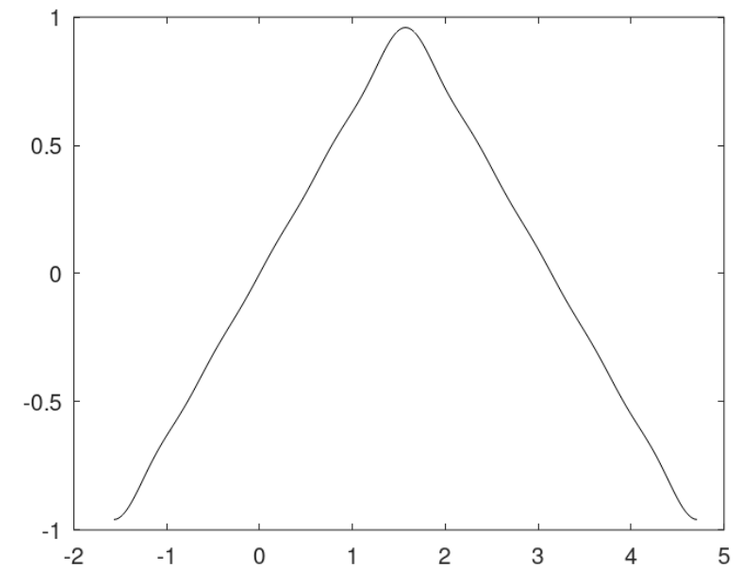
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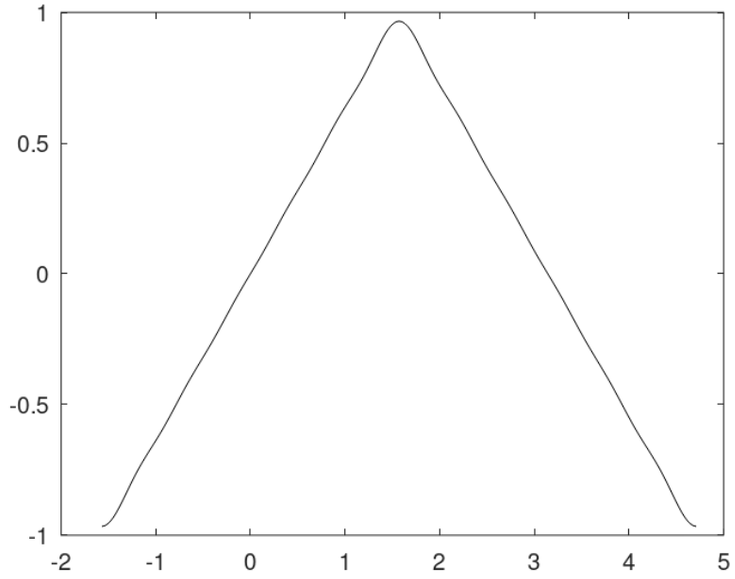
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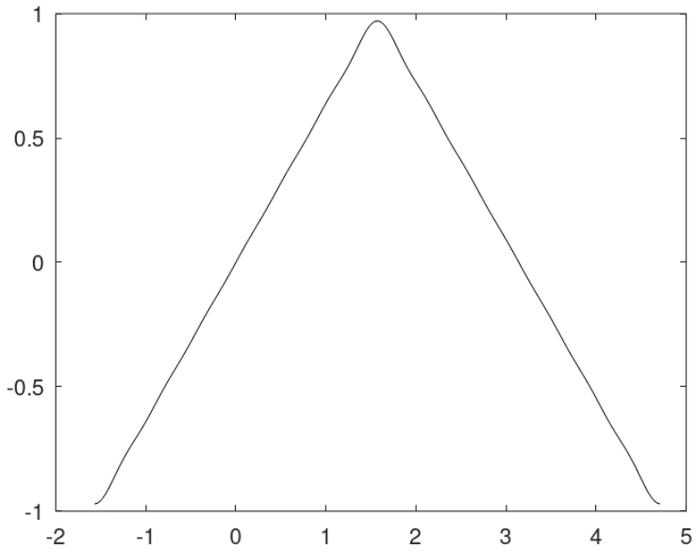
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-1
-2
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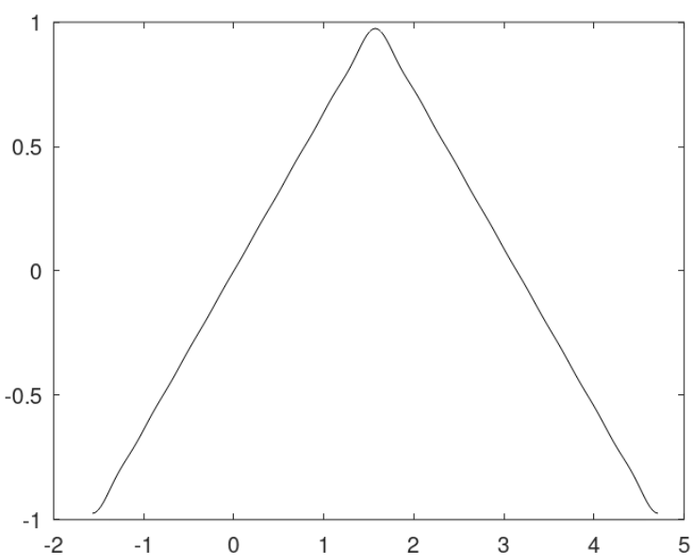
0
1
2
3
4
5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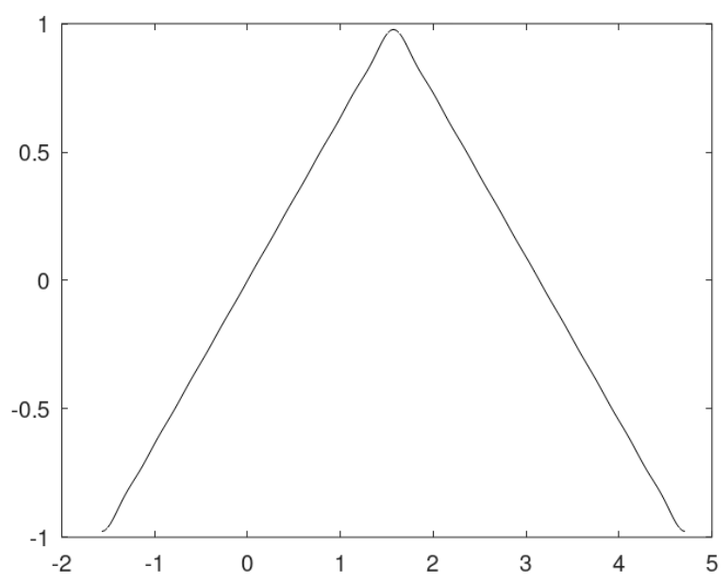
-0.5
-1
-2
-1
0
1
2
3
4
5


1
0.5
0
-0.5
-1
-2
-1
0
1
2
3
4
5

In the interval $[-\pi, \pi]$ we have

$$f(t) = \begin{cases} +1 & 0 \leq t \leq \pi \\ -1 & -\pi \leq t \leq 0 \end{cases}$$

Once again the basic period is $T_0 = 2\pi$ which again gives $\omega_n = n$.

Again this is an odd function so all the $a_n = 0$ and we find

$$b_n = \begin{cases} \frac{4}{n\pi} & n = 1, 3, 5, 6, ... \\ 0 & n = 2, 4, 6, 8, ... \end{cases}$$

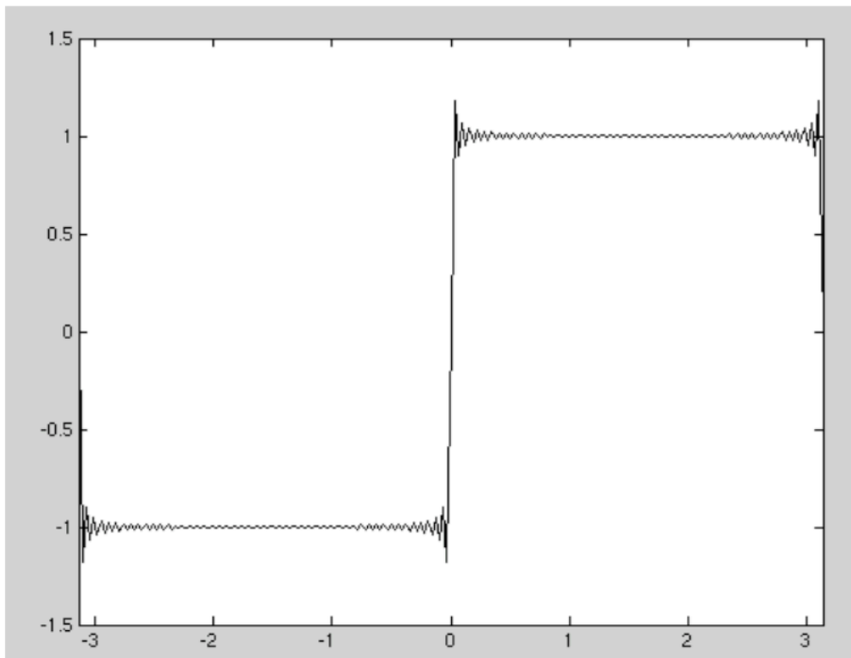
which gives

$$f(t) = \frac{4}{\pi} \sum_{n=odd} \frac{sinnt}{n}$$

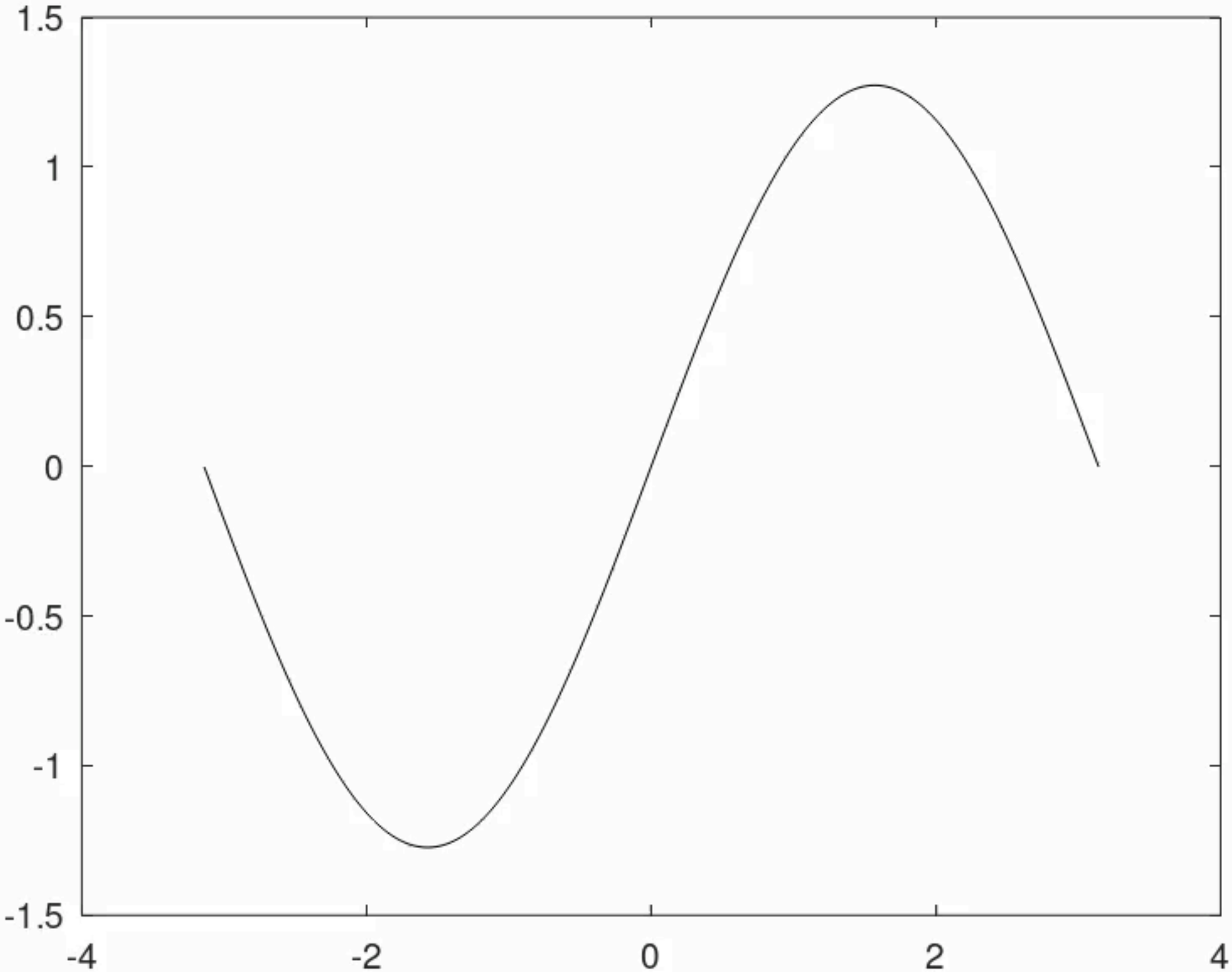
Illustrate in class with Octave program:

```
% illustrate Fourier Series for square wave pulse
% gives sequence of images building up to final curve x=-pi:pi/100:pi;
val = zeros(1,length(x));
figure(1);
for m=1:2:500
 f=4/(m*pi)*sin(m*x);
 val=val+f;
 m
 clf;
 plot(x,val,'-k');
 axis([-pi pi -1.5 1.5]);
 hold on;
 pause(1);
end
```

It looks like the figure below after including a 100 terms in the sum....



We will do better in class.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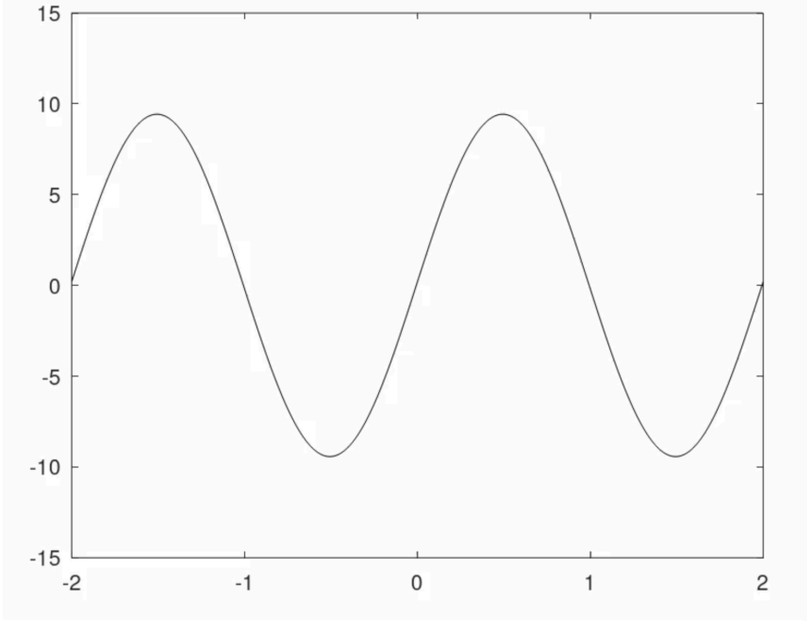
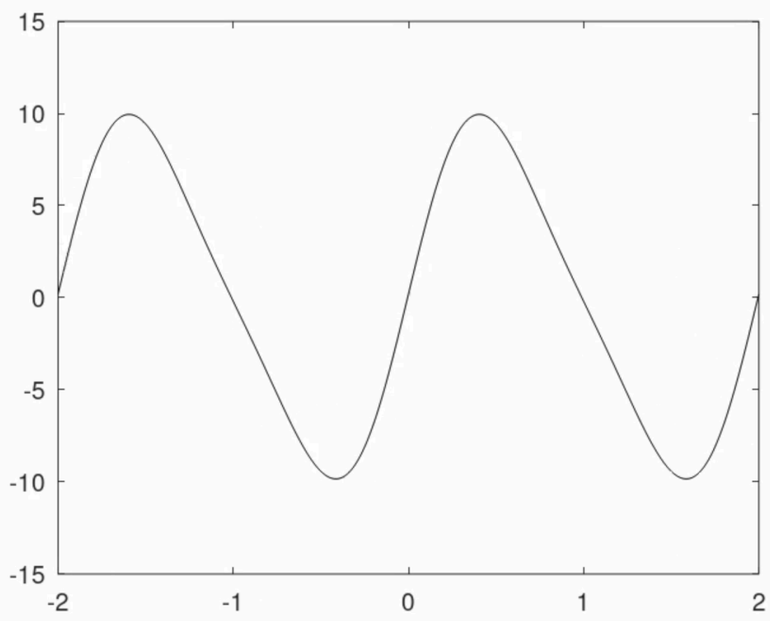
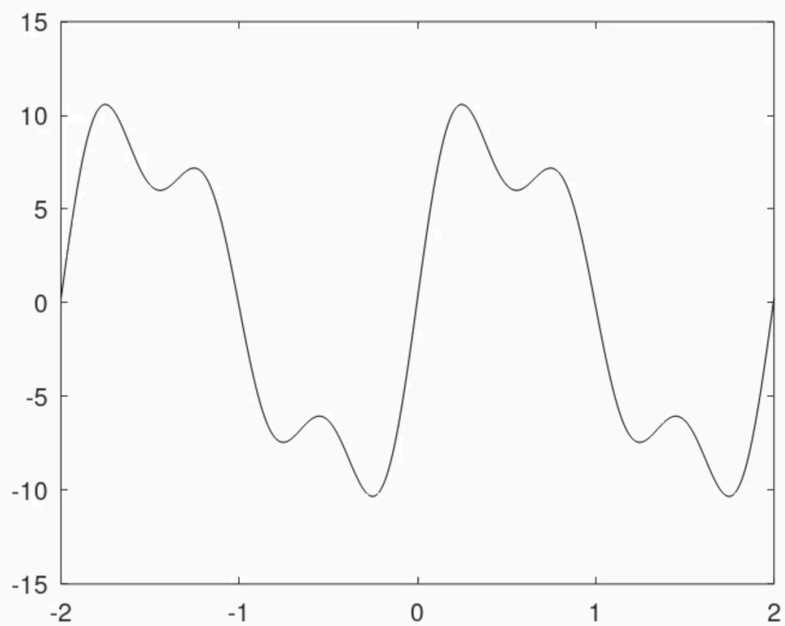
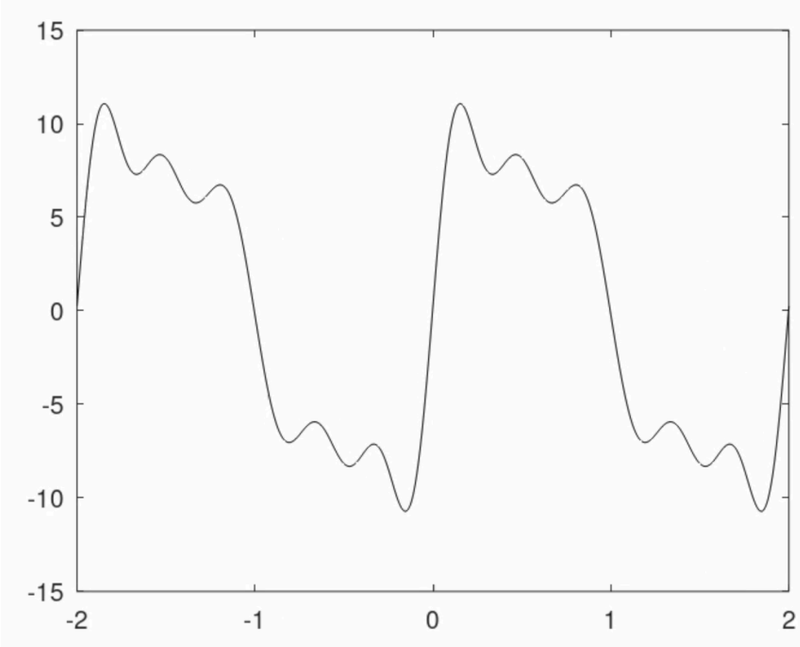
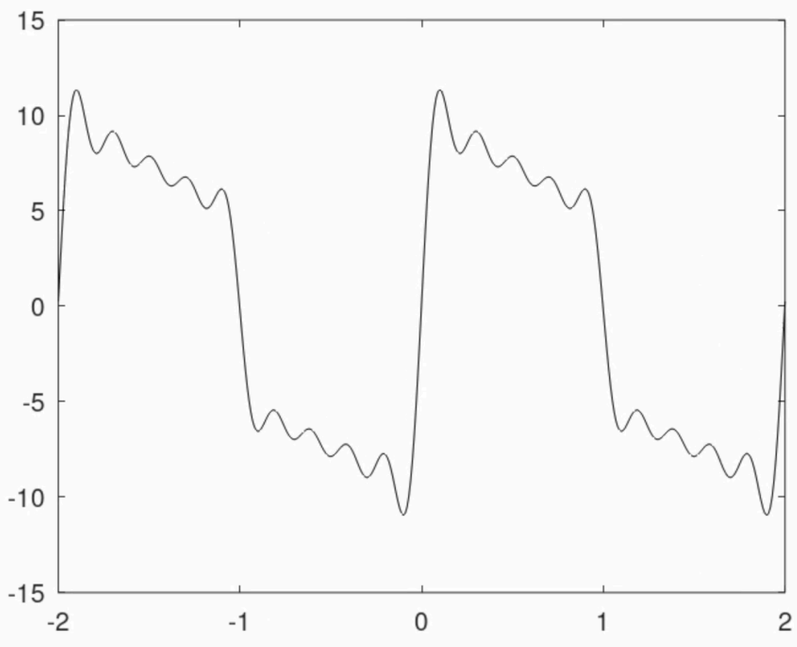
1
0.5
0
-0.5
-1
-1.5
-4
-2
0
2
4

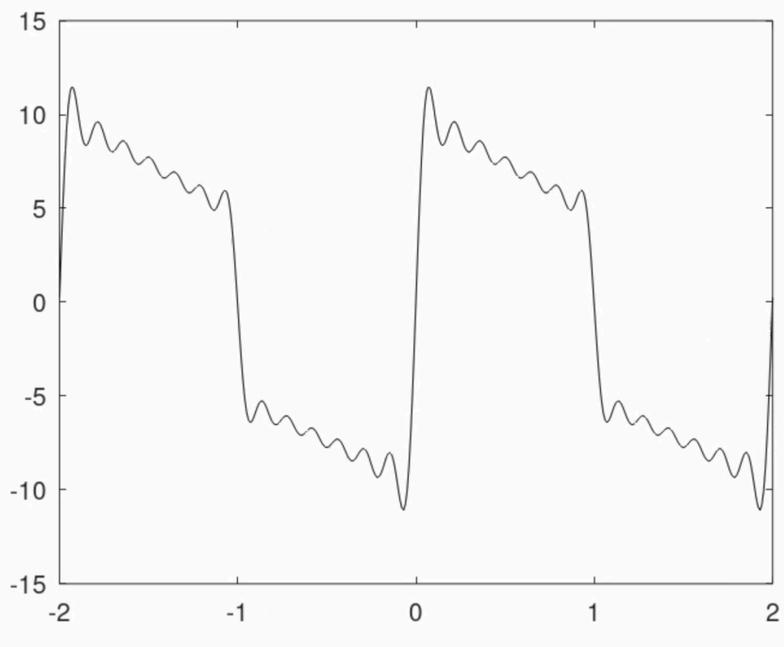




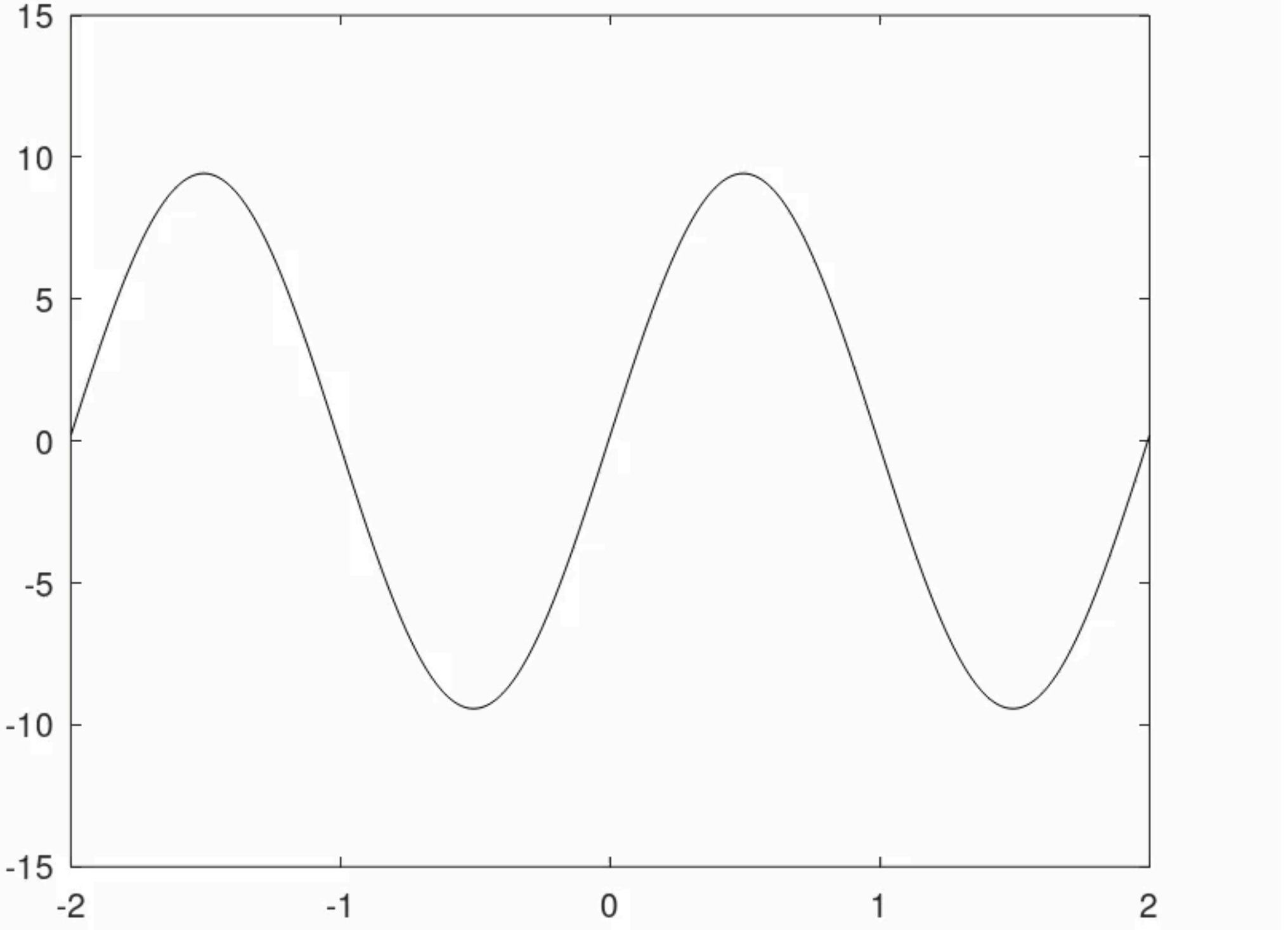








another example - first 6 slide because it happens fast


15
10
5
0
-5
-10
-15
-2
-1
0
1
2

Even and Odd Stuff

We can always rewrite any function as:

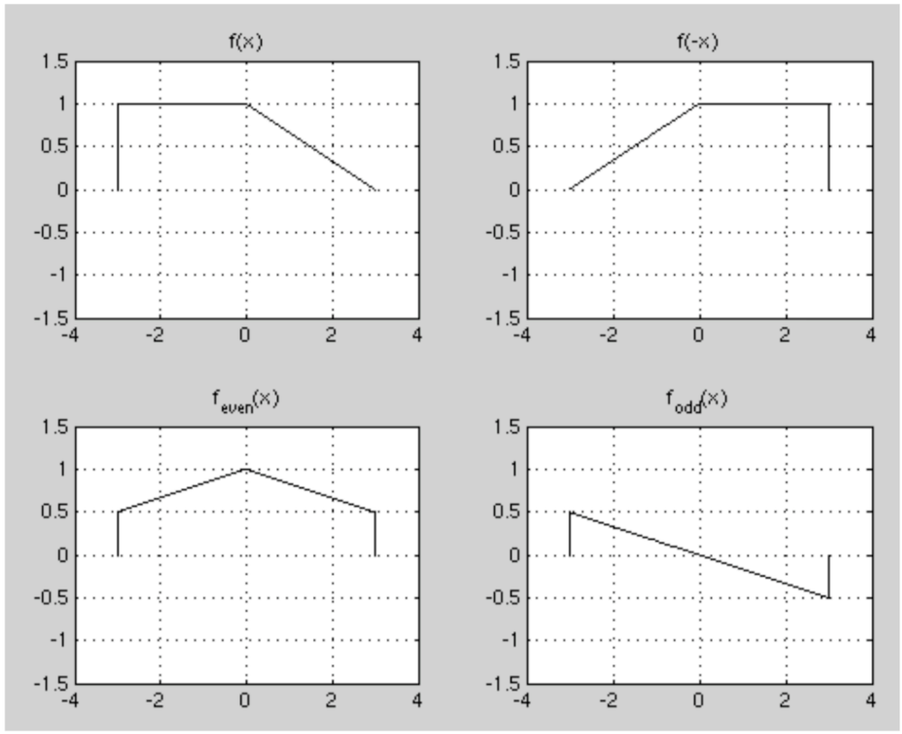
$$f(x) = \frac{1}{2}[f(x) + f(-x)] + \frac{1}{2}[f(x) - f(-x)] = f_{even}\ (x) + f_{odd}(x)$$

We can then use Fourier series to write:

$$f_{even}\ (x) = \frac{a_0}{2} \sum_n a_n \cos nx \quad , \quad f_{odd}(x) = \sum_n b_n \sin nx$$

where we have assumed that the function has a period $T_0 = 2\pi$.

Example:



Now we allow for an **Arbitrary Interval**.

If $f(x)$ is defined for an interval $[-L, L]$ of length(period) $2L$ instead of the standard interval of length (period) 2π, then a simple change of variable and integration range deals with the problem.

We have

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos \frac{2\pi n}{T_0} t + \sum_{n=1}^{\infty} b_n \sin \frac{2\pi n}{T_0} t$$

with

$$a_0 = \frac{2}{T_0} \int_{-T_0/2}^{T_0/2} dt\, f(t)\ ,\ a_n = \frac{2}{T_0} \int_{-T_0/2}^{T_0/2} dt\ \cos \frac{2\pi nt}{T_0} f(t)$$

$$b_n = \frac{2}{T_0} \int_{-T_0/2}^{T_0/2} dt\ \sin \frac{2\pi nt}{T_0} f(t)$$

We let $T_0 = 2L$ to get

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

with

$$a_0 = \frac{1}{L}\int_{-L}^{L} dx\, f(x)\ ,\ a_n = \frac{1}{L}\int_{-L}^{L} dx\, \cos\frac{\pi n x}{L} f(x)$$

$$b_n = \frac{1}{L}\int_{-L}^{L} dx\, \sin\frac{\pi n x}{L} f(x)$$

Another Example:

Suppose

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

The is a square pulse(wave).

We might imagine this is a signal being sent into some electronic apparatus.

We can calculate its Fourier coefficients

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} dx\ f(x)\frac{1}{\pi}\int_0^{\pi} h dx = h$$

$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} dx\ \cos nx f(x) = 0 \quad \text{for all} \quad n$$

$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} dx\ \sin nx f(x) = \frac{h}{n\pi}(1-\cos n\pi) = \begin{cases} 2h/n\pi & n \ \text{odd} \\ 0 & n \ \text{even} \end{cases}$$

which gives

$$f(x) = \frac{h}{2} = \frac{2h}{\pi}\left[\frac{\sin x}{1} + \frac{\sin 3x}{3} + \frac{\sin 5x}{5} + \cdots\right]$$

We note that the terms fall off only as $1/n$, which implies physically that a square wave contains lots of **high frequency components**.

This implies that if an electronic apparatus does not pass high-frequency components well, the square wave input will emerge with corners rounded off in the best case and, possibly, an amorphous blob in the worst case.

Complex Fourier Series and Return of the Dirac Delta Function

Let us rewrite our Fourier representation for $f(x)$ using

$$e^{i\beta t} = \cos\beta t + i\sin\beta t$$

as follows (using the interval $[-L, L]$):

$$\begin{aligned} f(x) &= \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \frac{e^{in\pi x/L} + e^{-in\pi x/L}}{2} + \sum_{n=1}^{\infty} b_n \frac{e^{in\pi x/L} - e^{-in\pi x/L}}{2i} \\ &= \sum_{-\infty}^{\infty} c_n e^{in\pi x/L} \end{aligned}$$

Note the change of limits on the summation.

The new coefficients are given by:

$$c_0 = \frac{a_0}{2} \quad , \quad c_{n>0} = \frac{1}{2}(a_n - ib_n) \quad , \quad c_{n<0} = \frac{1}{2}(a_{|n|} + ib_{|n|}) = \frac{1}{2}(a_{-n} + ib_{-n})$$

and in general, using the formulas for the a and b coefficients, we have:

$$c_n = \frac{1}{2L}\int_{-L}^{L} f(x)e^{-in\pi x/L}dx$$

This is called the **complex Fourier representation**.

Example: Let us repeat an example from earlier.

Let $g(x)$ be the square wave function

$$g(x) = \begin{cases} +1 & \text{for } 0 \le x \le \pi \\ -1 & \text{for } -\pi \le x \le 0 \end{cases}$$

We have $L = \pi$, so that

$$c_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} g(x)e^{-inx}dx = \frac{1}{2\pi}\int_{0}^{\pi} e^{-inx}dx - \frac{1}{2\pi}\int_{-\pi}^{0} e^{-inx}dx$$

$$= \frac{i}{2\pi n}[e^{-in\pi} - 1 + e^{in\pi} - 1] = i\frac{\cos n\pi - 1}{n\pi}$$

or

$$c_n = \begin{cases} -\frac{2i}{n\pi} & \text{n odd} \\ 0 & \text{n even} \end{cases}$$

This gives

$$g(x) = \sum_{n=-\infty}^{\infty} c_n e^{inx} = \sum_{n=[-\infty,\infty]\, odd} -\frac{2i}{n\pi} e^{inx}$$

$$= \sum_{n=[0,\infty]\, odd} \frac{1}{n}(e^{inx} - e^{-inx}) = \frac{4}{\pi} \sum_{n=[0,\infty]\, odd} \frac{\sin nx}{n}$$

which, of course, is the same as the earlier result.

Clearly, this calculation was more complicated.

The usefulness of the complex Fourier series comes when doing theoretical derivations.

Digression : The Dirac Delta Function

Let us substitute the expression for c_n back into the Fourier series.

We get:

$$
\begin{aligned}
f(x) &= \sum_{-\infty}^{\infty} c_n e^{in\pi x/L} = \sum_{-\infty}^{\infty} e^{in\pi x/L} \frac{1}{2L} \int_{-L}^{L} f(x') e^{-in\pi x'/L} dx' \\
&= \int_{-L}^{L} f(x') \left[\frac{1}{2L} \sum_{-\infty}^{\infty} e^{in\pi (x-x')/L} \right] dx' \\
&= \int_{-L}^{L} f(x') \delta(x - x') dx'
\end{aligned}
$$

where we have defined

$$
\delta(x - x') = \left[\frac{1}{2L} \sum_{-\infty}^{\infty} e^{in\pi (x-x')/L} \right] = \text{ Dirac delta function}
$$

This expression has all the standard properties of the Dirac delta function(listed below) and is a very important **representation** of the delta function.

Dirac Delta Function

Dirac, when faced with a mathematical dilemma during his development of quantum mechanics, solved his problem by introducing a new "function" defined by

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

$$\delta(x - x') = 0 \text{ if } x' \neq x$$

$$\int_{-\infty}^{\infty} f(x')\delta(x - x')dx' = f(x)$$

Clearly, this is not an ordinary "function" in any sense.

Some Properties:

(1)

$$\int_{0-}^{0+} dt'\delta(-t')f(t') = -\int_{-0-}^{-0+} dt'\delta(t')f(-t')$$
$$= -\int_{0+}^{0-} dt'\delta(t')f(-t') = \int_{0-}^{0+} dt'\delta(t')f(-t')$$
$$= f(0)$$

which implies that $\delta(-t) = \delta(t)$ if we are using it inside integrals, i.e.,

$$f(0) = \int \delta(-t)f(t)dt = \int \delta(t)f(t)dt$$

(2)

$$\int_{0-}^{0+} dt'\delta(at')f(t') = \frac{1}{|a|}\int_{0-/a}^{0+/a} dt''\delta(t'')f(t''/a) = \frac{1}{|a|}f(0)$$

which implies that

$$\delta(at) = \frac{1}{|a|}\delta(t)$$

if we are using it inside integrals, i.e.,

$$\frac{1}{|a|}f(0) = \int \delta(at)f(t)dt = \frac{1}{|a|}\int \delta(t)f(t)dt$$

(3)

$$\int_{0-}^{0+} dt't'\delta(t')f(t') = f(0)(0) = 0$$

If $f(0) \neq 0$, then this relation implies that

$$t\delta(t) = 0$$

if we are using it inside integrals.

(4)

$$\int_{-L}^{L} f(x)\delta(x^2 - b^2)dx = \int_{-L}^{0} f(x)\delta(x^2 - b^2)dx + \int_{0}^{L} f(x)\delta(x^2 - b^2)dx$$

$$= \int_{-L}^{0} f(x)\delta((x - b)(x + b))dx + \int_{0}^{L} f(x)\delta((x - b)(x + b))dx$$

$$= \int_{-L}^{0} f(x)\delta((-2b)(x + b))dx + \int_{0}^{L} f(x)\delta((x - b)(2b))dx$$

$$= \frac{1}{2|b|}\int_{-L}^{0} f(x)\delta(x + b)dx + \frac{1}{2|b|}\int_{0}^{L} f(x)\delta(x - b)dx$$

$$= \frac{1}{2|b|}(f(-b) + f(b))$$

which implies that

$$\delta(x^2 - b^2) = \frac{1}{2|b|}(\delta(x - b) + \delta(x + b))$$

Example: if $a > 0$, then

$$\int_{-a}^{a} e^{-x}\delta(x^2 - a^2)dx = \int_{-a}^{a} e^{-x}\frac{1}{2a}(\delta(x - a) + \delta(x + a))dx$$

$$= \frac{e^{-a} + e^{a}}{2a} = \frac{1}{a}\cosh(a)$$

Fourier Series Extended.....

Let us extend Fourier series somewhat .....

Remember a vector $\vec{A}$ in n-dimensions has n cartesian components

$$\vec{A} = \sum_{i=1}^{n} A_i \hat{e}_i = \sum_{i=1}^{n} (\hat{e}_i \cdot \vec{A})\hat{e}_i$$

The Fourier series has a **similar** structure!

Consider

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \psi_n(x)$$

This is also a sum of terms, each of which is made up of a Fourier coefficient c_n (the **analog** of the vector component A_i) and a unique (basis) function

$$\psi_n(x) = e^{in\pi x/L}$$

which plays the role of $\hat{e}_i$. The functions $\psi_n(x)$ satisfy the integral relations

$$\int_{-L}^{L} \psi_m^*(x)\psi_n(x)dx = \int_{-L}^{L} e^{i(n-m)\pi x/L}dx$$

$$= \begin{cases} 2L & m = n \\ \frac{2L}{(n-m)\pi}\sin(n-m)\pi & m \neq n \end{cases}$$

$$= 2L\delta_{mn}$$

which corresponds to the inner product relations of the unit vectors

$$\hat{e}_m \cdot \hat{e}_n = \delta_{mn}$$

Note the different normalizations. The coefficients c_n are given by

$$\int_{-L}^{L} \psi_m^*(x)f(x)dx = \sum_n c_n \int_{-L}^{L} \psi_m^*(x)\psi_n(x)dx = \sum_n c_n 2L\delta_{mn} = 2Lc_m$$

which corresponds to the component relations $A_i = \vec{A} \cdot \hat{e}_i$.

We can make the agreement exact by defining a **unit function** (equivalent to a unit basis vector) as

$$e_n(x) = \frac{1}{\sqrt{2\pi}} e^{in\pi x/L}$$

This unit function has the inner product

$$(e_m, e_n) = \int_{-L}^{L} e_m^*(x) e_n(x) dx = \delta_{mn}$$

which then gives

$$f(x) = \sum_n f_n e_n(x) \rightarrow f_n = (e_n, f) = \int_{-L}^{L} e_n^*(x) f(x) dx$$

in direct analogy to the relations

$$\vec{A} = \sum_{i=1}^{n} A_i \hat{e}_i = \sum_{i=1}^{n} (\hat{e}_i \cdot \vec{A}) \hat{e}_i$$

The unit functions are a set of orthonormal basis functions.

They are a basis because they span the space of all functions (since that is what a Fourier series is designed to do).

The Dirac delta-function is given by

$$\delta(x - x') = \sum_{n=-\infty}^{\infty} e_n(x) e_n^*(x')$$

$$\rightarrow \int f(x')\delta(x - x')dx' = \sum_{n=-\infty}^{\infty} e_n(x) \int e_n^*(x')\delta(x - x')dx' = \sum_{n=-\infty}^{\infty} f_n e_n(x) = f(x)$$

as it should.

The number of basis functions is infinite, so we have an infinite dimensional space.

Since an **inner product** is defined it is an **inner product space**.

For regular vectors, a different choice of axes implies a different set of unit basis vectors.

In the case of functions, a different choice of **coordinate axes** implies the use of a different set of **"orthonormal"** functions.

For the complex Fourier series in the interval $[-1, 1]$ corresponding to $L = 1$, the basis functions are

$$\psi_n(x) = e^{in\pi x} \quad , \quad \omega_n = \frac{2\pi n}{T_0} = \frac{2\pi n}{2L} = \pi n$$

where

$$e^{in\pi x} = 1 + (in\pi x) + \frac{1}{2!}(in\pi x)^2 + ...$$

which is a **convergent infinite power series** in x.

Since powers of x are much easier to work with than exponentials, let us attempt to use the powers of x, instead of the $\psi_n(x)$ as our basis functions for a generalized Fourier series.

Let us take the first two basis functions to be

$$P_0(x) = 1 \quad , \quad P_1(x) = x \quad , \quad \text{in the range } [-1, 1]$$

The orthogonality relations are

$$(P_0, P_0) = \int_{-1}^{1} dx = 2$$

$$(P_0, P_1) = (P_1, P_0) = \int_{-1}^{1} x dx = 0$$

$$(P_1, P_1) = \int_{-1}^{1} x^2 dx = \frac{2}{3}$$

The next power x^2 is orthogonal to $P_1(x)$

$$(P_1, x^2) = (x^2, P_1) = \int_{-1}^{1} x^3 dx = 0$$

but not to $P_0(x)$

$$(P_0, x^2) = (x^2, P_0) = \int_{-1}^{1} x^2 dx = \frac{2}{3}$$

This implies that x^2 **cannot** be one of the set of mutually orthogonal functions that is to be used as a basis for our so-called generalized Fourier series.

Let us now use the **Gram-Schmidt(GS) orthogonalization procedure** to create an orthogonal function.

If x^2 is not orthogonal to $P_0(x)$, then part of it must be parallel to $P_0(x)$.

Indeed the parallel component is given by

$$(P_0, x^2) = \frac{2}{3}$$

The **GS** procedure creates an orthogonal function by subtracting off the parallel part as follows

$$P_2(x) = x^2 - \frac{(x^2, P_0)}{(P_0, P_0)} P_0 = x^2 - \frac{1}{3}$$

We then have the orthogonality relations

$$(P_2, P_1) = (P_1, P_2) = 0 \quad , \quad (P_2, P_0) = (P_0, P_2) = 0$$

$$(P_2, P_2) = \int_{-1}^{1} \left(x^2 - \frac{2}{3} x^2 + \frac{1}{9} \right) dx = \frac{8}{45}$$

Now

$$(x^2, P_2) = (x^3, P_0) = 0 \quad \text{but} \quad (x^3, P_1) \neq 0$$

$$P_3(x) = x^3 - \frac{(x^3, P_1)}{(P_1, P_1)} P_1 = x^3 - \frac{3}{5}x$$

It is customary to normalize all basis functions to 1, which entails multiplication by the factor

$$\frac{1}{\sqrt{(P_i, P_i)}}$$

or by defining their value at a point, say $P_n(x = 1) = 1$.

This gives (using the **latter** normalization procedure) us a set of orthonormal basis functions (polynomials in this case) which are identical to the **Legendre functions or Legendre polynomials**.

$$P_0(x) = 1 \ , \ \ P_1(x) = x \ , \ \ P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}$$

$$P_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x \ , \ \ P_4(x) = \frac{35}{8}x^4 - \frac{15}{4}x^2 + frac38$$

$$P_5(x) = \frac{63}{8}x^5 - \frac{35}{4}x^23 + frac158x \quad \text{and so on}$$

where we have

$$(P_n, P_m) = \int_{-1}^{1} P_n(x)P_m(x)dx = \frac{2}{2n+1}\delta_{mn} \ , \ \ P_m(1) = 1$$

We then have using these as basis functions

$$f(x) = \sum_{n=0}^{\infty} c_n P_n(x)$$

$$\rightarrow \int_{-1}^{1} P_m(x) f(x) dx = \sum_{n=0}^{\infty} c_n \int_{-1}^{1} P_m(x) P_n(x) dx$$

$$= \sum_{n=0}^{\infty} c_n \frac{2}{2n+1} \delta_{mn} = \frac{2}{2m+1} c_m$$

or

$$c_n \frac{2n+1}{2} \int_{-1}^{1} P_n(x) f(x) dx$$

Example:

$$f(x) = \begin{cases} +1 & \text{for } 0 \leq x \leq 1 \\ -1 & \text{for } -1 \leq x \leq 0 \end{cases}$$

Now $f(x)$ is odd, which implies that all $n =$ even terms will $= 0$.

For odd n we have

$$c_1 = \frac{3}{2}\int_{-1}^{1} xf(x)dx = 3\int_{0}^{1} xdx = \frac{3}{2}$$

$$c_3 = \frac{7}{2}\int_{-1}^{1} \left(\frac{5}{2}x^3 - \frac{3}{2}x\right) f(x)dx = \frac{7}{2}\int_{0}^{1} \left(\frac{5}{x}^3 - 3x\right) dx = -\frac{7}{8}$$

$$c_5 = \frac{11}{16} \quad \text{and so on}$$

The Legendre series is then

$$f(x) = \frac{3}{2}P_1(x) - \frac{7}{8}P_3(x) + \frac{11}{16}P_5(x) + ...$$

The corresponding Fourier series in the interval $[-1, 1]$ is given by

$$a_n = 0 \quad , \quad b_n = \frac{1}{1}\int_{-1}^{1} f(x)\sin(n\pi x)dx = 2\int_{0}^{1} \sin(n\pi x)dx = \frac{4}{n\pi}$$

and the corresponding Fourier series is

$$f(x) = \frac{4}{\pi}\sin(\pi x) + \frac{4}{3\pi}\sin(3\pi x) + \frac{4}{5\pi}\sin(5\pi x) + ...$$

Such expansion can also be made in terms of other special functions such as Bessel functions, etc and we will use this fact to great advantage when solving partial differential equations.

Fourier Transforms

Transforms The complex Fourier series has an important limiting form when the period approaches infinity, i.e., $T_0 \to \infty$ or $L \to \infty$.

Suppose that in this limit

(1) $k = \frac{n\pi}{L}$ remains large (ranging from $-\infty$ to ∞) and

(2) $c_n \to 0$ since it is proportional to L, but

$$g(k) = \lim_{\substack{L\to\infty \\ c_n\to 0}} \frac{L}{\pi} c_n = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx = \quad \text{finite}$$

then we have

$$f(x) = \sum_{-\infty}^{\infty} c_n e^{ikx} = \lim_{\substack{L\to\infty \\ c_n\to 0}} \frac{1}{\sqrt{2\pi}} \sum_{-\infty}^{\infty} \frac{\pi}{L} g(k) e^{ikx}$$

where $k - \frac{n\pi}{L}$.

The sum over n is in steps of $\Delta n = 1$.

Thus, we can write using

$$\Delta k = \frac{\pi}{L} \Delta n$$

which becomes infinitesimally small when L becomes large, as a sum over k, which becomes an integral in the limit

$$\begin{aligned} f(x) &= \lim_{\substack{L\to\infty \\ c_n\to 0}} \frac{1}{\sqrt{2\pi}} \sum_{-\infty}^{\infty} \frac{\pi \Delta n}{L} g(k) e^{ikx} = \lim_{\Delta k\to 0} \frac{1}{\sqrt{2\pi}} \sum_{-\infty}^{\infty} \Delta k g(k) e^{ikx} \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} dk \end{aligned}$$

We call $g(k)$ the Fourier Transform of $f(x)$

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

and the last equation is the so-called Fourier inversion formula.

We can now obtain an integral representation of the delta-function.

This corresponds to the orthogonality condition for the complex exponential Fourier series.

We substitute the definition of $g(k)$ into the inversion formula to get

$$
\begin{aligned}
f(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} dk \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{ikx} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x') e^{-ikx'} dx' \\
&= \int_{-\infty}^{\infty} dx' f(x') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} dk \right] \\
&= \int_{-\infty}^{\infty} dx' f(x') \delta(x - x')
\end{aligned}
$$

where

$$
\delta(x - x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} dk
$$

Properties

The evaluation of the integrals involved in many Fourier transforms involves complex integration, which we shall learn later.

We will just state some properties

Examples:

(1) The Fourier transform of the box function

$$f(x) = \begin{cases} 1 & |x| \leq a \\ 0 & |x| \geq a \end{cases}$$

is

$$F(f) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} e^{-ikx} dx$$
$$= \frac{1}{\sqrt{2\pi}} \left. \frac{e^{-kx}}{ik} \right|_{-a}^{a} = \frac{1}{\sqrt{2\pi}} \frac{2 \sin ka}{k}$$

(2) The Fourier transform of the derivative of a function is

$$\begin{aligned} F\left(\frac{df}{dx}\right) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{df(x)}{dx}e^{-ikx}dx \\ &= \frac{1}{\sqrt{2\pi}}\left[f(x)e^{-ikx}\Big|_{-\infty}^{\infty} - (-ik)\int_{-\infty}^{\infty}f(x)e^{-ikx}dx\right] \\ &= \frac{ik}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x)e^{-ikx}dx = ikF(f) \end{aligned}$$

where we have assumed that $f(x) \to 0$ as $|x| \to \infty$.

This generalizes to

$$F\left(\frac{d^n f}{dx^n}\right) = (ik)^n F(f)$$

(3) Other useful properties of the Fourier transform are:

$$F(f(x)) = g(k) \quad , \quad F(f(x-a)) = e^{-ika} g(k) \quad , \quad F(f(x)e^{ax}) = g(k+ia)$$

A short table of Fourier Transforms is shown below:

$f(x)$	$g(k)$
$\delta(x)$	$\frac{1}{\sqrt{2\pi}}$
$\begin{cases} 0 & x>0 \\ e^{-\lambda x} & x<0 \end{cases}$	$\frac{1}{\sqrt{2\pi}} \frac{1}{a+ik}$
$e^{-\frac{cx^2}{2}}$	$\frac{1}{\sqrt{c}} e^{-\frac{k^2}{2c}}$
$\frac{1}{1+x^2}$	$\sqrt{\frac{\pi}{2}} e^{-\lvert k \rvert}$

Convolutions

In general, we define the **convolution integral** by

$$h(t) = \int_0^t f(t-\tau)g(\tau)d\tau \equiv f * g \equiv \text{ convolution integral}$$

Now, the Fourier transform of the product of two functions can be given in terms of the Fourier transforms of the individual functions.

$$F[f(t)g(t)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt\, e^{-i\omega t} f(t)g(t)$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt\, e^{-i\omega t} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega' e^{i\omega' t} G(\omega') \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega'' e^{i\omega'' t} F(\omega'')$$

$$= \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} d\omega'' [G(\omega')F(\omega'')] \int_{-\infty}^{\infty} dt\, e^{i(\omega'+\omega''-\omega)t}$$

$$= \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} d\omega'' [G(\omega')F(\omega'')] 2\pi\delta(\omega' + \omega'' - \omega)$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega' G(\omega')F(\omega - \omega') = G(\omega) * F(\omega)$$

This just the convolution of the Fourier transforms $G(\omega)$ and $F(\omega)$.

It is the fundamental construction needed to solve ODEs using Green's functions later, as we shall see later.

Clearly, it gives a measure of the overlap of two signals as a function of t.

The symmetry of the Fourier transform and its inverse operation gives the results

$$F^{-1}[G(\omega)F(\omega)] = \mathcal{I}[G(\omega)F(\omega)]$$
$$= \frac{1}{\sqrt{2\pi}} f(t) * g(t) \rightarrow \mathcal{I}[f(t) * g(t)] = \sqrt{2\pi} F(\omega)G(\omega)$$

Correlation

The correlation process gives a measure of the similarity of two signals.

One of its most important applications is to pick a known signal out of a sea of noise.

The **cross-correlation** between $f(t)$ and $g(t)$ is defined as

$$\psi_{fg}(t) = \int_{-\infty}^{\infty} d\tau\, f(\tau)g(\tau - t)$$

The cross-correlation of a function with itself

$$\psi_{ff}(t) = \int_{-\infty}^{\infty} d\tau\, f(\tau)f(\tau - t)$$

is called an **autocorrelation**.

This operation is similar to the convolution operation except that the second function is not inverted.

It is just as tricky as the convolution operation.

We can write

$$F[\psi_{fg}(t)] = F\left[\int_{-\infty}^{\infty} d\tau\, f(\tau)g(\tau - t)\right] = \sqrt{2\pi}F(\omega)G(-\omega)$$

Fourier Transform Examples:

(1) **The Square Pulse** - Consider the function

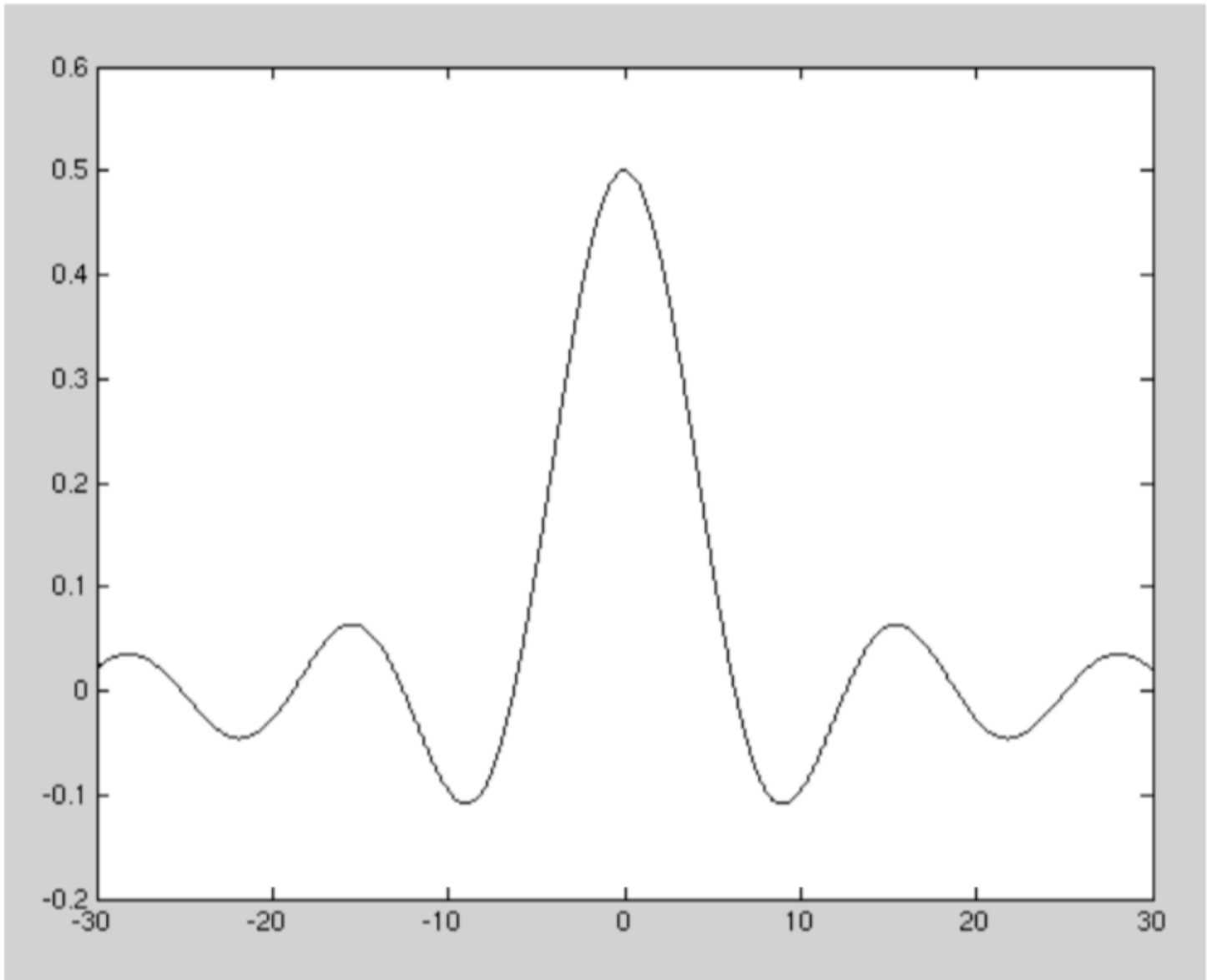
$$f(x) = \begin{cases} 1 & -T/2 < t < T/2 \\ 0 & \text{otherwise} \end{cases}$$

f(t) is absolutely integrable so it has a valid Fourier transform.

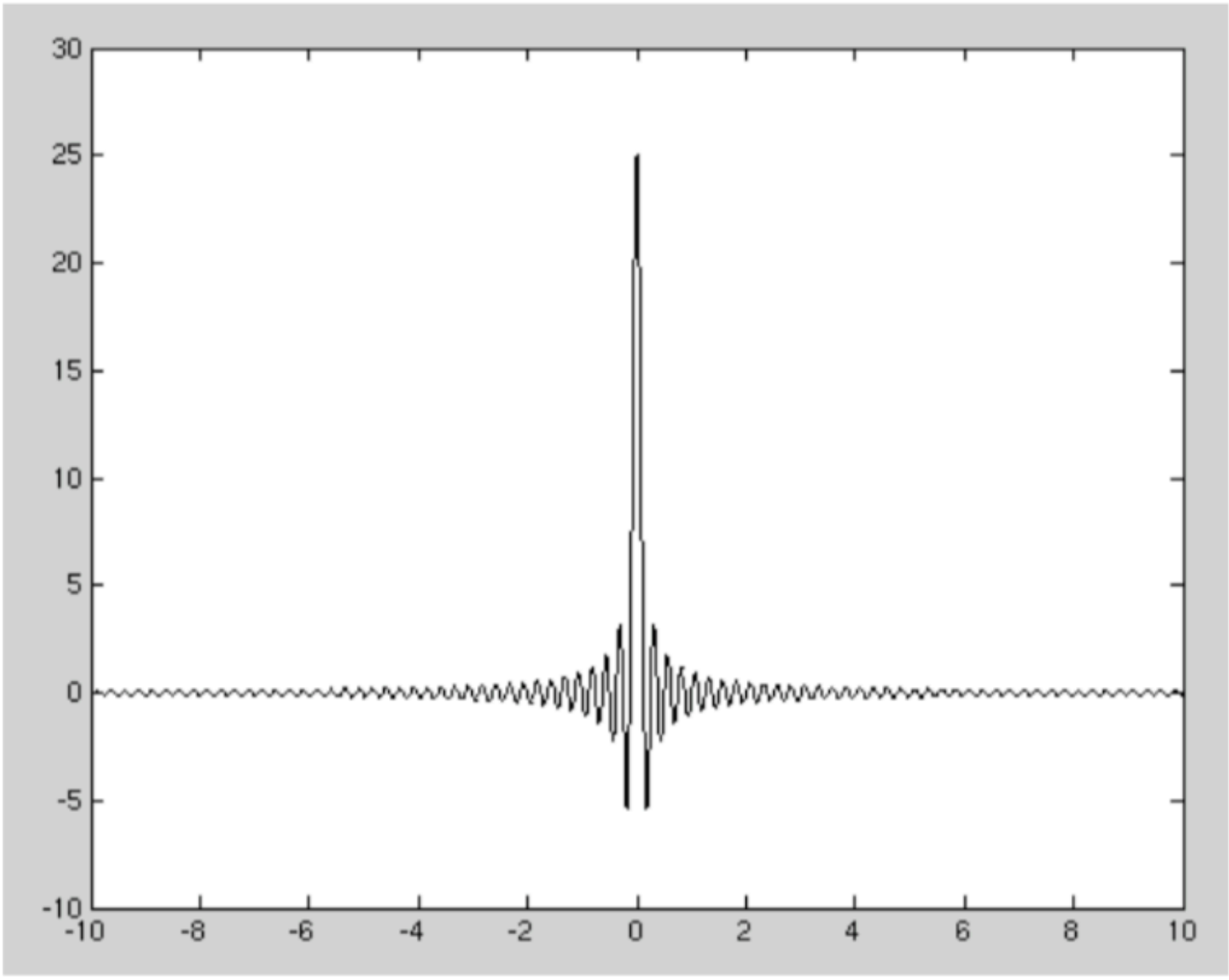
It is given by

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-T/2}^{T/2} dt\, e^{-i\omega t} = \sqrt{\frac{2}{\pi}} \left[\frac{\sin\frac{\omega T}{2}}{\omega}\right]$$

which looks like (for $T = 1$)



In the limit $T \to \infty$ we have ($T = 50$, in fact, here)



We get a sharp spike, but the area remains constant.

This implies that as $T \to \infty$

$$F(\omega) \to \delta(\omega)$$

Formally, we have

$$F(\omega) = \lim_{T\to\infty} \frac{1}{\sqrt{2\pi}} \int_{-T/2}^{T/2} dt\, e^{-i\omega t} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt\, e^{-i\omega t} = \sqrt{2\pi}\delta(\omega)$$

(2) **Transform of a Delta-Function** - Consider the function

$$f(t) = \delta t$$

The transform is

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt\, e^{-i\omega t}\delta(t) = \frac{1}{\sqrt{2\pi}}$$

The inverse transform is

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dt\, e^{-i\omega t}\frac{1}{\sqrt{2\pi}} = \delta(t)$$

Now

$$F\left(\frac{df}{dt}\right) = i\omega F(f) = i\omega F(\omega)$$

Therefore for the square pulse we have

$$\frac{df}{dt} = \delta(t + T/2) - \delta(t - T/2)$$

$$\mathcal{I}\left(\frac{df}{dt}\right) = \mathcal{I}(\delta(t + T/2) - \delta(t - T/2))$$

But

$$F(f(t - t_0)) = e^{-i\omega t_0}F(f(t))$$

Thus,

$$F\left(\frac{df}{dt}\right) = (e^{-i\omega(-T/2)} - e^{-i\omega(T/2)} F(\delta(t)) = i\sqrt{\frac{2}{\pi}} \sin\frac{\omega T}{2} = i\omega F(\omega)$$

$$\rightarrow F(\omega) = sqrt\frac{2}{\pi}\left[\frac{\sin\frac{\omega T}{2}}{\omega}\right] \quad \text{for the square pulse (as before)}$$

Remember this only makes sense inside an integral.

(3) **Transform of a Gaussian** - Consider the function

$$f(t) = \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 t^2} = \quad \text{normalized Gaussian pulse}$$

We choose $\alpha = 1$.

The peak is at α/π .

The 1/2 maximum points are separated by $\Delta t = 1/\alpha$.

The area under the curve is $= 1$.

The Fourier transform is

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt \, \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 t^2} e^{-i\omega t} = \frac{\alpha}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt \, e^{(\alpha^2 t^2 + i\omega t)}$$

We complete the square to evaluate the integral. We have

$$\alpha^2 t^2 + i\omega t = \alpha^2 t^2 + i\omega t + \gamma - \gamma = (\alpha t + \beta)^2 - \gamma$$

$$\rightarrow 2\alpha\beta = i\omega t \rightarrow \beta = \frac{i\omega}{2\alpha}$$

$$\rightarrow \gamma = \beta^2 = -\frac{\omega^2}{4\alpha^2}$$

We thus have

$$F(\omega) = \frac{\alpha}{\sqrt{2\pi}} e^{-\frac{\omega^2}{4\alpha^2}} \int_{-\infty}^{\infty} dt\, e^{-\left(\alpha t + \frac{i\omega}{2\alpha}\right)^2}$$

Let

$$x = \alpha t + \frac{i\omega}{2\alpha} \rightarrow dx = \alpha dt$$

then

$$F(\omega) = \frac{1}{\pi\sqrt{2}} e^{-\frac{\omega^2}{4\alpha^2}} \int_{-\infty}^{\infty} dx\, e^{-x^2} = \frac{1}{\sqrt{2\pi}} e^{-\frac{\omega^2}{4\alpha^2}}$$

which is a different Gaussian.

An important feature is

$$f(t) \rightarrow \Delta t \approx \frac{1}{\alpha}$$

$$F(\omega) \leftarrow \Delta\omega \approx 2\alpha$$

$$\rightarrow \Delta\omega\Delta t \approx 2$$

In general for any $f(t)$ we have $\Delta\omega\Delta t \approx c = \text{constant}$.

In the wave theory of quantum mechanics, this corresponds to the Heisenberg Uncertainty Principle.

The Laplace Transform

Another important integral transform is the **Laplace transform**.

For a function $f(t)$, we define the Laplace transform by

$$F(s) = \int_0^\infty dt\, e^{-st} f(t) = L(f(t))$$

The Laplace transform is a **linear** operator so that

$$L(af(t) + bg(t)) = aL(f(t)) + bL(g(t))$$

The Laplace transform has a **first shifting** property expressed as

$$\text{If } \; L(f(t)) = F(s), \text{ then } L(e^{at} f(t)) = F(s-a)$$

The Laplace transform has a **second shifting** property expressed as

$$\text{If} \quad L(f(t)) = F(s)$$

$$\text{and } g(t) = \begin{cases} f(t-a) & t > a \\ 0 & t < a \end{cases} \quad \text{then} \quad L(g(t)) = e^{-as}F(s)$$

If we let $t = \tau/a$, then

$$F(s) = \int_0^\infty dt\, e^{-st} f(t) = \frac{1}{a}\int_0^\infty d\tau e^{-s\tau/a} f(\tau/a)$$

and if $a\sigma = s$ we get

$$aF(a\sigma) = \int_0^\infty d\tau e^{-\sigma\tau} f(\tau/a)$$

$$\frac{1}{a}\int_0^\infty d\tau e^{-s\tau/a} f(\tau/a)$$

Examples:

(1) Heaviside unit step function

$$H(t) = \begin{cases} 1 & t \geq 0 \\ 0 & t < 0 \end{cases}$$

$$L(H(t)) = \int_0^\infty dt\, e^{-st} H(t) = \int_0^\infty dt\, e^{-st} = \frac{1}{s} = F(s)$$

Since integration is only between $\to \infty$, this also says that

$$L(H(t)) = \int_0^\infty dt\, e^{-st} 1 = \int_0^\infty dt\, e^{-st} 1 = \int_0^\infty dt\, e^{-st} = \frac{1}{s}$$

(2) Exponential function $f(t) = e^{at}$

$$L(e^{at}) = \int_0^\infty dt\, e^{(a-s)t} = \frac{1}{s-a} = F(s-a)$$

or by first shifting

$$L(e^{at} f(t)) = F(s-a)$$

$$L(1) = \frac{1}{s}$$

$$L(e^{at} 1) = L(e^{at}) = \frac{1}{s-a}$$

(3) Shifted Step function

$$H_a(t) = \begin{cases} 1 & t \geq a \\ 0 & t < a \end{cases}$$

Note original Heaviside function is then $H_0(t)$

By second shifting

$$L(H_a(t)) = L(H_0(t-a)) = e^{-as}L(H_0(t)) = \frac{e^{-as}}{s}$$

(4) Euler function $e^{i\theta} = \cos\theta + i\sin\theta$.

From (2) we have

$$L(e^{i\omega t}) = \frac{1}{s - i\omega} = L(\cos\omega t + i\sin\omega t) = L(\cos\omega t) + iL(\sin\omega t)$$

$$= \frac{1}{s - i\omega}\frac{s + i\omega}{s - i\omega} = \frac{s}{s^2 + \omega^2} + i\frac{\omega}{s^2 + \omega^2}$$

$$\rightarrow L(\cos\omega t) = \frac{s}{s^2 + \omega^2}$$

$$\rightarrow L(\sin\omega t) = \frac{\omega}{s^2 + \omega^2}$$

(5) Power function t^k

$$L(t^k) = \int_0^\infty t^k e^{-st} dt = \frac{1}{s^{k+1}} \int_0^\infty x^k e^{-x} dx \qquad \text{using } x = st$$
$$= \frac{1}{s^{k+1}} \Gamma(k+1) = \frac{k!}{s^{k+1}}$$

(6) Power series

$$f(t) = \sum_{n=0}^{\infty} a_n t^n$$

$$F(s) = L(f(t)) = \sum_{n=0}^{\infty} a_n L(t^n) = \sum_{n=0}^{\infty} a_n \frac{n!}{s^{n+1}}$$

(7) Bessel Function - we will see later that the Bessel function of zero order can be written as

$$J_0(t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{2^{2k}(k!)^2 t^{2k}} = \quad \text{Bessel function of order 0}$$

We have

$$L(J_0(t)) = \sum_{k=0}^{\infty} \frac{(-1)^k}{2^{2k}(k!)^2} L(t^{2k}) = \sum_{k=0}^{\infty} \frac{(-1)^k}{2^{2k}(k!)^2} \frac{(2k)!}{s^{2k+1}}$$

Now

$$\begin{aligned}(2k)! &= 1 \cdot 2 \cdot 3 \cdots 2k = 2 \cdot 4 \cdot 6 \cdots 2k \cdot 1 \cdot 3 \cdot 5 \cdots (2k-1) \\ &= 2^k k! 1 \cdot 3 \cdot 5 \cdots (2k-1)\end{aligned}$$

so

$$L(J_0(t)) = \sum_{k=0}^{\infty} \frac{(-1)^k}{2^{2k}(k!)^2} L(t^{2k}) = \sum_{k=0}^{\infty} \frac{(-1)^k}{2^{2k}(k!)^2} \frac{(2k)!}{s^{2k+1}}$$

$$= \frac{1}{s}\left[1 + \sum_{k=1}^{\infty} \frac{(-1)^k}{2^{2k}k!} \frac{1 \cdot 3 \cdot 5 \cdots (2k+1)}{s^{2k}}\right]$$

Now using the binomial theorem

$$(1+x)^n = 1 + \frac{n}{1!}x + \frac{n(n-1)}{2!}x^2 + \ldots + \frac{n(n-1)\ldots.(n-k+1)}{k!}x^k + \ldots\ldots.$$

$$\left(1 + \frac{1}{s^2}\right)^{-1/2} = 1 + \frac{(-1)\left(\frac{1}{2}\right)}{1!}\left(\frac{1}{s^2}\right) + \frac{(-1)^2\left(\frac{1}{2}\right)\left(\frac{3}{2}\right)}{2!}\left(\frac{1}{s^2}\right)^2$$

$$+ \ldots + \frac{(-1)^k\left(\frac{1}{2}\right)\left(\frac{3}{2}\right)\ldots.\left(\frac{2k-1}{2}\right)}{k!}\left(\frac{1}{s^2}\right)^k$$

or

$$L(J_0(t)) = \frac{1}{s}\left(1 + \frac{1}{s^2}\right)^{-1/2} = \frac{1}{\sqrt{s^2+1}}$$

Wow!!!

(8) Dirac Delta Function

$$L[\delta(t - t_0)] = \int_0^\infty \delta(t - t_0)e^{-st}dt = e^{-st_0}$$

There exist extensive tables of Laplace transforms

More examples - Some typical electric circuit input functions:

(1) Consider the square pulse (height = A) , i.e.,

$$f(t) = \begin{cases} 0 & t < a \\ 1 & a < t < b \\ 0 & t > b \end{cases}$$

remember

$$H_a(t) = \begin{cases} 1 & t \geq a \\ 0 & t < a \end{cases}$$

We rewrite this function as

$$f(t) = AH_a(t) - AH_b(t)$$

and then using linearity and example (3) above we have

$$L(f(t)] = A\frac{e^{-as}}{s} - A\frac{e^{-bs}}{s} = \frac{A}{s}[e^{-as} - e^{-bs}]$$

(2) Consider the time-dependent pulse

$$f(t) = \begin{cases} 0 & 0 < t < 1 \\ t^2 & 1 < t < 2 \\ 0 & t > 2 \end{cases}$$

We rewrite this function as

$$f(t) = H_1(t)t^2 - H_2(t)t^2$$

$g(t) = t^2$ is not in the proper form to use the second shift property.

We fix it by the following algebra

$$f(t) = H_1(t)[(t-1)^2 + 2(t-1) + 1] - H_2(t)[(t-2)^2 + 4(t-2) + 4]$$

Now using the second shift property and linearity we have

$$\begin{aligned}
L(f(t)] &= L\left(H_1(t)[(t-1)^2+2(t-1)+1]\right) \\
&\qquad - L\left(H_2(t)[(t-2)^2+4(t-2)+4]\right) \\
&= \int_1^\infty [(t-1)^2+2(t-1)+1]e^{-st}dt \\
&\qquad - \int_2^\infty [(t-2)^2+4(t-2)+4]e^{-st}dt \\
&= e^{-s}\int_0^\infty [x^2+2x+1]e^{-sx}dx - e^{-2s}\int_0^\infty [x^2+4x+4]e^{-sx}dx \\
&= e^{-s}\left[\frac{2}{s^3}+\frac{2}{s^2}+\frac{1}{s}\right] - e^{-2s}\left[\frac{2}{s^3}+\frac{4}{s^2}+\frac{4}{s}\right]
\end{aligned}$$

Finally, let us use a table to find the **inverse** Laplace transform. (1) Consider

$$F(s) = \frac{2s}{s^2+4}$$

Now

$$L(\cos \omega t) = \frac{s}{s^2 + \omega^2} L(2 \cos 2t) = \frac{2s}{s^2 + 4}$$

$$\rightarrow f(t) = 2 \cos 2t = L^{-1}\left(\frac{2s}{s^2 + 4}\right)$$

(2) Consider

$$F(s) = \frac{6s}{s^2 + 4s + 13}$$

Now

$$F(s) = \frac{6s}{s^2 + 4s + 13} = \frac{6s}{(s+2)^2 + 9} = 6L(e^{-2t} \cos 3t) - 4L(e^{-2t} \sin 3t)$$

$$\rightarrow f(t) = 6e^{-2t} \cos 3t - 4e^{-2t} \sin 3t$$

(3) Consider

$$F(s) = \frac{4e^{-2s}}{s^2 - 16} = e^{-2s}\left[\frac{4}{s^2 - 16}\right]$$

Now

$$L(\sinh 4t) = \frac{4}{s^2 - 16} \rightarrow L^{-1}\left(\frac{4}{s^2 - 16}\right) = \sinh 4t$$

The second shift property then gives

$$L(\sinh 4(t-2)) = e^{-2s}L(\sinh 4t) = e^{-2s}\left[\frac{4}{s^2 - 16}\right]$$

or

$$f(t) = L^{-1}\left(\frac{4e^{-2s}}{s^2 - 16}\right) = \begin{cases} \sinh 4(t-2) & t > 2 \\ 0 & t < 2 \end{cases}$$

Other Properties of the Laplace Transform

Laplace Transform of Derivatives and Integrals

I will just quote some results here without proof.

$$L(f') = sL(f) - f(0)$$

$$L(f^{(n)}) = s^n L(f) - s^{n-1} f(0) - s^{n-2} f'(0) - .... - f^{(n-1)}(0)$$

$$L\left(\int_0^t f(\tau) d\tau\right) = \frac{1}{s} L(f)$$

Examples:

(1) Consider $f(t) = t \sin t$. We have

$$f'(t) t \cos t = \sin t \quad \text{and} \quad f''(t) = -t \sin t + 2 \cos t$$

Now

$$L(f'') = s^2 L(f) - sf(0) - f'(0) = s^2 L(f)$$

$$L(t\sin t) = \frac{1}{s^2} L(2\cos t - t\sin t) = \frac{1}{s^2}[L(2\cos t) - L(-t\sin t)]$$

$$\left(1 + \frac{1}{s^2}\right) L(t\sin t) = \frac{1}{s^2} L(2\cos t) = \frac{2}{s^2}\frac{s}{s^2+1}$$

$$\rightarrow L(t\sin t) = \frac{2s}{(s^2+1)^2}$$

(2) If

$$L(t\sin 2t) = \frac{2s}{(s^2+4)^2}$$

$$F(s) = \frac{8}{(s^2+4)^2}$$

$$L(f) = F(s) = \frac{8}{(s^2+4)^2} = \frac{1}{s}\frac{8s}{(s^2+4)^2}$$

$$L\left(\int_0^t f(\tau)d\tau\right) = \frac{1}{s}L(f) \to L\left(\int_0^t \tau \sin 2\tau d\tau\right)$$

$$= \frac{1}{s}L(t\sin 2t) = \frac{1}{s}\frac{2s}{(s^2+4)^2}$$

or

$$L(f) = 4L\left(\int_0^t \tau \sin 2\tau d\tau\right)$$

$$\to f(t) = 4\int_0^t \tau \sin 2\tau d\tau = -2t\cos 2t + \sin 2t$$

Derivatives and Integrals of the Laplace Transform

$$L(t^n f(t)) = (-1)^n F^{(n)}(s)$$

$$L\left(\frac{f(t)}{t}\right) = \int_s^\infty F(\sigma)d\sigma$$

Laplace Transforms of Periodic Functions

We now consider functions that are periodic with period a, i.e.,

$$f(t) = f(t + na) \quad n = 1, 2, 3, ...$$

The transform is

$$
\begin{aligned}
L(f(t)) &= \int_0^{\infty} f(t)e^{-st}dt = \int_0^{a} f(t)e^{-st}dt \\
&\quad + \int_a^{2a} f(t)e^{-st}dt + \int_a^{3a} f(t)e^{-st}dt + \ldots\ldots \\
&= \int_0^{a} f(t)e^{-st}dt + \int_0^{a} f(t+a)e^{-s(t+a)}dt \\
&\quad + \int_0^{a} f(t+2a)e^{-s(t+2a)}dt + \ldots\ldots \\
&= \int_0^{a} f(t)e^{-st}dt + \int_0^{a} f(t)e^{-s(t+a)}dt \\
&\quad + \int_0^{a} f(t)e^{-s(t+2a)}dt + \ldots\ldots \\
&= (1 + e^{-sa} + e^{-2sa} + \ldots\ldots) \int_0^{a} f(t)e^{-st}dt \\
&= \frac{1}{1 - e^{-sa}} \int_0^{a} f(t)e^{-st}dt
\end{aligned}
$$

Inverse Laplace Transforms

Partial Fractions

(1) Consider two polynomials $P(s)$ and $Q(s)$ such that

$$\text{degree}(Q) > \text{degree}(P)$$

and $Q(s) = (s - a_1)(s - a_2)(s - a_3).....(s - a_n)$ with all the roots a_i **distinct**.

We saw earlier that we can then write

$$F(s) = \frac{P(s)}{Q(s)} = \frac{A_1}{s - a_1} + \frac{A_2}{s - a_2} + \frac{A_3}{s - a_3} + ... + \frac{A_n}{s - a_n}$$

We then have

$$\lim_{s\to a_k} \frac{P(s)}{Q(s)}(s-a_k) = A_k$$

$$= \lim_{s\to a_k} \frac{(s-a_k)}{Q(s)} P(s) = P(a_k) \lim_{s\to a_k} \frac{(s-a_k)}{Q(s)} = P(a_k) \lim_{s\to a_k} \frac{\frac{d}{ds}(s-a_k)}{\frac{d}{ds}Q(s)}$$

$$= P(a_k) \lim_{s\to a_k} \frac{1}{Q'(s)} = \frac{P(a_k)}{Q'(a_k)}$$

Example:

Suppose we know

$$F(s) = \frac{s^3 + 3s^2 - 2s + 4}{s(s-1)(s-2)(s^2+4s+3)}$$

then what is $f(t)$ or how do we find the **inverse Laplace transform**?

We have

$$F(s) = \frac{s^3 + 3s^2 - 2s + 4}{s(s-1)(s-2)(s+1)(s+3)}$$
$$= \frac{A_1}{s} + \frac{A_2}{s-1} + \frac{A_3}{s-2} + \frac{A_4}{s+1} + \frac{A_5}{s+3}$$

Using

$$A_k = \frac{P(a_k)}{[Q(s)/(s-a_k)]_{s=a_k}}$$

we get

$$A_1 = \frac{2}{3}\,,\ A_2 = -\frac{3}{4}\,,\ A_3 = \frac{2}{3}\,,\ A_4 = -\frac{2}{3}\,,\ A_5 = \frac{1}{12}$$

so that

$$F(s) = \frac{2/3}{s} - \frac{3/4}{s-1} + \frac{2/3}{s-2} - \frac{2/3}{s+1} + \frac{1/12}{s+3}$$

Using

$$L(e^{at}) = \frac{1}{s-a}$$

we have

$$f(t) = \frac{2}{3} - \frac{3}{4}e^{t} + \frac{2}{3}e^{2t} - \frac{2}{3}e^{-t} + \frac{1}{12}e^{-3t}$$

When the roots of Q(s) are not all distinct we get a different result.

Suppose there is a repeated factor $(s-a_1)^m$, i.e.,

$$Q(s) = (s-a_1)^m(s-a_2)(s-a_3).....$$

We then get

$$F(s) = \frac{P(s)}{Q(s)}$$

$$= \frac{B_m}{(s-a_1)^m} + \frac{B_{m-1}}{(s-a_1)^{m-1}}$$

$$+ .... + \frac{B_2}{(s-a_1)^2} + \frac{B_1}{(s-a_1)} + \frac{A_2}{(s-a_2)} + \frac{A_3}{(s-a_3)} + ...$$

where

$$A_k = \frac{P(a_k)}{[Q(s)/(s-a_k)]_{s=a_k}}$$

and

$$B_i = \frac{1}{(m-1)!} \frac{d^{(m-1)}}{ds^{(m-1)}} \left[\frac{P(s)}{[Q(s)/(s-a_1)^m]} \right]_{s=a_1}$$

$$B_m = \frac{P(a_1)}{[Q(s)/(s-a_1)^m]_{s=a_1}}$$

Two final cases are:

$$Q(s) = ((s-a)^2 + b^2)(s-a_1)(s-a_2)(s-a_3).....$$

$$F(s) = \frac{P(s)}{Q(s)} = \frac{B_1 s + B_2}{(s-a)^2 + b^2} + \frac{A_1}{s-a_1} + \frac{A_2}{s-a_2} + ...$$

$$A_k = \frac{P(a_k)}{[Q(s)/(s-a_k)]_{s=a_k}}$$

$$B_1(a_i b) + B_2 = \left[\frac{P(s)}{Q(s)/[(s-a)^2 + b^2]}\right]_{s=a+ib}$$

and

$$Q(s) = ((s-a)^2 + b^2)^2(s-a_1)(s-a_2)(s-a_3).....$$

$$F(s) = \frac{P(s)}{Q(s)} = \frac{C_1 s + C_2}{((s-a)^2 + b^2)^2} + \frac{B_1 s + B_2}{(s-a)^2 + b^2} + \frac{A_1}{s - a_1} + \frac{A_2}{s - a_2} + \ldots\ldots$$

$$A_k = \frac{P(a_k)}{[Q(s)/(s - a_k)]_{s=a_k}}$$

$$C_1(a + ib) + C_2 = \left[\frac{P(s)}{Q(s)/[(s-a)^2 + b^2]}\right]_{s=a+ib}$$

$$B_1(a_i b) + B_2 = \frac{d}{ds}\left[\frac{P(s)}{Q(s)/[(s-a)^2 + b^2]}\right]_{s=a+ib}$$

A Convolution Theorem

Suppose that we have two functions $f(t)$ and $g(t)$. We define the integral

$$h(t) = \int_0^t f(t-\tau)g(\tau)d\tau \equiv f * g \equiv \text{ convolution integral}$$

If

$$L(f(t)) = F(s) \quad \text{and} \quad L(g(t)) = G(s)$$

then we have

$$H(s) = \int_o^\infty dt\, e^{-st} h(t) = F(s)G(s) = L(f * g)$$

Ordinary Differential Equations(ODE)

ODEs are equations involving derivatives in various ways. The highest derivative specifies the order of the equation. Single variable equations are ODEs and multi-variable equations are Partial Differential Equations(PDE)s.

An ODE

$$L(y(x)) = R(x)$$

is linear if the differential operator L is a linear operator satisfying the linearity property

$$L(a_1 y_1(x) + a_2 y_2(x)) = a_1 L(y_1(x)) + a_2 L(y_2(x))$$

where a_1 and a_2 are constants.

Examples:

The **1st order ODE**

$$L(y(x)) = \frac{dy(x)}{dx}$$

is linear since

$$L(ay(x)) = \frac{d(ay(x))}{dx} = a\frac{dy(x)}{dx}$$

but the 1st order ODE

$$L(y(x)) = \sqrt{\frac{dy(x)}{dx}}$$

is nonlinear since

$$L(ay(x)) = \sqrt{\frac{d(ay(x))}{dx}} = \sqrt{a}\sqrt{\frac{dy(x)}{dx}} \neq a\sqrt{\frac{dy(x)}{dx}}$$

The **2nd order ODE**

$$\frac{d^2\theta(t)}{dt^2} + \frac{g}{L}\sin\theta(t) = 0$$

which describes the large amplitude motion of a pendulum is non-linear because

$$\sin(\lambda\theta_1 + \mu\theta_2) \neq \lambda\sin(\theta_1) + \mu\sin(\theta_2)$$

We note that if θ is always small, then $\sin\theta \approx \theta$ and the new ODE

$$\frac{d^2\theta(t)}{dt^2} + \frac{g}{L}\theta(t) = 0$$

is a linear ODE.

It describes the small amplitude motion of a pendulum.

All physical systems not far from **EQUILIBRIUM** (small displacements)are linear systems.

Linear ODEs are simpler to solve than non-linear ODEs.

This is a consequence of the following two superposition principles which apply only to linear ODEs:

(1) If $y_1(x)$ and $y_2(x)$ are **any** two solutions of a **homogeneous linear ODE**

$$L(y(x)) = 0$$

then

$$y_h(x) = c_1 y_1(x) + c_2 y_2(x) \qquad c_1, c_2 = \text{ constants}$$

is also a solution, i.e.,

$$Ly_h(x) = L(c_1 y_1(x) + c_2 y_2(x)) = c_1 L(y_1(x)) + c_2 L(y_2(x)) = 0$$

(2) If $y_h(x)$ is a (i.e.,any) solution of the homogeneous linear ODE, $L(y_h(x)) = 0$ and $y_p(x)$ is a solution of the inhomogeneous linear ODE

$$L(y_p(x)) = R(x)$$

then the linear combination

$$y(x) = y_p(x) + Ay_h(x) \qquad A = \text{ constant}$$

is a solution of the inhomogeneous linear ODE

$$L(y(x)) = R(x)$$

i,e,

$$L(y(x)) = L(y_p(x) + Ay_h(x)) = L(y_p(x)) + AL(y_h(x)) = R(x)$$

Solutions of ODEs

1st order ODEs can be solved by **direct integration** if the equation is **SEPARABLE**:

$$\frac{dy}{dx} = \frac{p(x)}{q(y)} \rightarrow \int q(y)dy = \int p(x)dx$$

Example:

$$\frac{dy}{dx} - x\sqrt{1-y^2} = 0 \rightarrow \frac{dy}{\sqrt{1-y^2}} = xdx$$

$$\int \frac{dy}{\sqrt{1-y^2}} = \sin^{-1} y = \int xdx = \frac{1}{2}x^2 + C \rightarrow y = \sin\left(\frac{1}{2}x^2 + C\right)$$

This works for both linear and nonlinear ODEs.

It is not always easy to separate the variables.

Sometimes a change of variables helps.

Example:

$$\frac{dy}{dx} - = (x - y + 3)^2$$

$$z = x - y + 3 \rightarrow \frac{dz}{dx} = 1 - \frac{dy}{dx} = 1 - z^2$$

$$\int \frac{dz}{1 - z^2} = \tanh^{-1} z = \int dx = x + c \rightarrow z = \tanh(x + c)$$

$$y = x + 3 - z \rightarrow y = x + 3 - \tanh(x + c)$$

The next best thing one can do to a nonlinear ODE is to change it into a linear ODE by a change of variable.

This is because (as we shall see later) linear ODEs can ALWAYS be solved in closed form.

Example:

$$\frac{dy}{dx} + f(x)y = g(x)y^n \qquad n \neq 1 \rightarrow \text{ nonlinear in } y(x)$$

$$\frac{1}{y^n}\frac{dy}{dx} + f(x)y^{1-n} = g(x)$$

$$v(x) = y^{1-n}(x) \rightarrow \frac{dv}{dx} = (1-n)y^{-n}(x)\frac{dy}{dx}$$

$$\rightarrow \frac{dv}{dx} + (1-n)f(x)v(x) = (1-n)g(x)$$

which is linear in $v(x)$.

Now consider the following general form for a 1st-order inhomogeneous linear ODE:

$$\left(\frac{d}{dx} + p(x)\right) y(x) = R(x)$$

which is homogeneous if $R(x) = 0$.

We can solve the homogeneous form of this equation formally as follows:

$$\left(\frac{d}{dx} + p(x)\right) y(x) = R(x)$$

R=0

$$\frac{dy(x)}{y(x)} = -p(x)dx$$

$$\int_a^x \frac{dy(x)}{y(x)} = \int_a^x d(\ln y(x') = -\int_a^x p(x')dx'$$

$$\ln y(x) - \ln y(a) = \ln \frac{y(x)}{y(a)} = -\int_a^x p(x')dx'$$

$$y(x) = y(a) \exp\left[-\int_a^x p(x')dx'\right]$$

The number $y(a) =$ **boundary condition** at the point $y = a$.

Example:

$$\left(\frac{d}{dx} + x\right) y(x) = 0 \rightarrow y(x) = y(0) \exp\left[-\int_0^x x'dx'\right]$$

$$\rightarrow y(x) = y(0)e^{-x^2/2}$$

Now, given a solution $y_h(x)$ of the homogeneous equation, a particular solution of the inhomogeneous equation can **always** be obtained as follows:

Let

$$y_p(x) = c(x)y_h(x) \qquad \text{multiply by a function } c(x)$$

Substituting we get

$$L(y_p(x)) = R(x) = \left(\frac{d}{dx} + x\right) y_p(x) = \left(\frac{d}{dx} + x\right) c(x)y_h(x)$$

$$R(x) = y_h(x)\frac{dc(x)}{dx} + c(x)\left(\frac{d}{dx} + x\right) y_h(x) = y_h(x)\frac{dc(x)}{dx}$$

since the last term

$$\left(\frac{d}{dx} + x\right) y_h(x) = 0$$

This implies that

$$\frac{dc(x)}{dx} = \frac{R(x)}{y_h(x)} \rightarrow c(x) = c(a) + \int_a^x \frac{R(x)}{y_h(x)} dx'$$

This means that

$$y_p(x) = \left[c(a) + \int_a^x \frac{R(x)}{y_h(x)} dx' \right] y_h(x)$$

and

$$\begin{aligned} y(x) &= A y_h(x) + y_p(x) = A y_h(x) + \left[c(a) + \int_a^x \frac{R(x)}{y_h(x)} dx' \right] y_h(x) \\ &= A' y_h(x) + \left[\int_a^x \frac{R(x)}{y_h(x)} dx' \right] y_h(x) \end{aligned}$$

where

$$A' = A + c(a)$$

This method is called **variation of constants** since $y_p(x)$ is proportional to $y_h(x)$, but the proportionality constant is itself a function of x.

Example: Consider the 1st-order linear ODE

$$\left(\frac{d}{dx} + s\right) y(x) = e^{-tx} \qquad t \neq s$$

(1) get a homogeneous solution

$$\left(\frac{d}{dx} + s\right) y_h(x) = 0 \rightarrow \frac{dy_h}{y_h} = -sdx \rightarrow y_h(x) = e^{-sx}$$

(2) get the proportional function $c(x)$

$$\frac{dc(x)}{dx} = \frac{R(x)}{y_h(x)} = \frac{e^{-tx}}{e^{-sx}} \rightarrow c(x) = c(0) + \int_0^x e^{-(t-s)x'} dx'$$

$$c(x) = c(0) - \frac{1}{t-s}(e^{-(t-s)x} - 1)$$

(3) get final answer

$$y_p(x) = c(x)y_h(x) = \left[c(0) - \frac{1}{t-s}(e^{-(t-s)x} - 1)\right] y_h(x)$$
$$= -\frac{1}{t-s}e^{-tx} + \left(c(0) + \frac{1}{t-s}\right) y_h(x)$$

(4) check answer

$$y(x) = Ay_h(x) - \frac{1}{t-s}e^{-tx} + \left(c(0) + \frac{1}{t-s}\right) y_h(x)$$
$$= A'y_h(x) - \frac{1}{t-s}e^{-tx}$$

$$\left(\frac{d}{dx} + s\right) y(x) = A' \left(\frac{d}{dx} + s\right) y_h(x) - \left(\frac{d}{dx} + s\right) \frac{1}{t-s}e^{-tx}$$
$$= -\frac{1}{t-s}[-t+s]e^{-tx} = e^{-tx}$$

as it should.

Uniqueness of Solutions

The solution of an n^{th} order linear ODE is uniquely determined by n boundary conditions that can be taken to be

$$y(b), y'(b), y''(b), ..., y^{(n-1)}(b)$$

at any point $x = b$.

In the example above, the 1st-order linear ODE required only the value of $y(b)$ for a complete solution, i.e.,

$$y(x) = A' y_h(x) - \frac{1}{t-s} e^{-tx} \rightarrow y(b) = A' y_h(b) - \frac{1}{t-s} e^{-tb}$$

which determines the unknown constant A'.

You are also familiar with the physical fact that a 2nd-order linear ODE like those that come from Newton's laws, requires 2 boundary conditions $y(b)$ and $y'(b)$ or that we specify both the position and the velocity at some instant of time.

1st order Equations - Integrating factors

Now suppose we have the differential equation

$$p(x,y)dx + q(x,y)dy = 0$$

It is called **exact** if

$$\frac{\partial p}{\partial y} = \frac{\partial q}{\partial x}$$

This implies that there exists a function $f(x,y)$ such that

$$p(x,y) = \frac{\partial f}{\partial x} \quad , q(x,y) = \frac{\partial f}{\partial y}$$

$$\rightarrow \frac{\partial p}{\partial y} = \frac{\partial^2 f}{\partial y \partial x} \quad , \quad \frac{\partial q}{\partial x} = \frac{\partial^2 f}{\partial x \partial y}$$

and in physics

$$\frac{\partial^2 f}{\partial y \partial x} = \frac{\partial^2 f}{\partial x \partial y}$$

always! Therefore we get

$$p(x,y)dx + q(x,y)dy = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy = df$$

We then have the solution

$$df = 0 \rightarrow f(x,y) = \text{ constant}$$

An equation that is not exact may often be made exact by multiplying it by an appropriate factor called an **integrating factor**.

For example:

$$xdy - ydx = 0$$

is not exact.

But the equation

$$\frac{xdy - ydx}{x^2} = \frac{1}{x}dy - \frac{y}{x^2}dx = 0$$

is exact, and its solution is

$$f(x, y) = \frac{y}{x} = \text{ constant}$$

Integrating factors can sometimes be used to solve linear, inhomogeneous first-order ODEs of the form

$$\frac{dy(x)}{dx} + P(x)y(x) = G(x)$$

We seek an $\alpha(x)$ such that

$$\alpha(x)\left[\frac{dy(x)}{dx} + P(x)y(x)\right] = \frac{d}{dx}[\alpha(x)y(x)] = \alpha(x)G(x)$$

or

$$\alpha(x)P(x) = \frac{d\alpha(x)}{dx}$$

$$P = \frac{d\alpha}{\alpha} \rightarrow \int P(x)dx = \int \frac{d\alpha(x)}{\alpha(x)} = \ln \alpha(x) \rightarrow \alpha(x) = e^{\int P(x)dx}$$

We then have

all steps

$$P(x)dx = \frac{d\alpha(x)}{\alpha(x)} \rightarrow \alpha(x) = \exp\left[\int dx\, P(x)\right]$$

Finally,

$$\frac{d}{dx}[\alpha(x)y(x)] = \alpha(x)G(x)$$

or

$$\alpha(x)y(x) = \int \alpha(x)G(x)dx + C_0$$

or

$$y(x) = \frac{\int \alpha(x)G(x)dx + C_0}{\alpha(x)}$$

$$\alpha(x) = \exp\left(\int dx\right) = e^x$$

$$y(x) = \frac{\int e^{2x} dx + C_0}{e^x} = \frac{1}{2} e^x + C_0 e^{-x}$$

$$y(0) = 1 = \frac{1}{2} + C_0 \rightarrow C_0 = -\frac{1}{2}$$

$$\rightarrow y(x) = \cosh(x)$$

2nd-Order Homogeneous ODEs with Constant Coefficients

Consider the ODE

$$\frac{d^2y}{dx^2} + 5\frac{dy}{dx} + 4y = 0$$

If we let

$$D = \frac{d}{dx}$$

then we have the equation

$$(D^2 + 5D + 4)y = 0$$

These equations can be solved by **substitution(guessing)** and converting the ODE into an **algebraic (quadratic)** equation.

We choose(guess) the solution

$$y = ce^{ax}$$

Substitution gives the allowed values of a (corresponding to possible solutions)

$(a^2 + 5a + 4)ce^{ax} = 0 \rightarrow a^2 + 5a + 4 = 0 \rightarrow a = -1$ and $a = -4$

The most general solution is a superposition of all possible solutions with arbitrary multiplicative constants (number of possible solutions = order of ODE) so

$$y = c_1 e^{-x} + c_2 e^{-4x}$$

The arbitrary constants c_1 and c_2 are determined by boundary conditions where we specify

$$y(x_0) \text{ and } \frac{dy(x_0)}{dx} \quad , \quad x_0 = \text{ arbitrary point}$$

For example suppose,

$$x_0 = 0 \text{ and } y(0) = 2 \text{ and } \frac{dy(0)}{dx} = -3$$

then we have

$$y(0) = 2 = c_1 + c_2$$

$$\frac{dy(0)}{dx} = -3 = -c_1 - 4c_2$$

$$\rightarrow c_1 = \frac{5}{3} \quad \text{and} \quad c_2 = \frac{1}{3}$$

and the general solution with these boundary conditions is

$$y(x) = \frac{5}{3}e^{-x} + \frac{1}{3}e^{-4x}$$

The solutions for a can be imaginary numbers (trigonometric solutions) or complex numbers (mixed trigonometric and exponential solutions).

Example: Simple Harmonic Oscillator

In this case:

$$\frac{d^2y}{dt^2} + \omega^2 y = 0 \quad , \quad D = \frac{d}{dt} \rightarrow (D^2 + \omega^2)y(t) = 0$$

Choosing

$$y = c_1 e^{at} \rightarrow a^2 + \omega^2 = 0 \rightarrow a = \pm i\omega$$

which gives the general solution

$$y(t) = c_1 e^{i\omega t} + c_2 e^{-i\omega t}$$

With boundary conditions

$$y(0) = 0 \quad \text{and} \quad \frac{dy(0)}{dt} = 4\omega \qquad \text{(what is the oscillator doing?)}$$

we get

$$c_1 + c_2 = 0$$

$$i\omega(c_1 - c_2) = 4\omega \rightarrow c_1 - c_2 = -4i$$

$$\rightarrow c_1 = -2i \quad \text{and} \quad c - 2 = 2i$$

so that

$$y(t) = -2i(e^{i\omega t} - e^{-i\omega t}) = 4\sin(\omega t)$$

Example:Equal Roots

Suppose we have

$$(D^2 - 6D + 9)y = 0 \rightarrow a = 3, 3$$

$\longrightarrow$ These solutions are linearly dependent.

The rule is then to choose a solution of the form

$$y(x) = (Ax + B)e^{3x}$$

since we **must have** 2 constants because it is a 2nd-order ODE.

Clifford-Euler Equation

We have a homogeneous equation of the form

$$x^2\frac{d^2u}{dx^2} + ax\frac{du}{dx} + bu = 0$$

The solutions take the form

$$u = x^m$$

Substitution gives

$$[m(m-1) + am + b]x^m = 0 \rightarrow m(m-1) + am + b = 0$$

$$\rightarrow 2 \text{ roots } \; m_1 \; \text{ and } \; m_2$$

and the solution is

$$u(x) = Ax^{m_1} + Bx^{m_2}$$

Second-Order Homogeneous ODEs in General

Suppose $y_1(x)$ and $y_2(x)$ are two solutions of the homogeneous equation with boundary conditions

$$y_1(a) = 1 \;\;,\quad y_1'(a) = 0 \;\;,\;\; y_2(a) = 0 \;\;,\;\; y_2'(a) = 1$$

It is clear that $y_1(x)$ and $y_2(x)$ can never be proportional to each other, since they already differ at the boundary $x = a$. This means that they are linearly independent.

They are also the only linearly independent solutions because 2nd-order ODEs have only two independent boundary conditions $y(a)$ and $y'(a)$.

A general solution satisfying the boundary conditions

$$y(a) = \;\; c_1 \quad\;\; ,\;\; y'(a) = c_2$$

is given by

$$y(x) = c_1 y_1(x) + c_2 y_2(x)$$

Test of Linear Independence of Solutions: The Wronskian

How do we determine the linear independence of 2 given homogeneous solutions? In the simple case, it is easy, just look ... if they are not proportional, then they are linearly independent. This simple procedure cannot be used for n given homogeneous solutions of the nth-order linear ODE when $n > 2$.

We need a more general procedure, applicable to an ODE of any order. I will illustrate the method in the 2nd-order case for simplicity.

If $y_1(x)$ and $y_2(x)$ are linearly independent, then it turns out that any solution $y(x)$ of a 2nd-order linear ODE

$$\left(\frac{d^2}{dx^2} + p(x)\frac{d}{dx} + q(x)\right) y(x) = R(x)$$

(where we assume $R(x) = 0$ for now) and its slope $y'(x)$ can be written as

$$c_1 y_1(x) + c_2 y_2(x) = y(x)$$

$$c_1 y_1'(x) + c_2 y_2'(x) = y'(x)$$

with unique linear coefficients c_1 and c_2.

Let us write these equations in matrix form

$$\begin{pmatrix} y_1(x) & y_2(x) \\ y_1'(x) & y_2'(x) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} y(x) \\ y'(x) \end{pmatrix} \rightarrow MC = Y$$

A solution of these equations is given by $C = M^{-1}Y$.

A **unique solution** requires that the determinant

$$W(x) = \begin{vmatrix} y_1(x) & y_2(x) \\ y_1'(x) & y_2'(x) \end{vmatrix}$$

does not vanish, where $W(x) =$ **Wronskian**.

This requirement corresponds to the existence of the inverse M^{-1}.

Now suppose $W(x = a) \neq 0$.

Then we can determine the coefficients c_1 and c_2 at $x = a$, which, in turn, implies that $W(x) \neq 0$ at all other x.

We show this as follows:

$$\frac{dW(x)}{dx} = \frac{d}{dx}(y_1 y_2' - y_2 y_1') \underset{\cdot}{=} y_1' y_2' + y_1 y_2'' - y_2' y_1' = y_1 y_2'' - y_2 y_1''$$
$$= -y_1(p(x)y_2' + q(x)y_2) + y_2(p(x)y_1' + q(x)y_1) = -p(x)W(x)$$

Therefore,

$$W(x) = W(a) \exp\left(-\int_a^x p(x')dx'\right)$$

This implies that

(1) if $W(a) \neq 0$, then $W(x) \neq 0$ everywhere

(2) if $W(a) = 0$, then $W(x) = 0$ everywhere

For higher order linear ODEs

$$W(x) = \begin{vmatrix} y_1 & y_2 & y_3 & \cdots & y_n \\ y_1' & y_2' & y_3' & \cdots & y_n' \\ y_1'' & y_2'' & y_3'' & \cdots & y_n'' \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ y_1^{(n-1)} & y_2^{(n-1)} & y_3^{(n-1)} & \cdots & y_n^{(n-1)} \end{vmatrix}$$

An Example: Consider the equation

$$\left(\frac{d^2}{dx^2} + k^2 \right) y(x) = 0$$

This has two linearly independent solutions given by

$$y_1(x) = \cos kx \quad , \quad y_2(x) = \frac{1}{k} \sin kx$$

The $1/k$ factor in the second solution is necessary for these solutions to agree with the solutions when $k = 0$, i.e.,

$$\left(\frac{d^2}{dx^2}\right) y(x) = 0$$

which has the two linearly independent solutions

$$y_1(x) = 1 \quad , \quad y_2(x) = x$$

which are the limits of the first solutions as $k \to 0$.

The Wronskian, in this case, is

$$W(x) = \begin{vmatrix} \cos kx & \frac{1}{k}\sin kx \\ -k\sin kx & \cos kx \end{vmatrix}$$

The 2nd Homogeneous Solution

Now, if one solution $y_1(x)$ of a 2nd order homogeneous linear ODE is known, a second solution $y_2(x)$, linearly independent of the first, can be constructed with the help of the Wronskian:

$$\frac{d}{dx}\left[\frac{y_2}{y_1}\right] = \frac{y_1 y_2' - y_2 y_1'}{y_1^2} = \frac{W(x)}{y_1^2(x)}$$

A simple integration then gives

$$\frac{y_2(x)}{y_1(x)} - \frac{y_2(b)}{y_1(b)} = \int_b^x \frac{W(x')}{y_1^2(x')} dx' = g(x)$$

$$y_2(x) = g(x) y_1(x) + \frac{y_2(b)}{y_1(b)} y_1(x)$$

Now we can drop the last term since it is proportional to $y_1(x)$ and we already have a term proportional to $y_1(x)$ in the general solution

$$y(x) = a y_1(x) + b y_2(x)$$

Therefore, we have

$$y_2(x) = g(x)y_1(x)$$

Since

$$W(x) = W(b)\exp\left(-\int_b^x p(x')dx'\right)$$

we get

$$g(x) = \int_b^x \frac{W(x')}{y_1^2(x')}dx' = W(b)\int_b^x \frac{\exp\left(-\int_b^{x'} p(x'')dx''\right)}{y_1^2(x')}dx'$$

Does this procedure work?

A Simple Example:

$$\frac{d^2}{dx^2}\psi(x) = 0$$

If one solution is $\psi_1(x) = 1$, then we can find a second linearly independent solution by

$$\psi_2(x) = g(x)\psi_1(x) = g(x)$$

We choose $b = 0$ and get (since $p(x) = 0$ in this case), $W(x) = W(0)$ and

$$g(x) = \int_0^x \frac{W(0)}{1^2} dx' = W(0)x \rightarrow \psi_2(x) = x$$

$\rightarrow$ correct second linearly independent homogeneous solution.

Inhomogeneous Solutions

The solution of the inhomogeneous 2nd order linear ODE

$$Ly(x) = R(x)$$

has the general form

$$y(x) = y_p(x) + [c_1 y_1(x) + c_2 y_2(x)]$$

where

$$y_p(x) = \text{ any particular solution}$$

$$[c_1 y_1(x) + c_2 y_2(x)] = \text{ complementary solution}$$

The complementary solution is a combination of 2 linearly independent solutions of the homogeneous equation.

Why do we bother creating $y(x)$ if we already know $y_p(x)$?

The reason is that $y_p(x)$ satisfies the boundary conditions $y_p(a)$, $y_p'(a)$ (a) at $x = a$.

Suppose instead that we want a solution satisfying the boundary conditions $y_p(a) = \alpha$, $y_p(a) = \beta$.

We do not want to spend time looking for a particular solution with JUST the right boundary conditions because they are very hard to obtain in general. Anyway we are unlikely to find one with exactly the correct boundary conditions.

The complementary function now comes to our rescue.

Using it we can change the boundary conditions without contributing anything to the inhomogeneity of the ODE(i.e., without changing the fact that we have a solution of the inhomogeneous ODE).

So we choose

$$c_1 y_1(a) + c_2 y_2(a) = \alpha - y_p(a)$$

$$c_1 y_1'(a) + c_2 y_2'(a) = \beta - y_p'(a)$$

The existence of the coefficients c_1 and c_2 is guaranteed by the linear independence of the homogeneous solutions y_1 and y_2, since then the Wronskian $W(a) \neq 0$ and the inverse matrix needed to solve

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} y_1(a) & y_2(a) \\ y_1'(a) & y_2'(a) \end{pmatrix}^{-1} \begin{pmatrix} \alpha - y_p(a) \\ \beta - y_p'(a) \end{pmatrix}$$

exists.

A Particular Solution: Method of Variation of Constants

We still need one (any one) particular solution $y_p(x)$ of the inhomogeneous ODE.

To obtain this, we first observe that the function $y_p(x)$ contains 2 degrees of freedom in the sense that at a point $x = x_1$, its value $y_p(x_1)$ and its slope $y_p'(x_1)$ can be chosen arbitrarily.

These two arbitrary numbers may be expressed in terms of the values and slopes of the **two linearly independent homogeneous solutions** $y_i(x)$, $i = 1, 2$

$$y_p(x) = v_1 y_1(x) + v_2 y_2(x)$$

$$y_p'(x) = v_1 y_1'(x) + v_2 y_2'(x)$$

because the RHSs also describe a system with 2 degrees of freedom, as represented by the 2 linear coefficients v_1 and v_2.

However, these linear coefficients v_1 and v_2 cannot be constants independent of x, for then $y_p(x)$ solves the homogeneous linear ODE, not the inhomogeneous equation.

We therefore must have (need)

$$v_i = v_i(x) \quad , \quad i = 1, 2$$

This method is called **variation of constants**.

However, by direct differentiation we have

$$\frac{dy_p(x)}{dx} = y_p'(x) = \frac{d}{dx}[v_1 y_1(x) + v_2 y_2(x)] = v_1 y_1' + v_2 y_2' + [v_1' y_1 + v_2' y_2]$$

which is not correct unless $[.....] = 0$.

It turns out that this single requirement is insufficient to determine the 2 unknowns v_i'.

We need another relation, which we can obtain from the original ODE:

$$\left(\frac{d^2}{dx^2} + p(x)\frac{d}{dx} + q(x)\right) y(x) = R(x)$$

As before, using

$$y_p(x) = v_1 y_1(x) + v_2 y_2(x)$$

$$y_p'(x) = v_1 y_1'(x) + v_2 y_2'(x)$$

we get

$$y_p'(x) = v_1 y_1' + v_1' y_1 + v_2' y_2 + v_2 y_2'$$

$$\frac{d^2 y_p}{dx^2} = v_1'' y_1 + 2v_1' y_1' + v_1 y_1'' + v_2'' y_2 + 2v_2' y_2' + v_2 y_2''$$

or

$$v_1''y_1 + 2v_1'y_1' + v_1y_1'' + v_2''y_2 + 2v_2'y_2' + v_2y_2'' + p(v_1y_1' + v_1'y_1 + v_2'y_2 + v_2y_2') + q(v_1y_1 + v - 2y_2) = R$$

$$[v_1y_1'' + pv_1y_1' + qv_1y_1] + [v_2y_2'' + pv_2y_2' + qv_2y_2] + [pv_1'y_1 + pv_2'y_2] + v_1''y_1 + 2v_1'y_1' + v_2''y_2 + 2v_2'y_2' = R$$

$$[0] + [0] + [0] + v_1''y_1 + 2v_1'y_1' + v_2''y_2 + 2v_2'y_2' = R$$

$$[v_1''y_1 + v_1'y_1' + v_2''y_2 + v_2'y_2'] + v_1'y_1' + v_2'y_2' = R$$

$$\left[\frac{d}{dx}(v_1'y_1 + v_2'y_2)\right] + v_1'y_1' + v_2'y_2' = R$$

$$[0] + v_1'y_1' + v_2'y_2' = R$$

and we thus get a second relation.

These two relations

$$v_1'(x)y_1(x) + v_2'(x)y_2(x) = 0$$

$$v_1'(x)y_1'(x) + v_2'(x)y_2'(x) = R(x)$$

along with $W(x) = y_1(x)y_2'(x) - y_2(x)y_1'(x) \neq 0$ give the results

$$v_1(x) = -\int_a^x \frac{y_2(x')R(x')}{W(x')}dx'$$

$$v_2(x) = \int_a^x \frac{y_1(x')R(x')}{W(x')}dx'$$

where integration constants have been chosen **arbitrarily** to give $v_1(a) = v_2(a) = 0$.

With this choice, the particular solution satisfies the boundary conditions $y_p(a) = y_p'(a) = 0$. any choice works!

An Example:

$$\left(\frac{d^2}{dx^2} + k^2\right) y(x) = A \sin qx$$

We know the 2 homogeneous solutions from our earlier discussions

$$y_1(x) = \cos kx \quad , \quad y_2(x) = \frac{1}{k} \sin kx \quad , \quad W(x) = 1$$

This gives

$$v_1(x) = -\int_{-L}^{x} \frac{A}{k} \sin kx \sin qx dx = -\frac{A}{k}\left[\frac{\sin(k-q)x}{2(k-q)} - \frac{\sin(k+q)x}{2(k+q)}\right] + C$$

$$v_2(x) = \int_{-L}^{x} \frac{A}{k} \cos kx \sin qx dx = \begin{cases} \frac{A}{k}\left[\frac{\cos(k-q)x}{2(k-q)} - \frac{\cos(k+q)x}{2(k+q)}\right] + C & k \neq q \\ \frac{A}{2k} \sin^2 kx + C & k = q \end{cases}$$

Thus, a particular solution is, for $k \neq q$

$$\begin{aligned} y_p(x) &= \frac{A}{2k(k-q)}[\sin{(k-q)x}\cos{kx} - \cos{(k-q)x}\sin{kx}] \\ &\quad + \frac{A}{2k(k+q)}[\sin{(k+q)x}\cos{kx} - \cos{(k+q)x}\sin{kx}] \\ &= -\frac{A}{2k(k-q)}\sin{qx} + \frac{A}{2k(k+q)}\sin{qx} = \frac{A}{k^2-q^2}\sin{qx} \end{aligned}$$

For $k = q$,

$$\begin{aligned} y_p(x) &= -\frac{A}{k}\cos{kx} + \frac{A}{2k^2}\sin^3{kx} \\ &= -\frac{A}{2k}x\cos{kx} + \frac{A}{2k^2}[\cos^2{kx} + \sin^2{kx}]\sin{kx} \\ &= -\frac{A}{2k}x\cos{kx} + \frac{A}{2k^2}\sin{kx} \end{aligned}$$

where we can drop the last term because it is proportional to $y_2(x)$ which is already included in the solution. Similarly for the extra integration constants.

The general solution is then

$$y(x) = -\frac{A}{2k} x \cos kx + c_1 \cos kx + c_2 \sin kx$$

and **any boundary conditions** can be met by adjusting the two arbitrary constants.

Now consider again the **Heaviside step function** defined by

$$H(x-a) = \begin{cases} 0 & x < a \\ 1 & x > a \end{cases}$$

Now since

$$\int_{-\infty}^{\infty} \frac{dH(x-a)}{dx}\delta(x-a)f(x)dx$$

$$= H(x-a)f(x)|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} H(x-a)df(x)$$

$$= f(\infty)(1) - f(-\infty)(0) - \int_{a}^{\infty} df(x)$$

$$= f(\infty) - f(\infty) + f(a) = f(a)$$

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

we have

$$\frac{dH(x-a)}{dx} = \delta(x-a)$$

Therefore, when we have an inhomogeneous equation with

$$R(x) = \delta(x-x')$$

we have

$$v_1(x) = -\frac{y_2(x')}{W(x')}H(x-x') \quad , \quad v_2(x) = \frac{y_1(x')}{W(x')}H(x-x')$$

This solution of an inhomogeneous ODE with a **delta-function inhomogeneity** is called a **Green Function**.

We have

$$G(x,x') = G_p(x,x') + c_1 y_1(x) + c_2 y_2(x)$$

where

$$G_p(x.x') = \frac{-y_1(x)y_2(x') + y_1(x')y_2(x)}{W(x')}H(x-x')$$

More about Green functions later.

Series Solution of Homogeneous 2nd Order Linear ODEs: Method of Frobenius

We have seen

(1) given one solution of a homogeneous 2nd order ODE we can generate a second linearly independent solution integration

(2) if we are given both solutions, then a particular solution of the inhomogeneous ODE also can be calculated by integration

Thus, it remains for us to obtain at least 1 solution for the homogeneous equation.

A method, with which it is usually possible to do so, is to obtain the solution $y(x)$ of the homogeneous ODE

$$Ly(x) = 0$$

using a **power series** in x.

We choose

$$y(x) = x^s \sum_{\lambda=0}^{\infty} a_\lambda x^\lambda \qquad a_0 \neq 0$$

We then have

$$\frac{dy}{dx} = \sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s) x^{\lambda+s-1}$$

$$\frac{d^2y}{dx^2} = \sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s)(\lambda + s - 1) x^{\lambda+s-2}$$

Substitution back into the homogeneous ODE produces a powers series which sums to zero.

In this case, because each term in the series is linearly independent, each coefficient must separately $= 0$.

This allows us to determine the values of s and the a-coefficients and hence the solution to the problem.

Let us illustrate the method with some examples.

Consider the equation

$$\frac{d^2u}{dx^2} + x^2u = 0$$

Let us first use the simpler method which is valid for certain equations where $s =$ integer.

$$y(x) = x^s \sum_{\lambda=0}^{\infty} a_\lambda x^\lambda \qquad a_0 \neq 0$$

In this case, we can choose

$$u(x) = \sum_{\lambda=0}^{\infty} a_\lambda x^\lambda \qquad a_0 \neq 0$$

i.e., we can use the simpler series when $s =$ integer.

We then have

$$\frac{d^2u}{dx^2} = \sum_{\lambda=0}^{\infty} a_\lambda(\lambda)(\lambda-1)x^{\lambda-2}$$

Substitution gives

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

or

$$a_2(1)(2)x^0 + a_3(2)(3)x^3 + [a_4(3)(4) + a_0]x^2$$
$$+ .... + [a_{k-2} + a_{k+2}(k+2)(k+1)]x^k = ... = 0$$

We then have

$$a_0 \neq 0$$

$$a_1 \neq 0$$

$$a_2 = 0$$

$$a_3 = 0$$

$$a_k + a_{k+4}(k+3)(k+4) = 0$$

$$a_{k+4} = -\frac{a_k}{(k+3)(k+4)}$$

$$a_2 = 0 \rightarrow a_6 = a_{10} = a_{14} = ... = 0$$

$$a_3 = 0 \rightarrow a_7 = a_{11} = a_{15} = ... = 0$$

Starting with a_0 we get

$$a_4 = -\frac{a_0}{(3)(4)}$$

$$a_8 = -\frac{a_4}{(7)(8)} = \frac{a_0}{(3)(4)(7)(8)}$$

Starting with a_1 we get

$$a_5 = -\frac{a_1}{(4)(5)}$$

$$a_9 = -\frac{a_5}{(8)(9)} = \frac{a_1}{(4)(5)(8)(9)}$$

and the general solution is

$$u(x) = c_1\left(1 - \frac{1}{12}x^4 + \frac{1}{672}x^8 - ....\right) + c_2\left(x - \frac{1}{20}x^5 + \frac{1}{1440}x^9 - .....\right)$$

Let us now do this same equation with s left in (more general).

We choose

$$u(x) = \sum_{\lambda=0}^{\infty} a_\lambda x^{\lambda+s} \qquad a_0 \neq 0$$

We then have

$$\frac{d^2u}{dx^2} = \sum_{\lambda=0}^{\infty} a_\lambda (s+\lambda)(s+\lambda-1) x^{\lambda-2+s}$$

Substitution gives

$$\sum_{\lambda=0}^{\infty} a_\lambda (s+\lambda)(s+\lambda-1) x^{\lambda-2+s} + \sum_{\lambda=0}^{\infty} a_\lambda x^{\lambda+s+2} = 0$$

or

$$a_0 s(s-1)x^{s-2} + a_1 s(s+1)x^{s-1} + a_2(s+1)(s+2)x^s$$
$$+ a_3(s+2)(s+3)x^{s+1}$$
$$+ [a_4(s+3)(s+4) + a_0]x^{s+2} + ...$$
$$+ [a_{k-2} + a_{k+2}(s+k+2)(s+k+1)]x^{s+k} + ... = 0$$

We then have

$$a_0 s(s-1) = 0 \rightarrow a_0 \neq 0, s = 0, 1$$

$$a_1 s(s+1) = 0 \rightarrow a_1 \neq 0, s = 09 \quad \text{and} \quad a_1 = 0, s = 1$$

$$a_2(s+1)(s+2) = 0 \rightarrow a_2 = 0$$

$$a_3(s+2)(s+3) = 0 \rightarrow a_3 = 0$$

$$[a_{k-2} + a_{k+2}(s+k+2)(s+k+1) = 0$$

$$a_{k+4} = -\frac{a_k}{(s+k+3)(s+k+4)}$$

$$a_2 = 0 \rightarrow a_6 = a_{10} = a_{14} = ... = 0$$

$$a_3 = 0 \rightarrow a_7 = a_{11} = a_{15} = ... = 0$$

Starting with $s = 0$ and choosing $a_0 = a_1 = 1$ we get

$$a_4 = -\frac{a_0}{(3)(4)}\ ,\ a_8 = -\frac{a_4}{(7)(8)} = \frac{a_0}{(3)(4)(7)(8)}\ ,\ .....$$

$$a_5 = -\frac{a_1}{(4)(5)}\ ,\ a_9 = -\frac{a_5}{(8)(9)} = \frac{a_1}{(4)(5)(8)(9)}\ ,\ .....$$

The case $s = 1$ does not generate any new series (always happens if $s =$ integer).

The general solution is the same as earlier

$$u(x) = c_1\left(1 - \frac{1}{12}x^4 + \frac{1}{672}x^8 - ....\right) + c_2\left(x - \frac{1}{20}x^5 + \frac{1}{1440}x^9 - .....\right)$$

We now consider the equation

$$8x^2\frac{d^2u}{dx^2} + 6x\frac{du}{dx} + (x-1)u = 0$$

Assume

$$u(x) = x^s\sum_{\lambda=0}^{\infty} a_\lambda x^\lambda \qquad a_0 \neq 0$$

Substitution gives

$$8\sum_{\lambda=0}^{\infty} a_\lambda(\lambda+s)(\lambda+s-1)x^{\lambda+s} + 6\sum_{\lambda=0}^{\infty} a_\lambda(\lambda+s)x^{\lambda+s} + \sum_{\lambda=0}^{\infty} a_\lambda x^{\lambda+s+1}$$
$$- \sum_{\lambda=0}^{\infty} a_\lambda x^{\lambda+s} = 0$$

$$[8a_0 s(s-1) + 6a_0 s - a_0]x^s + [8a_1 s(s+1) + 6a_1(s+1) - a_1 + a_0]x^{s+1}$$
$$+ [8a_2(s+1)(s+2) + 6a_2(s+2) - a_2 + a_1]x^{s+2} + ...$$
$$+ [8a_n(s+n-1)(s+n) + 6a_n(s+n) - a_n + a_{n-1}]x^{s+n} + ... = 0$$

The coefficient of x^s is called the **indicial equation**.

It determines the allowed values of s.

We choose $a_0 = 1$ for simplicity.

We get

$$8s(s-1)+6s-1 = 0 = 8s^2 - 2s - 1 \rightarrow s = \frac{2 \pm \sqrt{4+32}}{16} = \frac{1}{2}, -\frac{1}{4}$$

These two allowed s values will generate the two linearly independent homogeneous solutions.

We have from the other coefficients

$$8a_n(s+n-1)(s+n)+6a_n(s+n)=a_n+a_{n-1}=0$$

$$a_n=-\frac{a_{n-1}}{8(s+n-1)(s+n)+6(s+n)-1}$$

This last relation is a recursion relation and determines all higher order coefficients(for each allowed s value) in terms of a_0.

We get

$$s=\frac{1}{2}$$

$$\begin{aligned}u_1(x)&=x^{1/2}-\frac{1}{8(1/2)(3/2)+6(3/2)-1}x^{3/2}\\&+\frac{1}{(8(3/2)(5/2)+6(5/2)-1)(8(1/2)(3/2)+6(3/2)-1)}x^{5/2}-\ldots\\&=x^{1/2}-\quad\frac{1}{14}x^{3/2}+\frac{1}{616}x^{5/2}-\ldots.\end{aligned}$$

$$s = -\frac{1}{4}$$

$$u_2(x) = x^{-1/4} - \frac{1}{2}x^{3/4} + \frac{1}{40}x^{7/4} - .....$$

and the most general solution is

$$u(x) = au_1(x) + bu_2(x)$$

A second example is slightly trickier(even though equation is simpler).

Consider the equation

$$\left(\frac{d^2}{dx^2} + k^2\right) y(x) = 0$$

Remember we already know the solutions to this equation and that will help us to figure out what is going on with the method.

Substitution gives

$$\sum_{\lambda=0}^{\infty} a_\lambda(\lambda+s)(\lambda+s-1)x^{\lambda+s-2} + k^2\sum_{\lambda=0}^{\infty} a_\lambda x^{\lambda+s} = 0$$

or

$$a_0 s(s-1)x^{s-2} + a_1 s(s+1)x^{s-1} + [a_0 k^2 + a_2(s+2)(s+1)]x^s + \ldots\ldots$$
$$+ [a_\lambda k^2 + a_{\lambda+2}(s+\lambda+2)(s+\lambda+1)]x^{s+\lambda} + \ldots. = 0$$

Since the coefficient of each power must separately be $= 0$, we have

$$a_0 s(s-1) = 0 \rightarrow s = 0 \;\text{ or }\; 1 \quad \text{since} \quad a_0 \neq 0$$

This is always STEP #1: determine the possible values of s.

It is at this point that we use the assumption $a_0 \neq 0$.

Then look at next coefficient

$$a_1 s(s+1) = 0 \rightarrow \begin{cases} \text{if } s = 0, \text{ then } a_1 \text{ can be nonzero} \\ \text{if } s = 1, \text{ then } a_1 = 0 \end{cases}$$

In general, the coefficient of the other higher powers are given by

$$a_{\lambda+2} = -\frac{k^2}{(s+\lambda+2)(s+\lambda+1)} a_\lambda$$

This is a **recursion relation**, which allows an ordered step-by-step determination of all coefficients in terms of a_0 or a_1 i.e.,

$$a_2 = -\frac{k^2}{(s+2)(s+1)} a_0$$

$$a_3 = -\frac{k^2}{(s+3)(s+2)} a_1$$

and so on.

The particular recurrence relation for this equation contains the special feature that it steps λ by 2.

As a result, the coefficients a_λ are separated into two disjoint groups, one with even λ and another with odd λ.

For the even chain we find

(a) For $s = 0$

$$a_2 = -\frac{k^2}{2!}a_0 \quad , \quad a_4 = -\frac{k^2}{12}a_2 = \frac{k^2}{4!}a_0 \quad , \quad \ldots\ldots\ldots$$

(b) For $s = 1$

$$a_2 = -\frac{k^2}{3!}a_0 \quad , \quad a_4 = -\frac{k^2}{20}a_2 = \frac{k^2}{5!}a_0 \quad , \quad \ldots\ldots\ldots$$

or we get solutions

(a)

$$y_1(x) = y_{even}(x) = 1 - \frac{k^2}{2!}x^2 + \frac{k^2}{4!}x^4 - \ldots = \cos kx$$

(b)

$$y_2(x) = y_{odd}(x) = x\left(1 - \frac{k^2}{3!}x^2 + \frac{k^2}{5!}x^4 - \ldots.\right)$$
$$= \frac{1}{k}\left(x - \frac{k^2}{3!}x^3 + \frac{k^2}{5!}x^5 - \ldots.\right) = \frac{1}{k}\sin kx$$

where we have used $a_0 = 1$.

What about the odd chain of coefficients? There is no solution in that case for $s = 1$, since $a_1 = 0$ and therefore all higher order odd coefficients vanish.

For $s = 0$ however, $a_1 \neq 0$ and this gives

$$a_3 = -\frac{k^2}{3!}a_1 \quad , \quad a_5 = -\frac{k^2}{20}a_3 = \frac{k^2}{5!}a_1 \quad , \quad \ldots\ldots\ldots$$

which is the same solution as $y_{odd}(x)$ from before, so we get nothing new.

In fact, we should not have expected anything new since we already have found the 2 allowed linearly independent solutions.

The solutions are, of course, the same as we found earlier.

Parity Property

even **parity**

It can easily be seen that

odd **parity**

$$y_{even}(-x) = y_{even}(x) \rightarrow \text{ even function } \rightarrow \text{ even } \textbf{parity}$$

$$y_{odd}(-x) = -y_{odd}(x) \rightarrow \text{ odd function } \rightarrow \text{ odd } \textbf{parity}$$

For a solution of a linear ODE to have a definite parity, the linear operator L must be even (or invariant under inversion or parity operation $x \rightarrow -x$ or

$$L(-x) = L(x)$$

An example is a classical oscillator with **damping**

$$L(t)y(t) = \left(\frac{d^2}{dt^2} + 2\beta\frac{d}{dt} + \omega_0^2\right) y(t) = 0 \rightarrow L(t) \neq L(-t)$$

which means that solutions do not have definite parity.

For practice, let us do another example where $s \neq$ integer.

Consider the equation

$$16x^2\frac{d^2u}{dx^2} + 3(1+x)u = 0$$

Assuming

$$u(x) = x^s \sum_{\lambda=0}^{\infty} a_\lambda x^\lambda$$

Substitution gives

$$16\sum_{\lambda=0}^{\infty} a_\lambda(\lambda+s)(\lambda+s-1)x^{\lambda+s}+3\sum_{\lambda=0}^{\infty} a_\lambda)x^{\lambda+s+1}+3\sum_{\lambda=0}^{\infty} a_\lambda)x^{\lambda+s} = 0$$

$$\begin{aligned}
&[16a_0s(s-1)+3a_0]x^s + [16a_1s(s+1)+3a_0+3a_1]x^{s+1} \\
&\quad + [16a_2(s+1)(s+2)+3a_1+3a_2]x^{s+2} + ... \\
&\quad + [16a_n(s+n+1)(s+n)3a_{n-1}+3a_n]x^{s+n} + ...
\end{aligned}$$

We choose $a_0 = 1$ for simplicity. We get

$$16s(s-1)+3 = 0 = 16s^2-16s+3 \rightarrow s = \frac{16 \pm \sqrt{256-192}}{32} = +\frac{3}{4}, +\frac{1}{4}$$

These two allowed s values will generate the two linearly independent homogeneous solutions we need.

We have from the other coefficients

$$16a_n(s+n-1)(s+n) + 3a_{n-1} + 3a_n = 0$$

$$a_n = -\frac{3}{16(s+n-1)(s+n)+3} a_{n-1}$$

The recursion relation determines all higher order coefficients (for each allowed s value) in terms of $a_0 = 1$.

We get

$$s = \frac{1}{4} \rightarrow u_1(x) = x^{1/4}\left[1 - \frac{3}{20}x + \frac{1}{160}x^2 - .....\right]$$

$$s = \frac{3}{4} \rightarrow u_2(x) = x^{3/4}\left[1 - \frac{1}{8}x + \frac{3}{640}x^2 - .....\right]$$

and the most general solution is

$$u(x) = au_1(x) + bu_2(x)$$

Legendre Equation This ODE arises in many physical systems that we shall investigate later

$$(1-x^2)\frac{d^2u}{dx^2} - 2x\frac{du}{dx} + \ell(\ell+1)u = 0$$

We choose

$$u(x) = x^s \sum_{\lambda=0}^{\infty} a_\lambda x^\lambda$$

We then have

$$\frac{du}{dx} = \sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s) x^{\lambda+s-1}$$

$$\frac{d^2u}{dx^2} = \sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s - 1)(\lambda + s) x^{\lambda+s-2}$$

Substitution gives

$$\sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s)(\lambda + s - 1) x^{\lambda+s-2} - \sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s)(\lambda + s - 1) x^{\lambda+s}$$

$$- 2 \sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s) x^{\lambda+s} + \ell(\ell+1) \sum_{\lambda=0}^{\infty} a_\lambda x^{\lambda+s} = 0$$

$$[a_0 s(s-1)] x^{s-2} + [a_1 s(s+1)] x^{s-1}$$
$$+ [a_2 (s+1)(s+2) - a_0 (s(s-1) + 2s - \ell(\ell+1)] x^s$$
$$[a_{n+2}(s+n+2)(s+n+1) - a_n ((s+n)(s+n-1)$$
$$+ 2(s+n) - \ell(\ell+1)] x^{s+n} + ... = 0$$

or

$$a_0 s(s-1) = 0 \rightarrow s = 0, 1$$

$$a_1 s(s=1) = 0 \rightarrow s = 1, a_1 = 0 \quad \text{and} \quad s = 0, a_1 \neq 0$$

$$a_{n+2}(s+n+2)(s+n+1) - a_n((s+n)(s+n-1) + 2(s+n) - \ell(\ell+1) = 0$$

or

$$a_{n+2} = \frac{(n+2)(n+1) - \ell(\ell+1)}{(n+3)(n+2)} a_n$$

The **even** and **odd** solutions are then

$$u_1(x) = 1 - \frac{\ell(\ell+1)}{2!}x^2 + \frac{(\ell-2)(\ell+1)(\ell+3)}{4!}x^4 - .....$$

$$u_2(x) = x - \frac{(\ell-1)(\ell+2)}{3!}x^3 + \frac{(\ell-3)(\ell-1)(\ell+2)(\ell+4)}{5!}x^5 - .....$$

As before the other case does not contribute anything new.

If ℓ is an **integer**, then the series **terminate** at a finite number of terms and the solutions are **polynomials**.

We have

$$\ell = 0 \ , \ \ u_1(x) = 1 \ , \ \ u_2(x) = \text{ infinite series}$$

$$\ell = 1 \ , \ \ u_1(x) = \text{ infinite series } , \ \ u_2(x) = x$$

$$\ell = 2 \ , \ \ u_1(x) = 1 - 3x^2 \ , \ \ u_2(x) = \text{ infinite series}$$

$$\ell = 3 \ , \ \ u_1(x) = \text{ infinite series } , \ \ u_2(x) = x - \frac{5}{3}x^3$$

$$\ell = 4 \ , \ \ u_1(x) = 1 - 10x^2 + \frac{35}{3}x^4 \ , \ \ u_2(x) = \text{ infinite series}$$

$$\ell = 5 \ , \ \ u_1(x) = 1 \ , \ \ u_2(x) = x - \frac{14}{3}x^3 + \frac{21}{5}x^5$$

If we multiply a solution by a constant, then it is still a solution.

If we multiply each polynomial above by a constant so that they have the value 1 at $x = 1$, then they are called the **Legendre polynomials** $P_\ell(x)$, where

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = \frac{1}{2}(3x^2 - 1)$$

$$P_3(x) = \frac{1}{2}(5x^3 - 3x)$$

$$P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)$$

$$P_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x)$$

In general we write

$$P_\ell(x) = \sum_{n=0}^{N} (-1)^n \frac{(2\ell - 2n)!}{2^\ell n!(\ell - n)!(\ell - 2n)!} x^{\ell - 2n}$$

where

$$N = \begin{cases} \frac{\ell}{2} & \ell \text{ even} \\ \frac{\ell-1}{2} & \ell \text{ odd} \end{cases}$$

The infinite series and the polynomials generate **Legendre's functions of the second kind** $Q_\ell(x)$ where

$$Q_\ell(x) = \begin{cases} u_1(1)u_2(x) & \ell \text{ even} \\ -u_2(1)u_1(x) & \ell \text{ odd} \end{cases}$$

and the most general solution of Legendre's equations is

$$u(x) = c_1 P_\ell(x) + c_2 Q_\ell(x)$$

All Legendre's functions of the second kind are **singular** (diverge) at $x = 1$; this will be important in physical problems.

If we make the substitution $x = \cos\theta$ Legendre's equation becomes

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{du}{d\theta}\right) + \ell(\ell+1)u = 0$$

which is the form that will arise most often when we solve problems in spherical-polar coordinates later.

Hermite Equation

Now we turn our attention to Hermite's equation

$$\frac{d^2u}{dx^2} - 2x\frac{du}{dx} + 2\alpha u = 0 \quad , \quad \alpha = \text{ nonnegative integer}$$

As we shall see, the solutions are polynomials called **Hermite polynomials**.

Legendre and Hermite polynomials are the first two examples of a large class of **special functions** that play a major role in the solutions of partial differential equations representing physical systems.

We choose

$$u(x) = x^s \sum_{\lambda=0}^{\infty} a_\lambda x^\lambda$$

We then have

$$\frac{du}{dx} = \sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s) x^{\lambda+s-1}$$

$$\frac{d^2u}{dx^2} = \sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s - 1)(\lambda + s) x^{\lambda+s-2}$$

Substitution gives

$$\sum_{\lambda=0}^{\infty} a_\lambda (\lambda+s-1)(\lambda+s) x^{\lambda+s-2} - 2\sum_{\lambda=0}^{\infty} a_\lambda (\lambda+s) x^{\lambda+s} + 2\alpha \sum_{\lambda=0}^{\infty} a_\lambda x^{\lambda+s} = 0$$

$$[a_0 s(s-1)]x^{s-2} + [a_1 s(s+1)]x^{s-1}$$
$$+ [a_2(s+1)(s+2) - a_0(s-2\alpha)]x^s + ...$$
$$[a_{n+2}(s+n+2)(s+n+1) - a_n((s+n) - 2\alpha)]x^{s+n} + ... = 0$$

or

$$a_0 s(s-1) = 0 \rightarrow s = 0, 1$$

$$a_1 s(s+1) = 0 \rightarrow s = 1, a_1 = 0 \quad \text{and} \quad s = 0. a_1 \neq 0$$

$$a_{n+2}(s+n+2)(s+n+1) - a_n((s+n) - 2\alpha) = 0$$

or

$$a_{n+2} = \frac{(s+n) - 2\alpha}{(s+n+2)(s+n+1)} a_n$$

For s = 0 we have

$$a_{n+2} = \frac{n - 2\alpha}{(n+2)(n+1)} a_n$$

For s = 1 we have

$$a_{n+2} = \frac{(1+n) - 2\alpha}{(n+3)(n+2)} a_n$$

The **even** and **odd** solutions are then

$$u_1(x) = 1 - \frac{2\alpha}{2!}x^2 + \frac{2^2\alpha(2-\alpha)}{4!}x^4 - .....$$

$$u_2(x) = x - \frac{2(1-\alpha)}{3!}x^3 + \frac{2^2(1-\alpha)(3-\alpha)}{5!}x^5 - .....$$

As before the other case does not contribute anything new.

Clearly the infinite series terminate if α is an integer.

The Hermite polynomials are

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

$$H_2(x) = 4x^2 - 2$$

$$H_3(x) = 8x^3 - 12x$$

or in general

$$H_n(x) = n! \sum_{k=0}^{N} \frac{(-1)^k}{k!(n-2k)!}(2x)^{n-2k}$$

where

$$N = \begin{cases} \frac{n}{2} & n \text{ even} \\ \frac{n-1}{2} & n \text{ odd} \end{cases}$$

The Hermite polynomials appear in the harmonic oscillator solution of the Schrödinger equation as shown below.

The Schrödinger equation for the 1-dimensional harmonic oscillator with a potential function

$$V(x) = \frac{1}{2}kx^2$$

is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}kx^2\psi(x) = E\psi(x)$$

The standard ODE solution of this equations goes as follows.

Let

$$\xi = \alpha x \quad , \quad \alpha^4 = \frac{mk}{\hbar^2}$$

$$\lambda = \frac{2E}{\hbar\omega_0} \quad , \quad \omega_0 = \left(\frac{k}{m}\right)^{1/2}$$

This gives the new equation

$$\frac{d^2\psi}{d\xi^2} + (\lambda - \xi^2)\psi = 0$$

If we consider the behavior of the equation as $\xi \to \pm\infty$ we can neglect λ and the equation becomes

$$\frac{d^2\psi}{d\xi^2} - \xi^2\psi = 0$$

which says that the large ξ behavior of the solution is

$$\psi = e^{-\xi^2/2}$$

This suggests that we try a solution of the form

$$\psi = H(\xi)e^{-\xi^2/2}$$

which should remove the large ξ behavior from the equation.

We get the equation

$$H'' - 2\xi H' + (\lambda - 1)H = 0$$

This is Hermite's equation. If we do not terminate the series solutions then the solutions are not square-integrable and cannot represent wave functions.

This can be seen as follows:

The series solutions we found earlier have the recursion relation

$$a_{k+2} = \frac{2k + 1 - \lambda}{(k+2)(k+1)} a_k$$

If the series does not terminate, then its dominant asymptotic behavior can be inferred from the coefficients of its higher order terms.

We have

$$\lim_{k \to \infty} \frac{a_{k+2}}{a_k} \to \frac{2}{k}$$

This ratio is the same as that of the series for $\xi^n e^{\xi^2}$ with any finite value of n.

Thus, the solution $\psi = H(\xi)e^{-\xi^2/2}$ will not be square-integrable unless the series is terminated.

Therefore, we choose $\lambda = 2n + 1$ and the solutions are the Hermite polynomials H_n.

For this choice of λ we get energy eigenvalues

$$E_n = \hbar\omega_0 \left(n + \frac{1}{2} \right)$$

with associated wave functions

$$\psi_n(x) = H_n(\alpha x)e^{-\alpha^2 x^2/2}$$

That is why we are studying all these special equations - we will then recognize them when we solve the equations for real physical systems and can just quote our earlier results to get solutions!

Gamma or Factorial Function

Consider the integrals below:

$$\int_0^\infty e^{-\alpha x} dx = \frac{1}{\alpha} \quad , \quad \int_0^\infty x e^{-\alpha x} dx = \frac{1}{\alpha^2} \quad ,$$

$$\int_0^\infty x^2 e^{-\alpha x} dx = \frac{2!}{\alpha^3} \quad , \quad \int_0^\infty x^3 e^{-\alpha x} dx = \frac{3!}{\alpha^4}$$

or

$$\int_0^\infty x^n e^{-\alpha x} dx = \frac{n!}{\alpha^{n+1}}$$

If we let $\alpha = 1$, then

$$n! = \int_0^\infty x^n e^{-\alpha x} dx$$

where we have defined

$$n! \equiv n(n-1)(n-2)....(2)(1) \quad \text{and} \quad 0! \equiv 1$$

Generalizing this result we have the Gamma Function

$$\Gamma(p) = \int_0^\infty x^{p-1} e^{-x} dx \quad \text{for} \;\; p > 0$$

and for $n =$ integer

$$\Gamma(n) = \int_0^\infty x^{n-1} e^{-x} dx = (n-1)! \rightarrow \Gamma(n+1) = n!$$

Now

$$\Gamma(p+1) = \int_0^\infty x^p e^{-x} dx \quad \text{for} \;\; p > -1$$

$$= -x^p e^{-x}\Big|_0^\infty + p \int_0^\infty x^{p-1} e^{-x} dx = p\Gamma(p)$$

This is a **recursion relation** for the Γ function.

What about negative numbers? We can use the recursion relation:

$$\Gamma(p) = \frac{1}{p}\Gamma(p+1)$$

which gives

$$\Gamma(-0.5) = \frac{1}{-0.5}\Gamma(-0.5+1) = -2\Gamma(0.5)$$

$$\Gamma(-1.5) = \frac{1}{-1.5}\Gamma(-1.5+1) = -\frac{2}{3}\Gamma(-0.5) = \frac{4}{3}\Gamma(0.5)$$

Now

$$\Gamma(0.5) = \int_0^\infty t^{-1/2}e^{-t}dt$$

$$t = y^2 \rightarrow dt = 2ydy \rightarrow \Gamma(0.5) = \int_0^\infty y^{-1}e^{-y^2}2ydy = 2\int_0^\infty e^{-y^2}dy$$

$$
\begin{aligned}
[\Gamma(0.5)]^2 &= 4\int_0^\infty e^{-x^2}dx \int_0^\infty e^{-y^2}dy \\
&= 4\int_0^\infty \int_0^\infty e^{-(x^2+y^2)}dxdy = 4\int_0^\infty \int_0^{\pi/2} e^{-r^2} rdrd\theta \\
&= 2\pi \int_0^\infty e^{-r^2} rdr = 2\pi \int_0^\infty d\left(-\frac{1}{2}e^{-r^2}\right) \\
&= \pi \rightarrow \Gamma(0.5) = \sqrt{\pi}
\end{aligned}
$$

In addition, since $\Gamma(1) = 1$ we have

$$
\lim_{p\to 0} \frac{\Gamma(p+1)}{p} = \infty \rightarrow \Gamma(p) = \infty \quad \text{for all negative integers}
$$

Laguerre Equation

The Laguerre equation takes the form

$$
x\frac{d^2u}{dx^2} + (1-x)\frac{du}{dx} + Nu = 0
$$

We choose

$$u(x) = x^s \sum_{\lambda=0}^{\infty} a_\lambda x^\lambda$$

We then have

$$\frac{du}{dx} = \sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s) x^{\lambda+s-1}$$

$$\frac{d^2u}{dx^2} = \sum^{\infty} a_\lambda (\lambda + s - 1)(\lambda + s) x^{\lambda+s-2}$$

Substitution gives

$$\sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s)(\lambda + s - 1) x^{\lambda+s-1} - \sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s) x^{\lambda+s}$$

$$+ \sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s) x^{\lambda+s-1} + N \sum_{\lambda=0}^{\infty} a_\lambda x^{\lambda+s} = 0$$

$$
\begin{aligned}
&[a_0 s(s-1) + a_0 s] x^{s-1} \\
&+ [a_1 s(s+1) - a_0 s + a_1(s+1) + N a_0] x^s + ... \\
&+ [a_{n+1}(s+n+1](s+n) - \\
&\quad a_n(s+n) + a_{n+1}(s+n+1) + N a_n] x^{s+n} + ...
\end{aligned}
$$

or

$$
a_0 s(s-1) + a_o s = 0 \rightarrow s^2 = 0 \rightarrow s = 0
$$

$$
a_{n+1}(s+n+1](s+n) - a_n(s+n) + a_{n+1}(s+n+1) + N a_n = 0
$$

or

$$
a_{n+1} = \frac{(s+n) - N}{(s+n+1](s+n) + (s+n+1)} a_n = \frac{(s+n) - N}{(s+n+1)^2} a_n
$$

For $s = 0$ we have

$$a_{n+1} = \frac{n - N}{(n+1)^2} a_n$$

or

$$a_1 = (-1)^1 \frac{N}{(1!)^2} \quad , \quad a_2 = \frac{1 - N}{2^2} a_1 = (-1)^2 \frac{N(N-1)}{(2!)^2} \quad , \quad a_0 = 1$$

$$\rightarrow a_k = (-10^k \frac{N(N-1)....(N-k+1)}{(k!)^2}$$

$$= (-1)^k \frac{1}{k!} \frac{N!}{k!(N-k)!} = (-1)^k \frac{\binom{N}{k}}{k!}$$

It is clear that if $k > N$, then $a_k = 0$.

Thus we get

$$u(x) = L_N(x) = 1 + \sum_{k=1}^{N} (-1)^k \frac{\binom{N}{k}}{k!} x^k = \sum_{k=0}^{N} (-1)^k \frac{\binom{N}{k}}{k!} x^k \rightarrow \text{ polynomial}$$

These are the Laguerre polynomials:

$$L_0(x) = 1, \quad L_1(x) = 1 - x, \quad L_2(x) = 1 - 2x + \frac{x^2}{2!}$$

They will appear in the hydrogen atom solution of the Schrödinger equation.

Before proceeding to the final example, namely, Bessel's equation, let us digress to study **generating functions**.

Generating Functions

Legendre Polynomials Redux

Let us consider the function

$$\phi(x,h) = \frac{1}{(1-2xh+h^2)^{1/2}} \quad , \quad |h| < 1$$

$$= \sum_{\ell=0}^{\infty} h^\ell f_\ell(x) \quad \text{(power series)}$$

Differentiation gives

$$(1-x^2)\frac{\partial^2\phi}{\partial x^2} - 2x\frac{\partial\phi}{\partial x} + h\frac{\partial^2(h\phi)}{\partial h^2} = 0$$

If we substitute the power series we get

$$(1-x^2)\sum_{\ell=0}^{\infty} h^\ell [f_\ell''(x) - 2x\sum_{\ell=0}^{\infty} h^\ell f_\ell'(x) + \sum_{\ell=0}^{\infty} \ell(\ell+1)h^\ell f_\ell(x) = 0$$

$$\rightarrow \sum_{\ell=0}^{\infty} h^\ell [(1-x^2)f_\ell''(x) - 2xf_\ell'(x) + \ell(\ell+1)f_\ell(x)] = 0$$

This says that the coefficient of each power of h must separately equal zero.

We get

$$(1-x^2)f_\ell''(x) - 2xf_\ell'(x) + \ell(\ell+1)f_\ell(x) = 0$$

This is **Legendre's equation**.

So the solutions are

$$f_\ell(x) = P_\ell(x) = \text{ Legendre polynomials}$$

and thus

$$\phi(x,h) = \frac{1}{(1-2xh+h^2)^{1/2}} = \sum_{\ell=0}^{\infty} h^\ell P_\ell(x)$$

$\phi(x,h) =$ **generating function** for the Legendre polynomials.

Let us generate the first couple of polynomials. Let $y = 2xh - h^2$.

Then

$$\begin{aligned}
\phi(x,h) &= \frac{1}{(1-y)^{1/2}} = 1 + \frac{1}{2}y + \frac{3}{8}y^2 + ... \\
&= 1 + xh + \left(\frac{3}{2}x^2 - \frac{1}{2}\right) h^2 + ... \\
&= P_0(x) + hP_1(x) + h^2 P_2(x) + ...
\end{aligned}$$

or

$$P_0(x) = 1 \ , \ \ P_1(x) = x \ , \ \ P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}$$

We can also write

$$P_\ell(x) = \frac{1}{\ell!}\left(\frac{\partial^\ell}{\partial x^\ell}\phi(x,h)\right)_{h=0}$$

Recursion Relations

Legendre polynomials of different ℓ (**degree**) are related to each other, i.e.

$$P_1(x) = xP_0(x)$$

via **recursion or recurrence relations**.

Now consider

$$\phi(x,t) = \frac{1}{(1-2xt+t^2)^{1/2}} = \sum_{n=0}^{\infty} t^n P_n(x)$$

We have

$$\frac{\partial\phi(x,t)}{\partial t} = \frac{x-t}{(1-2xt+t^2)^{3/2}} = \sum_{n=0}^{\infty} nt^{n-1}P_n(x)$$

$$(x-t)\phi(x,t) = (1-2xt+t^2)\sum_{n=0}^{\infty} nt^{n-1}P_n(x) = (x-t)\sum_{n=0}^{\infty} t^n P_n(x)$$

Rearranging we get

$$\sum_{n=0}^{\infty}(2n+1)xt^nP_n(x) = P_1(x) + \sum_{n=1}^{\infty} t^n(nP_{n-1}(x) + (n+1)P_{n+1}(x))$$

Equating coefficients of t^n we have

$$(2n+1)xP_n(x) = nP_{n-1}(x) + (n+1)P_{n+1}(x)$$

Therefore, given that $P_0(x) = 1$ and $P_1(x) = x$ we get (for $n = 1$)

$$3xP_1(x) = P_0(x) + 2P_2(x) \rightarrow P(2(x) = 3x^2 - 1$$

In a similar manner we can find

$$nP_n(x) = xP;_n(x) - P'_{n-1}(x)$$

Orthogonality Relations

We have

$$\int_{-1}^{1} \phi^2(x,t)dx = \int_{-1}^{1} (1 - 2xt + t^2)^{-1} dx = \frac{1}{t}[(\ln(1+t) - \ln(1-t))]$$

$$= \sum_{k=0}^{\infty} \frac{2}{2k+1} t^{2k}$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} t^{n+m} \int_{-1}^{1} P_n(x) P_m(x) dx$$

where we have used

$$\ln(1+h) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{h^n}{n}$$

Equating coefficients we get orthogonality relations

$$\int_{-1}^{1} P_n(x)P_m(x)dx = \frac{2}{2n+1}\delta_{nm}$$

Thus, it is clear that **generating functions are very powerful tools**.

Hermite Polynomials

As we have seen, families of functions can be defined by DiffEQs.

We have also seen that they can be defined by means of a generating function.

Finally, they can be defined by a **differential formula** of the form such as the Rodriguez formula for Hermite polynomials.

We have

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \quad , \quad n = 1, 2, 3, ...$$

which gives

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

$$H_2(x) = 4x^2 - 2$$

We can get the generating function from this formula by introducing a dummy variable t as follows:

$$H_n(x) = e^{x^2} \left(\frac{\partial^n}{\partial t^n} e^{-(x-t)^2} \right)_{t=0} = \left(\frac{\partial^n}{\partial t^n} e^{2x-t^2} \right)_{t=0}$$

Earlier we saw that

$$P_\ell(x) = \frac{1}{\ell!} \left(\frac{\partial^\ell}{\partial x^\ell} \phi(x, h) \right)_{h=0}$$

Therefore, by analogy, we have

$$e^{2x-t^2} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} = \phi(x, t) = \text{ generating function}$$

In the same way as before we can derive recursion and orthogonality relations.

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$

$$H'_n(x) = 2nH_{n-1}(x)$$

$$H_{n+1}(x) - 2xH_n(x) + H'_n(x) = 0$$

If we differentiate this last relation, we get

$$H'_{n+1}(x) - 2H_n(x) - 2xH'_n(x) + H''_n(x)$$

$$H''_n(x) - 2xH'_n(x) - 2nH_n(x) = 0$$

which is the Hermite DiffEQ.

The solutions are the Hermite polynomials.

We also have the orthogonality relations

$$\int_{-1}^{1} e^{-x^2} H_n(x)H_m(x)dx = 2^n n!\sqrt{\pi}\delta_{nm}$$

Laguerre Polynomials

A similar procedure gives

$$L_n(x) = \frac{1}{n!} e^x \frac{d^n}{dx^n}(e^{-x} x^n)$$

$$\phi(x,t) = \frac{1}{1-t} e^{\frac{xt}{t-1}} = \sum_{n=0}^{\infty} L_n(x) t^n$$

$$(n=1)L_{n+1}(x) = (2n+1)L_n(x) - xL_n(x) - nL_{n-1}(x)$$

$$xL'_n(x) = nL_n(x) - nL_{n-1}(x)$$

Differentiation then gives the Laguerre DiffEQ

$$xL''_n(x) + (1-x)L'_n(x) + nL_n(x) = 0$$

and finally, we have the orthogonality relations

$$\int_0^\infty e^{-x} L_n(x) L_m(x) dx = \delta_{nm}$$

Bessel's Equation

We now consider the one of the most important equation in physics.

$$L(x)u(x) = \left(x^2 \frac{d^2}{dx^2} + x\frac{d}{dx} + (x^2 - \mu^2) \right) u(x) = 0$$

$$L(x) = L(-x) \rightarrow \text{ exists even and odd solutions}$$

We choose

$$u(x) = x^s \sum_{\lambda=0}^{\infty} a_\lambda x^\lambda$$

We then have

$$\frac{du}{dx} = \sum_{\lambda=0}^{\infty} a_\lambda (\lambda + s) x^{\lambda+s-1}$$

$$\frac{d^2u}{dx^2} = \sum_{\lambda=0}^{\infty} a_\lambda(\lambda+s-1)(\lambda+s)x^{\lambda+s-2}$$

Substitution gives

$$\sum_{\lambda=0}^{\infty} a_\lambda(\lambda+s)(\lambda+s-1)x^{\lambda+s} + \sum_{\lambda=0}^{\infty} a_\lambda(\lambda+s)x^{\lambda+s}$$
$$+ \sum_{\lambda=0}^{\infty} a_\lambda x^{\lambda+s+2} - \mu^2 \sum_{\lambda=0}^{\infty} a_\lambda x^{\lambda+s} + ... = 0$$

or

$$[a_0 s(s-1) + a_0 s - \mu^2 a_0]x^s$$
$$+ [a_1 s(s+1) + a_1(s+1) - \mu^2 a_1]x^{s+1} + ...$$
$$+ [a_n(s+n)(s+n-1) + a_n(s+n) + a_{n-2} - \mu^2 a_n]x^{s+n} + ... = 0$$

or

$$a_0 s(s-1) + a_0 s - \mu^2 a_0 = 0 \rightarrow S^2 - \mu^2 = 0 \rightarrow s = \pm\mu$$

$$[a_1 s(s+1) + a_1(s+1) - \mu^2 a_1 = 0 \rightarrow (s62 + 2s + 1 - \mu^2) a_1 = 0 \rightarrow a_1 = 0$$

$$a_n(s+n)(s+n-1) + a_n(s+n) + a_{n-2} - \mu^2 a_n = 0$$

or

$$a_n = -\frac{1}{(s+n-1)(s+n) + (s+n) - \mu^2} a_{n-2} = -\frac{1}{(s+n)^2 - \mu^2} a_{n-2}$$

Since $a_1 = 0$ this last relation implies that all odd coefficients $= 0$.

For $s = \mu$ we have

$$a_n = -\frac{1}{(n+\mu)^2 - \mu^2} a_{n-2}$$

or after some algebra

$$a_{2n} = \frac{(-1)^n}{(2)^{2n+\mu} n! \Gamma(\mu + n + 1)} \quad , \quad a_0 = \frac{1}{2^\mu \Gamma(\mu + 1)}$$

and the solution is

$$J_\mu(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2)^{2n+\mu} n! \Gamma(\mu + n + 1)} s^{2n+\mu}$$

which is the Bessel function of the first kind of order μ.

For $s = -\mu$ we have

$$a_n = -\frac{1}{(n-\mu)^2 - \mu^2} a_{n-2}$$

or after some algebra

$$a_{2n} = \frac{(-1)^n}{(2)^{2n-\mu} n! \Gamma(n - \mu + 1)}$$

and the solution is

$$J_{-\mu}(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2)^{2n-\mu} n! \Gamma(n - \mu + 1)} s^{2n-\mu}$$

which is the Bessel function of the second kind of order μ.

It is singular at $x = 0$, which will be important in many physical problems.

The most general solution is then

$$u(x) = aJ_{\mu}(x) + bJ_{-\mu}(x)$$

Bessel functions appear in a staggering number of physical systems.

Bessel Function Properties

Orthogonal polynomials such as Legendre, Hermite and Laguerre polynomials are well-suited (can be used as basis functions) for expansions of functions or the description of physical system that are **localized near the origin** of coordinates.

The Bessel function $J_n(x)$ of integral order n satisfies the DiffEQ

$$x^2 J_n''(x) + x J_n'(x) + (x^2 - n^2) J_n(x) = 0$$

The generating function for Bessel functions is

$$G(x,t) = \exp\left[\frac{1}{2}x\left(t - \frac{1}{t}\right)\right] = \sum_{n=-\infty}^{\infty} t^n J_n(x)$$

To explicitly obtain the $J_n(x)$ we expand $G(x,t)$ in powers of t.

$$\begin{aligned}
\exp\left[\frac{1}{2}x\left(t - \frac{1}{t}\right)\right] &= \exp\left[\frac{1}{2}xt\right]\exp\left[-\frac{x}{2}\frac{1}{t}\right] \\
&= \left(\sum_{r=0}^{\infty}\left(\frac{x}{2}\right)^r \frac{t^r}{r!}\right)\left(\sum_{s=0}^{\infty}\left(-\frac{x}{2}\right)^r \frac{t^{-s}}{s!}\right) \\
&= \sum_{r,s}(-1)^s \left(\frac{x}{2}\right)^{r+s} \frac{t^{r-s}}{r!s!}
\end{aligned}$$

We change the summation indices to $n = r - s$ or $r = n + s$ and $r + s = n + 2s$ which gives

$$G(x,t) = \sum_{n=-\infty}^{\infty} \sum_{s=0}^{\infty} (-1)^s \left(\frac{x}{2}\right)^{n+2s} \frac{t^n}{(n+s)!s!} = \sum_{n=-\infty}^{\infty} t^n J_n(x)$$

$$J_n(x) = \sum_{s=0}^{\infty} \frac{(-1)^s}{(n+s)!s!} \left(\frac{x}{2}\right)^{n+2s} \qquad \text{for} \quad n \geq 0$$

or

$$J_n(x) = \left(\frac{x}{2}\right)^n \left[\frac{1}{n!} - \frac{x^2}{4}\frac{1}{1!}\frac{1}{(n+1)!} + \left(\frac{x^2}{4}\right)^2 \frac{1}{2!}\frac{1}{(n+2)!} - \ldots\ldots\right]$$

For $n < 0$ a similar analysis gives

$$J_{-|n|}(x) = \sum_{s=|n|}^{\infty} \frac{(-1)^s}{(s-|n|)!s!} \left(\frac{x}{2}\right)^{2s-|n|} \qquad \text{for} \quad n < 0$$

since $\frac{1}{\Gamma(n)} = 0$ for the negative integers.

We also have

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

for integer n.

The generating function gives the recursion relations

$$\frac{1}{2}(J_{n-1} + J_{n+1}) = \frac{n}{x} J_n$$

$$\frac{1}{2}(J_{n-1} - J_{n+1}) = J'_n$$

Adding and subtracting we get the **ladder** operators

$$R_n J_n = \left(\frac{n}{x} - \frac{d}{dx}\right) J_n = J_{n+1}$$

$$N_n J_n = \left(\frac{n}{x} + \frac{d}{dx}\right) J_n = J_{n-1}$$

Since

$$L_{n+1}R_nJ_n = L_{n+1}J_{n+1} = J_n$$

we get

$$(L_{n+1}R_n - 1)J_n = 0$$

which is Bessel's equation.

One can easily verify that the expansion for $J_n(x)$ can have ν substituted for n where ν is any real number and then direct differentiation shows that $J_\nu(x)$ satisfies Bessel's equation with ν in place of n.

The factorials in the expansion do not present a problem since they are defined for non-integer values by

$$z! = \Gamma(Z+1) = \int_0^\infty e^{-t}t^z\,dt$$

In many cases, instead of the $J_{-\nu}(x)$ functions, one uses the Neuman functions defined by

$$N_\nu(x) = \frac{\cos\nu\pi\, J_\nu(x) - J_{-\nu}(x)}{\sin\nu\pi}$$

$N_\nu(x)$ is linearly independent of $J_\nu(x)$.

This means it is also a solution of Bessel's equation. It is the second linearly independent solution, i.e.,

$$W = \text{ Wronskian } = J_\nu N'_\nu - J'_\nu N_\nu = \frac{(-J_\nu J'_{-\nu} + J'_\nu J_{-\nu})}{\sin\nu\pi} = \frac{2}{\pi x}$$

The result is independent of ν. This also holds for $\nu = n$ which says the two solutions are linearly independent.

We also have the relations

$$\frac{d}{dx}(x^p J_p(x)) = x^p J_{p-1}(x)$$

$$\int_0^1 x J_p(ax) J_p(bx) dx = \begin{cases} 0 & a \neq b \\ \frac{1}{2} J_{p+1}^2(a) = \frac{1}{2} J_{p-1}^2(a) = \frac{1}{2} J''^2_p(a) & a = b \end{cases}$$

Relationship of the Cylindrical and Spherical Bessel Functions

The **spherical Bessel functions** are defined by:

$$j_\ell(z) = \left(\frac{\pi}{2z}\right)^{1/2} J_{\ell+1/2}(z)$$

$$\eta_\ell(z) = \left(\frac{\pi}{2z}\right)^{1/2} N_{\ell+1/2}(z)$$

Some simple ones are:

$$j_0(z) = \frac{\sin z}{z}$$

$$n_0(z) = -\cos z$$

$$j_1(z) = -j_0'(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}$$

$$j_2(z) = \frac{j_1}{z} j_1'(z) = \left(\frac{3}{z^3} - \frac{1}{z}\right) \sin z - \frac{3}{z^2} \cos z$$

In general:

$$j_{\ell-1} + j_{\ell+1} = \frac{2\ell+1}{z} j_\ell$$

$$\ell j_{\ell-1} - (\ell+1) j_{\ell+1} = (2\ell+1) j_\ell'$$

Some Odd Topics

Beta Function

$$B(p,q) = \int_0^1 x^{p-1}(1-x)^{q-1} dx \quad p > 0, q > 0$$

Other Forms:

$$B(q,p) = B(p,q)$$

$$x = y/a \rightarrow B(p,q) = \int_0^a y^{p-1}(a-y)^{q-1}dy$$

$$x = \sin^2\theta \rightarrow B(p,q) = 2\int_0^{\pi/2} (\sin\theta)^{p-1}(\cos\theta)^{q-1}d\theta$$

$$x = \frac{y}{1+y} \rightarrow B(p,q) = \int_0^{-1} \frac{y^{p-1}}{(1+y)^{q-1}}dy$$

$$B(p,q) = \frac{\Gamma_p\,\Gamma q}{\Gamma(p+q)}$$

Error Function

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt$$

Stirling's Formula (Factorial function for large arguments)

From the definition

$$\Gamma(p+1) = p! = \int_0^\infty x^p e^{-x} dx = \int_0^\infty e^{p \ln x - x} dx$$

Now let

$$x = p + y\sqrt{p} : x = 0 \to y = -\sqrt{p} \ , \ \ dx = \sqrt{p} dy$$

We then have

$$p! = \int_{-\sqrt{p}}^\infty e^{p \ln (p + y\sqrt{p}) - p - y\sqrt{p}} \sqrt{p} dy$$

Now

$$\ln (p + y\sqrt{p}) = \ln p \left(1 + \frac{y}{\sqrt{p}}\right) = \ln p + \ln \left(1 + \frac{y}{\sqrt{p}}\right)$$

For p very large

$$\ln(p + y\sqrt{p}) \approx \ln p + \frac{y}{\sqrt{p}} - \frac{y^2}{2p} + \text{.....}$$

so that

$$p! = e^{p \ln p - p}\sqrt{p}\int_{-\sqrt{p}}^{\infty} e^{-y^2/2}dy = p^p e^{-p}\sqrt{p}\left[\int_{-\infty}^{\infty} e^{-y^2/2}dy - \int_{-\infty}^{-\sqrt{p}} e^{-y^2/2}dy\right]$$

$$= p^p e^{-p}\sqrt{p}\int_{-\infty}^{\infty} e^{-y^2/2}dy = p^p e^{-p}\sqrt{2\pi p} \quad \text{for large } p$$

or more exactly

$$\Gamma(p+1) = p! = p^p e^{-p}\sqrt{2\pi p}\left(1 + \frac{1}{12p} + \frac{1}{288p^2} + \text{.....}\right)$$

And now for something completely different....

Expansions in Orthonormal Functions Gram-Schmidt in place of DiffEQs - (partial repeat of earlier material)

Definitions:

1. Expansion interval $[a, b]$: the variable x is confined to the interval $a \leq x \leq b$
2. Given two functions $f(x)$ and $g(x)$ defined on the interval $[a, b]$, the inner product of f and g is denoted by (f, g) and is given by

$$(f, g) = \int_a^b f^*(x) g(x) dx$$

   Over the space of complex functions.

   Note that order is important since $(f, g) = (g, f)^*$.
3. If $(f, g) = 0$ the functions f and g are **orthogonal**.
4. The norm of a function is (f, f).

   If the norm is finite, the function is square-integrable.

   If the function has norm $= 1$, then it is normalized.

In addition we have Any square-integrable function can be normalized by multiplication by a constant.

A set of functions $\varphi_1(x), \varphi_2(x), \ldots\ldots$ defined on the interval $[a, b]$ is said to be orthonormal if

$$(\varphi_i, \varphi_j) = \delta_{ij} \qquad \text{all i , j}$$

If we have an orthonormal set of functions on the interval $[a, b]$ then we can write any other square-integrable function $f(x)$ in terms of that set by

$$f(x) = \sum_j a_j \varphi_j \quad \text{where} \quad (\varphi_k, f) = \sum_j a_j (\varphi_k, \varphi_j) = \sum_j a_j \delta_{jk} = a_k$$

If this is true for any function $f(x)$, then set of functions $\varphi_1(x), \varphi_2(x), \ldots\ldots$ is **complete** and is called a **basis set**.

Gram-Schmidt Orthogonalization Method.

It turns out that to be a basis set, a set of functions only has to be linearly independent.

Linear independence implies that there exists no relation

$$\sum_{\lambda=1}^{n} c_\lambda f_\lambda(x) = 0$$

valid for all x, except the trivial one of all $c_\lambda = 0$.

They do not have to be orthonormal...that is only a **convenience**.

Suppose we have a set of n linearly independent, square integrable functions

$$f_\lambda(x) \quad \lambda = 1, 2, 3, 4, ..., n$$

on the interval $[a, b]$.

How do we construct an orthonormal set $\varphi_1(x), \varphi_2(x), ...\varphi_n(x)$?

There is a systematic process for doing this.

It goes as follows:

1. Choose
$$\varphi_1 = \frac{1}{\sqrt{N_1}} \quad \text{where} \quad N_1 = (f_1, f_2)$$
2. Choose φ_2 as a linear combination of f_1 and f_2 that is orthogonal to φ_1 and normalized to 1.
$$\varphi_2 = \frac{1}{\sqrt{N_2}}[f_2 - (\varphi_1, f_2)\varphi_1] \quad \text{where} \quad N_1 = (f_2, f_2) - |(\varphi_1, f_2)|^2$$
We have just subtracted off the **non-orthogonal part!**
3. This generalizes as
$$\varphi_k = \frac{1}{\sqrt{N_k}}[f_k - \sum_{j=1}^{k-1}(\varphi_j, f_k)\varphi_j] \quad \text{where} \quad N_k = (f_k, f_k) - |(\varphi_j, f_k)|^2$$

Legendre Polynomials Redux Redux

Consider the set of linearly independent functions which are the non-negative integral powers of x on the interval $[-1, 1]$

$$f_\lambda(x) = x^\lambda \quad \lambda = 0, 1, 2, 3, 4, ..., n$$

Using the orthogonalization procedure above we get the new set of functions

$$\varphi_0 = \frac{1}{\sqrt{N_0}} f_0 = \frac{1}{\sqrt{N_0}} \quad \text{where} \quad N_0 = (f_0, f_0) = \int_{-1}^{1} dx = 2 \rightarrow \varphi_0 = \frac{1}{\sqrt{2}}$$

$$\varphi_1 = \frac{1}{\sqrt{N_1}}[f_1 - (\varphi_0, f_1)\varphi_0] = \frac{1}{\sqrt{N_1}} \left[x - \left(\frac{1}{\sqrt{2}} \int_{-1}^{1} x dx \right) \frac{1}{\sqrt{2}} \right] = \frac{x}{\sqrt{N_1}}$$

where

$$N_1 = (f_1, f_1) - |(\varphi_0, f_1)|^2 = \int_{-1}^{1} x^2 dx - (0)^2 = \frac{2}{3} \rightarrow \varphi_1 = \sqrt{\frac{3}{2}} x$$

and in the same manner

$$\varphi_2 = \sqrt{\frac{5}{2}}\left(\frac{3}{2}x^2 - \frac{1}{2}\right)$$

$$\varphi_3 = \sqrt{\frac{7}{2}}\left(\frac{5}{2}x^3 - \frac{3}{2}x\right)$$

$$\varphi_4 = \sqrt{\frac{9}{2}}\left(\frac{35}{8}x^4 - \frac{15}{4}x^2 + \frac{3}{8}\right)$$

Apart from normalization these are the Legendre polynomials, i.e.,

$$\varphi_j(x) = \sqrt{\frac{2j+1}{2}}P_j(x)$$

Thus, we can construct the orthogonal polynomials using linear algebra instead of DiffEQs.

Finally, let us look at some weird numbers that have a habit of popping up in real world systems.

Bernoulli Numbers

Consider the series

$$\frac{x}{e^x - 1} = \sum_{n=0}^{\infty} \frac{B_n}{n!} x^n$$

We can use the relation

$$B_n = \left[\frac{d^n}{dx^n} \left(\frac{x}{e^x - 1} \right) \right]_{x=0}$$

to determine the **Bernoulli numbers** B_n.

This is a difficult direct process, however.

An easier method is to use the uniqueness property of the power series expansions.

We can write

$$\frac{e^x-1}{x}=\frac{x+\frac{1}{2!}x^2+\frac{1}{3!}x^3+....}{x}=1+\frac{1}{2!}x+\frac{1}{3!}x^2+\frac{1}{4!}x^3+...$$

We then get

$$\left(1+\frac{1}{2!}x+\frac{1}{3!}x^2+\frac{1}{4!}x^3+...\right)(\left(B_0+B_1x+\frac{1}{2!}B_2x^2+....\right)=1$$

which gives(by uniqueness or equating coefficients of like powers of x)

$$B_0=1$$

$$\frac{1}{2!}B_0+B_1=0\rightarrow B_1=-\frac{1}{2}$$

$$\frac{1}{3!}B_0+\frac{1}{2!}B_1++\frac{1}{2!}B_2=0\rightarrow B_2=\frac{1}{6}$$

and so on....

In general we have,

$$\sum_{k=0}^{n-1} \binom{n}{k} B_{2k} = 0$$

We obtain

$$B_{2n+1} = 0 \quad , \quad n = 1, 2, 3, ...$$

$$B_{2n} = \frac{(-1)^{n-1} 2(2n)!}{(2\pi)^{2n}} \sum_{p=1}^{\infty} p^{-2n} \quad , \quad n = 1, 2, 3, ...$$

These numbers are very divergent, i.e.,

$$B_{20} = -5.291 \times 10^{2} \quad ,, \quad B_{200} = -3.647 \times 10^{215}$$

The Bernoulli numbers appear all over the place, i.e.,

$$\tan x = x + \frac{1}{6} x^3 + \frac{2}{15} x^5 + ... + \frac{(-1)^{n-1} 2^{2n} (2^{2n} - 1)}{(2n)!} B_{2n} x^{2n-1} + ...$$

Bernoulli Functions

The functions are defined by

$$\frac{xe^{xs}}{e^x - 1} = \sum_{n=0}^{\infty} B_n(s) \frac{x^n}{n!}$$

It is clear that

$$B_n = \text{ Bernoulli number } B_n(0)$$

Other useful properties are:

$$B_n'(s) = nB_{n-1}(s) \quad , \quad n = 1, 2, 3, ...$$

$$B_n(1) = (-1)^n B_n(0) \quad , \quad n = 1, 2, 3, ...$$

Solving ODEs using Fourier Transforms

The formulas for derivatives are particularly useful because they reduce ODEs to algebraic expressions.

Consider the following ODE

$$\left(\frac{d^2}{dx^2} + p\frac{d}{dx} + q\right) f(x) = R(x) \qquad -\infty \leq x \leq \infty$$

where p and q are constants.

Transform both sides of the equations

$$F\left(\frac{d^2 f(x)}{dx^2} + p\frac{df(x)}{dx} + \quad \right) = ((ik)^2 + p(ik) + q)\tilde{f}(k)$$

$$= F(R(x)) = \tilde{R}(k)$$

where ˜ denotes the Fourier transform.

We then have

$$\tilde{f}(k) = \frac{\tilde{R}(k)}{-k^2 + ipk + q}$$

so that the solution (particular) is

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \tilde{f}(k) dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \frac{\tilde{R}(k)}{-k^2 + ipk + q} dk$$

This very formal solution to the problem is called the **integral representation** of the solution.

In general, we need complex integration techniques to evaluate these integrals.

We will see how later.

Solving ODEs with the Laplace Transform

We now have all the necessary tools to solve ODEs using the Laplace transform.

We consider an ODE with constant coefficients

$$\frac{d^2y}{dt^2} + a\frac{dy}{dt} + by = r(t)$$

Now if

$$L(y(t)) = Y(s)$$

we then have

$$L\left(\frac{d^2y}{dt^2} + a\frac{dy}{dt} + by\right) = L(r(t)) = R(s)$$

Our rules then give

$$[s^2Y(s) - sy(0) - y'(0)] + a[sY(s) - y(0)] + bY(s) = Rs$$

which is now an algebraic equation.

The solution is

$$Y(s) = \frac{(s+a)y(0) + y'(0)}{s^2 + as + b} + \frac{R(s)}{s^2 + as + b}$$

and

$$y(t) = L^{-1}(Y(s))$$

Examples:

(1) Consider the homogeneous ODE

$$\frac{d^2y}{dt^2} + 4\frac{dy}{dt} + 8y = 0$$

with initial conditions $y(0) = 2$, $y'(0) = 0$.

We have

$$Y(s) = \frac{2s+8}{s^2+4s+8} = \frac{2(s+2)}{(s+2)^2+4} + \frac{4}{(s+2)^2+4}$$

Now

$$L(e^{at}f(t)) = F(s-a) \quad \text{and} \quad L(\cos\omega t) = \frac{s}{s^2+\omega^2)}$$

or

$$L(e^{-2t}\cos 2t) = L(\cos 2(t+2)) = \frac{s+2}{(s+2)^2+4}$$

and

$$L(e^{at}f(t)) = F(s-a) \quad \text{and} \quad L(\sin\omega t = \frac{\omega}{s^2+\omega^2)}$$

or

$$L(e^{-2t}\sin 2t) = L(\sin 2(t+2)) = \frac{2}{(s+2)^2+4}$$

Therefore

$$Y(s) = \frac{2(s+2)}{(s+2)^2+4} + \frac{4}{(s+2)^2+4} = 2L(e^{-2t}\cos 2t) + 2L(e^{-2t}\sin 2t)$$

Thus,

$$L(y(t)) = L(2e^{-2t}(\cos 2t + \sin 2t)) \rightarrow y(t) = 2e^{-2t}(\cos 2t + \sin 2t)$$

(2) Consider the nonhomogeneous ODE

$$2\frac{d^2q}{dt^2} + 50q = 100 \sin \omega t$$

with initial conditions $q(0) = 0$, $\frac{dq(0)}{dt} = i(0) = 0$.

This ODE arises from a series circuit with an AC voltage source, a capacitor and an inductance.

We have

$$\begin{aligned} Q(s) &= \frac{(s+a)q(0) + i(0)}{s^2 + 25} + \frac{L(50 \sin \omega t)}{s^2 + 25} \\ &= \frac{L(50 \sin \omega t)}{s^2 + 25} = \frac{50\omega}{(s^2 + \omega^2)(s^2 + 25)} \end{aligned}$$

or using the partial fraction rules when a quadratic remains

$$Q(s) = \frac{50\omega}{(s^2+\omega^2)(s^2+25)} = \frac{A_1 s + A_2}{s^2+\omega^2} + \frac{B_1 s + B_2}{s^2+25}$$

Now for this form

$$B_1(a+ib) + B_2 = \left[\frac{P(s)}{Q(s)/[(s-a)^2+b^2]}\right]_{s=a+ib}$$

or

$$A_1(i\omega) + A_2 = \left[\frac{50\omega}{s^2+25}\right]_{s=i\omega} = \frac{50\omega}{-\omega^2+25} \rightarrow A_1 = 0\ ,\ A_2 = \frac{50\omega}{25-\omega^2}$$

$$B_1(5i) + B_2 = \left[\frac{50\omega}{s^2+\omega^2}\right]_{s=5i} = \frac{50\omega}{\omega^2-25} \rightarrow B_1 = 0\ ,\ A_2 = \frac{50\omega}{\omega^2-25}$$

Therefore,

$$Q(s) = \frac{50\omega}{25-\omega^2}\left[\frac{\omega}{s^2+\omega^2} - \frac{\omega}{s^2+25}\right]$$

or

$$q(t) = \frac{50\omega}{25-\omega^2}\left[\sin\omega t - \sin 5t\right]$$

Clearly, this form of the solution is valid only if $\omega \neq 5$ since the amplitude becomes unbounded.

This corresponds to resonance in the circuit and we have an unbounded amplitude because there is no damping in this circuit (no resistors).

If $\omega = 5$, we go back to $Q(s)$

$$Q(s) = \frac{50\omega}{(s^2+25)^2} = \frac{A_1 s + A_2}{(s^2+25)^2} + \frac{B_1 s + B_2}{s^2+25} \rightarrow \frac{250}{(s^2+25)^2}$$

which using the same procedure gives

$$q(t) = 250[\sin 5t - 5t\cos 5t] \rightarrow \text{ unbounded as } t \text{ gets large}$$

Green Function and Convolution

Consider the special equation shown below:

$$\left(\frac{d^2}{dx^2} + p\frac{d}{dx} + q\right) G(x - x') = \delta(x - x') \qquad -\infty \leq x \leq \infty$$

In this equation the inhomogeneous function is a delta-function, x' is an arbitrary point, and we denote this special solution as $G(x)$.

It is called the **Green function**.

We now show that the solution of the equation

$$\left(\frac{d^2}{dx^2} + p\frac{d}{dx} + q\right) f(x) = R(x)$$

is easily expressed in terms of the Green function.

We now show that the solution of the inhomogeneous ODE can be written as the expression

$$f(x) = \int_{-\infty}^{\infty} G(x - x')R(x')dx'$$

Substituting into the ODE we get

$$\left(\frac{d^2}{dx^2} + p\frac{d}{dx} + q\right) \int_{-\infty}^{\infty} G(x - x')R(x')dx'$$

$$= \int_{-\infty}^{\infty} \left(\frac{d^2}{dx^2} + p\frac{d}{dx} + q\right) G(x - x')R(x')dx'$$

$$= \int_{-\infty}^{\infty} \delta(x - x')R(x')dx' = R(x)$$

as it should! So the Green function representation of the solution is valid.

This means if we solve for $G(x - x')$ for a particular differential operator, then we have solved for **all** inhomogeneous solutions of the ODE given by that particular differential operator.

As we saw earlier, an integral of the form above involving $G(x-x')$ is called a **convolution**, and is denoted by the symbol $(*)$.

$$f(x) = \int_{-\infty}^{\infty} G(x-x')R(x')dx' = (G*R)_x$$

The Fourier transform of a convolution is always the product of the transforms(same as for Laplace transforms)

$$F((G*R)_x) = \frac{1}{\sqrt{2\pi}} \int dx\, e^{-ikx} \left[\frac{1}{\sqrt{2\pi}} \int G(x-x')R(x')dx' \right]$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2\pi}} \int dx \int dx'\, e^{-ikx} G(x-x')R(x')$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2\pi}} \int dx \int dx'\, e^{-ik(x-x')} e^{-ikx'} G(x-x')R(x')$$

$$= \frac{1}{\sqrt{2\pi}} \int dx' e^{-ikx'} R(x') \frac{1}{\sqrt{2\pi}} \int dx e^{-ik(x-x')} G(x-x')$$

$$= F(G)F(R)$$

In **Linear Response Theory**, the inhomogeneity function $R(x)$ is called the **input to**, the solution $f(x)$ is called the **output from**, the system, while the Green function is called the **response function**, since it describes how the system responds to the input.

Examples:

Consider Newton's 2nd law,

$$m\frac{d^2x(t)}{dt^2} = F(t) = \text{ force function}$$

This is a 2nd-order inhomogeneous ODE with $p = q = 0$ and $R = F$.

The Green function satisfies this equation with the force function replaced by a delta-function.

A delta-function force is called an **impulsive** force.

Thus, the Green function also describes the response of a mechanical system to an impulsive driving force.

Now let us consider a damped, driven oscillator

$$\ddot{x}(t) + 2\beta\dot{x}(t) + \omega_0^2 x(t) = R(t)$$

The solution will be of the form

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

where

$$\frac{d^2G(t-t')}{dt^2} = 2\beta\frac{dG(t-t')}{dt} + \omega_0^2 G(t-t') = \delta(t-t')$$

Let the Fourier transform of $G(t-t')$ be given by

$$F(G(t-t')) = \tilde{G}(\omega) = \frac{1}{\sqrt{2\pi}}\int e^{-i\omega(t-t')}G(t-t')d(t-t')$$

Now take the Fourier transform of the Green function ODE

$$F\left(\frac{d^2G(t-t')}{dt^2} = 2\beta\frac{dG(t-t')}{dt} + \omega_0^2 G(t-t')\right) = F(\delta(t-t'))$$

or we have

$$[-\omega^2 + 2i\beta\omega + \omega_0^2]\tilde{G}(\omega) = \frac{1}{\sqrt{2\pi}}$$

or

$$\tilde{G}(\omega) = \frac{1}{\sqrt{2\pi}}\frac{1}{(\omega_0^2 - \omega^2) + 2i\beta\omega}$$

Finally we compute the Green function itself by taking the inverse Fourier transform

$$G(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega t}\tilde{G}(\omega)d\omega = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\omega t}\frac{1}{(\omega_0^2 - \omega^2) + 2i\beta\omega}d\omega$$

Complex integration(we will do this later) gives the result

$$G(t) = \frac{1}{\omega_1} e^{-\beta t} \sin(\omega_1 t) H(t)$$

where

$$\omega_1 = \sqrt{\omega_0^2 - \beta^2} \quad \text{and} \quad H(t) = \begin{cases} 1 & t > 0 \\ 0 & t < 0 \end{cases} = \text{ step function}$$

Finally, the solution of the original equation is

$$\begin{aligned} x(t) &= \frac{1}{\omega_1} \int_{-\infty}^{\infty} e^{-\beta(t-t')} \sin(\omega_1 (t-t') H(t-t') R(t') dt' \\ &= \frac{1}{\omega_1} \int_{-\infty}^{t} e^{-\beta(t-t')} \sin(\omega_1 (t-t') R(t') dt' \end{aligned}$$

Note the interesting feature that the integral over t' takes into account the effects of all driving forces occurring in the past ($t' < t$) due to the presence of the step function.

It contains no effect due to the driving force in the future ($t' > t$), because these forces have not yet occurred.

Hence, the result is explicitly consistent with the physical requirement of **causality**.

Is the answer correct?

Let us choose a driving force where we know the answer.

In the Introductory Mechanics course, we discussed sinusoidal driving forces; so we choose

$$R(t) = e^{i\Omega t}$$

Direct integration of the $x(t)$ equation then gives the result

$$x(t) = \frac{e^{-i\Omega t}}{(\omega_0^2 - \Omega^2) + 2i\beta\Omega}$$

which corresponds to the resonance amplitude formula of the damped, driven oscillator and agrees with the earlier result.

More details of these integration techniques later.

Examples:

Consider the equation

$$M\frac{d^2x}{dt^2} + \alpha\frac{dx}{dt} + Kx = d(t)$$

Assume the Fourier transform of $d(t)$ is $D(\omega)$ and that

$$X(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dt\, e^{-i\omega t}x(t) \rightarrow x(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\omega\, e^{i\omega t}X(\omega)$$

Substituting we get

$$(-M\omega^2 + i\alpha\omega + K)X(\omega) = D(\omega)$$

or

$$X(\omega) = \frac{-D(\omega)/M}{\omega^2 - i\alpha\omega/M - K/M}$$

Now defining

$$\omega_{\pm} = \frac{i\alpha}{2M} \pm \sqrt{\frac{K}{M} - \frac{\alpha^2}{4M^2}}$$

we have

$$\begin{aligned} x(t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega\, e^{i\omega t} \frac{-D(\omega)/M}{\omega^2 - i\alpha\omega/M - K/M} \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega\, \frac{-D(\omega)/M}{(\omega - \omega_+)(\omega - \omega_-)} e^{i\omega t} \end{aligned}$$

where $x(t)$ is the **response** of the oscillator to the forcing function $d(t)$.

Response to a Delta-Function Impulse

Consider

$$d(t) = I_0 \delta t \rightarrow D(\omega) = I_0 \frac{1}{\sqrt{2\pi}}$$

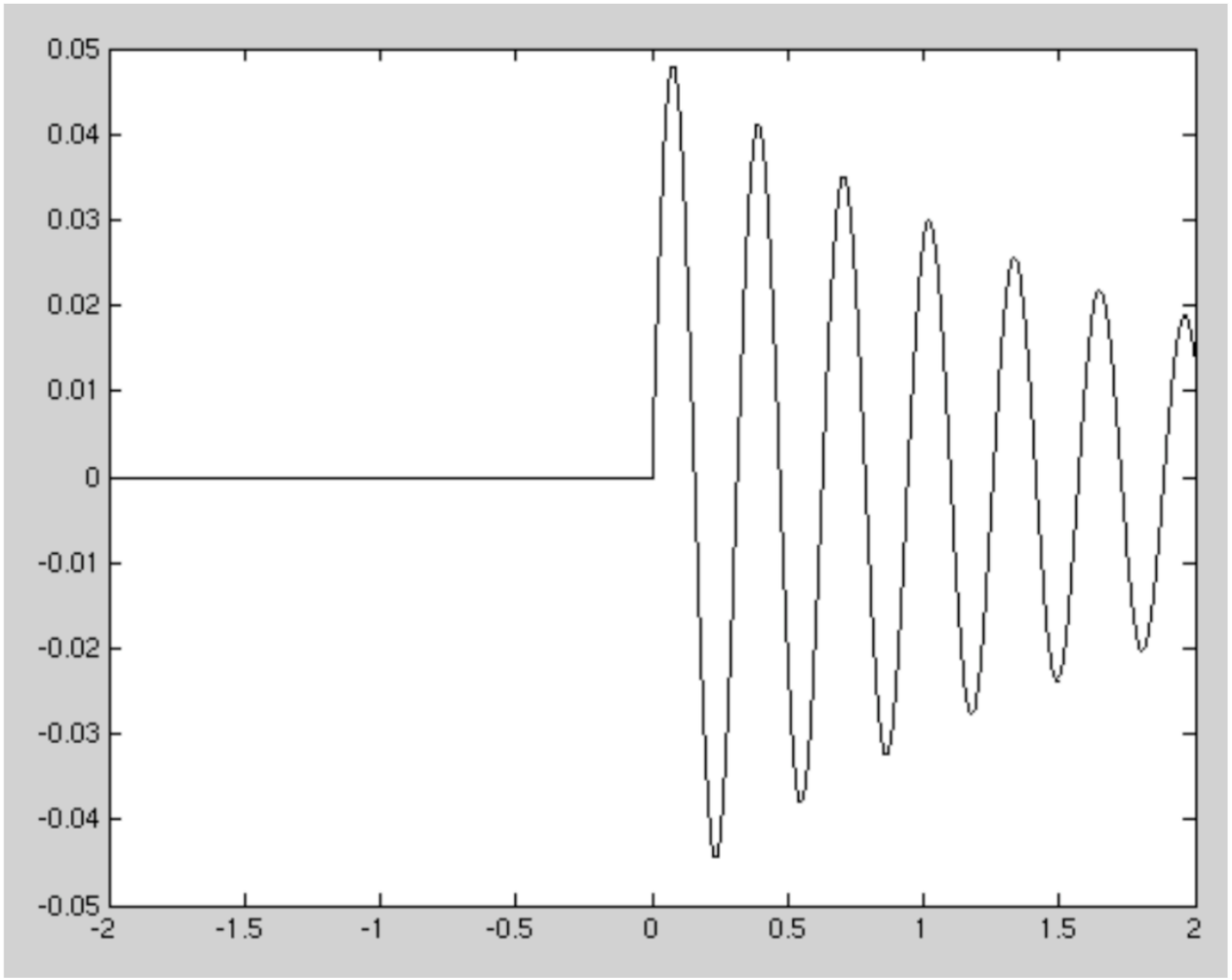
This gives

$$x(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{-I_0(\omega)/M}{(\omega - \omega_+)(\omega - \omega_-)} e^{i\omega t}$$

Using complex integration techniques which we learn later we get

$$x(t) = \begin{cases} 0 & t < 0 \\ \frac{I_0}{\sqrt{KM - \alpha^2}} e^{-\frac{\alpha t}{2M}} \sin \sqrt{\frac{K}{M} - \frac{\alpha^2}{4M^2}}\, t & t > 0 \end{cases}$$

The solution looks like



We note that the solution obeys causality, i.e., there is no motion until after the impulse is applied.

A delta-function impulse implies that

$$x(0) = 0 \quad \text{and} \quad v_x(0) \neq 0$$

Notice, however, that we have a solution with no unknown constants.

We started with a second-order equation.

Normally, that means we need to use 2 boundary conditions to completely define the solution.

Somehow we have already imposed them.

Where?

It turns out that the choice of integration path in the complex integration was the place!

We will see that later.

Effectively, we have done the following:

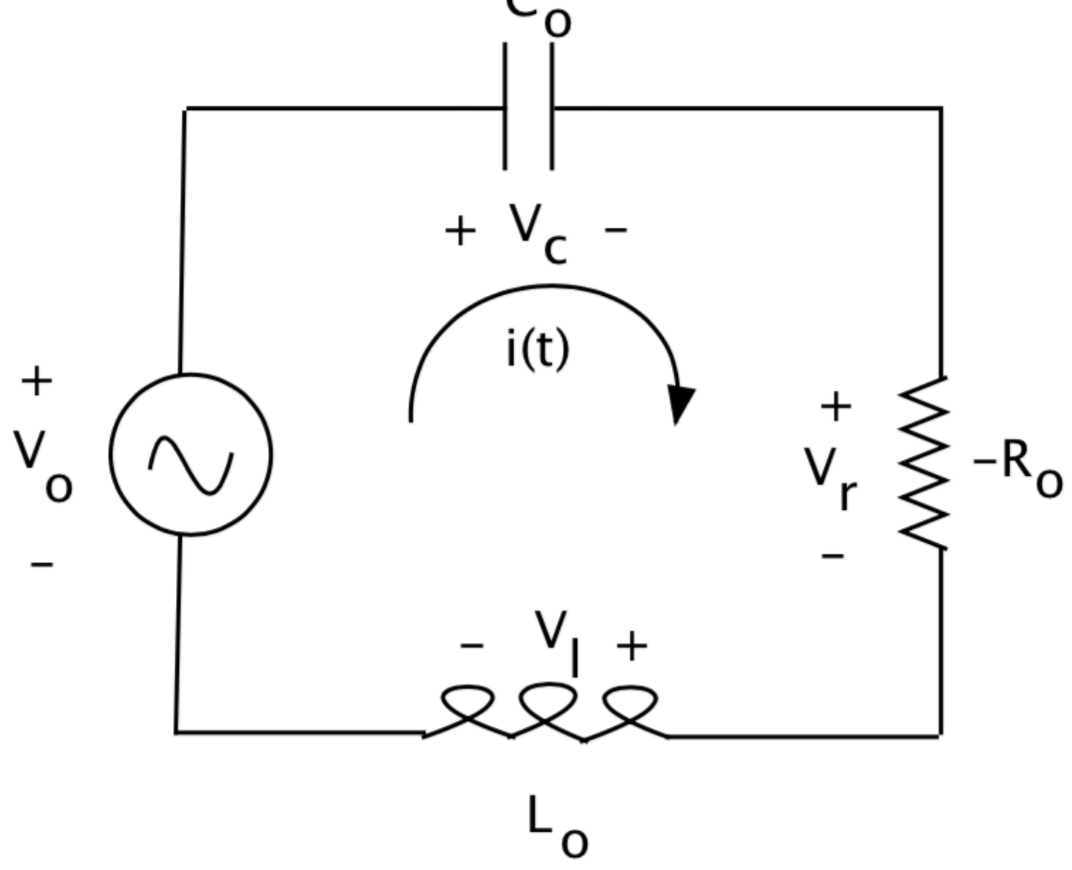
$$\text{causality} \ \rightarrow x(0) = 0$$

$$\delta\text{-function impulse} \ \rightarrow v_x(0) = I_0/M$$

Fourier methods fail where the response diverges(unstable systems).

In this case we must use the Laplace transform.

Example - Unstable Electric Circuit



This circuit has a negative resistance (a theorist's circuit) and is therefore unstable.

We let

$$V_s(t) = \begin{cases} 0 & t < 0 \\ V_0 \sin \omega_0 t & t > 0 \end{cases}$$

For $t < 0$, all voltages and $i(t) = 0$.

We have for $t > 0$ the integral-diffEQ

$$V_s(t) = V_c(t) + V_r(t) + V_l(t) = \frac{1}{C_0} \int dt\, i(t) - R_0 i(t) + L_0 \frac{di}{dt}$$

Taking the derivative wrt t we have

$$L_0 \frac{d^2 i}{dt^2} - R_0 \frac{di}{dt} + \frac{1}{C_0} i(t) = \frac{dV_s}{dt}$$

which is a second-order non-homogeneous diffEQ where $i(t) =$ dependent variable and $dV_s/\mathrm{dt\ is}$ the driving term.

Neither V_s nor dV_s/dt have a valid Fourier transform.

Thus, we use Laplace transforms.

We get

$$s^2 L_0 I(s) - s R_0 I(s) + \frac{1}{C_0} I(s) = s V_s(s)$$

where

$$I(s) = L(i(t)) \quad \text{and} \quad V_s(s) = L(V_s(t))$$

The initial conditions (due to causality) are

$$i(0) = 0 \quad \text{and} \quad \left.\frac{di}{dt}\right|_{t=0} = 0$$

Now

$$V_s(s) = \frac{V_0 \omega_0}{(s + i\omega_0)(s - i\omega_0)}$$

which gives

$$I(s) = \frac{V_0\omega_0 s}{(s+i\omega_0)(s-i\omega_0)\left(L_0 s^2 - R_0 s + \frac{1}{C_0}\right)}$$
$$= \frac{V_0\omega_0 s}{(s+i\omega_0)(s-i\omega_0)L_0(s-s_+)(s-s_-)}$$

where

$$s_\pm = \frac{R_0}{2L_0} \pm i\sqrt{\frac{1}{L_0 C_0} - \frac{R_0^2}{4L_0^2}}$$

Note that $R = -R_0 \rightarrow$ negative resistance $\rightarrow$ Real$(s+\pm) > 0$.

Inverting(using complex integration methods) we have

$$i(t) = \frac{1}{2\pi i}\int_{path} ds \frac{V_0\omega_0 s e^{st}}{(s+i\omega_0)(s-i\omega_0)L_0(s-s_+)(s-s_-)}$$

For simplicity we choose $\omega_0 = 1, L_0 = 1$ so that

$$i(t) = \frac{1}{2\pi i}\int_{path} ds \frac{V_0 s e^{st}}{(s+i)(s-i)L_0(s-1+2i)(s-1-2i)}$$

For $t < 0$ we get $i(t) = 0$.

For $t > 0$ (closing the contour to the left), we get

$$i(t) = \frac{V_0}{2\sqrt{5}} \cos(t + 0.15\pi) - \frac{V_0}{4} e^t \cos(2t + 0.2\pi)$$

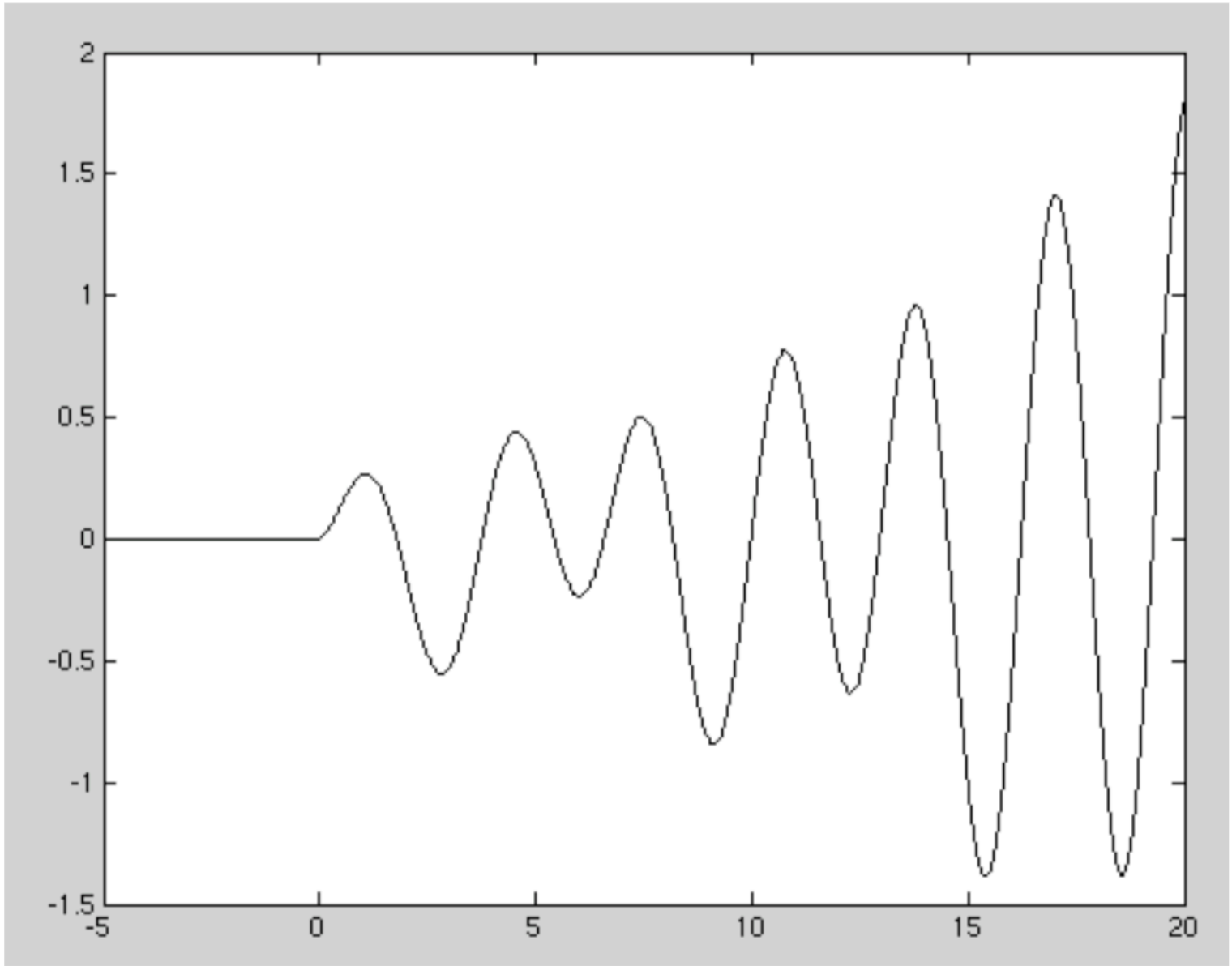
The first term is a result of the driving voltage at $\omega_0 = 1$.

It persists at a constant amplitude for all $t > 0$.

The second term is the characteristic response of the circuit (determined solely by R_0, L_0, C_0).

It grows exponentially in time because of $R < 0$ (an unstable circuit).

It looks like(where we have enhanced the initial interference terms by replacing e^t with $e^{0.1t}$)


2
1.5
1
0.5
0
-0.5
-1
-1.5
-5
0
5
10
15
20

Partial Differential Equations (PDEs) In Physics, there are differential equations of motion that describe the response of systems to external disturbances.

These are called ordinary differential equations (ODEs).

There are also differential equations of states, or field equations, whose solutions give the space-time dependence of physical properties.

These are called partial differential equations (PDEs) in the 4 variables x, y, z, t.

In general, the PDE's we will discuss describe three-dimensional situations. The independent variables are the position vector $\vec{r}$ and the time t.

The actual variables used to specify $\vec{r}$ are dictated by the coordinate system in use, i.e., (x, y, z), (ρ, ϕ, z), (r, θ, ϕ), etc.

The most important PDEs are:

(1) **The wave equation**

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

This equation describes as a function of position and time the displacement from equilibrium, $u(\vec{r}, t)$, of a vibrating string or membrane, or a vibrating solid, gas or liquid.

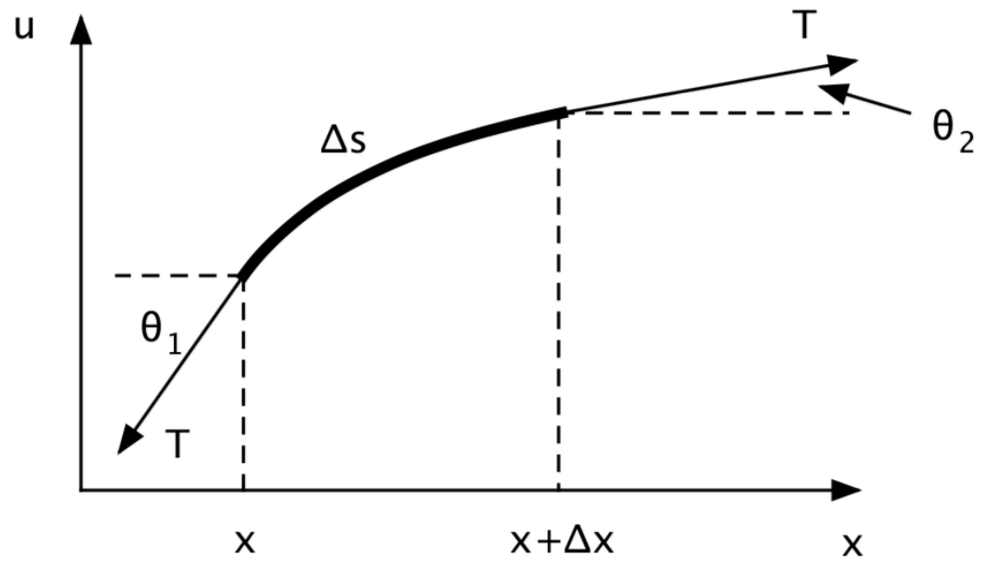
The equation also occurs in electromagnetism, where $u(\vec{r}, t)$ may be a component of the electric or magnetic field in an electromagnetic wave, or the current or voltage along a transmission line.

The quantity c is the speed of propagation of the waves.

We now derive the wave equation in a special case.

We consider the small transverse displacements $u(x, t)$ of a uniform string of mass per unit length ρ held under uniform tension T, assuming that the string is initially located along the x-axis in a Cartesian coordinate system.

The figure below shows the forces acting on an elemental length δs of the string.



If the tension T in the string is uniform along its length, the net upward vertical force on the element is

$$\Delta F = T \sin\theta_2 - T \sin\theta_1$$

Assuming that the angles θ_1 and θ_2 are both small, we may make the approximation $\sin\theta \approx \tan\theta$.

Since, at any point on the string the slope is

$$\tan\theta = \frac{\partial u}{\partial x}$$

the force can be written as

$$\Delta F = T\left(\frac{\partial u(x+\Delta x,t)}{\partial x} - \frac{\partial u(x,t)}{\partial x}\right) \approx T\frac{\partial^2 u(x,t)}{\partial x^2}\delta x$$

where we have used the standard definition of the partial derivative.

The upward force may be equated, by Newton's second law, to the product of the mass of the element and its upward acceleration.

The element has mass $\rho\Delta s$, which is approximately equal to $\rho\Delta x$ if the vibrations of the string are small, and so we have

$$\rho\Delta x\frac{\partial^2 u(x,t)}{\partial t^2} = T\frac{\partial^2 u(x,t)}{\partial x^2}\Delta x$$

$$\rightarrow \frac{\partial^2 u(x,t)}{\partial t^2} = \frac{1}{c^2}\frac{\partial^2 u(x,t)}{\partial x^2} \quad , \quad c^2 = \frac{T}{\rho}$$

which is the one-dimensional form of the wave equation.

(2) **The diffusion equation**

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

This equation describes the temperature $u(\vec{r}, t)$ in a region containing no heat sources or sinks.

It also applies to the diffusion of a chemical that has concentration $u(\vec{r}, t)$.

The constant D is called the diffusivity.

We now derive now derive the diffusion equation satisfied by the temperature $u(\vec{r}, t)$ at time t for a material of uniform thermal conductivity k, specific heat capacity s, and density ρ.

Let us consider an arbitrary volume V lying within a solid, and bounded by a surface S.

At any point in the solid the rate of heat flow per unit area in any given direction $\vec{r}$ is proportional to minus the component of the temperature gradient in that direction and is given by

$$(-k\nabla u)\cdot\vec{r}$$

The total flux of heat out of the volume V per unit time is given by

$$-\frac{dQ}{dt}=\iint_S(-k\nabla u)\cdot\hat{n}dS=\iiint_V\nabla\cdot(-k\nabla u)dV$$

where Q is the total heat energy in V at time t, and $\hat{n}$ is the outward-pointing unit normal to S; note that we have used the divergence theorem to convert the surface integral into a volume integral.

We can also express Q as the volume integral over V,

$$Q = \iiint_V s\rho u dV$$

and so its rate of change is given by

$$\frac{dQ}{dt} = \iiint s\rho \frac{\partial u}{\partial t} dV$$

Comparing the two expressions for dQ/dt and remembering the volume V is arbitrary, we obtain the three-dimensional diffusion equation

$$\nabla^2 u = \frac{1}{D}\frac{\partial u}{\partial t} \quad , \quad D = \frac{k}{s\rho}$$

(3) **Laplace equation**

$$\nabla^2 u = 0$$

This equation is obtained by setting

$$\frac{\partial u}{\partial t}$$

in the diffusion equation and describes (for example) the **steady-state** temperature of a solid in which there are no heat sources - i.e., the temperature after a long time has elapsed.

Laplace's equation also describes the gravitational potential in a region containing no matter, or the electrostatic potential in a charge-free region.

It also applies to the flow of an incompressible fluid with no sources, sinks or vortices - in this case $u(\vec{r}, t)$ is the velocity potential, from which the velocity is given by $\vec{v} = \nabla u$.

(4) **Poisson equation**

$$\nabla^2 u = \rho(\vec{r})$$

This equation describes the same physical situations as Laplace's equation, but in regions containing matter, charges, or sources of heat or fluid. The function $\rho(\vec{r})$ is called the source density, and in physical applications usually contains some multiplicative physical constants.

For example, if u is the electrostatic potential in some region of space, in which $\rho(\vec{r})$ is the density of electric charge, then

$$\nabla^2 u = -\frac{1}{\epsilon_0}\rho(\vec{r})$$

where ϵ_0 is the permittivity of free space.

Alternatively, u might represent the gravitational potential in some region where the matter density is given by $\rho(\vec{r})$; then

$$\nabla^2 u = 4\pi G \rho(\vec{r})$$

where G is the gravitational constant.

(5) **Schrödinger equation**

$$-\frac{\hbar^2}{2m}\nabla^2 u + V(\vec{r})u = i\hbar\frac{\partial u}{\partial t}$$

This equation describes the quantum mechanical wave function $u(\vec{r}, t)$ of a non-relativistic particle of mass m; $\hbar$ is Planck's constant divided by 2π. All of these equations are **linear**, They are all 2nd-order in the space variables and of 1st- or 2nd-order in time.

The use of these differential operators guarantees several things:

(1) differential operators imply invariance with respect to space and time translations and hence conservation of energy and momentum

(2) the differential operator ∇^2 is the simplest operator that will be invariant under the parity transformation (inversion)

(3) equations that are 2nd-order in time are invariant under time reversal ($t \to -t$) and hence, a movie of the system in time should represent a real physical system whether it is run forwards or backwards.

For example, the wave equation might have a solution representing a wave propagating to the right and if we run the movie backwards, we get a wave propagating to the left, which is also a valid solution.

In the diffusion or heat conduction, the field equation (for the density or temperature fields) is only 1st-order in time.

The equation does not, and should not, satisfy time-reversal invariance, since heat is known to flow from high temperature to low temperature and NEVER the other way around.

A movie of a pool of water solidifying into a block of ice on a hot day has obviously been run backwards.

The Schrödinger equation is a sort of diffusion equation with an imaginary diffusion constant; the wave function is a complex function.

There are many general methods for studying and solving for general aspects/properties of PDEs and their solutions.

We will concentrate in this course on one solution method, namely, **separation of variables.**

Separation of Variables and Eigenfunction Expansions

Under certain circumstances the solution of a PDE may be written as a sum of terms, each of which is the product of functions of only one of the variable.

This is called solution by **separation of variables (SOV)**.

Let us illustrate the procedure by an example:

Consider a 1-dimensional wave equation describing the transverse vibrations of a string

$$\frac{\partial^2 u(x,t)}{\partial t^2} = \frac{1}{c^2}\frac{\partial^2 u(x,t)}{\partial x^2}$$

In the SOV method we simply look for a solution of the form

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

Direct substitution then gives

$$\frac{\partial^2}{\partial t^2}u(x,t) = T(t)\frac{d^2X(x)}{dx^2} = \frac{1}{c^2}X(x)\frac{d^2T(t)}{dt^2}$$

or

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2} = \frac{1}{c^2}\frac{1}{T(t)}\frac{d^2T(t)}{dt^2}$$

It is clear that we have **separated the variables**.

Since the LHS is a function of x only and the RHS is a function of t only, both sides of this equation must be equal for all x and t.

The only way this is possible is for both of them to be equal to the same constant, say λ.

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2} = \lambda = \frac{1}{c^2}\frac{1}{T(t)}\frac{d^2T(t)}{dt^2}$$

which gives

$$\frac{d^2X(x)}{dx^2} - \lambda X(x) = 0 \quad , \quad \frac{d^2T(t)}{dt^2} - \lambda c^2 T(t) = 0$$

These are two separated ODEs (single variable).

They are not completely independent of each other since the same separation constant λ must appear in both.

They are both eigenvalue/eigenfunction equations.

The general solutions of these equations are:

$$X(x) = A\cos\left(\sqrt{-\lambda}x\right) + B\sin\left(\sqrt{-\lambda}x\right)$$

$$T(t) = D\cos\left(\sqrt{-\lambda}ct\right) + E\sin\left(\sqrt{-\lambda}ct\right)$$

As a rule, **all possible values** of the separation constant λ are allowed unless **explicitly forbidden** by the physics of the system. i.e., certain values of λ can be forbidden when the corresponding solution $X(x)$, which depends on λ, does not have the correct properties.

The properties in question, are the **boundary conditions** imposed by the physics of the system.

It may happen that one or more of these boundary conditions can be satisfied only when the separation constant takes on a set of special values. This set then contains the only permissible values, or **eigenvalues**, for the problem.

The corresponding solutions are called **eigenfunctions**.

Let us illustrate this with a particular example:

Suppose, as in the case of the Fourier series, we are interested in solutions with a period of 2π i.e.,

$$1 \quad , \quad \cos(nx) \quad , \quad \sin(nx) \quad , \quad n > 0 \text{ integer}$$

This implies that the only permissible constants are

$$\lambda_n^2 = -n^2 \quad , \quad n = 1, 2, 3, 4, ...$$

For each $\lambda = \lambda_n$ we then get a wave solution of the form

$$\begin{aligned} X_n(x)T_n(t) &= (A_n \cos(nx) + B_n \sin(nx))(D_n \cos(nct) + E_n \sin(nct)) \\ &= a_n \cos(nx)\cos(nct) + b_n \sin(nx)\cos(nct) \\ &\quad + d_n \cos(nx)\sin(nct) + e_n \sin(nx)\sin(nct) \end{aligned}$$

Since the 1-dimensional wave equation is linear, the general solution periodic in x with period 2π is then the linear superposition

$$u(x,t) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} X_n(x)\,T_n(t)$$

of all possible solutions.

Note that this is a **double Fourier series**.

Boundary and Initial Conditions

The complete determination of a solution of the PDE requires the specification of a suitable set of boundary and initial conditions.

The boundaries may not be just points, but, depending on the dimension of the system they can be lines or surfaces.

Let us return to the wave equation.

We now specialize the problem and consider the 1-dimensional vibrations of a string rigidly attached to a support at the points $x = 0$ and $x = L$.

$$X_n(x) = A_n \cos\left(\sqrt{-\lambda_n}x\right) + B_n \sin\left(\sqrt{-\lambda_n}x\right)$$

or

$$X_n(x) = A_n \cos k_n x + B_n \sin k_n x \quad \text{where} \quad k_n = \sqrt{-\lambda_n}$$

These boundary conditions then mean that

$$X(0) = 0 \to A_n = 0 \quad \text{for all } n$$

$$X(L) = 0 \to B_n \neq 0 \to \sin knL = 0 \to k_n = \frac{n\pi}{L} \quad \text{for all } n$$

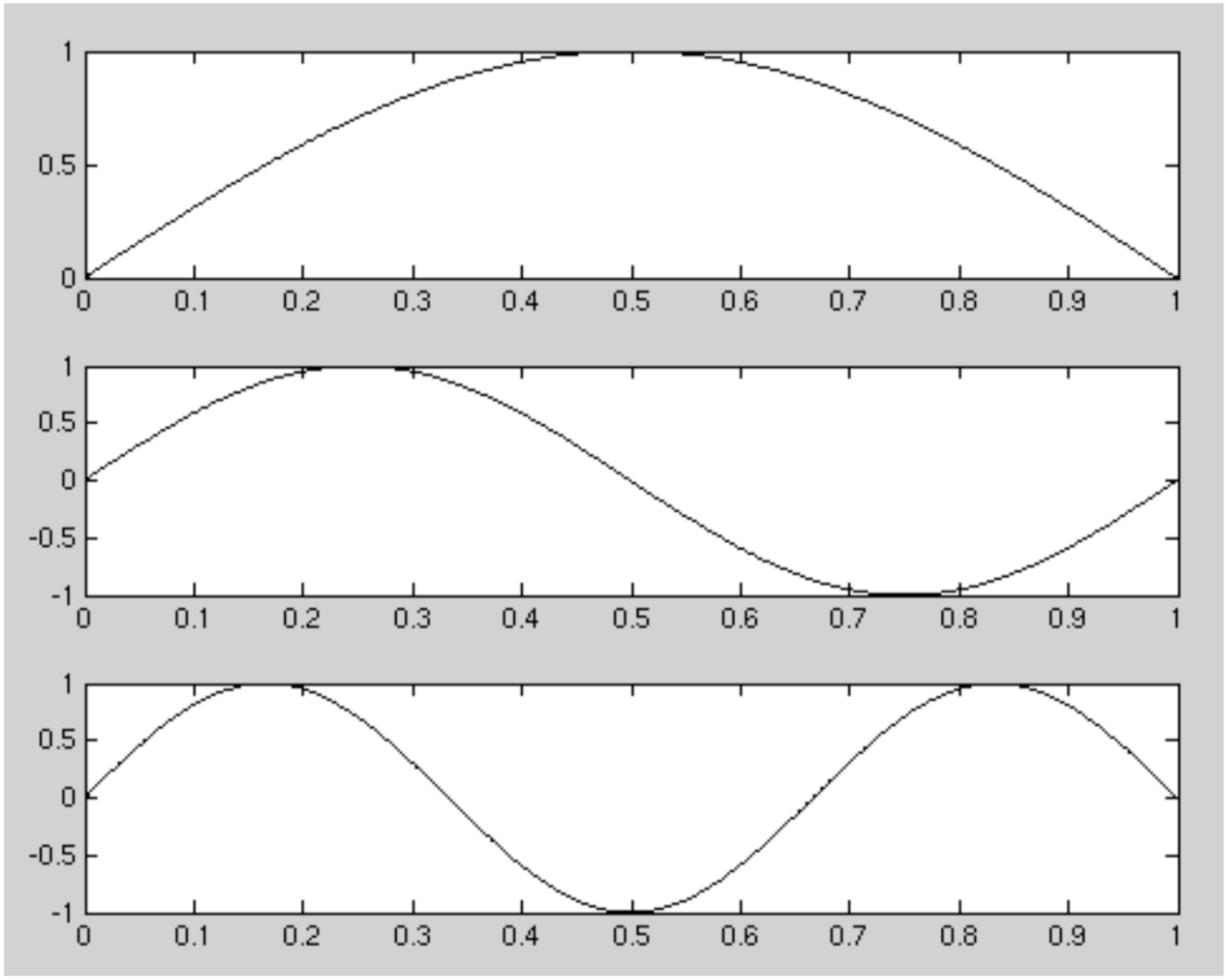
This gives as a solution

$$X_n(x) = B_n \sin\left(\frac{n\pi x}{L}\right)$$

where

$$\lambda_n = -\left(\frac{n\pi}{L}\right)^2 = \quad \text{allowed separation constants}$$

The eigenfunction $X_n(x)$ belongs to the eigenvalue λ_n and describes the nth eigenmode (or normal mode) of the vibration of the string (fixed at both ends)(see figure below)



These represent the **fundamental vibration** along with the **first and second harmonics**.

Note that there are points given by

$$x_m = \frac{mL}{n} \quad m = 1, 2, 3, 4, ..., n-1$$

where the displacement $u = 0$ or

$$X_n(x) = B_n \sin\left(\frac{n\pi x}{L}\right) = B_n \sin(m\pi) = 0$$

which are called **nodal points** of the wave.

The time factor $T_n(t)$ associated with $X_n(x)$ is given by

$$T_n(t) = D_n \cos(\omega_n t) + E_n \sin(\omega_n t)$$

where

$$\omega_n = \frac{nc\pi}{L}$$

is the frequency of vibration of the nth normal mode of the string (fixed at both ends).

Hence, the general wave amplitude function (shape) of the vibrating string fixed at $x = 0$ and $x = L$ is the general eigenfunction expansion (superposition of all solutions)

$$u(x,t) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} X_n(x)\,T_n(t)$$

$$= \frac{1}{2}a_0 + \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right)\left(D_n \cos(\omega_n t) + E_n \sin(\omega_n t)\right)$$

If we pluck the string at time t= 0, which mode(s) will be excited?

The answer depends on how we pluck the string or on the **initial conditions** at $t = 0$.

Since PDE is 2nd order in time, we need 2 initial conditions to completely specify the solution.

We usually choose them to be

$$u(x,0) = u_0(x) = \text{ initial displacement of the string at } t = 0$$

$$\left.\frac{\partial u(x,t)}{\partial t}\right|_{t=0} = v_0(x) = \text{ initial velocity profile of the string at } t = 0$$

or we have

$$u(x,0) = u_0(x) = \sum_{n=1}^{\infty} D_n \sin\left(\frac{n\pi x}{L}\right)$$

$$\left.\frac{\partial u(x,t)}{\partial t}\right|_{t=0} = v_0(x) = \sum_{n=1}^{\infty} E_n \omega_n \sin\left(\frac{n\pi x}{L}\right)$$

which implies that

$$D_m = \frac{2}{L}\int_0^L \sin\left(\frac{m\pi x}{L}\right) u_0(x)dx$$

$$E_m = \frac{2}{\omega_m L}\int_0^L \sin\left(\frac{m\pi x}{L}\right) v_0(x)dx$$

These coefficients determine which normal modes are excited and with what strength.

Real example of a vibrating string(we go back through everything again for practice):

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 y}{\partial t^2}$$

gives

$$y(x,t) = X(x)T(t)$$

$$\frac{X''}{X} = -\alpha^2 = \frac{1}{c^2}\frac{\ddot{T}}{T}$$

$$X'' + \alpha^2 X = 0 \quad , \quad \ddot{T} + \alpha^2 c^2 T = 0$$

Define

$$\alpha c = \omega = 2\pi\nu = \frac{2\pi c}{\lambda} \rightarrow \alpha = \frac{2\pi}{\lambda} = k = \text{ wave number}$$

The solution is (as before)

$$y = (a\sin(kx) + b\cos(kx))(d\sin(\omega t) + e\cos(\omega t))$$

The string is fastened at $x = 0$ and $x = L$, so that $y(0) = y(L) = 0$, which gives

$$y(0,t) = b(d\sin(\omega t) + e\cos(\omega t)) = 0 \rightarrow b = 0$$

$$y(L,t) = a\sin(kL)(d\sin(\omega t) + e\cos(\omega t)) = 0$$

$$\rightarrow \sin(kL) = 0 \rightarrow kL = n\pi$$

and

$$y_n(x,t) = a_n \sin\left(\frac{n\pi x}{L}\right)\left(d_n \sin\left(\frac{n\pi\nu t}{L}\right) + e_n \cos\left(\frac{n\pi\nu t}{L}\right)\right)$$

Now choose initial conditions at $t = 0$

$$y(x,0) = f(x) = \begin{cases} x/2 & 0 \le x \le L/2 \\ L/2 - x/2 & L/2 \le x \le L \end{cases}$$

and

$$\left.\frac{\partial y(x,t)}{\partial t}\right|_{t=0} = 0$$

The condition

$$\left.\frac{\partial y(x,t)}{\partial t}\right|_{t=0} = 0$$

$$\rightarrow a_n \sin\left(\frac{n\pi x}{L}\right)\frac{n\pi\nu}{L}\left(d_n \sin\left(\frac{n\pi\nu t}{L}\right) + e_n \cos\left(\frac{n\pi\nu t}{L}\right)\right)\Big|_{t=0}$$

$$0 = a_n \sin\left(\frac{n\pi x}{L}\right)\frac{n\pi\nu}{L}(d_n) \rightarrow d_n = 0$$

This means we physically pull the string into a triangular shape and let is go from rest.

The most general solution is then is

$$y(x,t) = \left(\sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi}{L}x\right)\right)\cos\left(\frac{n\pi\nu}{L}t\right)$$

Now using the other initial condition, we have

$$y(x,0) = f(x) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi}{L}x\right)$$

or the A_n are the Fourier coefficients of the sine series for the triangular pulse.

We have

$$\begin{aligned} A_m &= \frac{2}{L}\int_0^L \sin\left(\frac{m\pi}{L}x\right) f(x)dx = \frac{1}{L}\int_0^L \sin\left(\frac{m\pi}{L}x\right) x dx \\ &\quad + \frac{1}{L}\int_0^L \sin\left(\frac{m\pi}{L}x\right)(L-x)dx \\ &= \frac{1}{L}\frac{L^2}{m^2\pi^2}\int_0^{m\pi/2} y \sin y dy - \frac{1}{L}\frac{L^2}{m^2\pi^2}\int_{m\pi/2}^{m\pi} y \sin y dy \\ &\quad + \frac{L}{m\pi}\int_{m\pi/2}^{m\pi} \sin y dy \end{aligned}$$

$$
\begin{aligned}
&= \frac{L}{m^2\pi^2}\left(\sin y - y\cos y\right)\Big|_0^{m\pi/2} - \frac{L}{m^2\pi^2}\left(\sin y - y\cos y\right)\Big|_{m\pi/2}^{m\pi} \\
&\quad - \frac{L}{m\pi}\left(\cos y\right)\Big|_{m\pi/2}^{m\pi} \\
&= \frac{L}{m^2\pi^2}\left(\sin\left(\frac{m\pi}{2}\right) - \frac{m\pi}{2}\cos\left(\frac{m\pi}{2}\right) - \sin\left(0\right) + \left(0\right)\cos\left(0\right)\right) \\
&\quad - \frac{L}{m^2\pi^2}\left(\sin\left(m\pi\right) - m\pi\cos\left(m\pi\right) - \sin\left(\frac{m\pi}{2}\right) + \frac{m\pi}{2}\cos\left(\frac{m\pi}{2}\right)\right) \\
&\quad - \frac{L}{m\pi}\left(\cos\left(m\pi\right) - \cos\left(\frac{m\pi}{2}\right)\right)
\end{aligned}
$$

or

$$
A_m = \begin{cases} \left(\frac{2L}{m^2\pi^2}\right)\sin\left(\frac{m\pi}{2}\right) & m \text{ odd} \\ 0 & m \text{ even} \end{cases}
$$

and so on.

The other possible initial condition is

$$y(x,0) = 0$$

and

$$\left.\frac{\partial y(x,t)}{\partial t}\right|_{t=0} = f(x) = \begin{cases} x/2 & 0 \le x \le L/2 \\ L/2 - x/2 & L/2 \le x \le L \end{cases}$$

which corresponds to hitting the string when it is flat.

This gives

$$y(x,t) = \left(\sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right)\right) \sin\left(\frac{n\pi\nu}{L}t\right)$$

$$\left.\frac{\partial y(x,t)}{\partial t}\right|_{t=0} = f(x) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right) = \text{ initial velocity profile}$$

For each n (in either case) there is a different frequency

$$f_n = \frac{\omega_n}{2\pi} = \frac{n\pi\nu}{2\pi L} = \frac{n\nu}{2L}$$

which are the **normal mode frequencies**.

These frequencies **can be excited separately and would be stable**.

The string would vibrate in a single mode or one term of the general sum

$$\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{n\pi\nu}{L}t\right)$$

If we took a photograph at any given value of t, we get a picture of the string

$$y = \sin\left(\frac{n\pi x}{L}\right)$$

which are the shapes shown earlier.

At a fixed point x,

$$y = \sin\left(\frac{n\pi\nu}{L}t\right)$$

or a particular x point oscillates up and down with the normal mode frequency.

Fast Image Sequence (like a movie)

```
function z=acoeff(m,L)
if (2*floor(m/2) == m)
  z=0;
else
  z=(2*L/(m^2*pi^2))*sin(m*pi/2);
end
endfunction

function z=aterm(m,L,v,x,t)
z=acoeff(m,L)*sin(m*pi*x/L).*cos(m*pi*v*t/L);
endfunction
```

```
% m-file waveqxt.m
L=1;
v=1;
x=0:0.01:1;
for j = 1:201
  t=(j-1)*0.01; sum=0;
  for k=1:100
    sum=sum+aterm(k,L,v,x,t);
  end
  plot(x,sum,'-k');
  axis([-1 2 -.5 .5]);
  pause(0.01)
end
```

Run code….

Vibrations of a Rectangular Drum

We now choose to look at a rectangular drum because we can handle this boundary easily with a simple extension of our 1-dimensional solutions in cartesian coordinates.

We will look at a circular drum later.

The vibration of a 2-dimensional membrane fixed at the boundaries

$$x = 0,\ x = a,\ y = 0,\ y = b$$

can be described as follows:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}$$

We choose

$$u(x, y, t) = X(x)Y(y)T(t)$$

SOV substitution gives

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = \frac{1}{c^2}\frac{1}{T}\frac{\partial^2 T}{\partial t^2}$$

The separation constant assignment goes like

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = \lambda_x \quad , \quad \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = \lambda_y \quad , \quad \frac{1}{c^2}\frac{1}{T}\frac{\partial^2 T}{\partial t^2} = \lambda$$

with

$$\lambda_x + \lambda_y = \lambda \quad , \quad \text{all constants}$$

The solutions are

$$X(x) = A\cos k_x x + B\sin k_x x \quad , \quad k_x^2 = -\lambda_x$$

$$Y(y) = C\cos k_y y + D\sin k_y y \quad , \quad k_y^2 = -\lambda_y$$

$$T(t) = E\cos \alpha t + D\sin \alpha t \quad , \quad \alpha^2 = -\lambda$$

with

$$k_x^2 + k_y^2 = \frac{\alpha^2}{c^2}$$

The boundary conditions give

$$X(0) = 0 \to A = 0 \quad , \quad Y(0) = 0 \to C = 0$$

$$X(a) = 0 \to k_x = \frac{m\pi}{a} = k_m \quad , \quad Y(b) = 0 \to k_y = \frac{n\pi}{a} = k_n$$

or

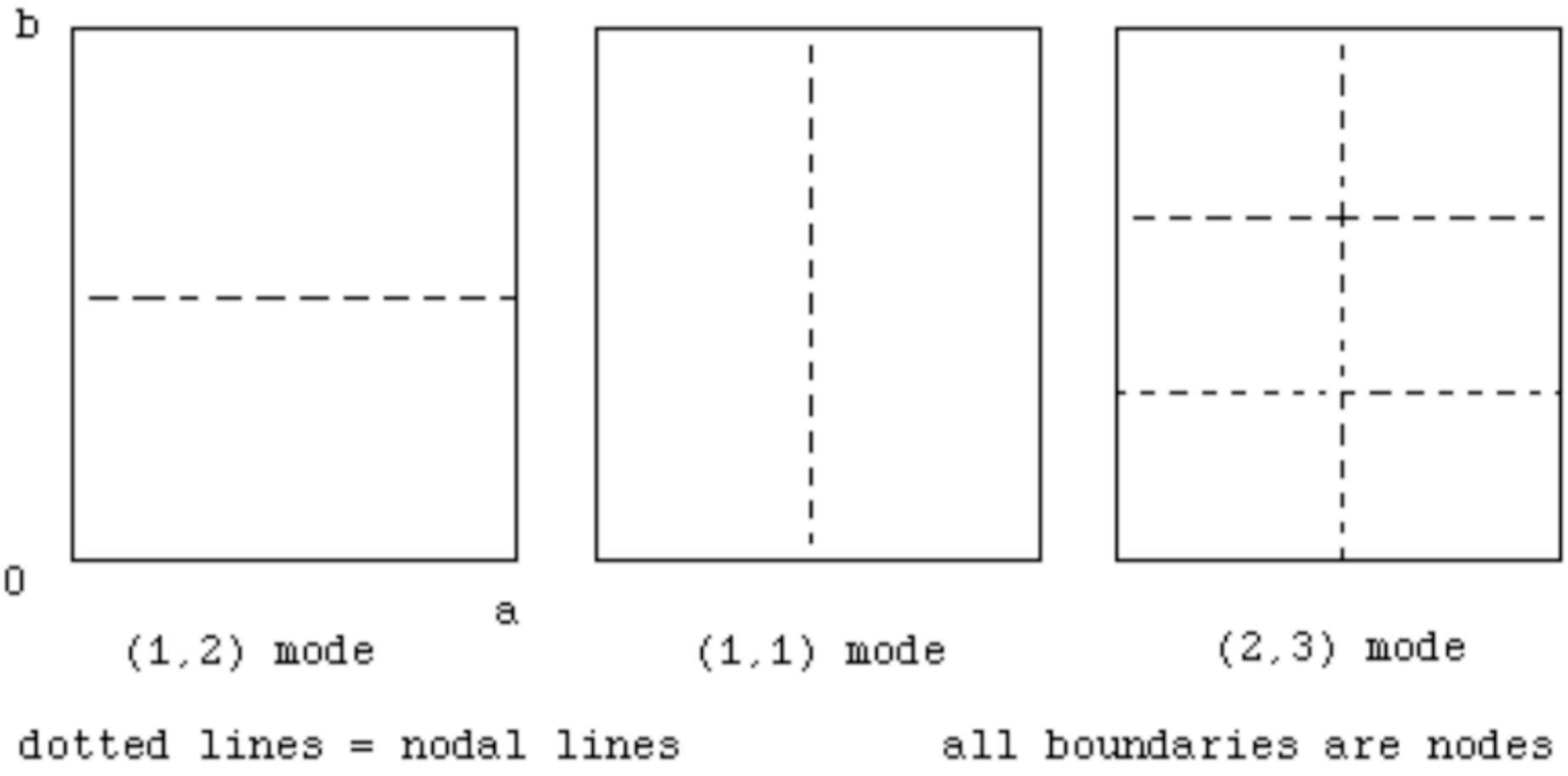
$$\frac{m^2\pi^2}{a^2} + \frac{n^2\pi^2}{a^2} = \frac{\alpha^2}{c^2} = \frac{\omega_{mn}^2}{c^2} \to \omega_{mn} = c\pi\sqrt{\frac{m^2}{a^2} + \frac{n^2}{a^2}}$$

The general solution is then a sum of all possible solutions (all m, n)

$$u(x, y, t) = \sum_{m,n=1}^{\infty} \sin\frac{m\pi x}{a} \sin\frac{n\pi y}{a}(c_{nmn}\cos\omega_{mn}t + c_{mn}\sin\omega_{mn}t)$$

where ω_{mn} = frequency of the (m, n) normal mode.

Some examples of modes are shown below:



As always, the strength with which various normal modes are excited depends on the exact initial conditions.

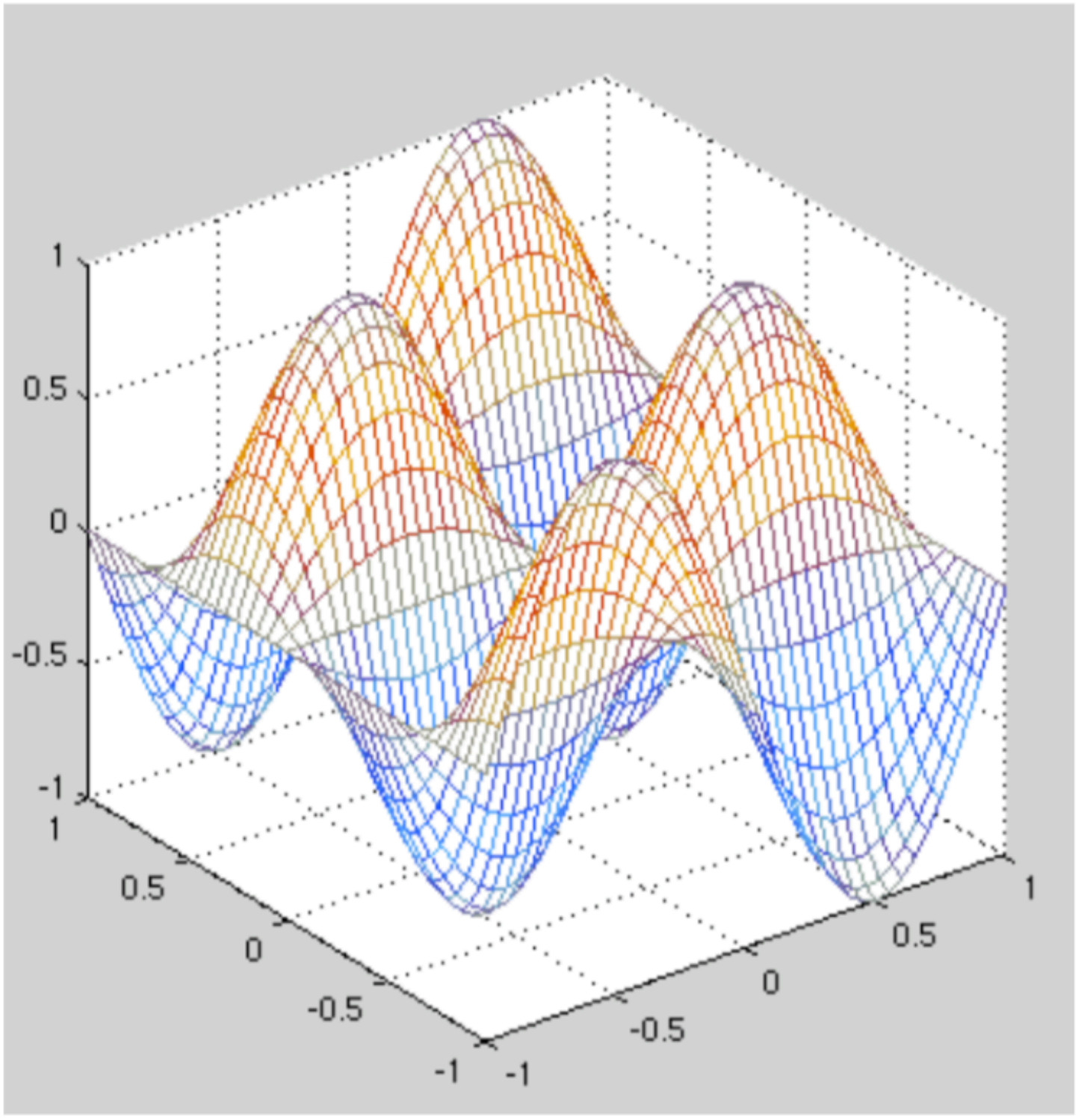
The OCTAVE program below sq-drum.m shows the (n, m) modes of the rectangular membrane (image sequence type movie).

sqdrum.m

```
x=-1:0.05:1;
y=-1:0.05:1;
[X,Y]=meshgrid(x,y);
c=1;a=2;b=2;
% (1,2) mode
;m=1;n=1;
% (1,1) mode
;m=2;n=3;
% (2,3) mode
m=2;n=3;
w=c*pi*sqrt(m^2/a^2+n^2/b^2);
Z=sin(m*pi*X/a).*sin(n*pi*Y/b);
lim=[-1 1 -1 1 -1 1];
figure('Position', [200 200 400 400])
for j=1:500
    t=(j-1)*.01;
    mesh(X,Y,Z*cos(w*t))
    axis(lim);
    colormap(waves);
    pause(0.01);
end
```

Run code….

An image from the sequence for the (2,3) mode looks like



Diffusion Equation

The 1-dimensional diffusion equation is

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{1}{D}\frac{\partial u(x,t)}{\partial t}$$

Using SOV we have

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

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = \frac{1}{D}\frac{1}{T}\frac{\partial T}{\partial t} = \lambda = \text{ separation constant}$$

We get equations and solutions

$$\frac{d^2X}{dx^2} - \lambda X = 0 \rightarrow X(x) = A\cos kx + B\sin kx$$

$$\frac{dT}{dt} - \lambda DT = 0 \rightarrow T(t) = Qe^{-k^2Dt} + Re^{k^2Dt}$$

with

$$k^2 = -\lambda$$

The positive exponential solution is not allowed physically since it would imply that, as

$$t \to \infty \Rightarrow T \to \infty$$

which makes no sense in a heat diffusion problem.

On the other hand for the negative exponential solution

$$t \to \infty \Rightarrow T \to 0$$

which does make physical sense.

This is just an example of the "physics of the problem" restricting or modifying the strictly mathematical solution.

Therefore, we have

$$T(t) = e^{-k^2 Dt}$$

Special case:

Consider a 1-dimensional rod of length a, at temperature T_0, which has both of its ends placed in contact with a heat reservoir at $T = 0$.

We have the possible solutions

$$u(x,t) = (A\cos kx + B\sin kx)e^{-k^2Dt}$$

Boundary Conditions

$$x = 0 \to u(0,t) = 0 \to (A)e^{-k^2Dt} = 0 \to A = 0$$

$$x = a \to u(a,t) = 0 \to (B\sin ka)e^{-k^2Dt} = 0$$

$$\to \sin ka = 0 \to k = k_n = \frac{n\pi}{a}$$

Therefore, a solution is given by

$$u_n(x,t) = B_n \sin k_n x e^{-k_n^2 Dt}$$

so that the most general solution is

$$u(x,t) = \sum_n B_n \sin k_n x e^{-k_n^2 Dt}$$

Initial Conditions At $t = 0$, we were in equilibrium such that $T = T_0$ everywhere.

This means that

$$\frac{\partial u}{\partial t} = 0 \quad \text{at} \quad t = 0$$

so that

$$\frac{\partial^2 u(x,0)}{\partial x^2} = \frac{1}{D}\frac{\partial u(x,0)}{\partial t} = 0 \rightarrow \text{ meaning of equilibrium or steady-state}$$

$$\frac{d^2 u(x,0)}{dx^2} =\rightarrow u(x,0) = F + Gx = T_0 \text{ for all } x \rightarrow G = 0, F = T_0$$

This gives

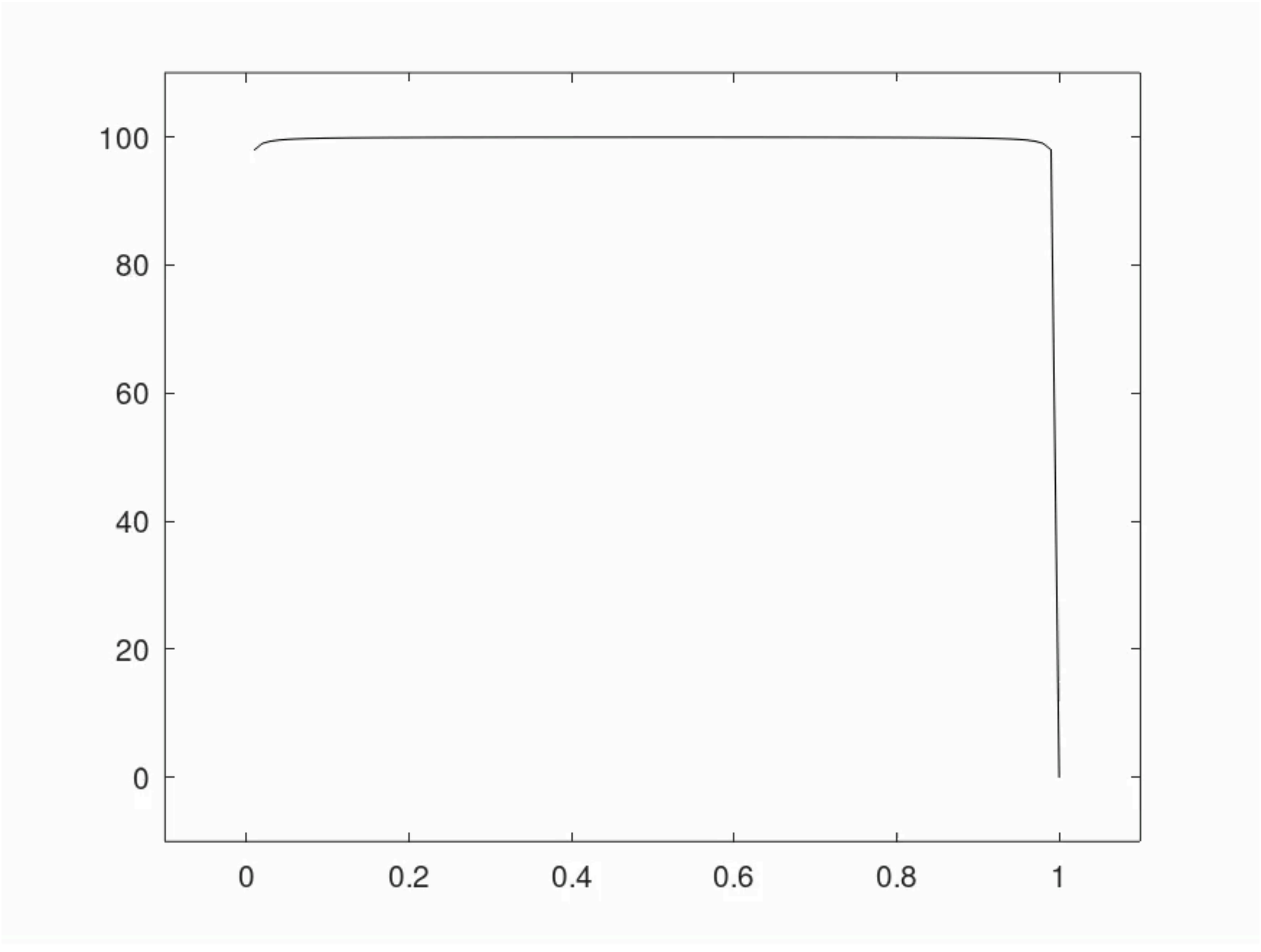
$$u(x,0) = T_0 = \sum_n B_n \sin k_n x$$

$$B_n = \frac{2}{a}\int_0^a T_0 \sin\frac{n\pi x}{a}dx = \frac{2T_0}{n\pi}(1-\cos n\pi) = \begin{cases} 4T_0/n\pi & n \text{ odd} \\ 0 & n \text{ even} \end{cases}$$

The final solution is then

$$u(x,t) = T_0 \sum_{n\ odd} \frac{4}{n\pi} \sin\frac{n\pi x}{a} e^{-\frac{n^2\pi^2}{a^2}Dt}$$

The OCTAVE program diff1.m, which generates a sequence of temperature profiles (in time), is given by

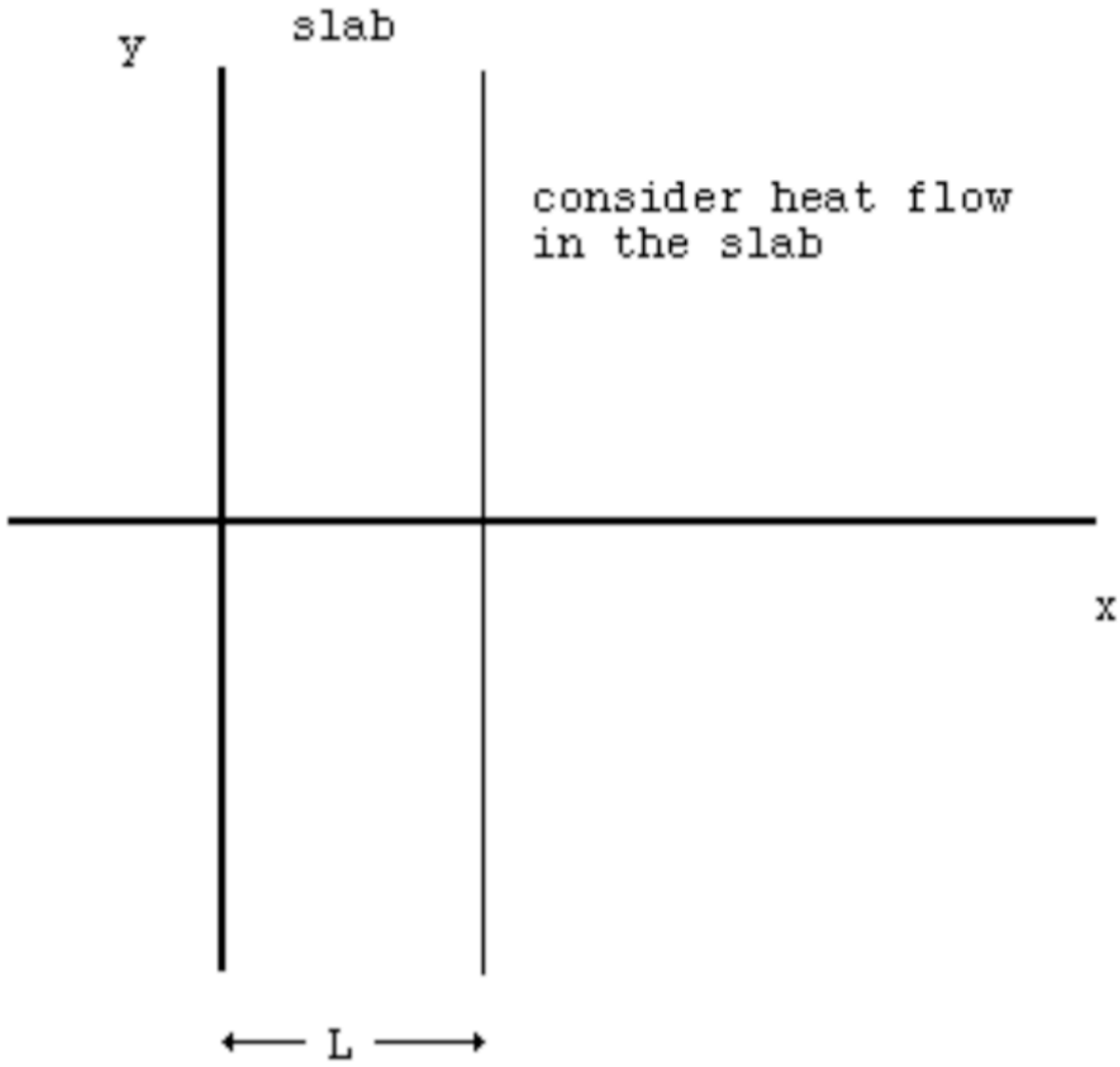

100
80
60
40
20
0
0
0.2
0.4
0.6
0.8
1

```
% m-file diff1.m
D=1.0;
a=1.0;
T0=100.0;
kk=100;
tdel=0.005;
x=(a/kk)*(1:kk);
numterms=500;
for i=1:201
  t=tdel*(i-1);
  z=0.0;
  for j=1:numterms
    jj=2*j-1;
    z=z+T0*(4.0/(jj*pi))*sin(jj*pi*x/a).*exp(-(jj*jj*pi*pi/a^2)*D*t);
  end
  plot(x,z,'-k');
  axis([-0.1 1.1*a -10.0 1.1*T0]);
  pause(0.05);
end
```

Another example:

We consider a slab, as shown below, which is infinite in the y-direction.

This means we only need to worry about the x and t variables.



We assume that initially ($t = 0$)

$$T = 0 \quad \text{at} \quad x = 0$$

$$T = 100 \quad \text{at} \quad x = L$$

and for $t > 0$ we assume

$$T = 0 \quad \text{at} \quad x = 0$$

$$T = 0 \quad \text{at} \quad x = L$$

and ask what happens in time?

The $T(t)$ solution is the same as before, namely,

$$T(t) = e^{-k^2\alpha^2 t}$$

where $D = \alpha^2$.

For the x solution, first we find the initial steady-state T distribution.

We have only x to worry about (everything must be uniform in y).

Now, steady-state means

$$\frac{\partial u}{\partial t} = 0$$

or

$$\frac{d^u(x,0)}{dx^2} = 0 \rightarrow u(x,0) = ax + b$$

$$u(0,0) = 0 \rightarrow b = 0$$

$$u(L,0) = 100 \rightarrow a = \frac{100}{L}$$

so that

$$u(x,0) = \frac{100x}{L}$$

For $t > 0$ we use the diffusion equation which gives

$$u(x,t) = (a\cos kx + b\sin kx)e^{-k^2Dt}$$

$$u(0,t) = 0 \rightarrow b = 0$$

$$u(L,t) = 0 \rightarrow \sin kL = 0 \rightarrow k = k_n = \frac{n\pi}{L}$$

Therefore the most general solution is

$$u(x,t) = \sum_{n=1}^{\infty} a_n e^{-\left(\frac{n\pi\alpha}{L}\right)^2 t} \sin\frac{n\pi x}{L}$$

Now

$$u(x,0) = \frac{100x}{L} = \sum_{n=1}^{\infty} a_n \sin\frac{n\pi x}{L}$$

which gives

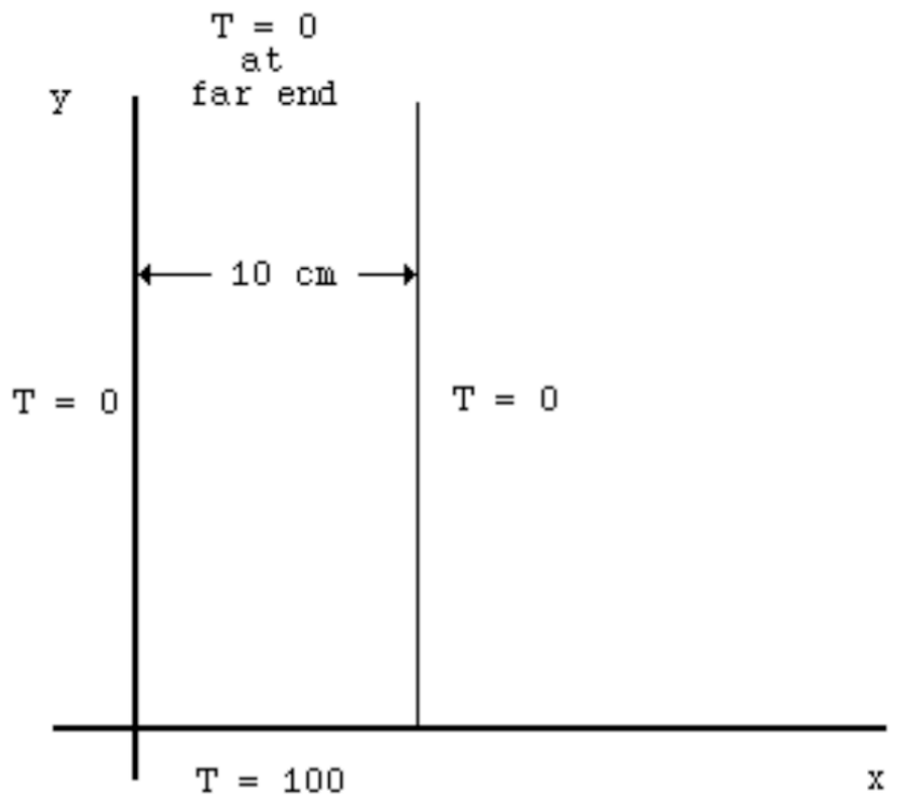
$$a_n = \frac{200}{\pi}\frac{(-1)^{n-1}}{n}$$

and the solution

$$u(x,t) = \frac{200}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n}e^{-\left(\frac{n\pi\alpha}{L}\right)^2 t}\sin\frac{n\pi x}{L}$$

Heat conduction example:

We consider a long rectangular metal plate which has the steady-state configuration as shown in the figure below:



We are looking for a solution of the 2-dimensional steady-state diffusion equation

$$\nabla^2 T(x,y) = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = \frac{1}{D}\frac{\partial T}{\partial t} = 0$$

We assume

$$T(x,y) = X(x)y(y) \rightarrow \frac{d^2X}{dx^2} = -\frac{d^2Y}{dy^2} = -k^2 \quad , \quad k \geq 0$$

The solutions are

$$X(x) = a\cos kx + b\sin kx$$

$$Y(y) = ce^{ky} + de^{-ky}$$

We made this particular choice of signs for the separation constant because we need X to be trigonometric functions and Y to be exponential functions for physical reasons,

i.e., X being trigonometric is the only way for us to be able to have $X = 0$ at **both** $x = 0$ and $x = 10$.

Therefore, the solution is

$$T(x, y) = (a \cos kx + b \sin kx)(ce^{ky} + de^{-ky})$$

The boundary conditions give

$$T(0, y) = 0 \rightarrow b = 0$$

$$T(10, y) = 0 \rightarrow \sin 10k = 0 \rightarrow k = k_n = \frac{n\pi}{10} \quad , \quad n = 1, 2, 3, ...$$

which gives the most general solution (sum of all possible solutions) as

$$T(x, y) = \sum_n \sin k_n x (c_n e^{k_n y} + d_n e^{-k_n y})$$

Now, if we let the far end be at $y = 30$, then we have

$$T(x, 30) = 0 = \sum_n \sin k_n x (c e^{30 k_n} + d e^{-30 k_n}) \rightarrow \frac{c_n}{d_n} = e^{-60 k_n}$$

Therefore

$$\begin{aligned} T(x, y) &= \sum_n d_n \sin k_n x (e^{-60 k_n} e^{k_n y} + e^{-k_n y}) \\ &= \sum d_n \sin \frac{n\pi x}{10} (e^{-3n\pi} e^{\frac{n\pi}{10}(y-30)} + e^{-\frac{n\pi}{10}(y-30)}) \\ &= \sum_n D_n sin \frac{n\pi x}{10} \sinh \frac{n\pi}{10}(y - 30) \end{aligned}$$

Finally, we have

$$T(x, 0) = 100 = -\sum_n D_n sin \frac{n\pi x}{10} \sinh 3n\pi$$

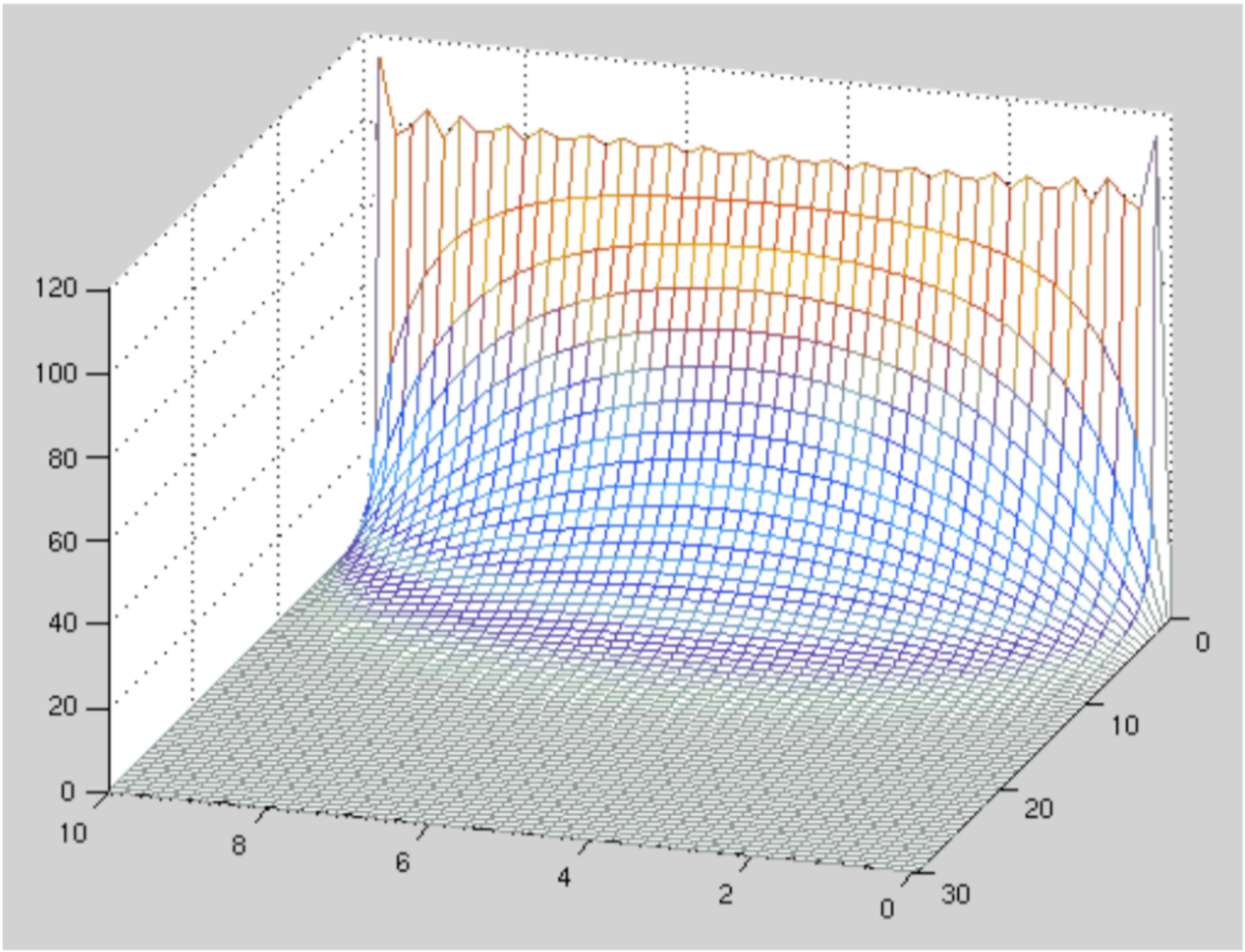
Solving for D_n we finally get

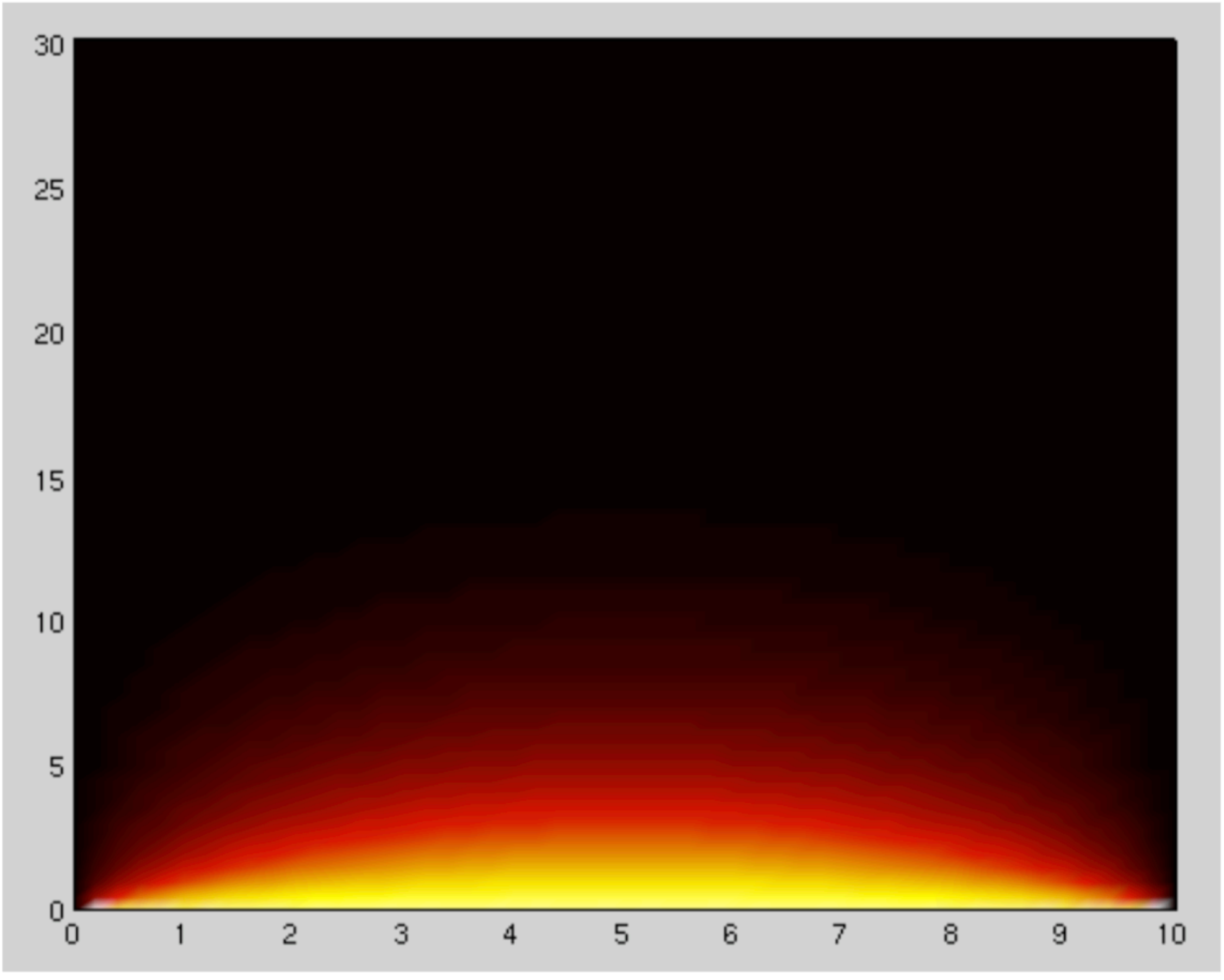
$$T(x,y) = -\sum_{n\,odd} \frac{400}{n\pi \sinh 3n\pi} \sin \frac{n\pi x}{10} \sinh \frac{n\pi}{10}(y-30)$$

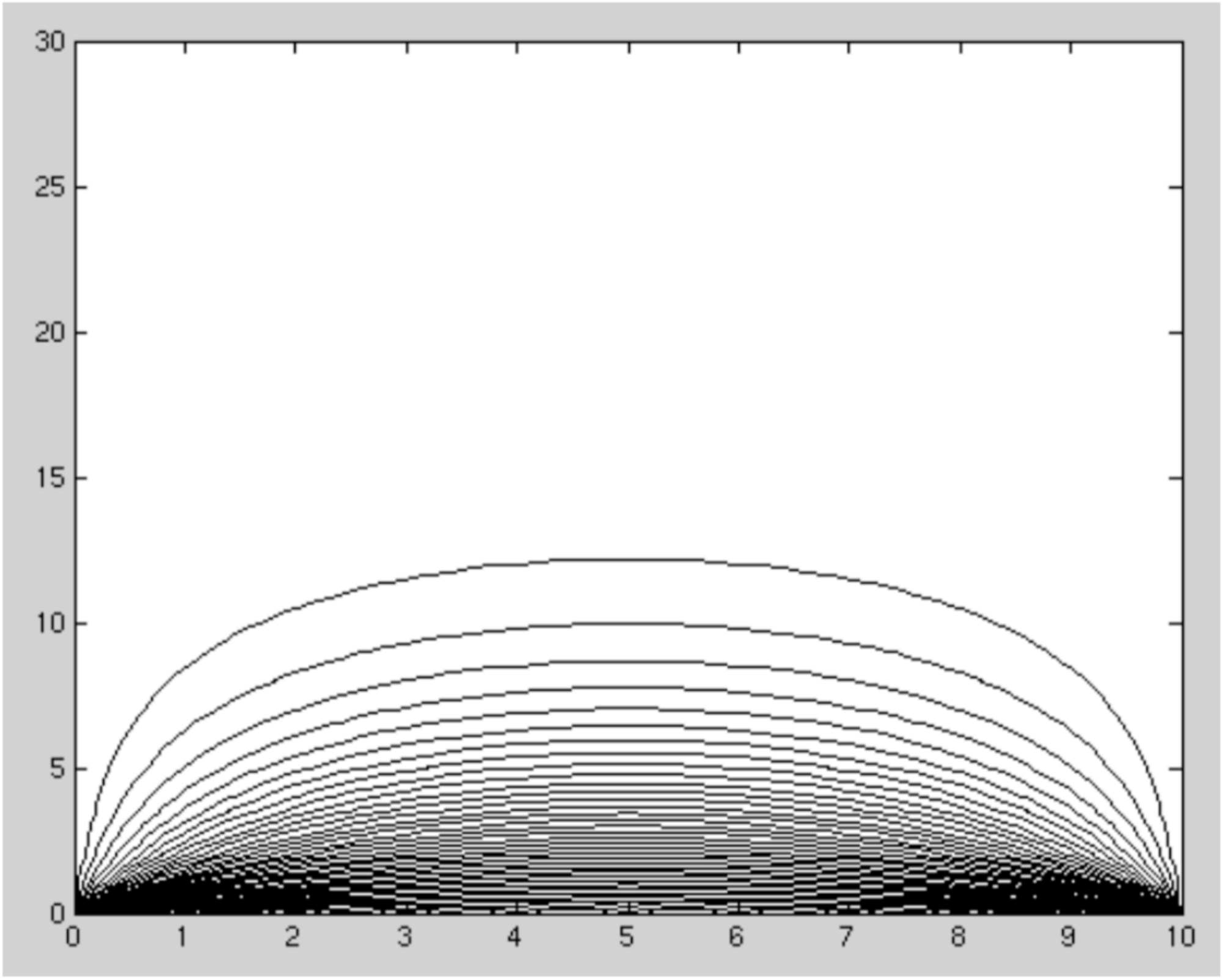
A OCTAVE program that plots the steady-state solution as a surface image is given by

```
function z=ssfunc1(x,y,n)
z=(400.0/(n*pi*sinh(3.0*n*pi)))*sin(n*pi*x/10.0).* sinh(n*pi*(30.0-y)/10.0);
endfunction
```

```
% m-file diff2.m
x=0.0:0.2:10.0;
y=0.0:0.5:30.0;
[X,Y]=meshgrid(x,y);
sum=zeros(length(y),length(x));
for ii=1:30
  jj=2*ii-1;
  sum=sum+ssfunc1(X,Y,jj);
end
figure
mesh(X,Y,sum);
colormap(waves);
view(120.0,30);
figure
pcolor(X,Y,sum);
colormap(hot);
shading interp
figure
contour(X,Y,sum,40,'-k');
```


120
100
80
60
40
20
0
10
8
6
4
2
0
0
10
20
30


30
25
20
15
10
5
0
0
1
2
3
4
5
6
7
8
9
10


30
25
20
15
10
5
0
0
1
2
3
4
5
6
7
8
9
10

Dealing with the Laplacian

To deal with other equations we must work with the full Laplacian operator. The first step is always to separate out the t dependence using the SOV procedure.

So we always assume

$$u(\vec{r}, t) = u(\vec{r})\, T(t)$$

Most of the PDEs of interest then reduce to the form

$$(\nabla^2 + k^2) u(\vec{r}) = 0$$

where

$$k^2 = 0 \quad \text{for the Laplace equation}$$

$$k^2 > 0 \quad \text{for the helmholtz equation}$$

$$k^2 < 0 \quad \text{for the diffusion equation}$$

The Schrödinger equation is an exception to the rule because of the appearance of an extra term due to the potential function

$$\frac{2m}{\hbar^2}V(\vec{r})$$

The Laplacian in Different Coordinate Systems

Cartesian:

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

Cylindrical Polar:

$$\nabla^2 = \frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho\frac{\partial}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}$$

Spherical Polar:

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

Cartesian SOV Solution: assuming

$$u(\vec{r}) = X(x)y(y)Z(z)$$

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2} + k^2 = 0$$

We then choose

$$\frac{1}{Y}\frac{d^2Y}{dy^2} = -m_y^2 \rightarrow \frac{d^2Y}{dy^2} + m_y^2 Y = 0$$

$$\frac{1}{Z}\frac{d^2Z}{dz^2} = -m_z^2 \rightarrow \frac{d^2Z}{dz^2} + m_z^2 Z = 0$$

which gives

$$\frac{d^2X}{dx^2} + (k^2 - k_y^2 - k_z^2)X = 0 = \frac{d^2X}{dx^2} + m_x^2 X$$

so that we end up with **three separate ODEs**.

Cylindrical Polar SOV Solution: assuming

$$u(\vec{r}) = R(\rho)\Phi(\phi)Z(z)$$

$$\frac{1}{\rho R}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial R}{\partial \rho}\right) + \frac{1}{\rho^2 \Phi}\frac{\partial^2 \Phi}{\partial \phi^2} + \frac{1}{Z}\frac{\partial^2}{\partial z^2} + k^2 = 0$$

We then choose

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2 \rightarrow \frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0$$

$$\frac{1}{Z}\frac{d^2}{dz^2} = \alpha^2 \rightarrow \frac{d^2}{dz^2} - \alpha^2 Z = 0$$

which gives

$$\rho^2 \frac{d^2 R}{d\rho^2} + \rho \frac{dR}{d\rho} + (\beta^2\rho^2 - m^2)R = 0 \quad , \quad \beta^2 = k^2 + \alpha^2$$

Again, we end up with **three separate ODEs**.

Spherical Polar SOV Solution: assuming

$$u(\vec{r}) = u(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{1}{r^2\sin\theta\,\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\frac{1}{r^2\sin\theta\,\Phi}\frac{\partial^2\Phi}{\partial\phi^2}+k^2=0$$

We then choose

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2 \rightarrow \frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0$$

$$\frac{1}{\sin\theta\,\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) - \frac{m^2}{\sin^2\theta}\Theta = -c$$

$$\rightarrow \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) - \frac{m^2}{\sin^2\theta}\Theta + c\Theta = 0$$

which gives

$$\frac{1}{r^2R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{c}{r^2}R + k^2R = 0$$

Again, we end up with **three separate ODEs**.

Solutions

Cartesian

The three ODEs for X, Y, and Z are all solved either by trigonometric functions or exponentials.

Cylindrical Polar The Z and Φ equations are solved either by trigonometric functions or exponentials.

The R or **radial equation** is

$$\left[z^2\frac{d^2}{dz^2} + z\frac{d}{dz} + (z^2 - m^2)\right] J_m(z) = 0 \quad , \quad z = \beta\rho$$

where $J_m(z)$ is the cylindrical Bessel function of order m.

It is the solution of this equation that behaves like

$$\left(\frac{z}{2}\right)^m$$

as $z \to 0$.

Spherical Polar

The Φ equation is solved either by trigonometric functions or exponentials.

The equation for θ is familiar.

Putting $x = \cos\theta$ we get

$$\left[(1-x^2)\frac{d^2}{dx^2} - 2z\frac{d}{dx} - \left(c - \frac{m^2}{1-x^2}\right)\right] P(x) = 0$$

which is the Associated Legendre equation.

The ODE Legendre equation we studied is a special case of this equation with $m = 0$.

This equation can be solved by a power series using the standard Frobenius method.

The infinite Frobenius series is only convergent for $|x| < 1$.

The solution at $x = 1$ is infinite(not good) unless

$$c = \ell(\ell + 1) \quad , \quad \ell = 0, 1, 2, 3, ...$$

With this choice of c the Frobenius infinite series terminates as a polynomial, which is called the associated Legendre polynomial $P_\ell^m(x)$.

Since physical solutions must be bounded, we choose always to terminate the series and get associated Legendre polynomials as the solutions with ℓ non-negative.

$$\left[(1-x^2)\frac{d^2}{dx^2} - 2z\frac{d}{dx} - \ell(\ell+1) + \frac{m^2}{1-x^2})\right] P_\ell^m(x) = 0$$

The r or radial equation is then

$$\left[z^2\frac{d^2}{dz^2} + 2z\frac{d}{dz} + (z^2 - \ell(\ell+1))\right] j_\ell(z) = 0$$

where $j_\ell(z)$ is the spherical Bessel function of order ℓ and

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

These Bessel functions are among the most useful of the so-called **"higher transcendental functions"**.

A transcendental function is one that is not **"algebraic"**.

An algebraic function of x is one that can be generated from x by a finite number of algebraic operations like $+, -, x, /$.

For example, a polynomial is algebraic but $\log(x)$ is not.

The elementary transcendental functions are exp, log, sin, cos, sinh, cosh, ...

Each of these equations has a second linearly independent solution

$$Q_\ell^m(z) = \text{ associated Legendre function of the second kind}$$

$$N_m(z) = \text{ associated Bessel function of the second kind}$$

$$\eta_\ell(z) = \text{ spherical Bessel function of the second kind}$$

They generally have divergent properties at the origin and are only included in the most general solution to a problem if the origin is excluded from the system under consideration.

The properties of the Bessel function, the Legendre polynomials, the Laguerre polynomials and the Hermite polynomials are available at `https://dlmf.nist.gov` and earlier in my class notes.

The important properties are:

(1) which ODE they solve

(2) recurrence formulas

(3) indefinite and definite integrals

(4) orthogonality relations

You will need to use all of these results to solve PDEs.

In addition, as you solve more problems, including those we will solve together in these notes later, you will learn how to use various other properties of these functions.

Now the special case $k = 0$ gives Laplace equation

We get in this special case $\frac{1}{r^2 R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{c}{r^2}R + k^2 R = 0$

$$\frac{1}{r^2 R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{\ell(\ell+1)}{r^2}R = 0 = \frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{\ell(\ell+1)}{r^2}R$$

We consider the solution $R = r^q$ where q is to be determined.

Substitution gives

$$(q(q-) + 2q - \ell(\ell+1))r^{q-2} = 0 \rightarrow q^2 + q - \ell(\ell+1) = 0$$

$$\rightarrow q = \ell, -(\ell+1)$$

Therefore the most general solution is

$$R(r) = a_1 r^{\ell} + a_2 r^{-(\ell+1)}$$

where the second term must be excluded if the origin ($r = 0$) is in the system.

All this theory can fry the brain..... so let us do a few examples.

Vibration of a Circular Membrane (drumhead)

The circular membrane is fixed at the rim(circular boundary).

We want to determine the characteristic frequencies and vibrational normal modes.

The membrane is in the $x - y$ or $r - \theta$ plane and z represents the vibration amplitude.

We choose the coordinate origin at the center of the membrane.

We have the wave equation

$$\nabla^2 z(\rho, \phi, t) = \frac{1}{\nu^2} \frac{\partial^2 z}{\partial t^2}$$

$$z = F(\rho,\phi)T(t) \rightarrow \frac{1}{F}\nabla^2 F = \frac{1}{\nu^2}\frac{d^2T}{dt^2} = -k^2$$

$$\nabla^2 F + k^2 F = 0 \rightarrow \text{ Helmholtz equation}$$

$$\ddot{T} + k^2\nu^2 T = 0$$

If we choose

$$F(\rho,\phi) = R(\rho)\Phi(\phi)$$

we can separate the Helmholtz equation as

$$\frac{1}{\rho R}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial R}{\partial\rho}\right) + \frac{1}{\rho^2\Phi}\frac{\partial^2\Phi}{\partial\phi^2} + k^2 = 0$$

We then let

$$\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2} = -n^2 \rightarrow \frac{d^\Phi}{d\phi^2} + n^2\Phi = 0$$

to obtain

$$\rho^2\frac{d^2R}{d\rho^2} + \rho\frac{dR}{d\rho} + (k^2\rho^2 - n^2)R = 0$$

We have solutions

$$T(t) = c \sin k\nu t + d \cos k\nu t$$

$$\Phi(\phi) = a \sin n\phi + b \cos n\phi$$

where n must be an integer so that

$$\Phi(\phi) = \Phi(\phi + 2\pi)$$

i.e., it makes no physical sense to get a different solution (different physics) if we change ϕ by 2π , and

$$R(\rho) = J_n(k\rho)$$

There is no contribution from the $N_n(k\rho)$ solution because it is singular at $\rho = 0$ which is the center of the membrane.

Thus, a solution for the circular membrane is

$$z(\rho, \phi, t) = J_n(k\rho)(a \sin n\phi + b \cos n\phi)(c \sin k\nu t + d \cos k\nu t)$$

At $\rho = 1$ we have the boundary condition $z = 0$ for all ϕ, t.

This implies that

$$J_n(k) = 0 \rightarrow k = k_{mn} = m^{th} \text{ zero of } J_n$$

The most general solution is then

$$z(\rho, \phi, t)$$
$$= \sum_{m,n} J_n(k_{mn}\rho)(a_{mn} \sin n\phi + b_{mn} \cos n\phi)(c_{mn} \sin k_{mn}\nu t + d_{mn} \cos k_{mn}\nu t)$$

To completely solve this problem, we would need to use a double Fourier series in ϕ and t to determine the allowed (n, m) values and the corresponding coefficients given appropriate initial conditions on the position and velocity of the membrane.

This is very tedious so, instead, we will look at some properties of the solutions.

With the circular membrane we also get normal modes with characteristic frequencies

$$\nu_{mn} = \frac{\omega_{mn}}{2\pi} = \frac{k_{mn}\nu}{2\pi}$$

There is a doubly infinite set of such modes and frequencies.

All frequencies are different and not equal to multiples of a fundamental as with a vibrating string.

This is the reason why a drum is different from a violin!

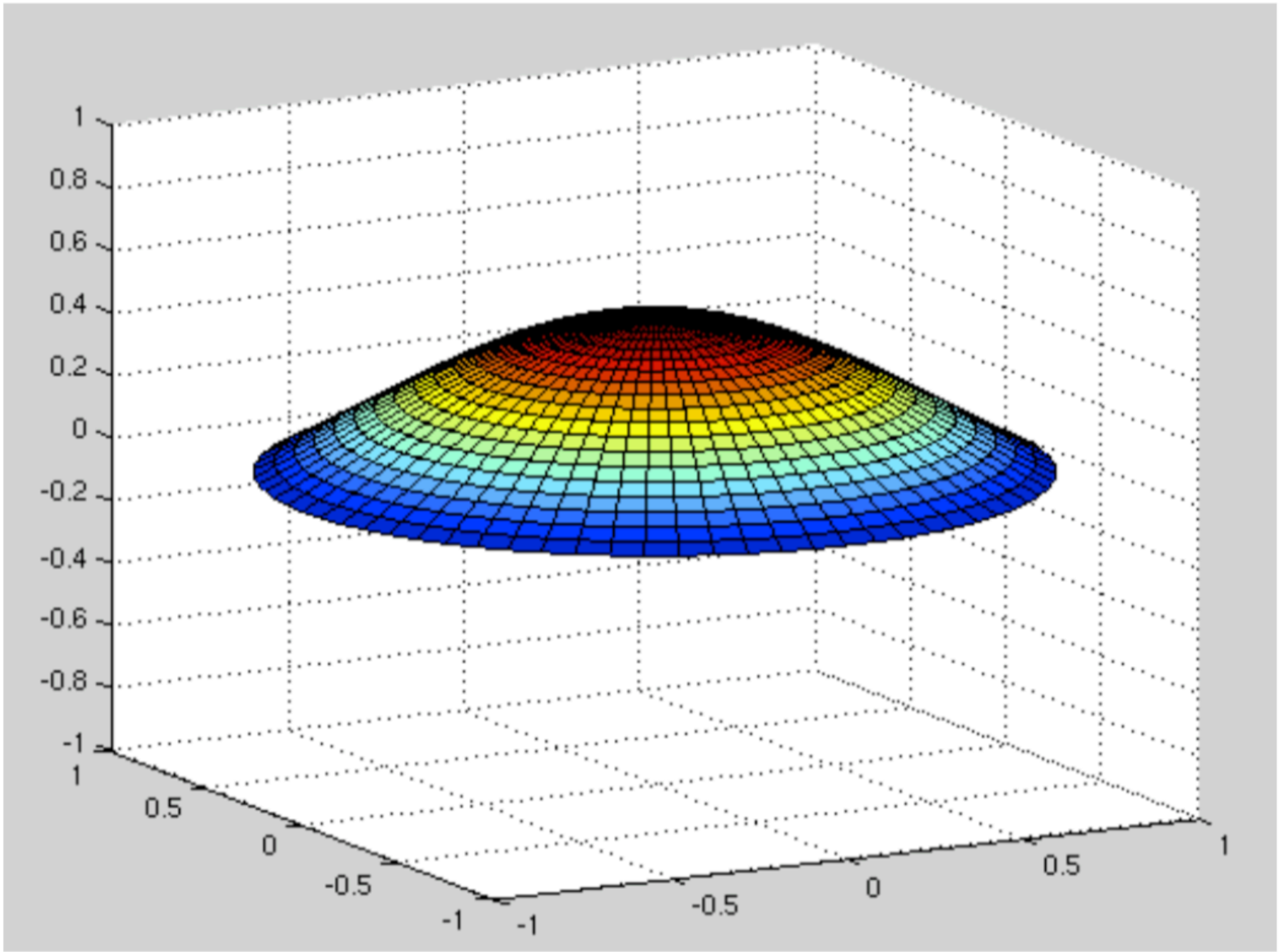
The OCTAVE program below generates the normal modes of the drumhead.

```
% m-file drumhead.m
Q=input('[m,n,ampl] :' )
m=Q(1);
n=Q(2);
ampl=Q(3);
kval=zeros(3,3);
kval(1,:)=[2.40483,5.52008,8.65373];
kval(2,:)=[3.83171,7.01559,10.17347];
kval(3,:)=[5.13562,8.41724,11.61984];
[TH,R] = meshgrid((0:5:360)*pi/180,0:.05:1);
Z=ampl*besselj(n,kval(m+1,n+1)*R).*cos(n*TH);
[X,Y,Z] = pol2cart(TH,R,Z);
surf(X,Y,Z)
axis([-1 1 -1 1 -1,1])
```

Some images are below:

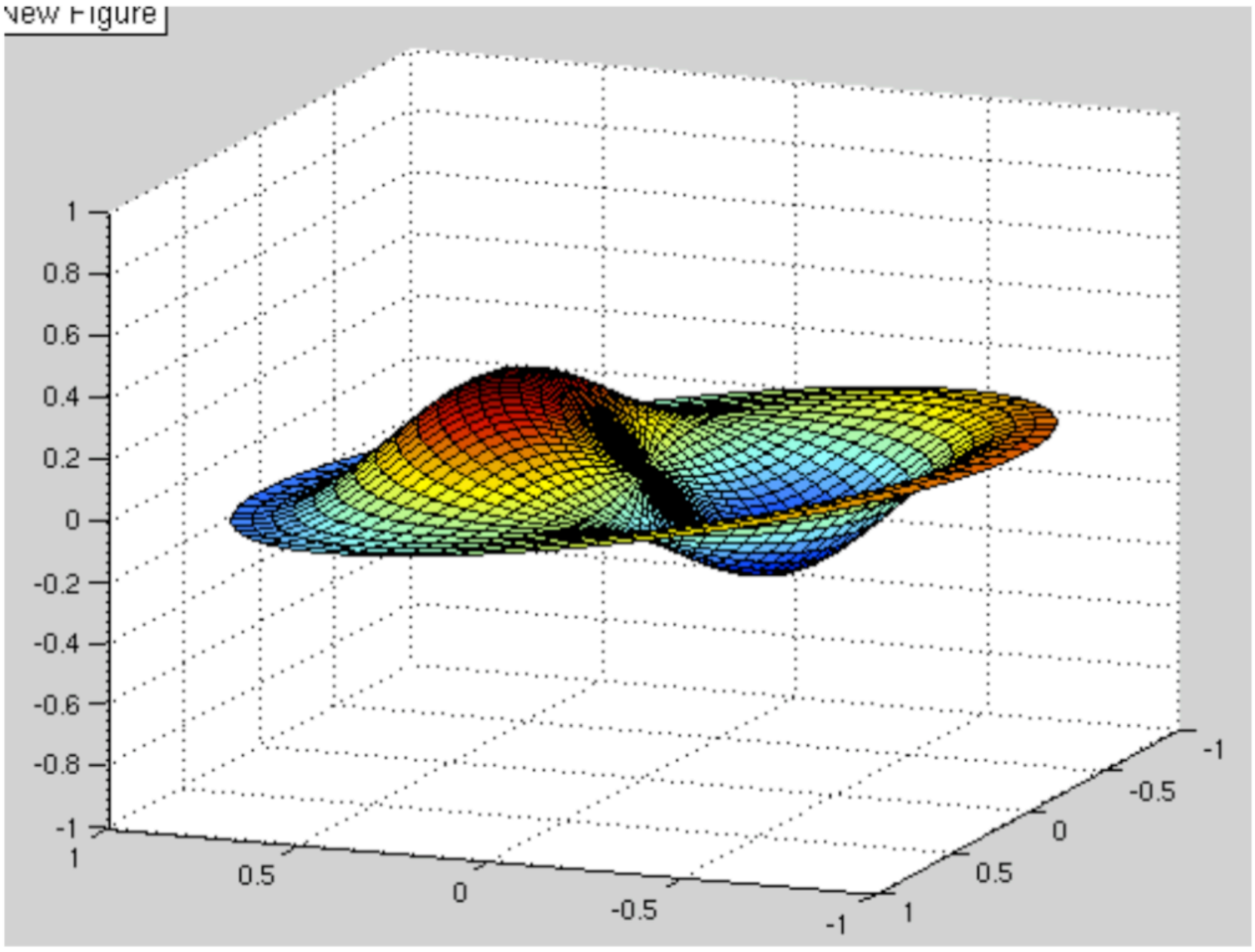
>> drumhead

[*m*, *n*, *ampl*] : [0, 0, 0.5]



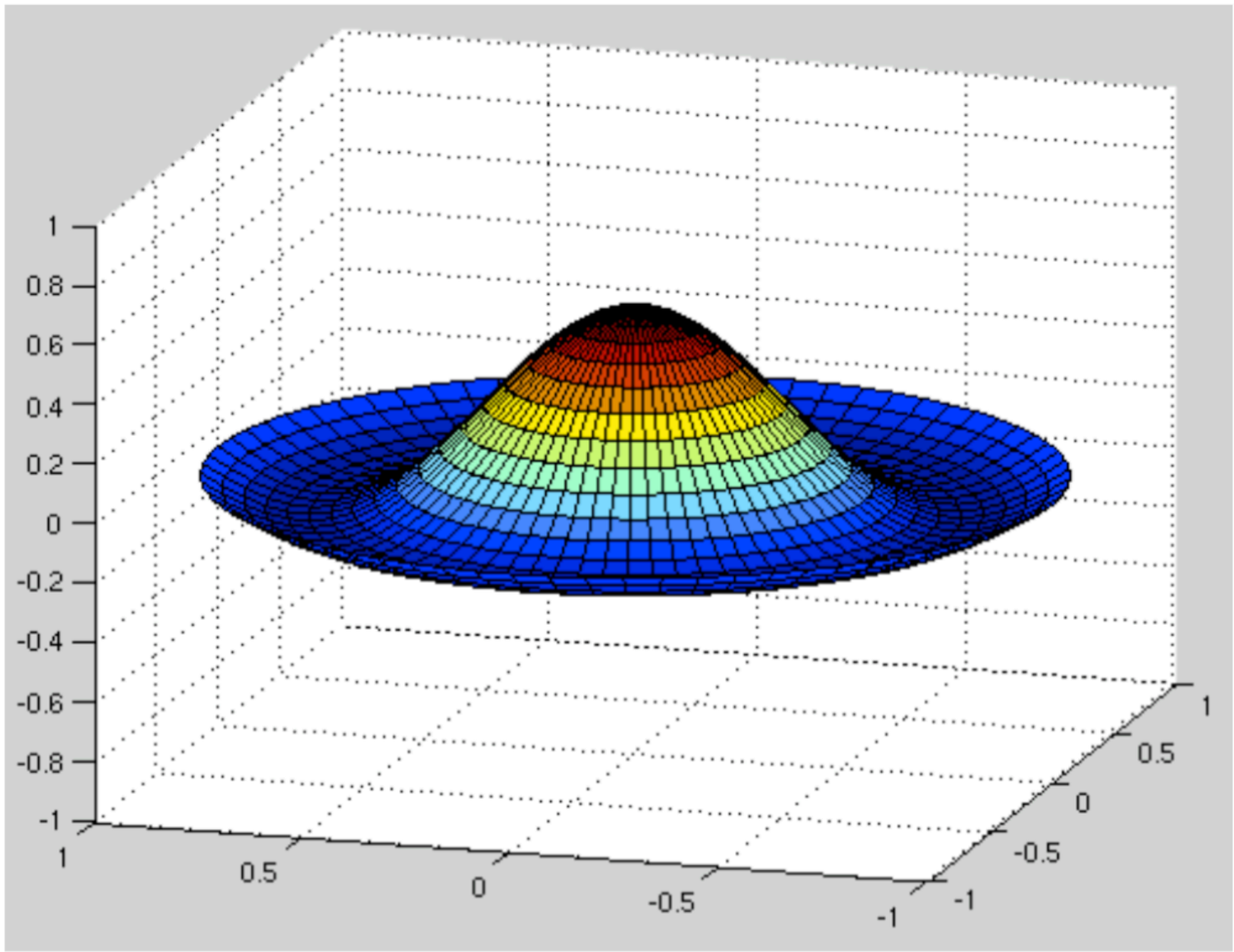
>> drumhead

$[m, n, ampl] : [0, 1, 0.5]$



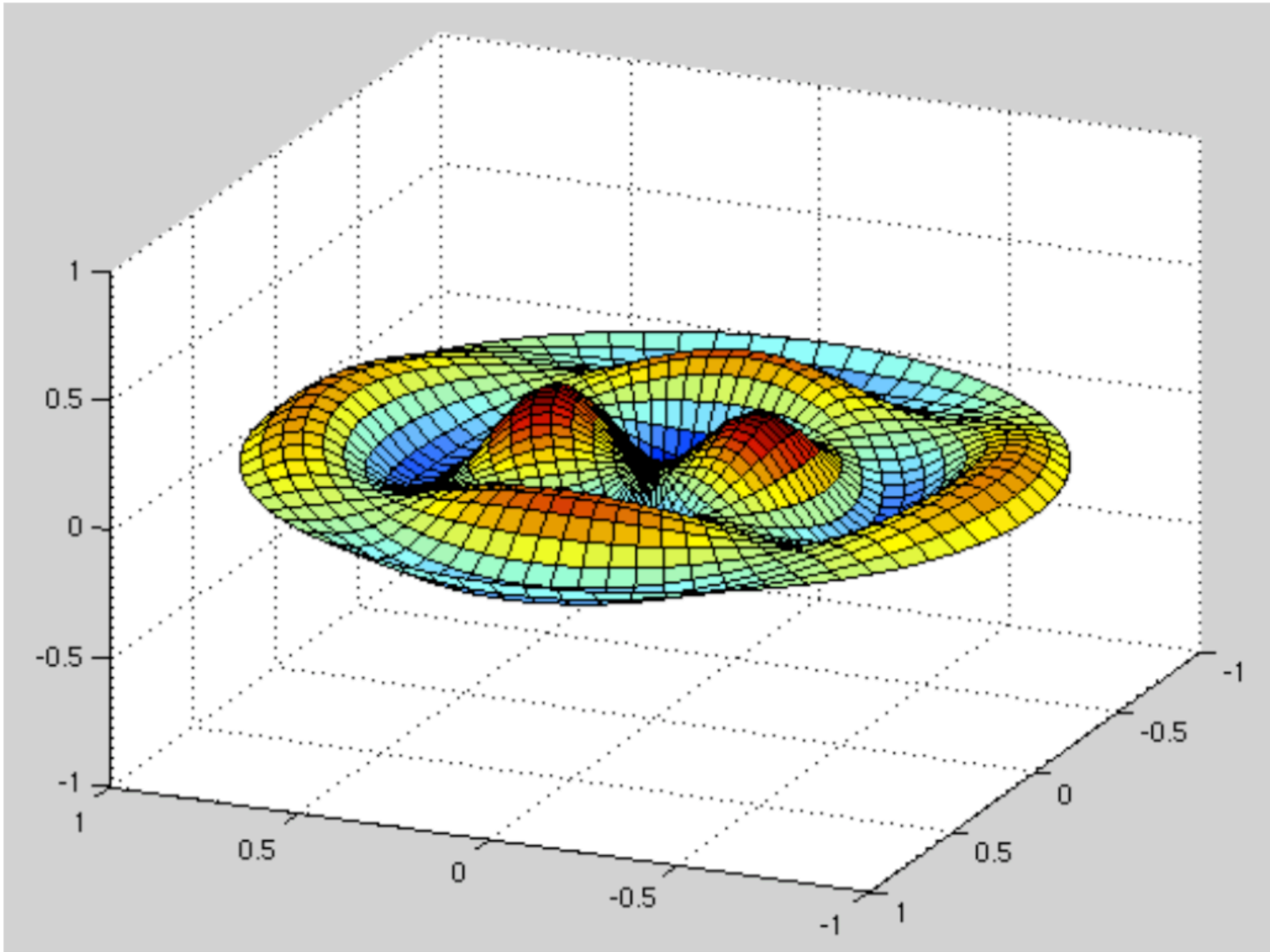
» drumhead

[*m*, *n*, *ampl*] : [2, 0, 0.5]



>> drumhead

[*m*, *n*, *ampl*] : [2, 2, 0.5]



Steady State Temperature in a Cylinder

In this example, we have a semi-infinite cylinder of radius $r = 1$ in the $r - \theta$ plane with one cap at $z = 0$ and extending to $z = \infty$.

The cap at $z = 0$ is kept at $T = 100$ and the cylindrical surface is kept at $T = 0$.

We also assume that because this is a steady-state problem

$$\frac{\partial T}{\partial t} = 0$$

and thus we have the equation

$$\nabla^2 T = 0 = \frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial T}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 T}{\partial \phi^2} + \frac{\partial^2 T}{\partial z^2}$$

We substitute the SOV solution

$$T(\rho,\phi,z) = R(\rho)\Phi(\phi)Z(z) \rightarrow \frac{1}{\rho R}\left(\rho\frac{\partial R}{\partial \rho}\right) + \frac{1}{\rho^2\Phi}\frac{\partial^2\Phi}{\partial\phi^2} + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = 0$$

We choose

$$\frac{1}{Z}\frac{d^2Z}{dz^2} = k^2 \rightarrow \frac{d^2Z}{dz^2} + k^2 Z = 0$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -n^2 \rightarrow \frac{d^2\Phi}{d\phi^2} + n^2\Phi = 0$$

which leads to

$$\rho^2\frac{d^2R}{d\rho^2} + \rho\frac{dR}{d\rho} + (k^2\rho^2 - n^2)R = 0$$

We then have the solutions

$$Z(z) = e^{-kz}$$

where we only include the negative exponential solutions since the positive exponential solutions make no physical sense for this system since $T \to 0$ as $z \to \infty$, and

$$\Phi(\phi) = a \sin n\phi + b \cos n\phi$$

where we must choose $n =$ integer so that

$$\Phi(\phi) = \Phi(\phi + 2\pi)$$

i.e., it makes no physical sense to get a different solution (different physics) if we change ϕ by 2π, and

$$R(\rho) = J_n(k\rho)$$

where we have not included the other solution $N_n(k\rho)$ because it is singular at $\rho = 0$ which is the center of the cylinder.

The boundary condition on the cylindrical surface gives

$$R(1) = J_n(k) = 0$$

so that the possible k-values are the zeroes of the Bessel function of order n, i.e., $k = k_{mn} = m^{th}$ zero of J_n.

Thus, a solution for the cylinder is

$$T_{mn}(\rho, \phi, z) = J_n(k_{mn}\rho)(a_{mn} \sin n\phi + b_{mn} \cos n\phi)e^{-k_{mn}z}$$

If we turn the cylinder through any angle, the boundary conditions on the top and bottom caps are the same (independent of ϕ).

Therefore, the solution cannot depend on ϕ.

This means that the only allowed value of $n = 0$.

The solutions are then

$$T_m(\rho, \phi, z) = b_m J_0(k_m\rho)e^{-k_m z}$$

where $k_m = m^{th}$ root of J_0.

The most general solution is the superposition

$$T(\rho, \phi, z) = \sum_{m=1}^{\infty} b_m J_0(k_m \rho) e^{-k_m z}$$

In this case, the b_m are determined by the exact temperature value on the bottom cap.

We have the boundary condition on the bottom cap

$$T(\rho, \phi, 0) = 100 = \sum_{m=1}^{\infty} b_m J_0(k_m \rho)$$

This should remind you of a Fourier series.

However, instead of expanding in trigonometric function, here we expand in Bessel functions.

Remember the earlier example where we expanded both in a Fourier series and in Legendre polynomials.

From the properties of the Bessel function we can determine the coefficients as follows:

$$100 = \sum_{m=1}^{\infty} b_m J_0(k_m \rho)$$

$$\int_0^1 100 \rho J_0(k_n \rho) d\rho = \sum_{m=1}^{\infty} b_m \int_0^1 \rho J_0(k_n \rho) J_0(k_m \rho) d\rho$$

$$= \sum_{m=1}^{\infty} b_m \delta_{mn} \int_0^1 \rho [J_0(k_n \rho)]^2 d\rho$$

$$= b_n \int_0^1 \rho [J_0(k_n \rho)]^2 d\rho = \frac{b_n}{2} [J_1(k_n)]^2$$

or

$$b_n = \frac{200}{[J_1(k_n)]^2} \int_0^1 \rho J_0(k_n \rho) d\rho$$

Now,

$$\frac{d}{dx}[xJ_1(x)] = xJ_0(0) \rightarrow \frac{1}{k_n}\frac{d}{d\rho}[k_n\rho J_1(k_n\rho)] = k_n\rho J_0(k_n\rho)$$

which gives

$$\int_0^1 \rho J_0(k_n\rho)d\rho = \frac{1}{k_n}\int_0^1 d[\rho J_1(k_n\rho)] = \left.\frac{1}{k_n}\rho J_1(k_n\rho)\right|_0^1 = \frac{1}{k_n}J_1(k_n)$$

and

$$b_n = \frac{200}{[J_1(k_n)]^2}\frac{1}{k_n}j_1(k_n) = \frac{200}{k_nJ_1(k_n)}$$

We finally get the solution

$$T(\rho,\phi,z) = \sum_{m=1}^{\infty}\frac{200}{k_mJ_1(k_m)}J_0(k_m\rho)e^{-k_mz}$$

Steady State Temperature in a Sphere

We have a sphere of radius $r = 1$.

The upper hemisphere is kept at $T = 100$ and the lower hemisphere is kept at $T = 0$.

We now know the process so we will just write down all of the steps.

Equations:

$$\nabla^2 T = 0$$

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

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

We choose

$$\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2} = -m^2 \rightarrow \frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0$$

$$\frac{1}{\sin\theta\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) - \frac{m^2}{\sin^2\theta} = -k$$

$$\rightarrow \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) - \frac{m^2}{\sin^2\theta}\Theta + k\Theta = 0$$

which gives

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - kR = 0$$

Solutions:

First,

$$\Phi(\phi) = a\sin m\phi + b\cos m\phi$$

where $m =$ integer so that

$$\Phi(\phi) = \Phi(\phi + 2\pi)$$

We then choose $k = \ell(\ell + 1)$ to get convergent polynomials, i.e.,

$$\Theta(\theta) = P_\ell^m(\cos\theta)$$

We neglect the Legendre functions of the second kind because they are singular at $\cos\theta = 1$.

Finally, we have

$$R(r) = cr^\ell + dr^{-(\ell+1)}$$

We must, however, choose $d = 0$ or the solution diverges at $r = 0$.

General Solution

$$T(r, \theta, \phi) = r^\ell P_\ell^m(\cos\theta)(a \sin m\phi + b \cos m\phi)$$

We have boundary condition that are independent of ϕ.

Therefore we can have $m = 0$ only and our general solution becomes

$$T(r, \theta, \phi) = \sum_{\ell=0}^{\infty} b_\ell r^\ell P_\ell(\cos\theta)$$

where $P_\ell(\cos\theta) =$ Legendre polynomial.

We determine the coefficients by using the boundary condition

$$T(1, \theta, \phi) = \sum_{\ell=0}^{\infty} b_\ell P_\ell(\cos\theta) = f(\theta) = \begin{cases} 100 & 0 \le \theta \le \pi/2 \\ 0 & \pi/2 \le \theta \le \pi \end{cases}$$

This is always possible to do because the Legendre functions are an orthonormal basis on the interval $[0, 1]$.

We finally get

$$\int_{-1}^{1} dx P_n(x) \sum_{\ell=0}^{\infty} b_\ell P_\ell(\cos\theta) = \int_{-1}^{1} dx P_n(x) f(x) = 100 \int_{0}^{1} dx P_n(x)$$

$$\sum_{\ell=0}^{\infty} b_\ell \int_{-1}^{1} dx P_n(x) P_m(x) = 100 \int_{0}^{1} dx P_n(x)$$

$$\sum_{\ell=0}^{\infty} b_\ell \delta_{n\ell} \frac{2}{2n+1} = 100 \int_{0}^{1} dx P_n(x) = \frac{2}{2n+1} b_n \to b_n = \frac{50(2n+1)}{\int_0^1 dx P_n(x)}$$

Therefore,

$$T(r,\theta,\phi) = 50 \sum_{\ell=0}^{\infty} \frac{50(2\ell+1)}{\int_0^1 dx P_\ell(x)} r^\ell P_\ell(\cos\theta)$$

Now,

$$\int_0^1 dx P_0(x) = \int_0^1 dx = 1 \quad , \quad \int_0^1 dx P_1(x) = \int_0^1 x dx = \frac{1}{2}$$

$$\int_0^1 dx P_2(x) = \frac{1}{2}\int_0^1 dx(3x^2 - 1) = 0$$

$$\int_0^1 dx P_3(x) = \frac{1}{8} \quad , \quad \int_0^1 dx P_4(x) = 0 \quad , \quad \int_0^1 dx P_5(x) = \frac{1}{16}$$

so that we get the final answer

$$T(r,\theta,\phi)$$
$$= 100\left[\frac{1}{2}P_0(\cos\theta) + \frac{3}{4}P_1(\cos\theta) - \frac{7}{16}P_3(\cos\theta) + \frac{11}{32}P_5(\cos\theta) + ...\right]$$

Nuclear Fission example

Assume that the neutron density n inside U_{235} obeys the differential equation

$$\nabla^2 n(r,\theta,\phi,t) + \lambda n(r,\theta,\phi,t) = \frac{1}{\kappa}\frac{\partial n(r,\theta,\phi,t)}{\partial t}$$

with $n = 0$ on the surface of the sphere.

Find the critical radius R_0 such that the neutron density inside a U_{235} sphere of radius R_0 or greater is unstable and increases exponentially with time (called **nuclear fission**).

We have

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial n}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial n}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 n}{\partial\phi^2} + \lambda n = \frac{1}{\kappa}\frac{\partial n}{\partial t}$$

We make the standard SOV substitution

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

to get

$$\frac{1}{r^2 R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{1}{r^2\sin\theta\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{1}{r^2\sin^2\theta\Phi}\frac{d^2n}{d\phi^2}+\lambda$$
$$=\frac{1}{\kappa}\frac{dT}{dt}=-k$$

Thus,

$$\frac{dT}{dt}+k\kappa T=0\rightarrow T=e^{-k\kappa t}$$

We choose

$$\frac{1}{\Phi}\frac{d^2n}{d\phi^2}=-m^2\rightarrow\frac{d^2n}{d\phi^2}+m^2\Phi=0\rightarrow\Phi(\phi)=a\sin m\phi+b\cos m\phi$$

Since there is no ϕ dependence in the system, we must choose $m=0$ so that

$$\Phi(\phi)=b$$

We choose

$$\frac{1}{\sin\theta\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = -c = -\ell(\ell+1) \rightarrow \Theta(\theta) = P_\ell(\cos\theta)$$

Since there is no θ dependence in the system, we must choose $\ell = 0$ so that

$$\Theta(\theta) = P_0(\cos\theta) = 1$$

This leaves us with only the radial equation remaining

$$\frac{1}{r^2 R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \lambda + k = 0 \rightarrow r^2\frac{d^2R}{dr^2} + 2r\frac{dR}{dr} + r^2(\lambda+k)R = 0$$

Remember the full solution for this system is

$$n(r,t) = R(r)e^{-k\kappa t}$$

We can change the radial equation to

$$z^2\frac{d^2R}{dz^2}+2z\frac{dR}{dz}+z^2R=0 \quad , \quad z=\sqrt{\lambda+k}r$$

which is the spherical Bessel function equation

$$\left[z^2\frac{d^2}{dz^2}+2z\frac{d}{dz}+\ z^2-\ell(\ell+1)\right]j_\ell(z)=0$$

for $\ell=0$.

The solution in this case is

$$R(z)=j_0(z)=\frac{\sin z}{z}=\frac{\sin\sqrt{\lambda+k}r}{\sqrt{\lambda+k}r}$$

The general solution is then

$$n(r,t)=\frac{\sin\sqrt{\lambda+k}r}{\sqrt{\lambda+k}r}e^{-k\kappa t}$$

The boundary condition is

$$n(R_0, t) = 0 \rightarrow \sin\sqrt{\lambda + k}R_0 = 0 \rightarrow \sqrt{\lambda + k_m}R_0 = m\pi$$

so that

$$k_m = \frac{m^2\pi^2}{R_0^2} - \lambda$$

Therefore our solution is

$$n_m(r, t) = \frac{\sin\frac{m\pi}{R_0}}{\frac{m\pi}{R_0}} e^{-\left(\frac{m\pi}{R_0} - \lambda\right)\kappa t}$$

The full general solution is a superposition of these solutions for all m values.

$$n(r, t) = \sum_m \frac{\sin\frac{m\pi}{R_0}}{\frac{m\pi}{R_0}} e^{-\left(\frac{m\pi}{R_0} - \lambda\right)\kappa t}$$

If

$$k_m = \frac{m^2\pi^2}{R_0^2} - \lambda < 0$$

then the solution is unstable (grows exponentially with time).

This condition becomes, if

$$R_0 > \frac{m\pi}{\lambda}$$

then we have unstable behavior.

The minimum value of m is 1.

Therefore, we have unstable behavior if

$$R_0 > \frac{\pi}{\lambda}$$

or we get a nuclear explosion if we bring too much U_{235} together.

The actual critical mass of U_{235} is 52 kg.

The density of U_{235} is 19.1 g/cm^3 $= 19.1 \times 10^3$ kg/m^3.

52 kg corresponds to a sphere of radius

$$\frac{4}{3}\pi R_0^3 \rho = M = 52kg$$

or

$$R_0 = \left(\frac{3M}{4\pi\rho}\right)^{1/3} = 0.87m = 8.7cm$$

and the parameter λ would be

$$\lambda > \frac{\pi}{R_0} = 0.115\, cm^{-1}$$

Worrying About the $k = 0$ Solutions

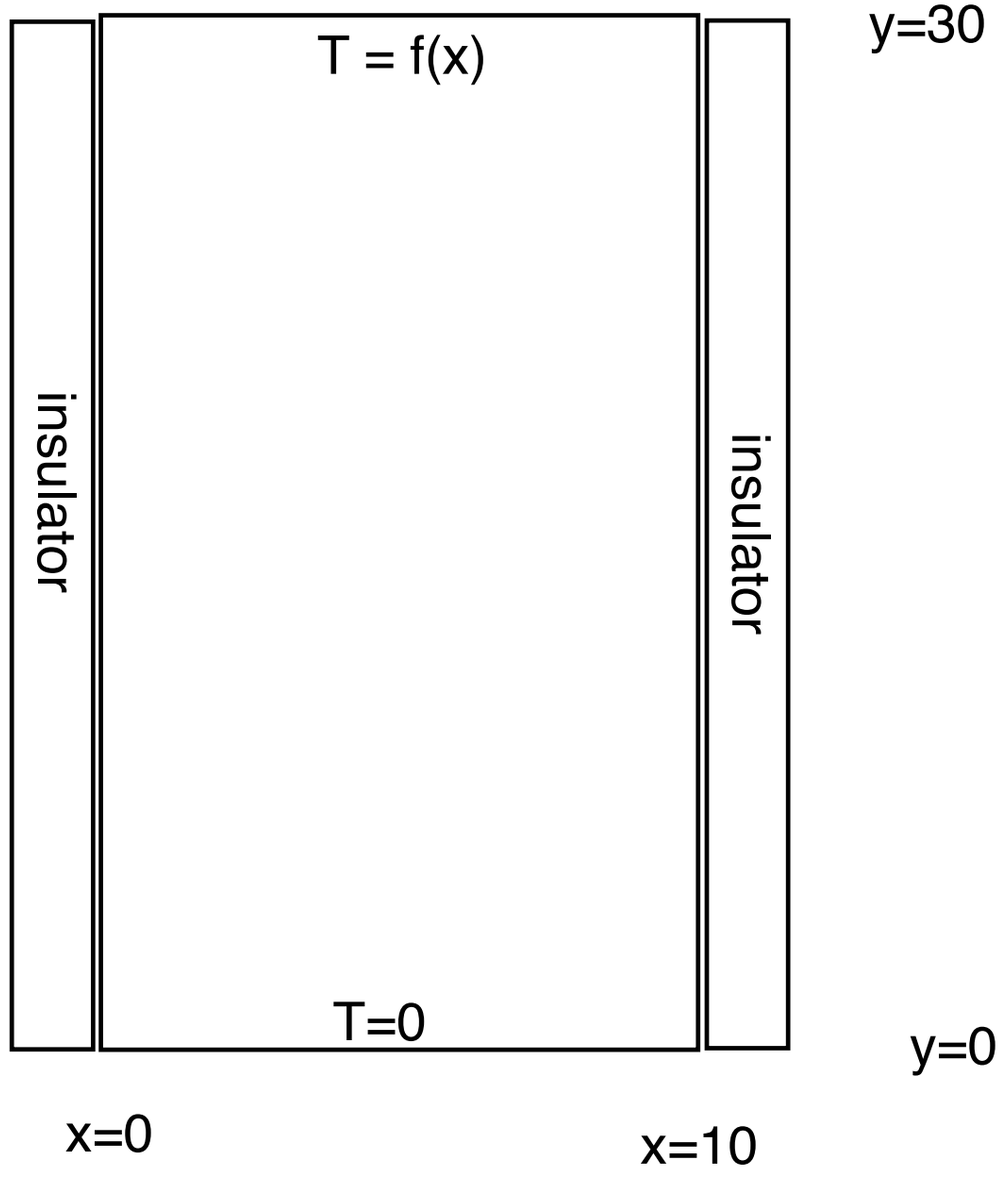
We consider a plate, 10cm by 30cm, with two insulated sides, one end held at $T = 0$ and the other held at a given temperature

$$T = f(x) = 100 \text{ or } T = f(x) = x \text{ (two different cases).}$$

Insulated sides means that

$$\frac{\partial T}{\partial x} = 0 \text{ at } x = 0 \text{ and } x = 10 \text{ (the sides)}$$

The plate looks like



As before we have the general solution

$$T(x,y) = ae^{ky}\sin kx + be^{-ky}\sin kx + ce^{ky}\cos kx + de^{-ky}\cos kx$$

Boundary conditions:

$$\frac{\partial T}{\partial x}(x=0) = 0 \rightarrow a = b = 0$$

$$\frac{\partial T}{\partial x}(x=10) = 0 \rightarrow k = \frac{n\pi}{10}$$

$$T(x, y=30) = 0 \rightarrow (ce^{30k} + de^{-30k})\cos kx = 0 \rightarrow ce^{30k} + de^{-30k} = 0$$

Thus, we have

$$T(x,y) = \sum_n A_n \sinh\frac{n\pi(30-y)}{10}\cos\frac{n\pi x}{10}$$

Thus, we have

$$T(x,y) = \sum_n A_n \sinh \frac{n\pi(30-y)}{10} \cos \frac{n\pi x}{10}$$

For $T = f(x)$, when $y = 0$, we expand $f(x)$ in a Fourier series on the interval $[0, 10]$.

Note, however, that there are no constant terms in the solution since for $n = 0$ has $sinh(0) = 0$. Now putting

$$k = \frac{n\pi}{10} = 0$$

in terms like $e^{\pm ky} \cos kx$ gives a constant as a possible solution of Laplace's equation.

We cannot, however, just add a constant to our solution because then $T \neq 0$ when $y = 30$. We must go back to the **original** equation and set $k = 0$ to determine what to do.

We have

$$\frac{d^2X}{dx^2} = 0 \rightarrow \frac{dX}{dx} = \text{ constant } \rightarrow X = a + bx$$

$$\frac{d^2Y}{dy^2} = 0 \rightarrow \frac{dY}{dy} = \text{ constant } \rightarrow Y = c + dy$$

Therefore, we must add

$$T_{add} = a + bx + cy + dxy$$

to our general solution for $k = 0$.

We were not careful enough in the $k = 0$ case.

Often this is a troublesome case and must be looked at with care.

Now

$$\frac{\partial T_{add}}{\partial x}(x=0)=0 \rightarrow b=d=0$$

$$T_{add}=a+cy$$

$$T_{add}(x,y=30)=0 \rightarrow a+30c=0$$

$$T_{add}=c(30-y)$$

and thus,

$$T(x,y)=c(30-y)+\sum_n A_n \sinh\frac{n\pi(30-y)}{10}\cos\frac{n\pi x}{10}$$

Now we can impose $T=f(x)$ at $y=0$ and get

$$f(x)=30c+\sum_n A_n \sinh 3n\pi \cos\frac{n\pi x}{10}=30c+\sum_n a_n \cos\frac{n\pi x}{10}$$

$$=\frac{a_0}{2}+\sum_n a_n \cos\frac{n\pi x}{10}$$

which says that

$$c = \frac{a_0}{60} \quad , \quad A_n = \frac{a_n}{\sinh 3n\pi}$$

Case #1: $f(x) = 100$

$$a_0 = \frac{2}{10}\int_0^{10} 100 dx = 200 \rightarrow c = \frac{10}{3}$$

$$a_n = \frac{2}{10}\int_0^{10} 100 \cos\frac{n\pi x}{10} dx = \frac{200}{n\pi}\int_0^{n\pi} \cos u du = 0$$

Therefore,

$$T(x, y) = \frac{10}{3}(30 - y)$$

which you should have been able to guess !!!!!

Case #2: $f(x) = x$ Same analysis as Case #1 except

$$a_0 = \frac{2}{10}\int_0^{10} x dx = 10 \to c = \frac{1}{6}$$

$$a_n = \frac{2}{10}\int_0^{10} \cos\frac{n\pi x}{10} dx = \frac{2}{10}\left(\frac{10}{n\pi}\right)^2 \left[\cos\frac{n\pi x}{10} + \frac{n\pi x}{10}\sin\frac{n\pi x}{10}\right]_0^{10}$$

$$= \frac{20}{n^2\pi^2}(\cos n\pi - 1) = \begin{cases} 0 & n \text{ even} \\ -\frac{40}{n^2\pi^2} & n \text{ odd} \end{cases}$$

Therefore,

$$T(x,y) = \frac{1}{6}(30-y) - \frac{40}{\pi^2}\sum_{n\,odd} \frac{1}{n^2 \sinh 3n\pi} \sinh\frac{n\pi(30-y)}{10}\cos\frac{n\pi x}{10}$$

Examples, Examples,, Examples, ...

#1 - A string of length L is initially stretched straight; its ends are fixed for all t.

At time $t = 0$, its is given the the following velocity profile:

$$v(x) = \left(\frac{\partial y}{\partial t}\right)_{t=0} = \begin{cases} 0 & 0 \leq x \leq L/2 - w \\ h & L/2 - w \leq x \leq L/2 + w \\ 0 & L/2 + w \leq x \leq L \end{cases}$$

which is a square pulse.

Determine the shape of the string at time t, that is, find the displacement y as a function of x and t in the form of a series.

As before the most general solution is of the form

$$y(x,t) = (A\sin kx + B\cos kx)(C\sin\omega t + D\cos\omega t)$$

where

$$y(x,0) = 0 \to D = 0 \quad , \quad v(x,0) = v(x)$$

The ends are fixed so that

$$y(0,t) = 0 \to B = 0$$

$$y(L,t) = 0 \to \sin kL = 0 \to k = k_n = \frac{n\pi}{L}$$

Therefore,

$$y(x,t) = \sum_{n=1}^{\infty} A_n \sin\frac{n\pi x}{L}\sin\frac{n\pi\nu t}{L}$$

Using the initial($t = 0$) velocity profile we have

$$v(x) = \sum_{n=1}^{\infty} A_n \frac{n\pi\nu t}{L} \sin \frac{n\pi x}{L}$$

$$\begin{aligned} A_n \frac{n\pi\nu t}{L} &= h \int_{L/2-w}^{L/2+w} \sin \frac{n\pi x}{L} dx = \frac{2h}{l} \left(-\frac{L}{n\pi} \cos \frac{n\pi x}{L} \right)_{L/2-w}^{L/2+w} \\ &= -\frac{2h}{n\pi} \left(\cos \left(\frac{n\pi}{2} + \frac{n\pi w}{L} \right) - cos \left(\frac{n\pi}{2} - \frac{n\pi w}{L} \right) \right) \\ &= \frac{4h}{n\pi} \sin \left(\frac{n\pi}{2} \right) \sin \left(\frac{n\pi w}{L} \right) \end{aligned}$$

or

$$A_n = \frac{4hL}{n^2\pi^2\nu} \sin \left(\frac{n\pi}{2} \right) \sin \left(\frac{n\pi w}{L} \right)$$

and

$$y(x,t) = \frac{4hL}{\pi^2\nu}\sum_{n=1}^{\infty}\frac{1}{n^2}\sin\left(\frac{n\pi}{2}\right)\sin\left(\frac{n\pi w}{L}\right)\sin\frac{n\pi x}{L}\sin\frac{n\pi\nu t}{L}$$

or since

$$\sin\left(\frac{n\pi}{2}\right) = 0 \quad \text{for } n \text{ even} \quad \text{and} \quad \sin\left(\frac{n\pi}{2}\right) = (-1)^{(n-1)/2} \quad \text{for } n \text{ odd}$$

we have

$$y(x,t) = \frac{4hL}{\pi^2\nu}\sum_{n\,odd}^{\infty}\frac{(-1)^{(n-1)/2}}{n^2}\sin\left(\frac{n\pi w}{L}\right)\sin\frac{n\pi x}{L}\sin\frac{n\pi\nu t}{L}$$

#2 - Find the steady-state temperature distribution in the sector of a circular plate of radius 10 and angle 45° if the temperature is maintained at 0° along the radii and at 100° along the curved edge.

As before these are the solutions of Laplace's equation:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 u}{\partial \phi^2}$$

$$u(r,\phi)=R(r)\Phi(\phi)$$

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

We choose

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=-n^2\rightarrow\frac{d^2\Phi}{d\phi^2}+n^2\Phi=0$$

which gives

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

We assume that

$$R = r^q \to r^q(q(q-1) + q - n^2) = 0 = q^2 - n^2 \to q = \pm n$$

We have the general solution

$$u_n(r, \phi) = (Ar^n + Br^{-n})(C_n \sin n\phi + D_n \cos n\phi)$$

Since $r = 0$ is on the plate we must choose $B = 0$ so that

$$u_n(r, \phi) = r^n(C_n \sin n\phi + D_n \cos n\phi)$$

At $\theta = 0$ we have $u(r, 0) = 0$, which says that we must choose $D_n = 0$.

$$u_n(r, \phi) = C_n r^n \sin n\phi$$

At $\theta = \pi/4$ we have $u(r, \pi/4) = 0$, which says that we must choose

$$\frac{n\pi}{4} = m\pi \quad , \quad m, n = \text{ integers} \quad \to n = 4m$$

Thus the most general solution is then

$$u(r,\phi) = \sum_{m=1}^{\infty} C_m r^{4m} \sin 4m\phi$$

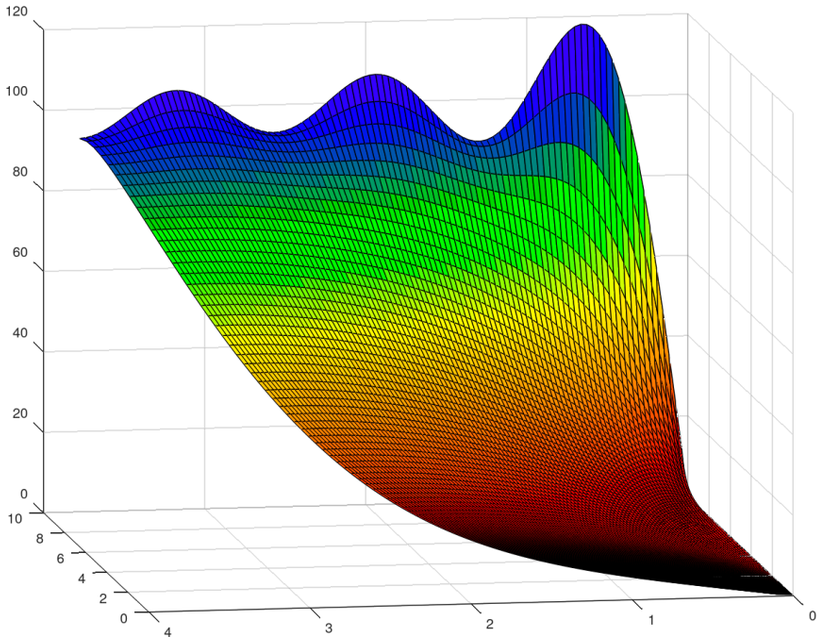
Finally,

$$u(10,\phi) = \sum_{m=1}^{\infty} C_m r^{4m} \sin 4m\phi$$

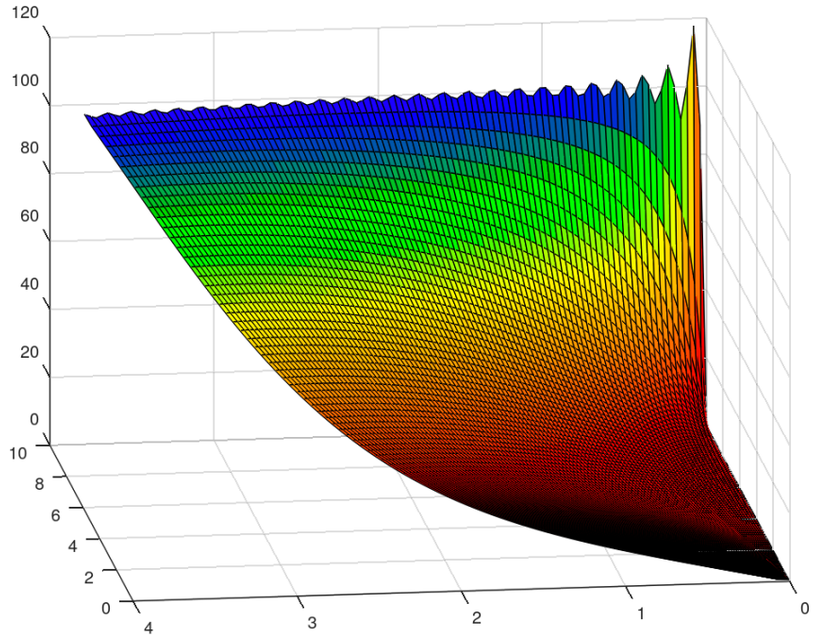
$$C_n 10^{4n} = \frac{200}{\pi/4} \int_0^{\pi/4} \sin 4n\phi d\phi = -\frac{200}{n\pi}(\cos n\pi - 1) = \begin{cases} 0 & n \text{ even} \\ \frac{400}{n\pi} & n \text{ odd} \end{cases}$$

or

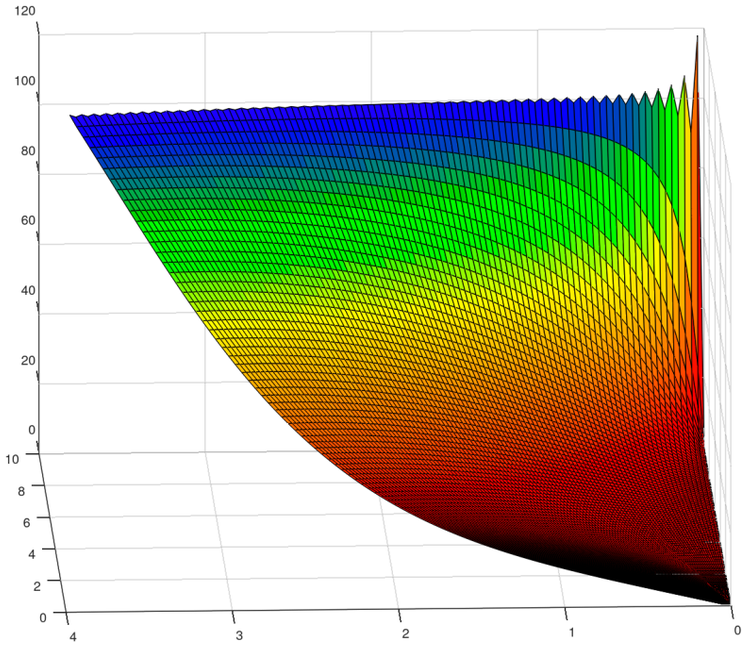
$$u(r,\phi) = \frac{400}{\pi} \sum_{m\,odd}^{\infty} \frac{1}{m} \left(\frac{r}{10}\right)^{4m} \sin 4m\phi$$



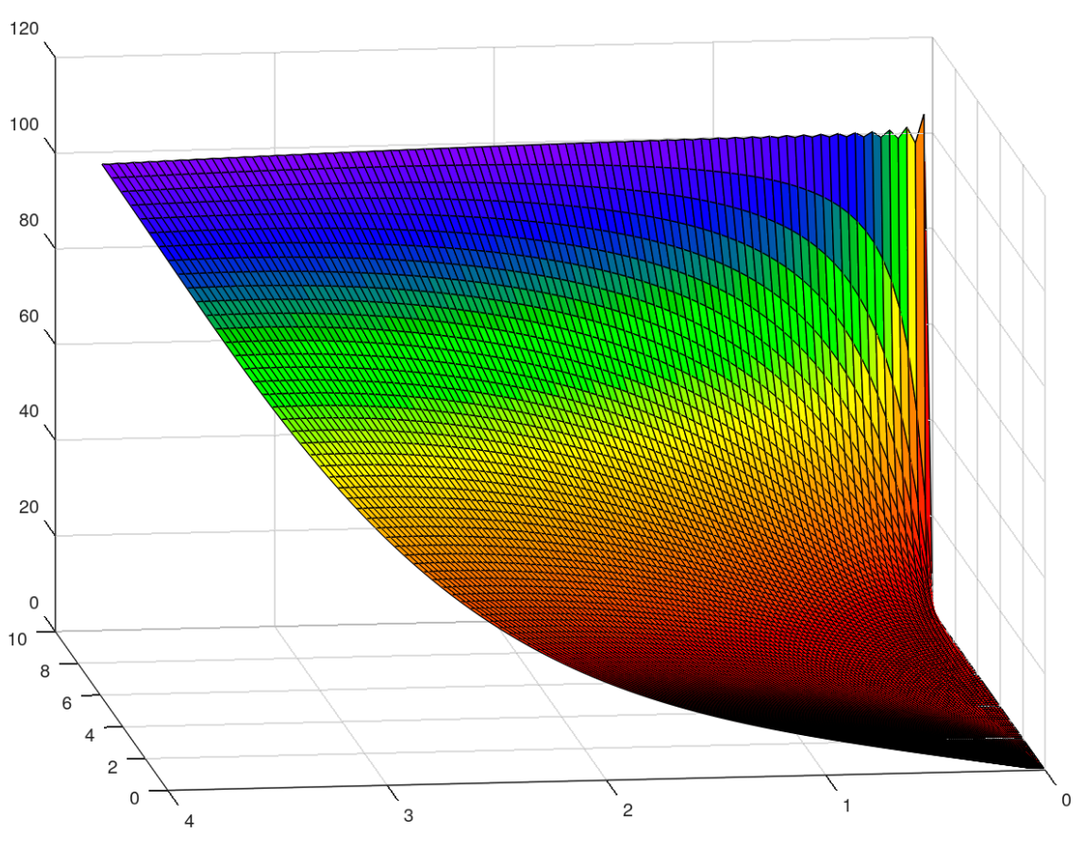
5 terms



50 terms



100 terms



500 terms

```
[r,phi] = ndgrid(0:0.1:10,linspace(0,pi/8,101));
u=0;
for j=[1:2:1001]
 u=u+(400/pi)*(1/j)*(r/10).^(4*j) .*sin((4*j)*phi);
end
[x,y] = pol2cart(phi,r);
surf(x,y,u);
colormap(rainbow)
```

3 - Find the steady-state temperature distribution inside a sphere of radius 1 when the surface temperature is given by

$$T(1,\theta,\phi) = \frac{\pi}{2} - \theta$$

The general solution is

$$T(r,\theta,\phi) = r^{\ell} P_{\ell}^{m}(\cos\theta)(A\sin m\phi + B\cos m\phi)$$

No ϕ dependence means that we must choose $m = 0$ to get

$$T(r,\theta,\phi) = \sum_{\ell=0}^{\infty} A_{\ell} r^{\ell} P_{\ell}(\cos\theta)$$

Now

$$T(1,\theta,\phi) = \sum_{\ell=0}^{\infty} A_{\ell} P_{\ell}(\cos\theta) = \frac{\pi}{2} - \theta$$

or

$$\sum_{\ell=0}^{\infty} A_{\ell} P_{\ell}(x) = \frac{\pi}{2} - \cos^{-1} x = \sin^{-1} x$$

We have

$$\sum_{\ell=0}^{\infty} A_\ell \int_{-1}^{1} P_\ell(x) P_n(x) dx = \int_{-1}^{1} \sin^{-1} x P_n(x) dx$$

$$= \sum_{\ell=0}^{\infty} A_\ell \delta_{n\ell} \frac{2}{2n+1} = \frac{2}{2n+1} A_n$$

or

$$A_n = \frac{2n+1}{2} \int_{-1}^{1} \sin^{-1} x P_n(x) dx$$

Now

$$\sin^{-1} x \text{ is an odd function of } x$$

$$P_n(x) \text{ is odd for } n \text{ odd and even for } n \text{ even}$$

Therefore,

$$A_n = \frac{2n+1}{2} \int_{-1}^{1} \sin^{-1} x P_n(x) dx = 0 \text{ for } n \text{ even}$$

$$A_n = (2n+1) \int_{0}^{1} \sin^{-1} x P_n(x) dx \text{ for } n \text{ odd}$$

Now from the tables

$$\int_0^1 \sin^{-1} x P_n(x) dx = \left. \frac{x^{n+1} \sin^{-1} x}{n+1} \right|_0^1 - \frac{1}{n+1} \int_0^1 \frac{x^{n+1}}{\sqrt{1-x^2}} dx$$
$$= \frac{1}{n+1} \left[\frac{\pi}{2} - \int_0^1 \frac{x^{n+1}}{\sqrt{1-x^2}} dx \right]$$

To evaluate

$$\int_0^1 \frac{x^{n+1}}{\sqrt{1-x^2}} dx$$

we let

$$x = \sin\theta$$

to get

$$\frac{dx}{\sqrt{1-x^2}} = d\theta$$

and

$$\int_0^1 \frac{x^{n+1}}{\sqrt{1-x^2}} dx = \int_0^{\pi/2} (\sin\theta)^{n+1} d\theta = \frac{1 \cdot 3 \cdot 5 \cdots n}{2 \cdot 4 \cdot 6 \cdots (n+1)} \frac{\pi}{2}$$

Finally,

$$A_1 = 3\int_0^1 \sin^{-1} x P_1(x)dx = \frac{3\pi}{8}$$

$$A_3 = 7\int_0^1 \sin^{-1} x P_3(x)dx = \frac{5\pi}{4}$$

$$A_5 = 11\int_0^1 \sin^{-1} x P_5(x)dx = \frac{11\pi}{192}$$

or

$$\sum_{\ell=0}^{\infty} A_\ell P_\ell(x) = \sin^{-1} x = \frac{\pi}{8}\left[3P_1(x) + \frac{7}{16}P_3(x) + \frac{11}{64}P_5(x) + ...\right]$$

so that

$$T(r,\theta,\phi) = \sum_{\ell=0}^{\infty} A_\ell r^\ell P_\ell(x)$$

$$= \frac{\pi}{8}\left[3rP_1(x) + \frac{7}{16}r^3P_3(x) + \frac{11}{64}r^5P_5(x) + ...\right]$$

#4 - Find the electrostatic potential outside a conducting sphere of radius a placed in an originally uniform electric field and maintained at zero potential. HINT: Let the original field $\vec{E}$ be in the negative z-direction so that

$$\vec{E} = -E_0 \hat{k}$$

Then since $\vec{E} = -\nabla\Phi$, where Φ is the potential, we have

$$\Phi = E_0 z = E_0 r \cos\theta$$

You then want a solution of Laplace's equation

$$\nabla^2 u = 0$$

which is zero at $r = a$ and becomes $u \approx \Phi$ for large r (far away from the sphere).

Select the solutions of Laplace's equation in spherical coordinates which have the right θ and ϕ dependence (there are just two such solutions) and find the combination that reduces to zero for $r \to \infty$.

$$\nabla^2 u = 0 \quad , \quad u(r = a, \theta, \phi) = 0 \quad , \quad u(r \to \infty, \theta, \phi) = E_0 r \cos\theta$$

The general solution is

$$u(r,\theta,\phi) = (Ar^{\ell} + Br^{-(\ell+1)})P_{\ell}^{m}(\cos\theta)(C\cos m\phi + D\sin m\phi)$$

No ϕ dependence means we must choose $m = 0$.

$$u(r,\theta,\phi) = \sum_{\ell=0}^{\infty}(A_{\ell}r^{\ell} + B_{\ell}r^{-(\ell+1)})P_{\ell}(\cos\theta)$$

We keep both radial solutions since $r = 0$ is not in system.

The boundary condition

$$u(r = a,\theta,\phi) = 0 \rightarrow A_{\ell}a^{\ell} + B_{\ell}a^{-(\ell+1)} = 0 \rightarrow B_{\ell} = -a^{2\ell+1}A_{\ell}$$

so that

$$u(r,\theta,\phi) = \sum_{\ell=0}^{\infty} A_{\ell}(r^{\ell} - a^{2\ell+1}r^{-(\ell+1)})P_{\ell}(\cos\theta)$$

The boundary condition

$$u(r \to \infty, \theta, \phi) = E_0 r \cos\theta$$

says that

$$A_\ell = 0 \;\; \ell \neq 1 \quad \text{and} \quad A_1 = E_0$$

Finally we have

$$u(r, \theta, \phi) = E_0 (r - a^3 r^{-2}) P_1(\cos\theta)$$

#5 - A hollow split conducting sphere of radius a is placed at the origin.

If one half of the surface is charged to a potential v_0 and the other half is kept at zero potential, find the potential inside and outside the sphere.

We choose the top hemisphere to be charged to v_0 and the bottom hemisphere at zero potential with the plane where the two hemispheres meet perpendicular to the polar (z) axis.

The boundary conditions are then

$$V(a,\theta,\phi) = \begin{cases} v_0 & 0 < \theta < \pi/2 \;\; (1 > \cos\theta > 0) \\ 0 & \pi/2 < \theta < \pi \;\; (0 > \cos\theta > -1) \end{cases}$$

This implies that the potential is independent of ϕ so that we choose $m = 0$ in the solution

$$\Phi(\phi) = A \sin m\phi + B \cos m\phi$$

and the θ solution is given by $P_\ell(\cos\theta)$.

Therefore,

$A_\ell a^\ell P_\ell(\cos\theta)$

$$V(r,\theta,\phi) = \sum_{\ell=0}^{\infty}(A_\ell r^\ell + B_\ell r^{-(\ell+1)})P_\ell(\cos\theta)$$

Inside the sphere $r < a$ ($r = 0$ in this region) so that we must choose $B_\ell = 0$ and therefore

$$V_{inside}(a,\theta,\phi) = \sum_{\ell=0}^{\infty} A_\ell a^\ell P_\ell(\cos\theta)$$

or using the orthogonality of the Legendre polynomials we have

$$A_\ell a^\ell = \frac{2\ell+1}{2}\int_{-1}^{1} V_{inside}(a,\theta,\phi)P_\ell(\cos\theta)d(\cos\theta)$$
$$= \frac{2\ell+1}{2}v_0\int_{0}^{1} P_\ell(\mu)d\mu$$

$A_\ell a^\ell$

which gives the results

$$A_0 = \frac{v_0}{2} \ , \ A_1 = \frac{3v_0}{4a} \ , \ A_2 = 0 \ , \ A_3 = -\frac{7v_0}{16a^3} \ , \ldots\ldots$$

and

$$V_{inside}(r,\theta,\phi) = \frac{v_0}{2}\left[1 + \frac{3r}{2a}P_1(\cos\theta) - \frac{7r^3}{8a^3}P_3(\cos\theta) + \ldots.\right]$$

Outside the sphere ($r > a$) the solution must approach zero as $r \to \infty$, which implies that $A_\ell = 0$ and thus

$$V_{outside}(a,\theta,\phi) = \sum_{\ell=0}^{\infty} B_\ell a^{-(\ell+1)} P_\ell(\cos\theta)$$

and similar to above we have

$$B_\ell a^{-(\ell+1)} = \frac{2\ell+1}{2} v_0 \int_0^1 P_\ell(\mu) d\mu$$

$$B_0 = \frac{v_0 a}{2} \ , \ B_1 = \frac{3 v_0 a^2}{4} \ , \ B_2 = 0 \ , \ B_3 = -\frac{7 v_0 a 64}{16} \ , ...$$

and

$$V_{outside}(r, \theta, \phi) = \frac{v_0 a}{2r} \left[1 + \frac{3a}{2r} P_1(\cos\theta) - \frac{7a^3}{8r^3} P_3(\cos\theta) + ... \right]$$

On the equator ($r = a, \theta = \pi/2$)

$$V(a, \pi/2, \phi) = \frac{v_0}{2}$$

or halfway between the top and bottom hemisphere values (the average).

Relaxation Methods

This is a way to approximate the Laplace Equation by finite differences and produce an iterated solution for the potential.

Cartesian Coordinates

$$= \frac{u(x+\Delta x, y, z) + u(x-\Delta x, y, z) - 2u(x, y, z)}{(\Delta x)^2}$$

$$\nabla^2 u(x, y, z) = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0$$

We approximate the derivatives by

$$\frac{\partial u}{\partial x}(x, y, z) = \frac{u(x+\Delta x/2, y, z) - u(x-\Delta x/2, y, z)}{\Delta x}$$

$$\frac{\partial^2 u}{\partial x^2}(x, y, z) = \frac{\frac{\partial u}{\partial x}(x+\Delta x/2, y, z) - \frac{\partial u}{\partial x}(x-\Delta x/2, y, z)}{\delta x}$$

$$= \frac{u(x+\Delta x, y, z) - u(x, y, z)}{(\Delta x)^2} - \frac{u(x, y, z) - u(x-\Delta x, y, z)}{(\Delta x)^2}$$

$$= \frac{u(x+\Delta x, y, z) + u(x-\Delta x, y, z) - 2u(x, y, z)}{(\Delta x)^2}$$

and so on for y and z .....

We then have (choosing $\Delta x = \Delta y = \Delta z = \Delta$) the finite difference equation

$$\begin{aligned}
&\nabla^2 u(x,y,z) = 0 \\
&= \frac{1}{\Delta^2}[u(x+\Delta,y,z) + u(x-\Delta,y,z) + u(x,y+\Delta,z) \\
&\quad + u(x,y-\Delta,z) + u(x,y,z+\Delta) + u(x,y,z-\Delta)] \\
&\quad - \frac{6u(x,y,z)}{\Delta^2}
\end{aligned}$$

or in 3 dimensions

$$\begin{aligned}
&u(x,y,z) \\
&= \frac{1}{6}\,[u(x+\Delta,y,z) + u(x-\delta,y,z) + u(x,y+\Delta,z) \\
&\quad + u(x,y-\Delta,z) + u(x,y,z+\Delta) + u(x,y,z-\Delta)]
\end{aligned}$$

and in 2 dimensions

$$u(x, y, z) = \frac{1}{4}\left[u(x + \Delta, y) + u(x - \Delta, y) + u(x, y + \Delta) + u(x, y - \Delta)\right]$$

The proceess (in 2 dimensions) is as follows:

1. Define a grid
2. Define the potential on the boundaries of the grid (boundary conditions)
3. Iterate the equation for $u(x, y, z)$ until the potential stops changing
4. The final configuration is the solution to the Laplace equation

Example 1: We start with these boundary conditions:

200×200 grid size

potential = 0 on the edges

potential = +15 on a line

potential = -15 on a parallel line

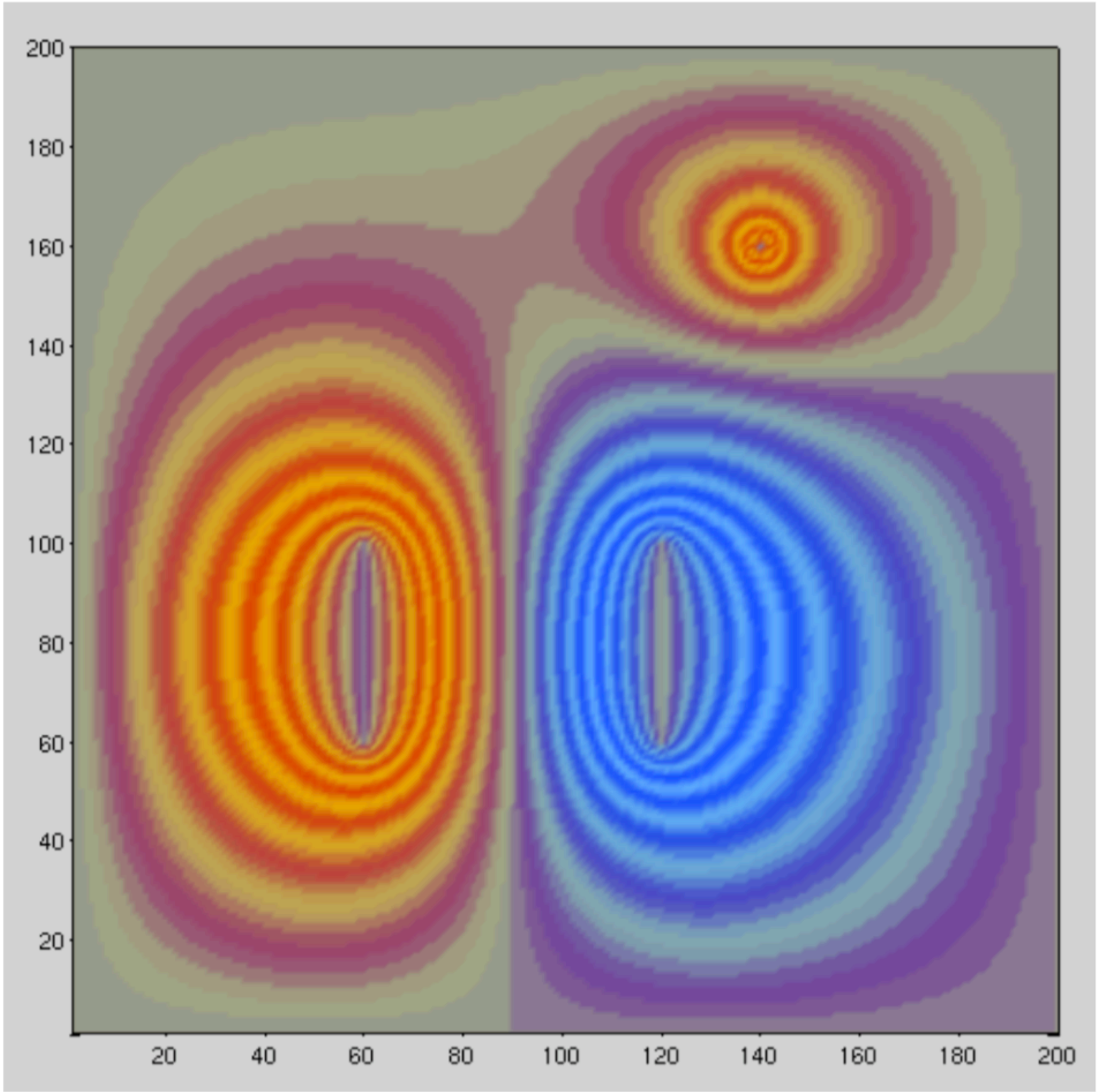
potential = +15 at a point

We are attempting to model a parallel plate + a point charge.

OCTAVE program relax1.m shown below.

```
n = 200;
pin=zeros(n); p=pin; b=pin;
pin(16*n/20,14*n/20)=15 ;
pin(6*n/20:10*n/20,6*n/20)=15*ones(size(pin(6*n/20:10*n/20,6*n/20))) ;
pin(6*n/20:10*n/20,12*n/20)=-15*ones(size(pin(6*n/20:10*n/20,12*n/20)));
b(:,[1,n])=1*ones(size(b(:,[1,n])));
b([1,n],:)=1*ones(size(b([1,n],:)));
b=b+(pin ~= 0);
p=pin;
for i=1:5000
  p=0.25*(p(:,[n,[1:(n-1)]])+p(:,[[2:n],1]) ...
         +p([n,[1:(n-1)]],:)+p([[2:n],1],:));
  p=p.*(1-b)+pin;
end
figure('Position',[300,300,600,600]);
pcolor(p);
axis square;
colormap(waves);
shading interp;
```

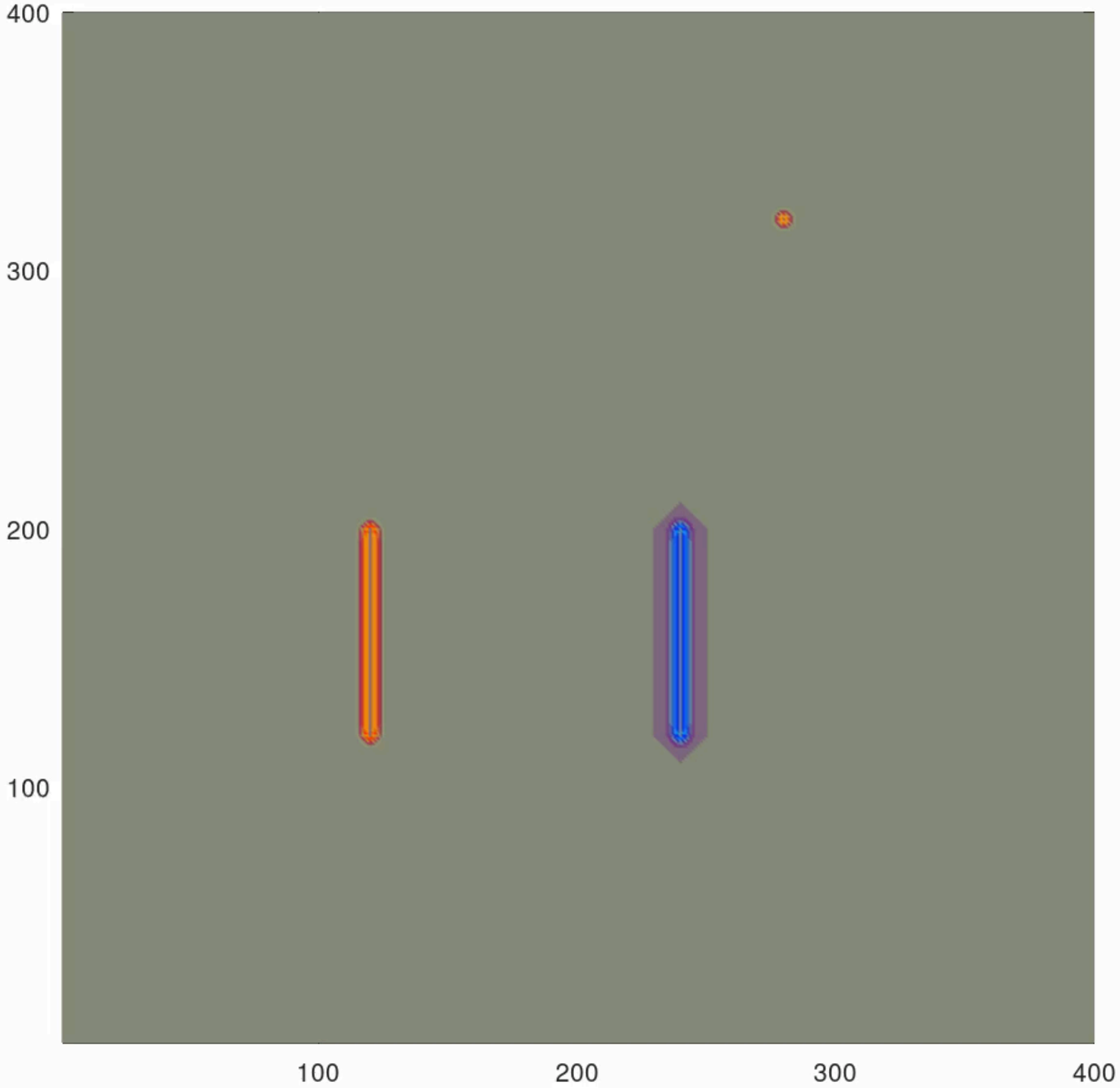
The final potential configuration is shown below.

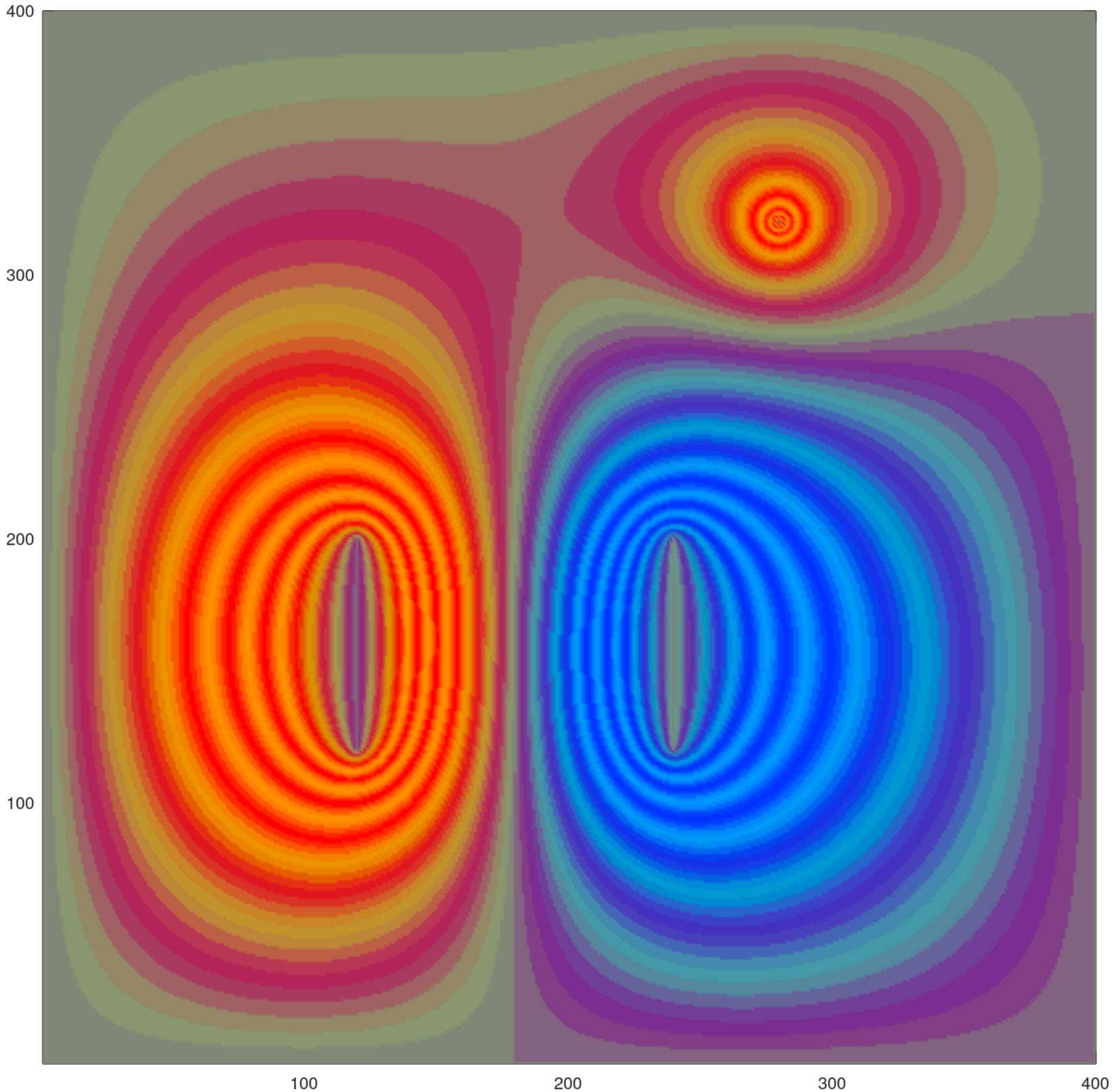


The code below(relax1mov.m) does the same calculation but show all the intermediate configurations leading to the final configuration.

```
n = 400;
figure('Position',[200,200,800,800]);
pin=zeros(n); p=pin; b=pin;
pin(16*n/20,14*n/20)=15 ;
pin(6*n/20:10*n/20,6*n/20)=15*ones(size(pin(6*n/20:10*n/20,6*n/20))) ;
pin(6*n/20:10*n/20,12*n/20)=-15*ones(size(pin(6*n/20:10*n/20,12*n/20)));
b(:,[1,n])=1*ones(size(b(:,[1,n])));
b([1,n],:)=1*ones(size(b([1,n],:)));
b=b+(pin ~= 0);
p=pin;
for i=1:5000
  if mod(i,100) == 0
    i
  endif
  p=0.25*(p(:,[n,[1:(n-1)]])+p(:,[[2:n],1]) ...
         +p([n,[1:(n-1)]],:)+p([[2:n],1],:));
  p=p.*(1-b)+pin;
  pcolor(p);
  axis square;
  colormap(waves);
  shading interp;
  pause(0.001)
end
```

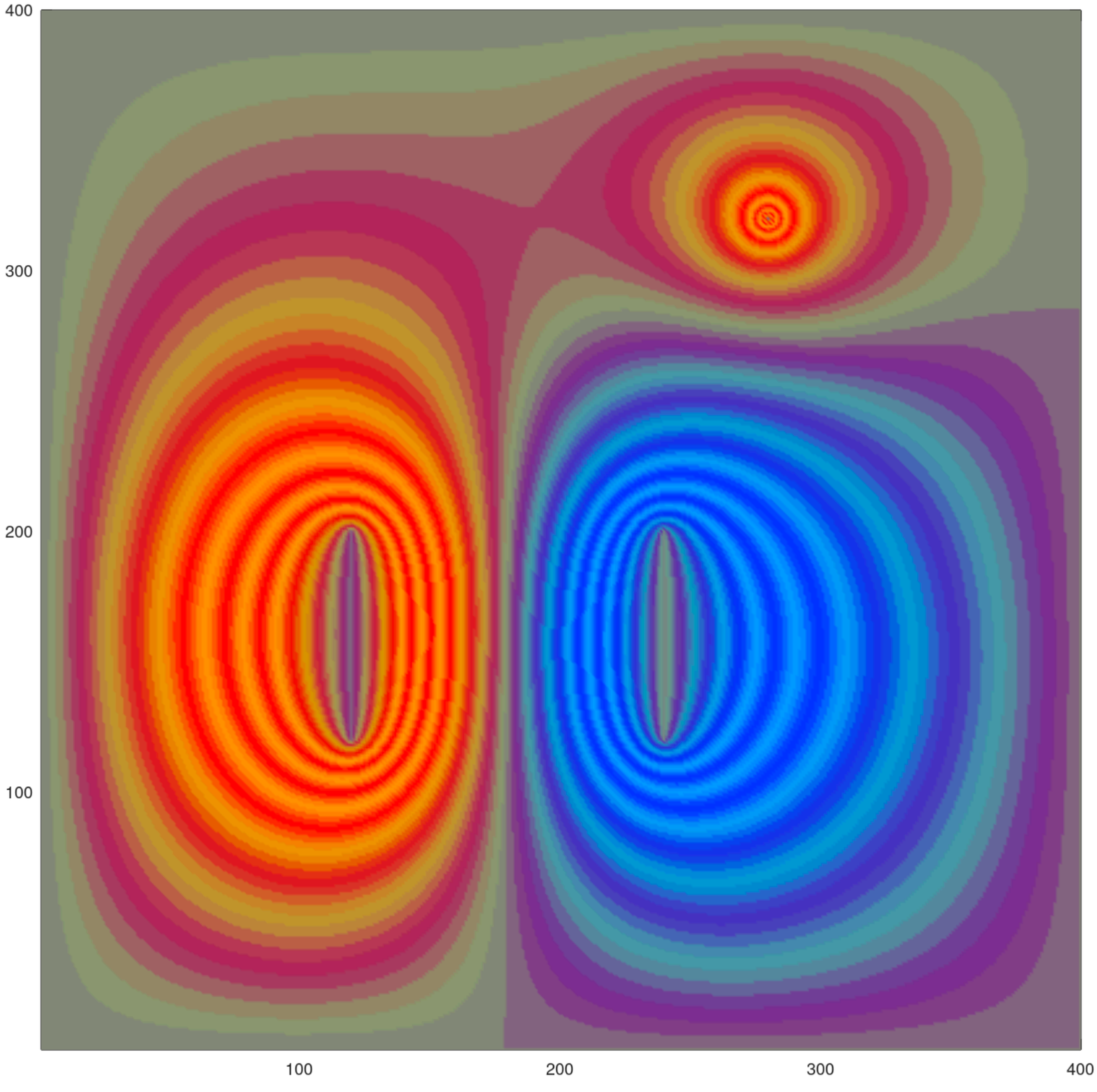
10000 steps



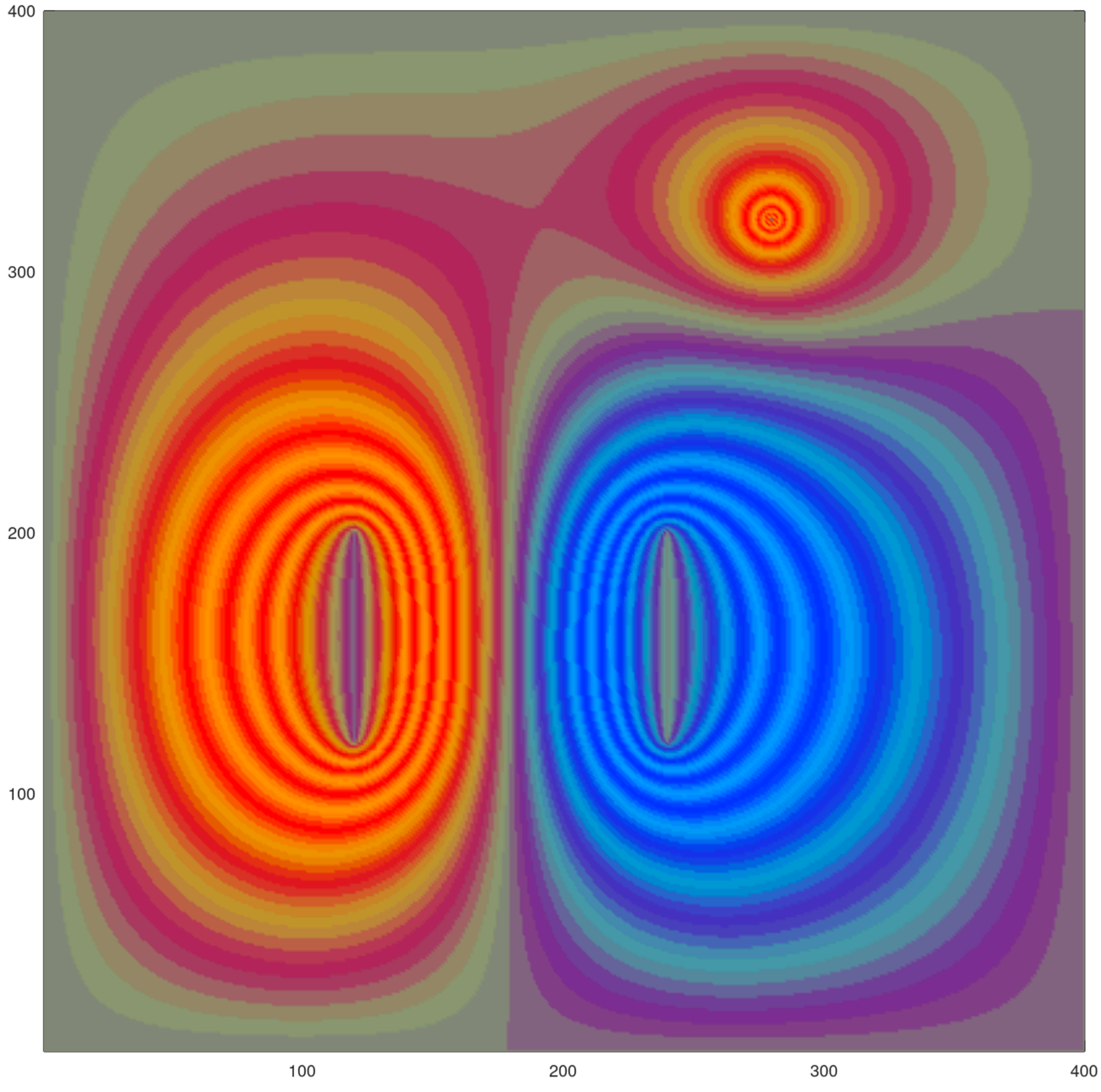


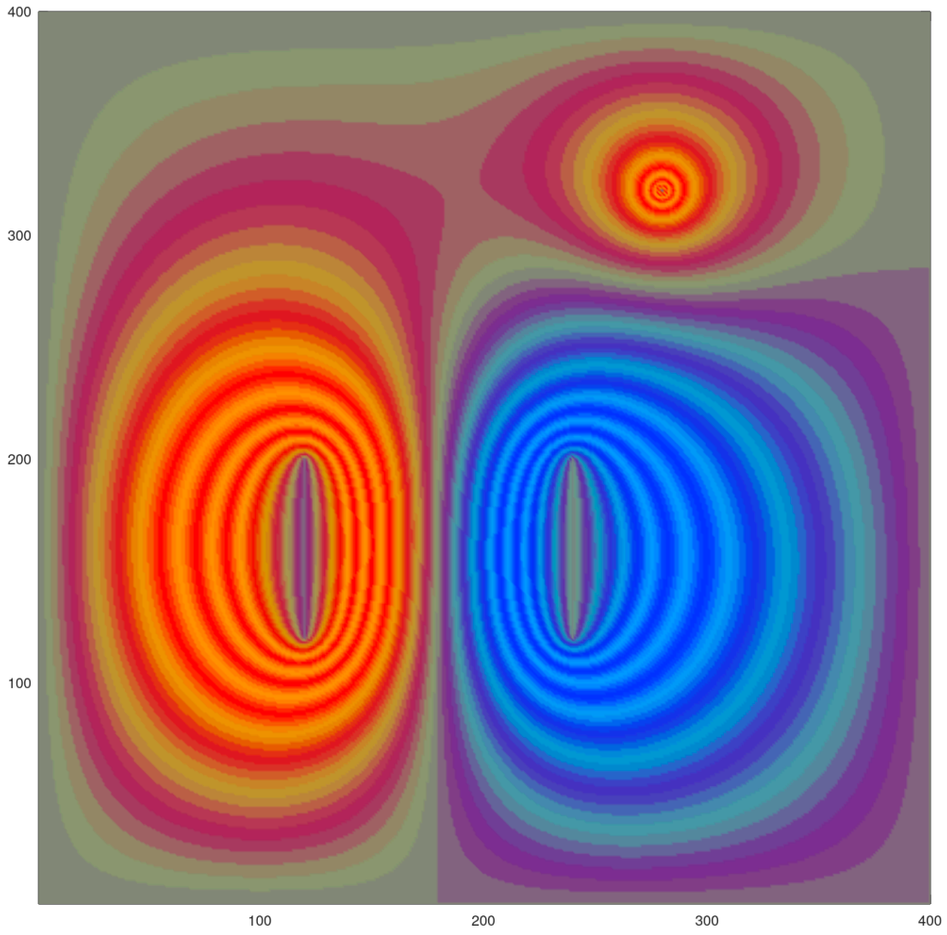
50000 steps

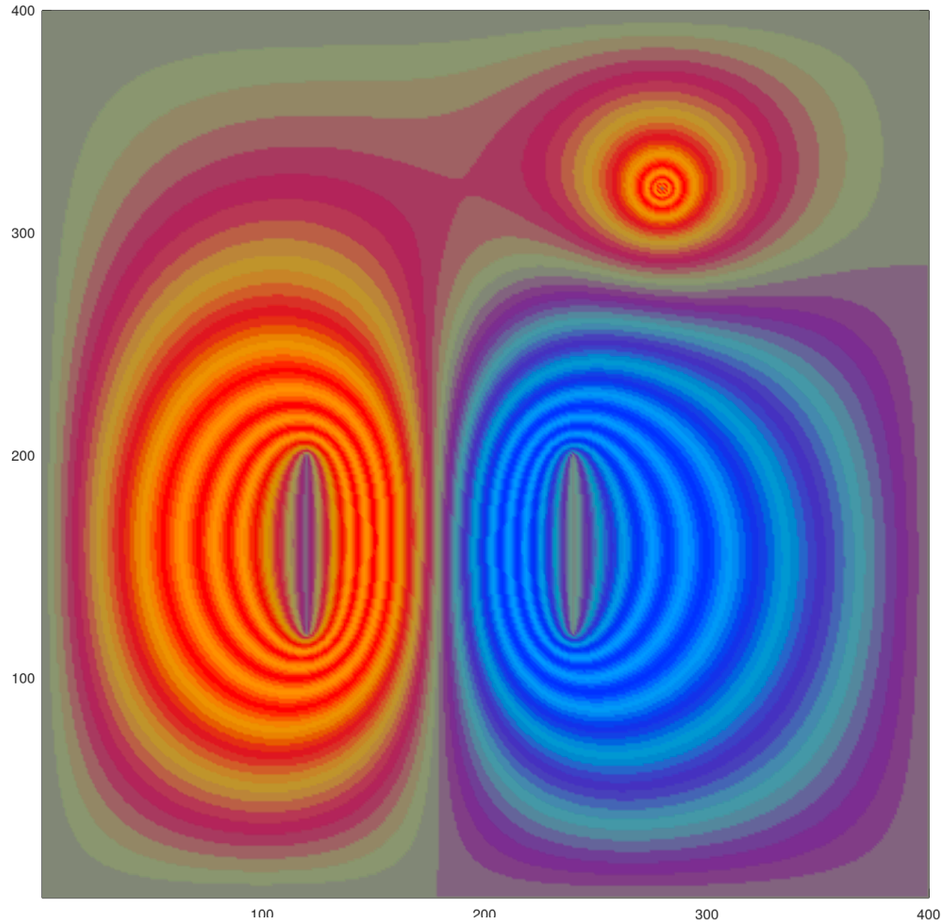
100000 steps



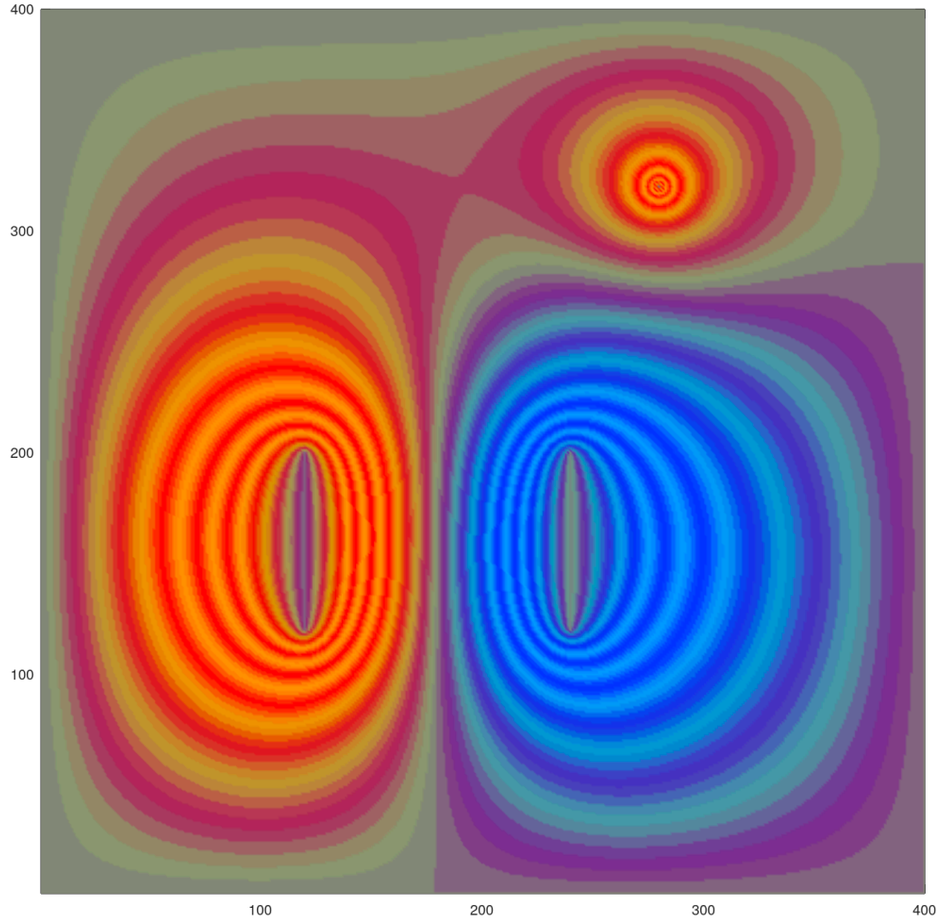
500000 steps







50000 steps



100000 steps

500000 steps

Plane-Polar Coordinates We now do the same derivation but in plane-polar coordinates.

$$\nabla^2 u(r,\theta) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} = 0$$

$$\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} = 0$$

We approximate the derivatives (as earlier) by

$$\frac{\partial u}{\partial r}(r,\theta) = \frac{u(r+\Delta r/2,\theta) - u(r-\Delta r/2,\theta)}{\Delta r}$$

$$\frac{\partial^2 u}{\partial r^2}(r,\theta) = \frac{u(r+\Delta r,\theta) + u(r-\Delta r,\theta) - 2u(r,\theta)}{(\Delta r)^2}$$

$$\frac{\partial^2 u}{\partial \theta^2}(r,\theta) = \frac{u(r,\theta+\Delta\theta) + u(\ r,\theta-\Delta\theta\ ) - 2u(r,\theta)}{(\Delta\theta)^2}$$

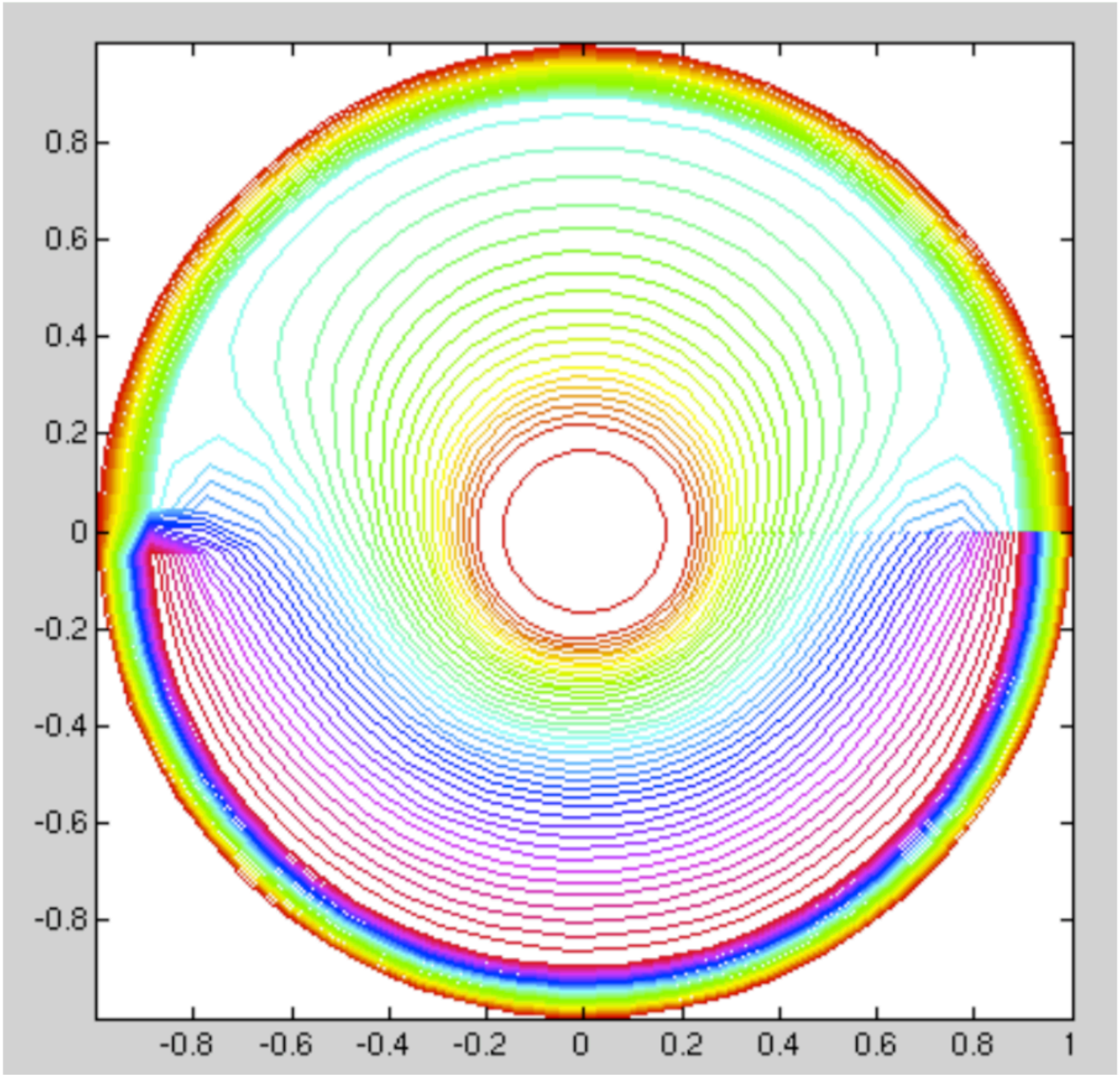
This gives the finite difference equation

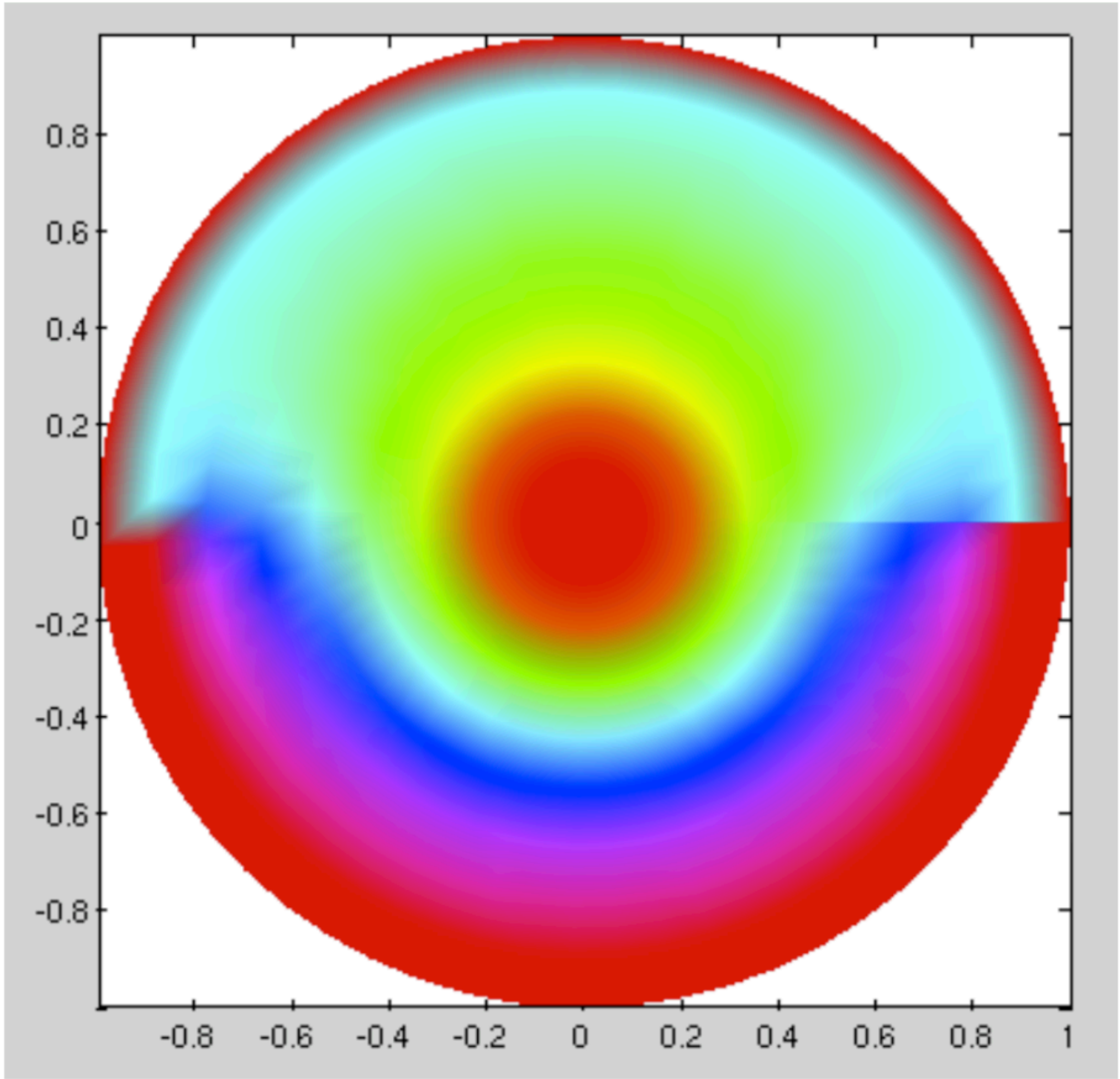
$$u(r,\theta) = \frac{1}{2(\Delta r)^2 + 2(\Delta\theta)^2}\,\big(r^2(\Delta\theta)^2(u(r+\Delta r,\theta) + u(r-\Delta r,\theta)) \\ r(\delta r)(\Delta\theta)^2(u(r+\Delta r,\theta) - u(r-\Delta r,\theta)) \\ (\Delta r)^2(u(r,\theta+\Delta\theta) + u(r\theta-\Delta\theta))\big)$$

The OCTAVE program relax2.m (below) iterates these equations (can you guess the boundary conditions?).

```
n=60;m=10;steps=1000;
dth=2.0*pi/59;dr=1.0/9;
theta=(0:59)*dth;r=(0:9)*dr;
pin=zeros(10,60); b=pin;
pin(1:2,:)=0.0;pin(3,:)=10.0;
pin(9,:)=100.0;
b(1:3,:)=1;b(9,:)=1;
p=pin;
for i=1:steps
i
for j=3:8
   for k=1:60
    coef=1.0/(2.0*((dr^2)+(r(j)^2)*(dth^2)));
    a2=((r(j)^2)*(dth^2))*(p(j+1,k)+p(j-1,k));
    a3=(dr*r(j)*(dth^2)/2.0)*(p(j+1,k)-p(j-1,k));
    a4=(dr^2)*(p(j,fixerp(k+1,n))+p(j,fixerm(k-1,n)));
    p(j,k)=coef*(a2+a3+a4);
   end
end
  p=p.*(1-b)+pin;
end
TH=zeros(10,60);RO=zeros(10,60);
for j=1:10
 TH(j,:)=theta;
end
for j=1:60
 RO(:,j)=r;
end
[X,Y,Z] = pol2cart(TH,RO,p);
figure;
contour(X,Y,Z,40);
colormap(hsv);
axis square
figure
pcolor(X,Y,Z);
shading interp;
colormap(hsv);
axis square
```

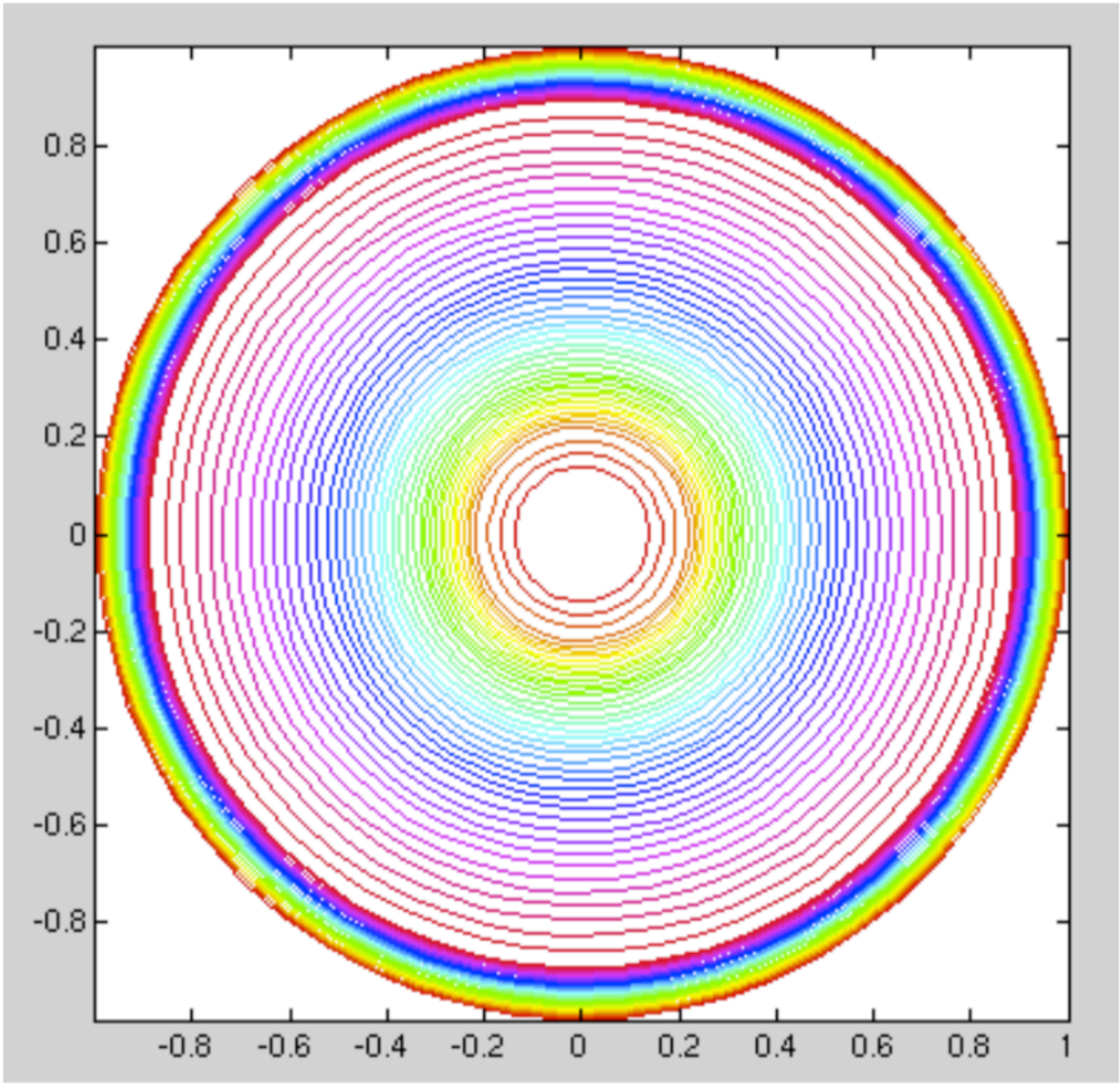
```
function z=fixerp(m,n)
if (m == (n+1))
   z=1;
else
   z=m;
end
endfunction

function z=fixerm(m,n)
if (m == 0)
    z=n;
else
    z=m;
end
endfunction
```

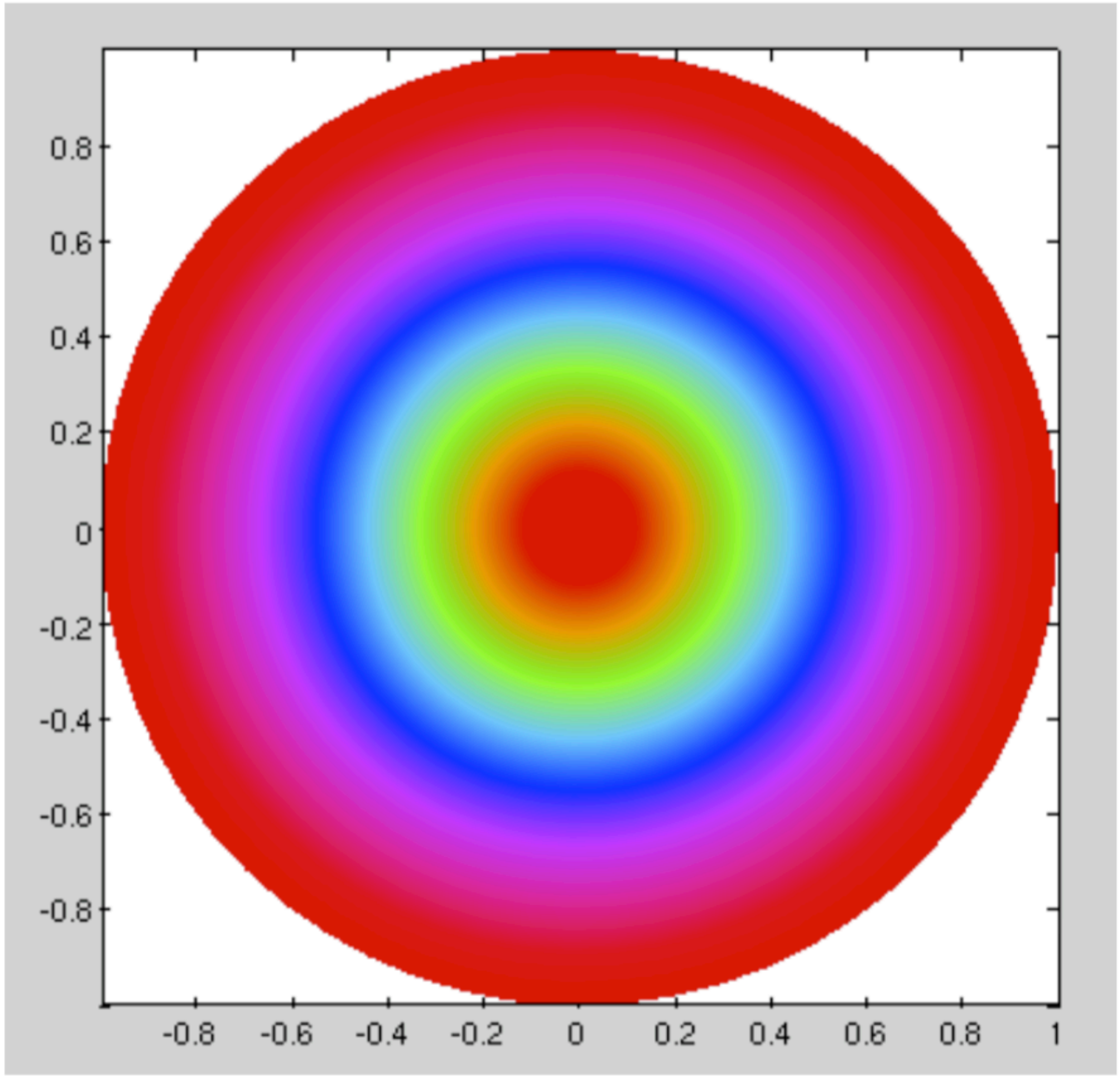

0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1


0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1

Changing the boundary conditions (Octave code relax3.m):

```
n=60;
m=10;
steps=1000;
dth=2.0*pi/59;
dr=1.0/9;
theta=(0:59)*dth;
r=(0:9)*dr;
pin=zeros(10,60); b=pin;
pin(1:2,:)=0.0;
pin(3,:)=10.0;
pin(9,1:30)=100.0;
pin(9,31:60)=200.0;
b(1:3,:)=1;
b(9,:)=1;
p=pin;
for i=1:steps
  i
  for j=3:8
   for k=1:60
    coef=1.0/(2.0*((dr^2)+(r(j)^2)*(dth^2)));
    a2=((r(j)^2)*(dth^2))*(p(j+1,k)+p(j-1,k));
    a3=(dr*r(j)*(dth^2)/2.0)*(p(j+1,k)-p(j-1,k));
    a4=(dr^2)*(p(j,fixerp(k+1,n))+p(j,fixerm(k-1,n)));
    p(j,k)=coef*(a2+a3+a4);
   end
  end
  p=p.*(1-b)+pin;
end
TH=zeros(10,60);
RO=zeros(10,60);
for j=1:10
 TH(j,:)=theta;
end
for j=1:60
 RO(:,j)=r;
end
[X,Y,Z] = pol2cart(TH,RO,p);
figure;
contour(X,Y,Z,40);
colormap(hsv);
axis square
figure
pcolor(X,Y,Z);
shading interp;
colormap(hsv);
axis square
```


0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1


0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1

Complex Variable — Existence of a Derivative

For a complex function of a complex variable given by $f(z) = u(z) + iv(z)$ where $z = x + iy$ and u, v are real functions, the derivative of $f(z)$ is defined by

$$f'(z) = \frac{df}{dz} = \lim_{\delta z \to 0} \frac{\delta f(z)}{\delta z} = \lim_{\delta z \to 0} \frac{f(z + \delta z) - f(z)}{\delta z}$$

provided that the limit is **independent** of the particular approach to the point z in the complex plane.

This is always true provided the following Cauchy-Riemann(C-R) conditions are satisfied:

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \quad , \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}$$

If these conditions are true at some point z and in the neighborhood of z, then they are necessary and sufficient conditions for the existence of the derivative of $f(z)$ or we say the function is differentiable in this region of the complex plane.

Analytic Functions

If $f(z)$ is differentiable at $z = z_0$ and in some small region around z_0, then we say that $f(z)$ is analytic at $z = z_0$.

Example:

$$w(z) = z^2 = (x + iy)^2 = x^2 - y^2 + 2xyi$$

$$u(x, y) = x^2 - y^2 \quad , \quad v(x, y) = 2xy$$

$$\frac{\partial u}{\partial x} = 2x = \frac{\partial v}{\partial y} \quad , \quad \frac{\partial u}{\partial y} = -2y = -\frac{\partial v}{\partial x}$$

This is true everywhere in the complex plane and thus $w(z)$ is analytic and differentiable everywhere and

$$\frac{dw}{dz} = 2z$$

Another example: Define $z^* = x - iy =$ complex conjugate.

$$w(z) = \frac{1}{z} = \frac{1}{z}\frac{z^*}{z^*} = \frac{x - iy}{x^2 + y^2}$$

$$u(x, y) = \frac{x}{x^2 + y^2} \quad , \quad v(x, y) = -\frac{y}{x^2 + y^2}$$

The Cauchy-Riemann conditions are satisfied everywhere but at $z = 0$.

Thus, the function $1/z$ is analytic everywhere but $z = 0$ and its derivative is

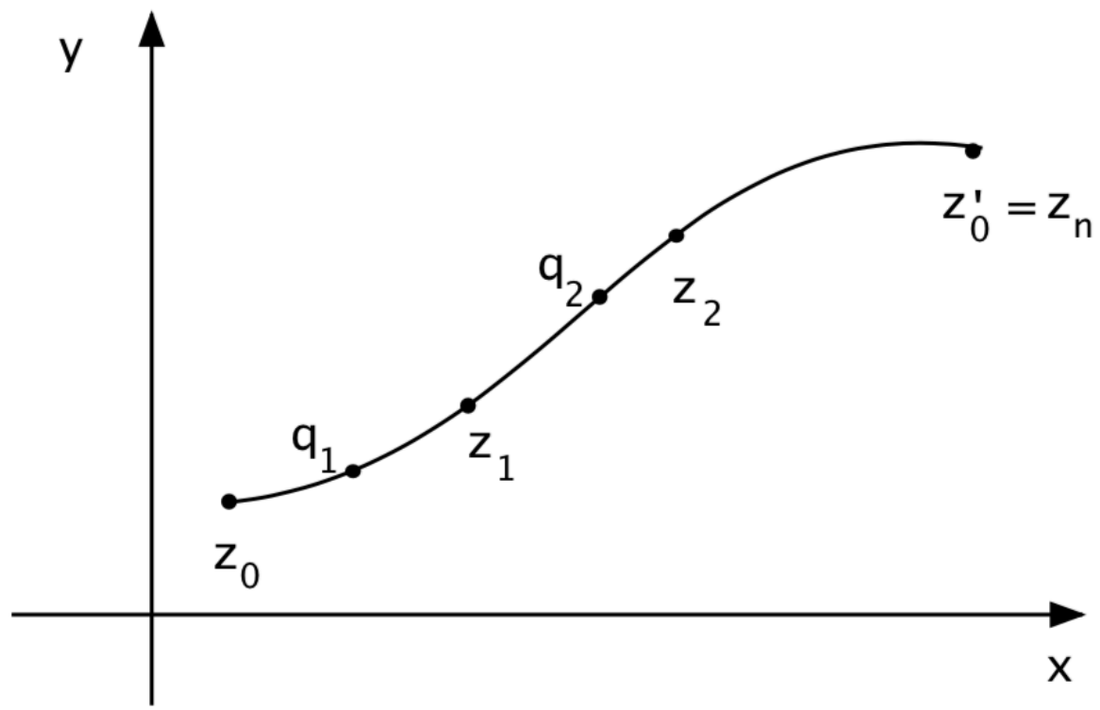
$$\frac{d(1/z)}{dz} = -\frac{1}{z^2}$$

in the analytic region.

Define a Contour Integral

The integral of a complex function over a contour(path) in the complex plane is defined in close analogy with the standard integral of a real function integrated along the real x-axis.

Divide the contour $z_0 \to z_0' = z_n$ into n intervals by picking $n-1$ intermediate points $z_1, z_2, \ldots$. on the contour (see figure)



Now consider the sum

$$S_n = \sum_{j=1}^{n} f(q_j)(z_j - z_{j-1})$$

where q_j is a point on the curve between z_j and z_{j-1}. Now let $n \to \infty$ with

$$|z_j - z_{j-1}| \to 0$$

for all j.

If the $\lim_{n\to\infty} S_n$ exists and is independent of the details of choosing the points z_j and q_j, then

$$\lim_{n\to\infty} \sum_{j=1}^{n} f(q_j)(z_j - z_{j-1}) = \int_{z_0}^{z_0'} f(z)dz$$

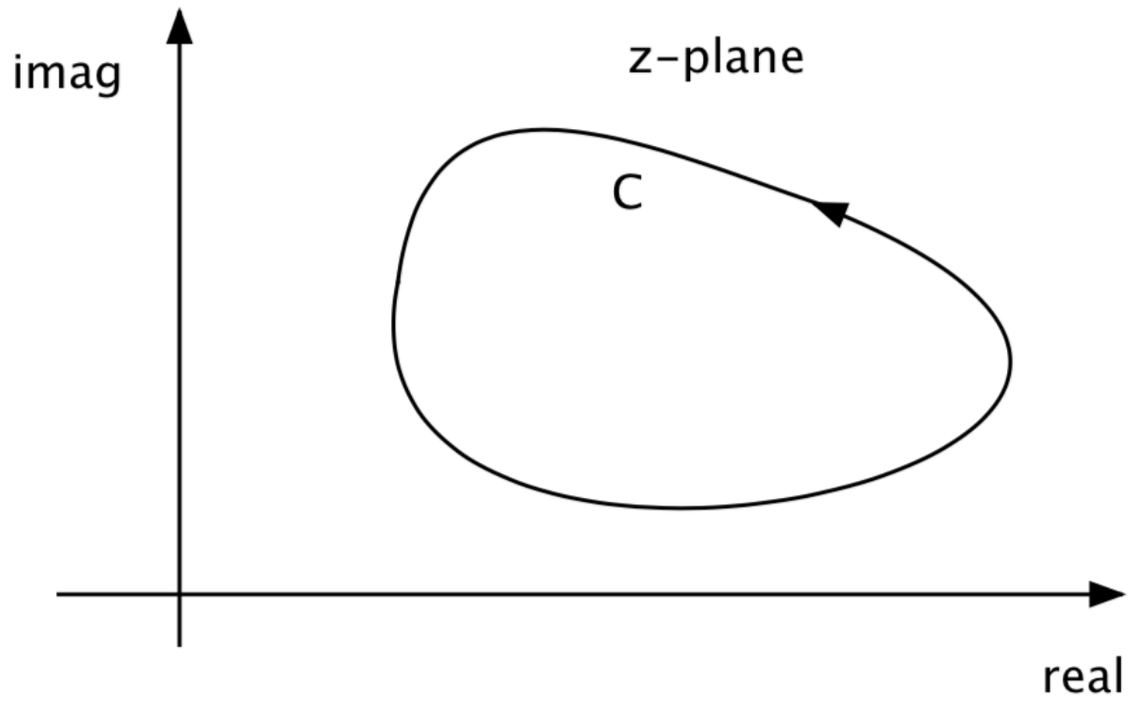
The RHS is called the **contour integral** of $f(z)$ (along the specified contour C from $z = z_0$ to $z = z_0'$.

Cauchy Integral Theorem

Now let $w(z)$ be a complex function which is analytic in some region of the complex plane and consider this integral

$$\oint_C w(z)dz$$

along a closed contour C which lies **entirely** within the analytic region as shown below:



Since $w(z)$ is analytic and obeys the C-R conditions, we have

$$\oint_C w(z)dz = \oint_C (u(z) + iv(z))d(x + iy)$$

$$= \oint_C (udx - vdy) + i \oint_C (vdx + udy)$$

$$= -\iint_R \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right) dxdy - i\iint_R \left(-\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) dxdy = 0$$

where R is are area inside the curve C and we have made use of Green's theorem. $\int_C Pdx + Qdy = \iint_D \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y}\right) dA$

So we have the **Cauchy Integral Theorem:**

If $f(z)$ is an analytic function whose derivative $f'(z)$ exists and is continuous at each point within and on the closed contour C, then

$$\oint_C f(z)dz = 0$$

We note that all integrations traverse the contour counterclockwise unless otherwise stated.

Contour Deformation

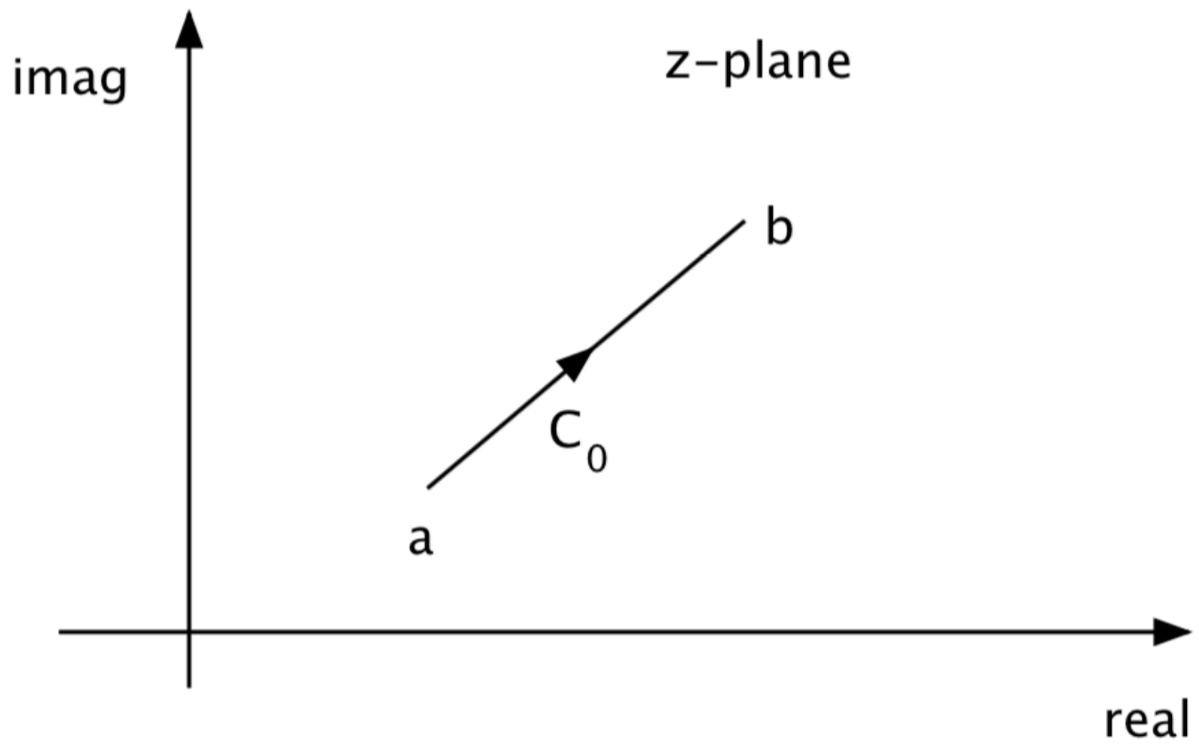
An important consequence of the Cauchy integral theorem is that

any contour of such complex integrals can be arbitrarily deformed within the analytic region without changing the value of the integral.

We can see this as follows: the integral

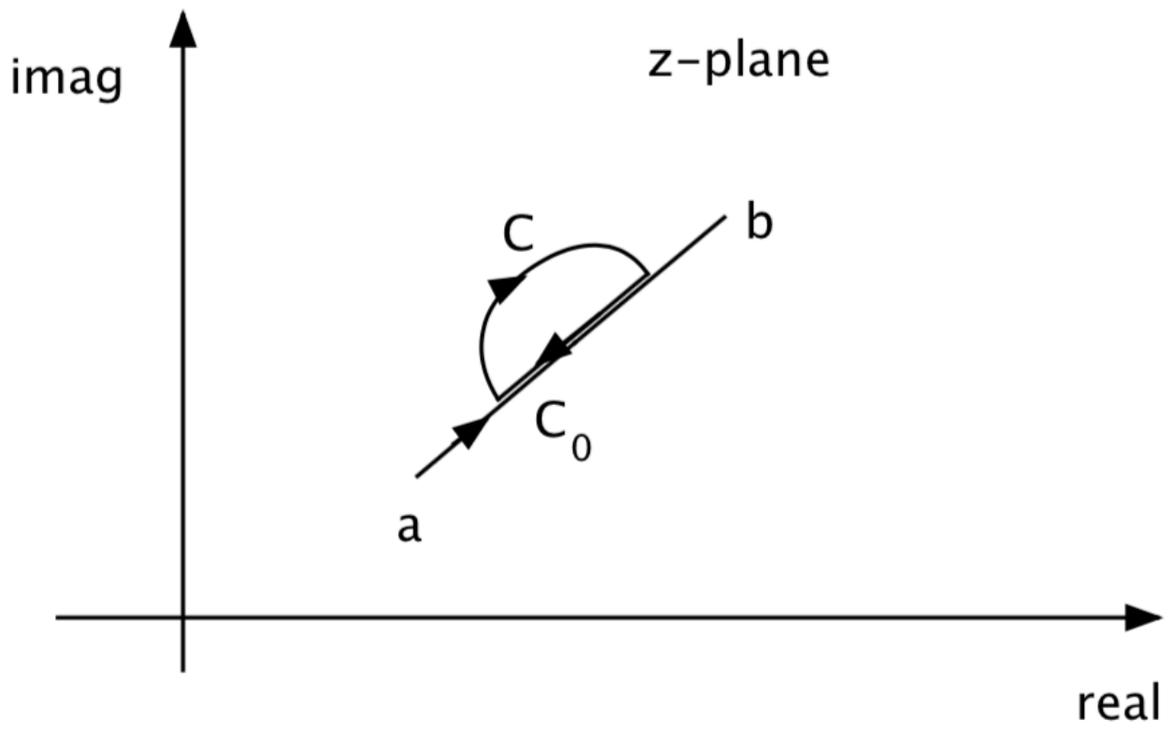
$$I = \int_{C_0} w(z)dz$$

is along the contour C_0 from a to b



We now add an integral with the same integrand but a different contour C

$$I = \int_{C_0} w(z)dz + \oint_C w(z)dz$$



The value is still I since $w(z)$ is analytic and thus

$$\oint_C w(z)dz = 0$$

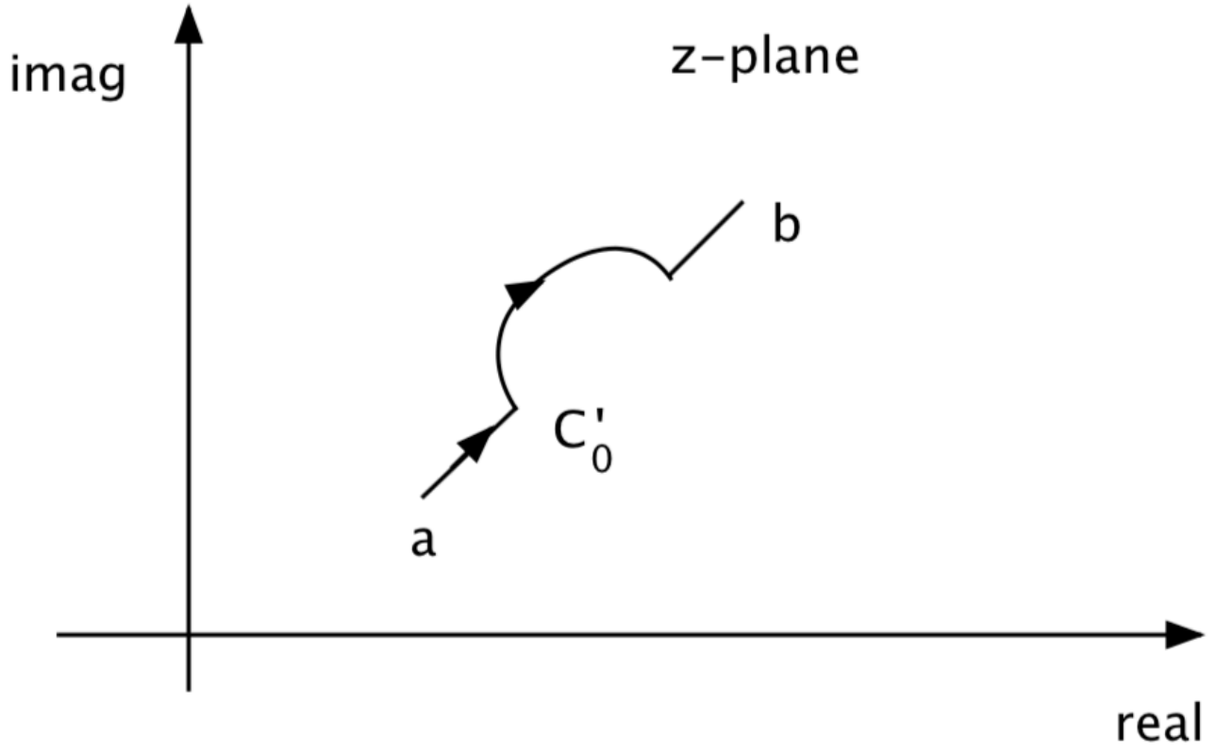
Notice, however, that two parts of the paths overlap.

The integral is the same over both of these paths but we are traversing them in opposite directions so they cancel out.

Therefore

$$I = \int_{C_0} w(z)dz = \int_{C_0'} w(z)dz$$

where C_0' is shown below:

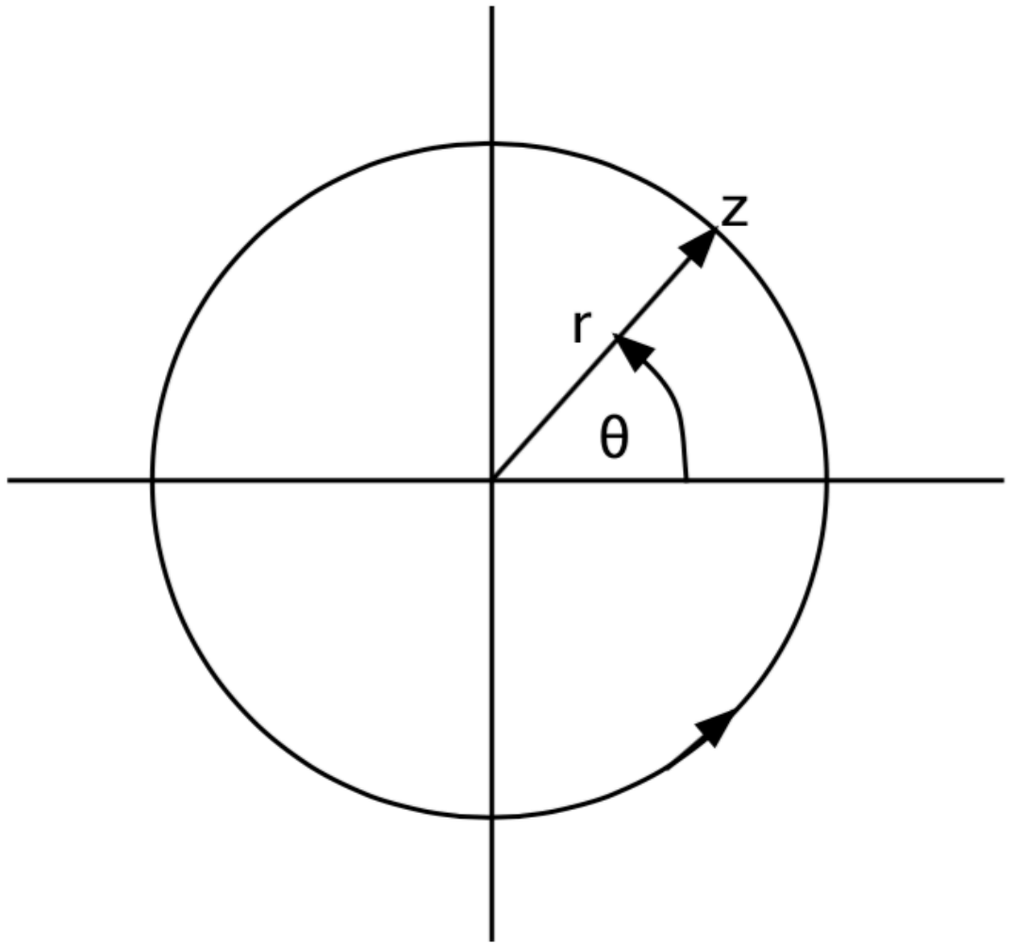


This means we can **freely deform** the contour in analytic regions.

An important example is the contour integral:

$$\int_C z^n dz$$

where C is a circle of radius $r > 0$ around the origin $z = 0$ in the positive mathematical sense (counterclockwise).



In polar coordinates we can parameterize z by

$$z = re^{i\theta} \rightarrow dz = ire^{i\theta}d\theta \text{ (on the circle where r = constant)}$$

For $n \neq 1$, we get

$$\frac{1}{2\pi i}\int_C z^n dz = \frac{r^{n+1}}{2\pi}\int_0^{2\pi} e^{i(n+1)\theta}d\theta = \frac{r^{n+1}}{2\pi i(n+1)}\left[e^{i(n+1)\theta}\right]_0^{2\pi} = 0$$

while for $n = 1$ we have

$$\frac{1}{2\pi i}\int_C = \frac{1}{2\pi}\frac{dz}{z}\int_0^{2\pi} d\theta = 1$$

Both results are **independent of** r.

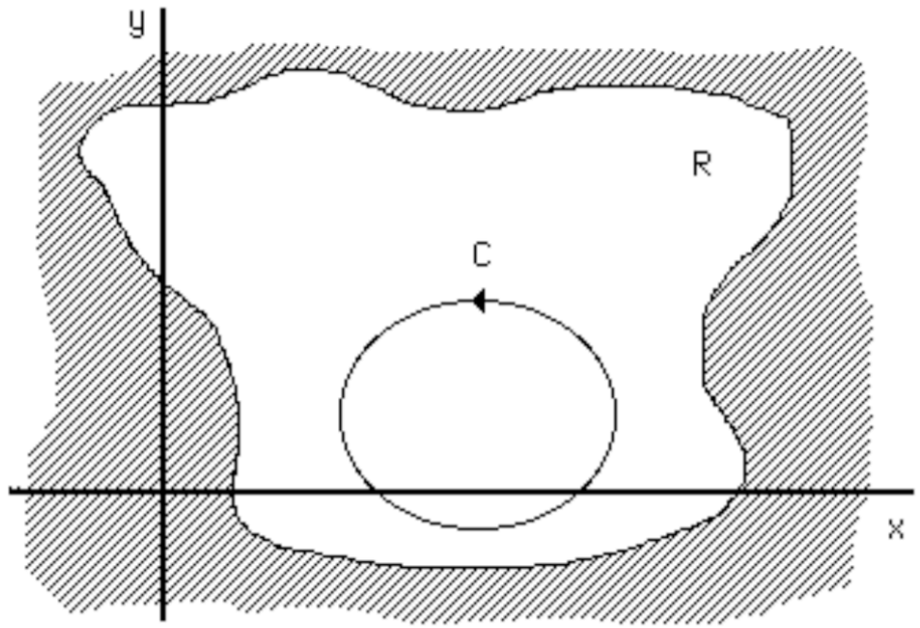
This is an example of the **Cauchy integral theorem**.

The Cauchy integral theorem is the first of **two basic theorems** in the study of complex variables.

Let us elaborate on our earlier definition:

Statement of the Theorem

If a function $f(z)$ is analytic (therefore single-valued) and its partial derivatives are continuous throughout some region R as shown in the figure,



then for every closed path C in R the contour integral of $f(z)$ around C is zero

$$\oint_C f(z)dz = 0$$

The Cauchy Integral Formula

Consider a function $f(z)$ that is analytic on and within a closed contour C.

Let us evaluate

$$\oint_C \frac{f(z)}{z - z_0} dz$$

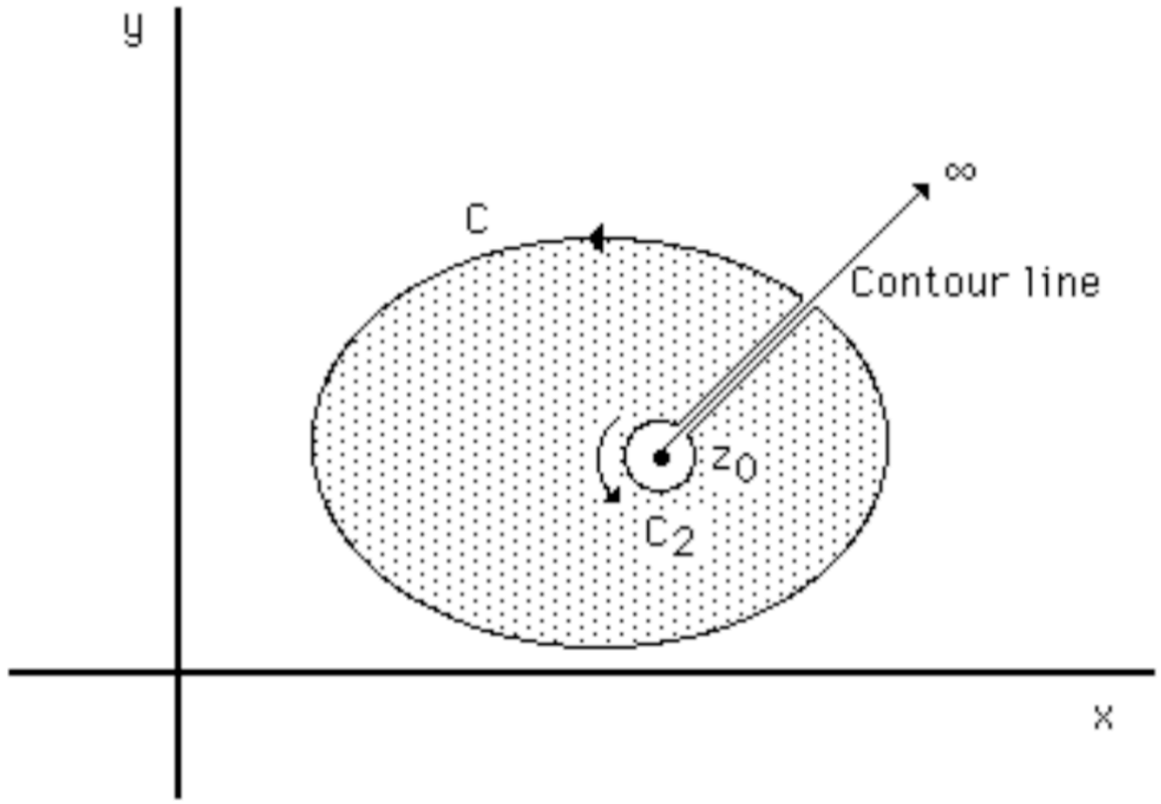
where z_0 is some point in the interior region bounded by C.

Although $f(z)$ is analytic, the integrand

$$\frac{f(z)}{z - z_0}$$

is not analytic at z_0 unless $f(z_0) = 0$.

If the contour is deformed as shown in the figure,



then Cauchy's integral theorem applies and we have

$$\oint_C \frac{f(z)}{z - z_0} dz - \oint_{C_2} \frac{f(z)}{z - z_0} dz = 0$$

where C is the original outer contour and C_2 is the circle surrounding the point z_0 (traversed in a counterclockwise direction).

If we let

$$z = z_0 + re^{i\theta}$$

on C_2, where eventually r will go to zero, then we have

$$\oint_C \frac{f(z)}{z - z_0} dz = \oint_{C_2} \frac{f(z)}{z - z_0} dz = \oint_{C_2} \frac{f(z_0 + re^{i\theta})}{re^{i\theta}} ire^{i\theta} d\theta$$

Taking the limit $r \to 0$, we get

$$\oint_C \frac{f(z)}{z - z_0} dz = if(z_0) \oint_{C_2} d\theta = 2\pi i f(z_0)$$

which is the **Cauchy integral formula**.

Here is a **remarkable result**.

The value of an analytic function $f(z)$ is given(by the formula) at an interior point $z = z_0$ once the values on the boundary C are specified. If z_0 is a point exterior to the region bounded by C , then the integral equals zero.

Summarizing the theorem:

Let $f(z)$ be be an analytic function within a closed contour C and continuous within and on C.

If a is any point within C, then

$$f(a) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z-a} dz$$

If a is any point outside C, then

$$0 = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z-a} dz$$

Derivatives of a Complex Function

We can write

$$f(z) = \frac{1}{2\pi i} \oint_C \frac{f(q)}{q-z} dq$$

where z is any point interior to C.

We then have

$$f'(z) = \lim_{h\to 0} \frac{f(z+h)-f(z)}{h} = \frac{1}{2\pi i} \lim_{h\to 0} \frac{\oint_C \frac{f(q)}{q-z-h}dq - \oint_C \frac{f(q)}{q-z}dq}{h}$$

$$= \frac{1}{2\pi i} \lim_{h\to 0} \frac{\oint_C f(q)\left(\frac{1}{q-z-h} - \frac{1}{q-z}\right)dq}{h}$$

$$= \frac{1}{2\pi i} \lim_{h\to 0} \frac{\oint_C f(q)\left(\frac{h}{(q-z-h)(q-z)}\right)dq}{h}$$

$$= \frac{1}{2\pi i} \lim_{h\to 0} \oint_C f(q)\left(\frac{1}{(q-z-h)(q-z)}\right)dq$$

$$= \frac{1}{2\pi i} \oint_C \frac{f(q)}{(q-z)^2}dq$$

In a similar manner we have

$$f^{(n)}(z) = \frac{n!}{2\pi i} \oint_C \frac{f(q)}{(q-z)^{n+1}}dq$$

Taylor Series

We have

$$f(z) = \frac{1}{2\pi i} \oint_C \frac{f(q)}{q - z} dq$$

where C is a circle centered at a and of radius $r < \delta$ and z lies inside C.

δ is the distance from a to the nearest point of C.

This means that

$$|z - a| < r$$

Now let

$$k = \frac{z - a}{q - a}$$

Then

$$1 - k = \frac{q - z}{q - a}$$

$$\frac{1}{1-k} = \frac{q-a}{q-z} = \sum_{n=0}^{\infty} k^n \quad , \quad |k| < 1$$

This implies that

$$\frac{1}{q-z} = \frac{1}{q-a} \sum_{n=0}^{\infty} \left(\frac{z-a}{q-a} \right)^n = \frac{1}{q-a} + \frac{z-a}{(q-a)^2} + \ldots + \frac{(z-a)^n}{(q-a)^{n+1}} + \ldots$$

Since, on the circle C

$$|k| = \left| \frac{z-a}{q-a} \right| = \frac{r}{\delta} < 1$$

this series converges uniformly on C.

This means that we can multiply by

$$\frac{f(q)}{2\pi i}$$

and integrate term by term around C.

We get

$$\oint_C \frac{f(q)}{q-z}dq = \oint_C dq\frac{f(q)}{q-a} + \oint_C dqf(q)\frac{z-a}{(q-a)^2}$$
$$+ .... + \oint_C dqf(q)\frac{(z-a)^n}{(q-a)^{n+1}} + ...$$

$$f(z) = \oint_C dq\frac{f(q)}{q-a} + (z-a)\oint_C dqf(q)\frac{1}{(q-a)^2}$$
$$+ .... + (z-a)n\oint_C dqf(q)\frac{1}{(q-a)^{n+1}} + ...$$

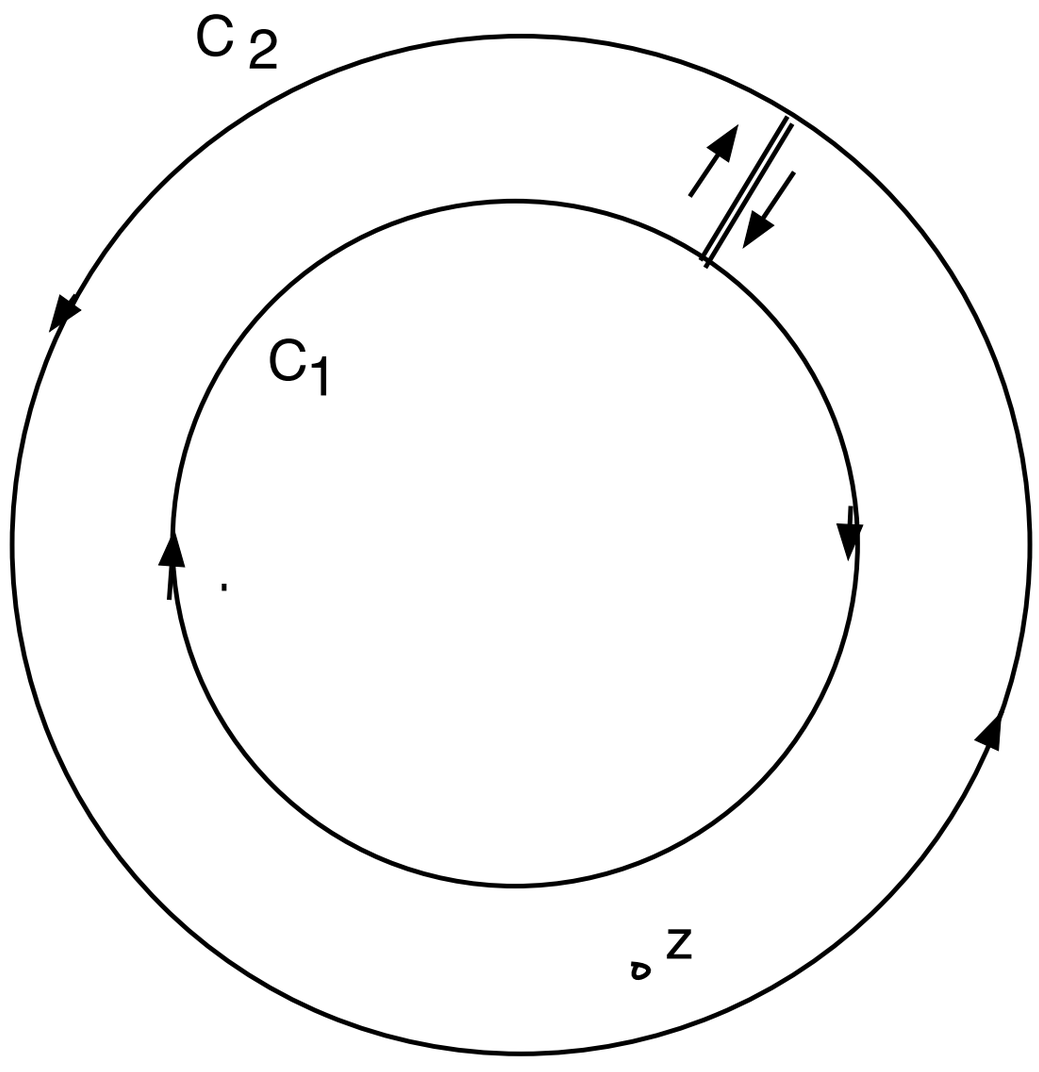
$$f(z) = f(a) + f'(a)(z-a) + ... + \frac{f(n)(a)}{n!}(z-a)^n + ...$$

which is the Taylor series.

Laurent Series

We assume that $f(z)$ is single-valued and analytic throughout the closed annulus bounded by the outer circle C_2 and the inner concentric circle C_1.

Let z be a point inside the annulus.



We then have

$$f(z) = \frac{1}{2\pi i} \oint_C \frac{f(q)}{q-z} dq$$

where C is the total boundary of the annulus traversed so that the interior of the annulus always lies to the left (counterclockwise around C_2 and clockwise around C_1).

This means that

$$f(z) = \frac{1}{2\pi i} \oint_{C_2} \frac{f(q)}{q-z} dq - \frac{1}{2\pi i} \oint_{C_1} \frac{f(q)}{q-z} dq$$

Now

$$\frac{1}{2\pi i} \oint_{C_2} \frac{f(q)}{q-z} dq = \sum_{n=0}^{\infty} a_n (z-a)^n$$

where a is the common center of C_1 and C_2 and

$$a_n = \frac{1}{2\pi i} \oint_{C_2} \frac{f(q)}{(q-a)^{n+1}} dq$$

We note that a_n is not in general equal to

$$\frac{f^{(n)}(a)}{n!}$$

since $f(z)$ is not necessarily analytic throughout the interior of C_2.

Now

$$\frac{1}{z-q} = \frac{1}{z-a} + \frac{q-a}{(z-a)^2} + ... + \frac{(q-a)^n}{(z-a)^{n+1}} + ...$$

This series converges uniformly on C_1. Therefore

$$\begin{aligned} -\frac{1}{2\pi i}\oint_{C_1} dq \frac{f(q)}{q-z} &= \frac{1}{2\pi i}\frac{1}{z-a}\oint_{C_1} dq f(q) \\ &+ \frac{1}{2\pi i}\frac{1}{(z-a)^2}\oint_{C_1} dq f(q)(q-a) \\ &+ ... + \frac{1}{2\pi i}\frac{1}{(z-a)^{n+1}}\oint_{C_1} dq f(q)(q-a)^n + ... \end{aligned}$$

or

$$-\frac{1}{2\pi i}\oint_{C_1} dq \frac{f(q)}{q-z} = \sum_{n=1}^{\infty} \frac{b_n}{(z-a)^n}$$

where

$$b_n = \frac{1}{2\pi i}\oint_{C_1} dq f(q)(q-a)^{n-1}$$

Putting this all together we get

$$f(z) = \sum_{-\infty}^{\infty} a_n (z-a)^n$$

where

$$a_n = \frac{1}{2\pi i}\oint_{C} dq \frac{f(q)}{(q-a)^{n-1}}$$

for all values of n.

The contour C is any closed contour which passes around the annulus and lies between the two circles.

Notice that when $f(z)$ is analytic throughout the interior of the inner circle C_1, all the terms with negative n are absent (use the Cauchy theorem) and it reduces to a Taylor series.

Example: Let

$$f(q) = \frac{1}{q(q-1)}$$

Choose $a = 0$. We then have $r = 0$ and $R = 1$ as the radii of the two concentric circles defining the region of analyticity of $f(q)$.

We then obtain

$$a_n = \frac{1}{2\pi i}\oint_C dq \frac{f(q)}{(q-a)^{n-1}} = \frac{1}{2\pi i}\oint_C dq \frac{1}{(q)^{n+2}(q-1)}$$

$$= -\frac{1}{2\pi i}\oint_C \sum_{m=0}^{\infty} q^m \frac{dq}{(q)^{n+2}} = -\frac{1}{2\pi i}\sum_{m=0}^{\infty}\oint_C \frac{dq}{(q)^{n+2-m}}$$

Now we use the polar form of q to integrate around the circle

$$a_n = -\frac{1}{2\pi i}\sum_{m=0}^{\infty}\oint_C \frac{dq}{(q)^{n+2-m}} = -\frac{1}{2\pi i}\sum_{m=0}^{\infty}\oint_C \frac{ire^{i\theta}d\theta}{((r)^{n+2-m}}e^{i(n+2-m)\theta}$$

$$= -\frac{1}{2\pi i}\sum_{m=0}^{\infty}\delta_{n-m+2,1}$$

This gives

$$a_n = \begin{cases} -1 & n \geq -1 \\ 0 & n < -1 \end{cases}$$

The Laurent expansion becomes

$$\frac{1}{z(z-1)} = -\frac{1}{z} - 1 - z^2 - z^3 - ..... = -\sum_{n=-1}^{\infty} z^n$$

We have smashed a peanut with a sledgehammer, but the method is clear and works very well when a real sledgehammer is necessary.

Let us look at all this another way.

Laurent's Theorem

Let C_1 and C_2 be two concentric circles with centers at z_0.

Let $f(z)$ be analytic in the region R **between** the circles.

Then $f(z)$ can be expanded in a series of the form

$$f(z) = a_0 + a_1(z - z_0) + a_2(z - z_0)^2 + \ldots\ldots + \frac{b_1}{z - z_0} + \frac{b_2}{(z - z_0)^2} + \ldots\ldots$$

A Taylor series has only one circle about z_0 which implies that $b_i = 0$ so that

$$f(z) = a_0 + a_1(z - z_0) + a_2(z - z_0)^2 + \ldots\ldots$$

where

$$a_n = \frac{1}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{n+1}} \quad , \quad b_n = \frac{1}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{-n+1}}$$

and $C =$ any closed curve surrounding z_0 in R.

Example: We consider

$$W(z) = \frac{1}{1+z^2} = \frac{1}{(z+i)(z-i)} = \frac{i}{2}\left[\frac{1}{(z+i)} - \frac{1}{(z-i)}\right]$$

(a) Taylor series about $z = 0$: We have

$$\frac{1}{z-a} = -\sum_{n=0}^{\infty} \frac{1}{(a-z_0)^{n+1}}(z-z_0)^n \quad , \quad z_0 = \text{ expansion point}$$

Therefore,

$$\frac{1}{(z+i)} = -\sum_{n=0}^{\infty} \frac{(-1)^{n+1}}{(i+z_0)^{n+1}}(z-z_0)^n$$

$$\frac{1}{(z-i)} = -\sum_{n=0}^{\infty} \frac{1}{(i-z_0)^{n+1}}(z-z_0)^n$$

so that

$$W(z) = -\frac{i}{2} - \sum_{n=0}^{\infty}\left[\frac{(-1)^{n+1}}{(i+z_0)^{n+1}} - \frac{1}{(i-z_0)^{n+1}}\right](z-z_0)^n$$

inside the circle $|z| < 1$.

For $z_0 = 0$ we have

$$W(z) = -\frac{1}{2}\sum_{n=0}^{\infty}\frac{1}{i^n}\left[(-1)^n + 1\right]z^n$$

Now

$$\frac{1}{2}\left[(-1)^n + 1\right] = \begin{cases} 1 & n = \text{ even} \\ 0 & n = \text{ odd} \end{cases}$$

so that

$$W(z) = 1 - z^2 + z^4 - z^6 + ...$$

as expected.

(b) What is the Laurent series expansion of

$$f(z) = \frac{1}{z^2 - 3z + 2} = \frac{1}{(z-2)(z-1)} = \frac{1}{(z-2)} - \frac{1}{(z-1)}$$

valid in each of the regions

$$(1)\ 1 < |z| < 2 \ , \ \ (2)\ 2 < |z| \ , \ \ (3)\ |z| < 2$$

(1) To obtain a Laurent series expansion in this region, we expand about the origin.

We write

$$f(z) = -\frac{1}{2}\left(\frac{1}{1 - z/2}\right) - \frac{1}{z}\left(\frac{1}{1 - 1/z}\right)$$

The first fraction has a singularity at $z/2 = 1$ and can be expanded in a Taylor series that converges if $z < 2$.

The second fraction has a singularity at $1/z = 1$ and can be expanded in a Laurent series that converges if $1 < z$.

The two fractions are expressed in the appropriate series are

$$-\frac{1}{2}\left(\frac{1}{1-z/2}\right) = -\frac{1}{2}\left(1+\frac{z}{2}+\left(\frac{z}{2}\right)^2+\left(\frac{z}{2}\right)^3+....\right)$$
$$= -\frac{1}{2}-\frac{z}{4}-\frac{z^2}{8}-\frac{z^3}{16}-.....$$

$$-\frac{1}{z}\left(\frac{1}{1-1/z}\right) = -\frac{1}{z}\left(1+\frac{1}{z}+\left(\frac{1}{z}\right)^2+\left(\frac{1}{z}\right)^3+....\right)$$
$$= -\frac{1}{z}-\frac{1}{z^2}-\frac{1}{z^3}-\frac{1}{z^4}-.....$$

where the first series is valid for $|z| < 2$ and the second series is valid for $1 < |z|$. Adding the two series we get the Laurent series as

$$f(z) = \frac{1}{z^2-3z+2} = ...-\frac{1}{z^3}-\frac{1}{z^2}-\frac{1}{z}-\frac{1}{2}-\frac{z}{4}-\frac{z^2}{8}-\frac{z^3}{16}-....$$

valid for $1 < |z| < 2$.

(2) In this region we expand

$$\frac{1}{z-1} = \frac{1}{z}\left(\frac{1}{1-1/z}\right)$$

and as above

$$\frac{1}{z}\left(\frac{1}{1-1/z}\right) = \frac{1}{z} + \frac{1}{z^2} + \frac{1}{z^3} + \frac{1}{z^4} + \ldots\ldots$$

which is valid for $1 < |z|$.

However, we now write

$$\frac{1}{z-2} = \frac{1}{z}\left(\frac{1}{1-2/z}\right) = \frac{1}{z} + \frac{2}{z^2} + \frac{4}{z^3} + \frac{8}{z^4} + \ldots\ldots$$

which is valid for $2 < |z|$.

Thus we have the Laurent series

$$f(z) = \frac{1}{z^2-3z+2} = \frac{1}{z^2} + \frac{3}{z^3} + \frac{7}{z^4} + \frac{15}{z^5} + \ldots..$$

valid for $2 < |z|$.

(3) In this region, we expand about the point $z = 1$ to get

$$f(z) = \frac{1}{z^2 - 3z + 2} = \frac{1}{z-1}\left(-\frac{1}{2-z}\right) = \frac{1}{z-1}\left(\frac{-1}{1-(z-1)}\right)$$
$$= \frac{-1}{z-1}\left(1 + (z-1) + (z-1)^2 + (z-1)^3 + (z-1)^4 + ...\right)$$
$$= \frac{-1}{z-1} - 1 - (z-1) - (z-1)^2 - (z-1)^3 - (z-1)^4 - .....$$

valid for $0 < |z-1| < 1$.

Calculus Of Residues

Singularities: Poles

In the Laurent expansion of $f(z)$ about z_0

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z-a)^n$$

If $a_n = 0$ for $n < -m < 0$ and $a_m \neq 0$, we say that is a pole of order m.

For instance, if $m = 1$, that is, if

$$\frac{a_{-1}}{z - z_0}$$

is the first non-vanishing term in the Laurent series, then we have a **pole of order one, which is called a simple pole**.

Residue Theorem

If the Laurent expansion of a function

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - a)^n$$

is integrated term by term by using a closed contour that encircles one isolated singular point z_0 once in a counterclockwise sense, we obtain

$$\oint_C f(z)dz = \sum_{n=-\infty}^{\infty} a_n \oint_C (z - z_0)^n dz = \sum_{n=-\infty}^{\infty} a_n \left. \frac{(z - z_0)^{n+1}}{n+1} \right|_{z-1}^{z_1} = 0$$

for all $n \neq 1$.

However, for $n = -1$,

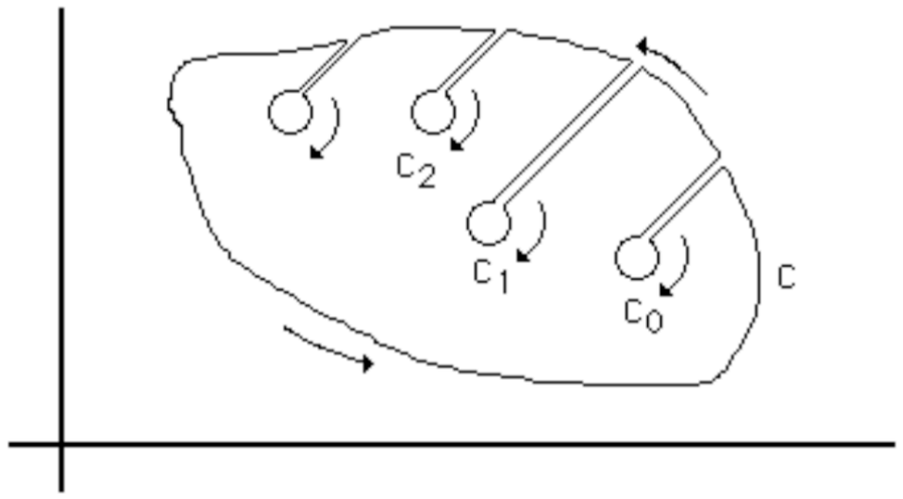
$$a_{-1} \oint_C (z - z_0)^{-1} dz = a_{-1} \oint_C \frac{ire^{i\theta}}{re^{i\theta}} d\theta = 2\pi i a_{-1}$$

Summarizing

$$\frac{1}{2\pi i} \oint_C f(z) dz = a_{-1}$$

The constant a_{-1}, which is the coefficient of $(z - z_0)^{-1}$ in the Laurent expansion , is called the **residue** of $f(z)$ at $z = z_0$.

If we have a set of isolated singularities, then we can handle them by deforming the our contour as shown in the figure



Cauchy's integral theorem then gives

$$\oint_C f(z)dz + \oint_{C_0} f(z)dz + \oint_{C_1} f(z)dz + \oint_{C_2} f(z)dz + ... = 0$$

The circular integral around any singular point is given by

$$\oint_{C_i} f(z)dz = -2\pi i a_{-1z_i}$$

(negative sign from clockwise integration as shown).

Putting this all together we get,

$$\oint_C f(z)dz = 2\pi i(a_{-1z_0} + a_{-1z_1} + a_{-1z_2} + a_{-1z_3} + ...)$$

$$= 2\pi i(\text{sum of enclosed residues})$$

This is the **residue theorem**.

The problem of evaluating one or more contour integrals is replaced by the algebraic problem of computing residues at the enclosed singular points.

The residues are obviously very important.

We need a general way to calculate them.

If we know the Laurent series for a function, then the residue is simply the coefficient of the $(z - z_0)^{-1}$ term.

But, often, we do not know the Laurent series.

We can always, however, assume that a Laurent series exists and then write

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n$$

$$a_n = \frac{1}{2\pi i} \oint_C \frac{f(z')}{(z' - z)^{n+1}} dz'$$

The coefficient a_{-1} or the residue for a pole of order n is then given by

$$a_{-1} = \frac{1}{(n-1)!} \lim_{z \to z_0} \frac{d^{n-1}}{dz^{n-1}} (f(z)(z - z_0)^n)$$

Examples:

First-order pole ($n = 1$):

$$f(z) = \frac{a_1}{z - z_0} + a_0 + a_1(z - z_0) + a_2(z - z_0)^2 + ...$$

We have

$$\lim z \to z_0 [f(z)(z - z_0)] = a_{-1}$$

Second-oder pole ($n = 2$):

$$f(z) = \frac{a_2}{(z - z_0)^2} + \frac{a_1}{z - z_0} + a_0 + a_1(z - z_0) + a_2(z - z_0)^2 + ...$$

We have

$$\lim z \to z_0 \frac{d}{dz} [f(z)(z - z_0)^2] = a_{-1}$$

Evaluation of Definite Integrals

now for the useful stuff after all those mathematical proof....

Integrals of the form

$$I = \int_0^{2\pi} f(\sin\theta, \cos\theta) d\theta$$

where f is a finite and single-valued function for all values of θ.

We let

$$z = re^{i\theta} \rightarrow dz = ire^{i\theta} \rightarrow d\theta = -i\frac{dz}{z}$$

$$\sin\theta = \frac{z - z^{-1}}{2i} \quad , \quad \cos\theta = \frac{z + z^{-1}}{2}$$

The integral becomes (choosing $r = 1$)

$$I = -i \oint_{\substack{unit \\ circle}} f\left(\frac{z - z^{-1}}{2i}, \frac{z + z^{-1}}{2}\right) \frac{dz}{z}$$

with the new path of integration(as indicated) the **unit circle**.

By the residue theorem we get

$$I = (-i)2\pi i \sum (\text{residues within the unit circle})$$

where we must find the residues of $f(z)/z$.

Example:

$$I = \int_0^{2\pi} \frac{d\theta}{1 + \epsilon \cos\theta} \quad , \quad |\epsilon| < 1$$

This becomes

$$I = -i \oint_{\substack{unit \\ circle}} \frac{dz}{z\left(1 + \frac{\epsilon}{2}(z + z^{-1})\right)} = i\frac{2}{\epsilon} \oint_{\substack{unit \\ circle}} \frac{dz}{z^2 + \frac{2z}{\epsilon} + 1}$$

The denominator has roots

$$z_{\pm} = -\frac{1}{\epsilon} \pm \sqrt{1 - \epsilon^2}$$

Now z_+ is within the unit circle and z_- is outside.

The integrand looks like

$$\frac{1}{(z - z_+)(z_+ - z_-)}$$

near $z = z_+$, and thus,

$$a_{-1} = \frac{1}{(z_+ - z_-)} = \frac{\epsilon}{2\sqrt{1 - \epsilon^2}}$$

The integral then becomes

$$I = -i\frac{2}{\epsilon}2\pi i\frac{\epsilon}{2\sqrt{1 - \epsilon^2}} = \frac{2\pi}{\sqrt{1 - \epsilon^2}} \quad , \quad |\epsilon| < 1$$

A truly amazing procedure!

Integrals of the form

$$I = \int_{-\infty}^{\infty} f(x)dx$$

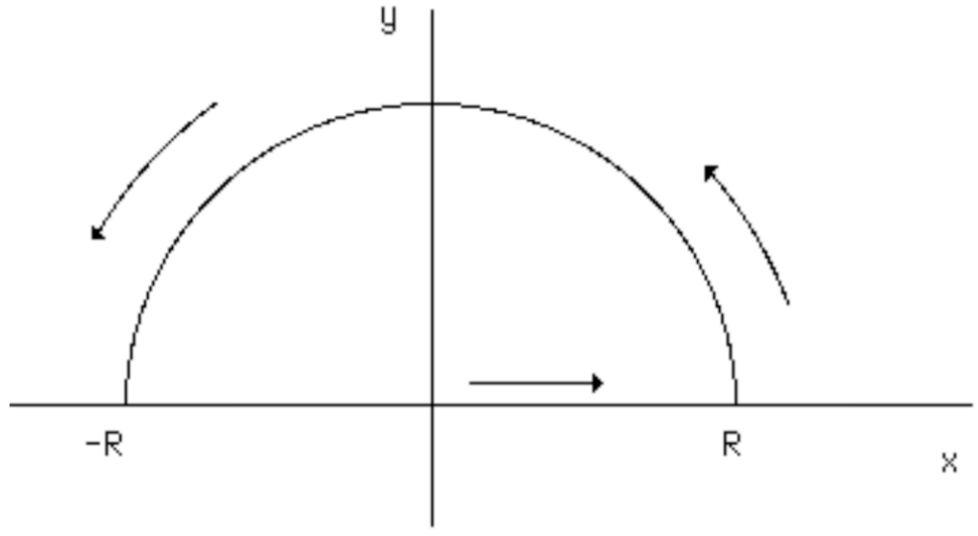
where

(a) $f(z)$ is analytic in the upper half plane except for a finite number of poles(no poles on the real axis)

(b) $f(z)$ vanishes as strongly as

$$\frac{1}{z^2} \quad \text{for} \quad |z| \to \infty \quad , \quad 0 \leq \arg(z) \leq \pi$$

With these conditions, we can take the contour of integration as the real axis $[-R, R]$ + a semi-circle in the upper half-plane as shown in the figure:



where we eventually let the radius R of the semicircle become infinitely large.

Then we have

$$\oint f(z)dz = \lim_{R\to\infty}\int_{-R}^{R} f(x)dx + \lim_{R\to\infty}\int_{0}^{\pi} f(Re^{i\theta})d(Re^{i\theta})$$
$$= 2\pi i \sum(\text{sum of residues in the upper half-plane})$$

where the integral over the semicircle generally vanishes(**see example below**) and we get

$$I = \int_{-\infty}^{\infty} f(x)dx = 2\pi i \sum(\text{sum of residues in the upper half-plane})$$

Example:

$$I = \int_{-\infty}^{\infty} \frac{dx}{1+x^2} = 2\pi i \sum (\text{sum of residues in the upper half-plane})$$

The first question is always...where are the poles?

$$\frac{1}{1+z^2} = \frac{1}{z+i} - \frac{1}{z-i} \rightarrow 2 \text{ simple poles at } \pm i$$

with

$$a_{-1} = \pm \frac{1}{2i}$$

We then get(since only the pole at $z = i$ lies within the contour)

$$I = \int_{-\infty}^{\infty} f(x)dx = 2\pi i \frac{1}{2i} = \pi$$

Show once: Vanishing of integral on upper semi-circle in limit $R \rightarrow \infty$.

On the upper semi-circle, $z = Re^{i\theta}$ so that

$$\lim_{R\to\infty}\int_0^{\pi}\frac{dz}{1+z^2} = \lim_{R\to\infty}\int_0^{\pi}\frac{iRe^{i\theta}}{1+R^2e^{2i\theta}}d\theta = i\lim_{R\to\infty}\frac{1}{R}\int_0^{\pi}d^{-i\theta}d\theta = 0$$

Integrals of the form

$$I = \int_{-\infty}^{\infty} f(x)e^{iax}dx \quad , \quad a \text{ real and positive}$$

This is just the Fourier transform we defined earlier.

We assume two conditions:

(a) $f(z)$ is analytic in the upper half plane except for a finite number of poles(no poles on the real axis)

(b)

$$\lim_{|z|\to\infty} f(z) = 0 \quad , \quad 0 \le \arg(z) \le \pi$$

We use the same contour as in the previous example(the real axis plus a large semicircle).

The application of the residue theorem is the same as before, except that it is more difficult to show that the integral goes to zero over the large semicircle.

On the semicircle the integral becomes

$$I_R = \int_0^\pi f(Re^{i\theta}) e^{iaR\cos\theta - aR\sin\theta} iRe^{i\theta} d\theta$$

We let R be so large that

$$|f(z)| = |f(Re^{i\theta})| < \epsilon$$

Then we get

$$|I_R| \leq \epsilon R \int_0^\pi e^{-aR\sin\theta} d\theta = 2\epsilon R \int_0^{\pi/2} e^{aR\sin\theta} d\theta$$

Now in the range $[0, \pi/2]$, $2\theta/\pi \leq \sin\theta$.

Thus, we have

$$|I_R| \leq \epsilon R \int_0^\pi e^{-2aR\theta/\pi} d\theta = 2\epsilon R \frac{1 - e^{-aR}}{2aR/\pi}$$

Finally,

$$\lim_{R\to\infty} |I_R| \leq \frac{\pi}{a}\epsilon \to 0 \quad \text{as} \quad \epsilon \to 0 (R \to \infty)$$

Using the contour we then have

$$I = \int_{-\infty}^{\infty} f(x) e^{iax} dx + \lim_{R\to\infty} |I_R|$$

$$= 2\pi i \sum (\text{sum of residues in the upper half-plane})$$

or for $a > 0$

$$\int_{-\infty}^{\infty} f(x) e^{iax} dx = 2\pi i \sum (\text{sum of residues in the upper half-plane})$$

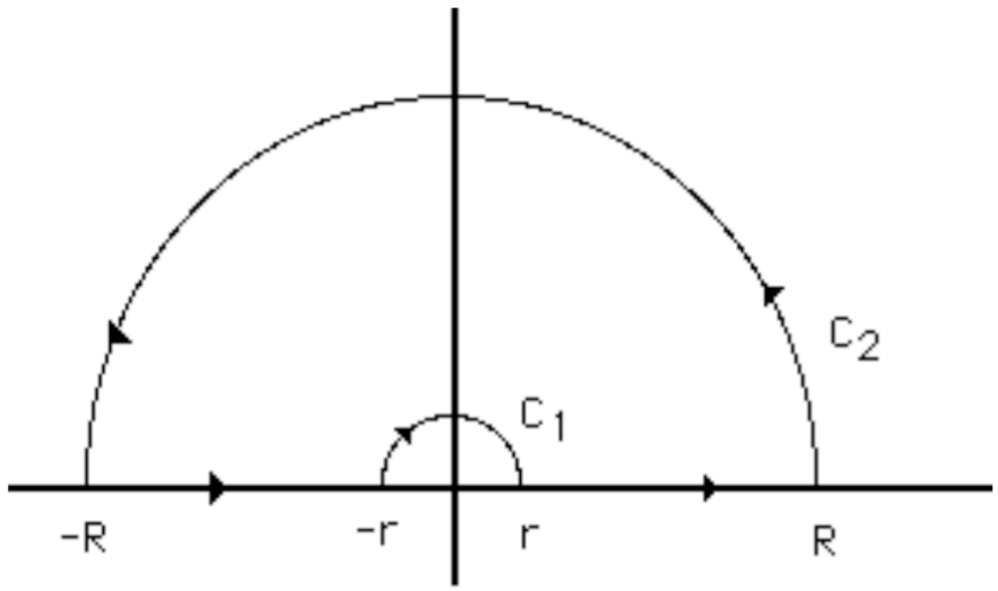
This allows us to evaluate many Fourier transform integrals.

Note that if $a < 0$, then we just close contour in **lower half-plane**.

Example:

$$I = \int_0^\infty \frac{\sin x}{x} dx$$

We use the contour shown in the figure below:



and evaluate

$$I_z = \oint \frac{e^{iz}}{z} dz$$

The original integral I is the **imaginary part** of I_z.

The only pole is a simple pole at $z = 0$ which is outside the chosen contour.

We therefore have

$$\oint \frac{e^{iz}}{z} dz = 0 = \int_{-R}^{-r} \frac{e^{ix}}{x} dx + \int_{C_1} \frac{e^{iz}}{z} dz + \int_{r}^{R} \frac{e^{ix}}{x} dx + \int_{C_2} \frac{e^{iz}}{z} dz$$

As before,

$$\int_{C_2} \frac{e^{iz}}{z} dz = 0$$

In the limits $r \to 0$ and $R \to \infty$, we have

$$I = -\frac{1}{2} \lim_{r \to 0} \int_{C_1} \frac{e^{iz}}{z} dz$$

There are two ways to do the integral around the small semicircle.

First, it is

$$-\pi i \text{ (residue at } z = 0) \text{ (1/2 full circle in wrong direction)} = -\pi i$$

or by explicit integration

$$
\begin{aligned}
-\lim_{r\to 0}\int_{C_1}\frac{e^{iz}}{z}dz &= \lim_{r\to 0}\int_{\pi}^{0}\frac{e^{ir\cos\theta - r\sin\theta}}{re^{i\theta}}ire^{i\theta}d\theta \\
&= -i\lim_{r\to 0}\int_{\pi}^{0} e^{ir\cos\theta - r\sin\theta}d\theta \\
&= -i\int_{\pi}^{0}\lim_{r\to 0} e^{ir\cos\theta - r\sin\theta}d\theta = -i\int_{\pi}^{0} d\theta = \pi i
\end{aligned}
$$

Thus,

$$
I = \int_0^{\infty}\frac{\sin x}{x}dx = \frac{1}{2}\text{Imag}(i\pi) = \frac{\pi}{2}
$$

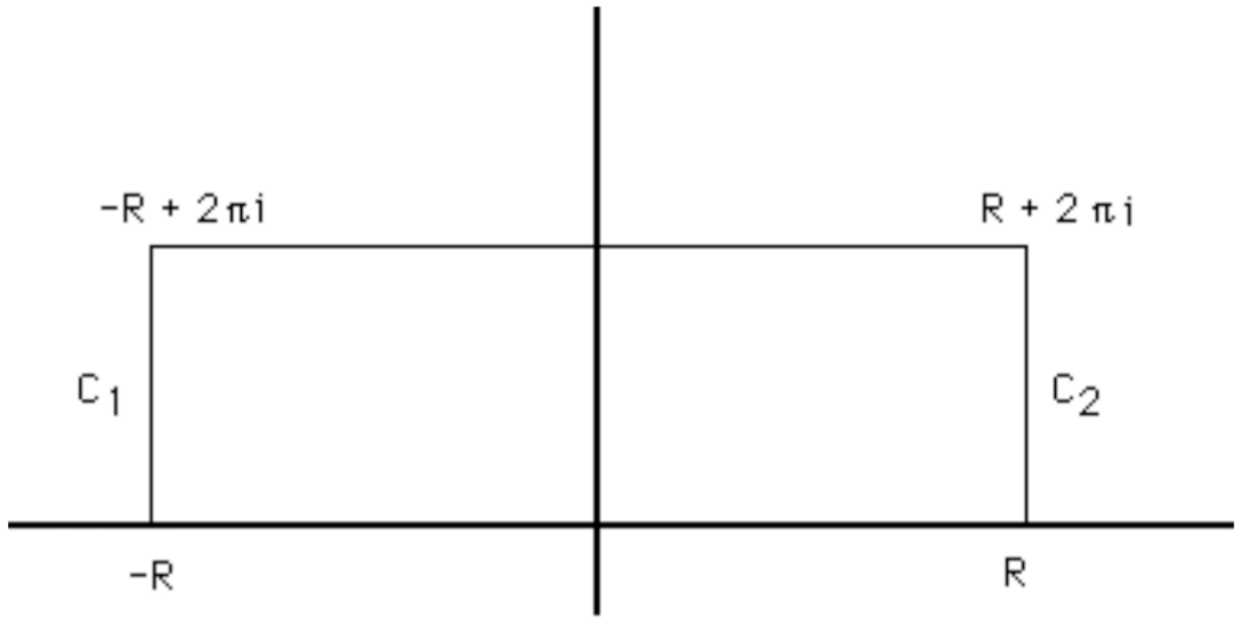
Integrals of exponential form

If we have real exponentials in the integrand, then we must choose a contour specifically for each separate problem.

We illustrate this with an example.

$$I = \int_{-\infty}^{\infty} \frac{e^{ax}}{1+e^{x}} dx \quad , \quad 0 < a < 1$$

The limits on a are necessary to avoid a divergent integral. We choose the contour



and evaluate

$$\oint \frac{e^{az}}{1+e^{z}} dz = \lim_{R\to\infty} \left(\int_{-R}^{R} \frac{e^{ax}}{1+e^{x}} dx + \int_{-R}^{R} \frac{e^{ax}}{1+e^{x}} dx + \int_{C_1} + \int_{C_2} \right)$$

The two vertical contours C_1 and C_2 vanish exponentially as $R \to \infty$.

We then have

$$\oint \frac{e^{az}}{1+e^z} dz = \lim_{R\to\infty} \left(\int_{-R}^{R} \frac{e^{ax}}{1+e^x} dx - e^{2\pi i a} \int_{-R}^{R} \frac{e^{ax}}{1+e^x} dx \right)$$

$$= \lim_{R\to\infty} \left((1 - e^{2\pi i a}) \int_{-R}^{R} \frac{e^{ax}}{1+e^x} dx \right)$$

$$= 2\pi i \sum (\text{residues inside the contour})$$

Where are the poles?

We have a pole when

$$e^z = -1 \to \text{ pole at } z = i\pi$$

A Laurent expansion in powers of $(z - i\pi)$ is

$$1 + e^z = 1 - e^{z-i\pi} = (z - i\pi)\left(1 - \frac{z - i\pi}{2!} + \frac{(z - i\pi)^2}{3!} + ...\right)$$

and thus it has a simple pole with residue $-e^{i\pi a}$.

We thus get

$$\lim_{R\to\infty}\left((1 - e^{2\pi ia})\int_{-R}^{R}\frac{e^{ax}}{1 + e^x}dx\right) = 2\pi i\sum(\text{residues inside the contour})$$
$$= 2\pi i(-e^{i\pi a})$$

and finally

$$\int_{-\infty}^{\infty}\frac{e^{ax}}{1 + e^x}dx = \frac{2\pi i(-e^{i\pi a})}{(1 - e^{2\pi ia})} = \frac{2\pi i(-e^{i\pi a})}{e^{i\pi a}(e^{-i\pi a} - e^{\pi ia})} = \frac{\pi}{\sin\pi a}$$

That is how many integrals are actually done!!!

Tensors

The quantitative description of physical processes cannot depend on the coordinate system in which they are represented.

On the other hand, physical results are independent of the choice of coordinate system.

What does this imply about the nature of the quantities involved in the description of physical processes?

(1) Notation

Einstein Summation Convention $\rightarrow$ **repeated indices** are summed over.

Examples:

$$a_j x_j = \sum_j a_j x_j = a_1 x_1 + a_2 x_2 + a_3 x_3 + ...$$

$$a_{ij} b_{jk} = \sum_j a_{ij} b_{jk} = a_{i1} b_{1k} + a_{i2} b_{2k} + a_{i3} b_{3k} + ...$$

$$\frac{\partial v_i}{\partial x_i} = \sum_i \frac{\partial v_i}{\partial x_i} = \frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \frac{\partial v_3}{\partial x_3} + ...$$

$$\frac{\partial^2 \phi}{\partial x_i \partial x_i} = \sum_i \frac{\partial^2 \phi}{\partial x_i \partial x_i} = \frac{\partial^2 \phi}{\partial x_1 \partial x_1} + \frac{\partial^2 \phi}{\partial x_2 \partial x_2} + \frac{\partial^2 \phi}{\partial x_3 \partial x_3} + ...$$

Subscripts that are summed over are called **dummy** subscripts and others are called **free** subscripts.

Defining the **Kronecker Delta**

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

we then have

$$a_{ij}\delta_{jk} = a_{ij}\delta_{kj} = a_{ik}$$
$$b_j\delta_{jk} = b_k$$
$$a_{ij}b_{jk}\delta_{ki} = a_{ij}b_{ji} = a_{kj}b_{jk}$$

(2) Change of Basis

A vector $\vec{A}$ with components (A_1, A_2, A_3) is written as

$$\vec{A} = A_i \hat{e}_i$$

with respect to the basis vectors $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$.

We introduce a new basis $\{\hat{e}'_1, \hat{e}'_2, \hat{e}'_3\}$ related to the old basis by the relations

$$\hat{e}'_j = S_{ij} \hat{e}_i$$

The coefficient S_{ij} is the ith component of the vector $\hat{e}'_j$ with respect to the original basis.

We then have

$$\vec{A} = A'_i \hat{e}'_i$$

or

$$\vec{A} = A'_i \hat{e}'_i = A'_i S_{ji} \hat{e}_j = A_j \hat{e}_j$$

$$A_j = S_{ji} A'_i$$

$$(S^{-1})_{ij} S_{ji} A'_i = (S^{-1})_{ij} A_j$$

$$(S^{-1}S)_{ii} A'_i = (I)_{ii} A'_i = (S^{-1})_{ij} A_j$$

$$A'_i = (S^{-1})_{ij} A_j$$

where we have denoted the matrix with elements S_{ij} by S.

In the special case where the transformation is a rotation of the coordinate axes(as we saw earlier), the transformation matrix S is **orthogonal** and we have

$$A'_i = (S^T)_{ij} A_j = S_{ji} A_j$$

Scalars, for example, the scalar or "dot" product of two vectors $\vec{A} \cdot \vec{B}$ (just a number), behave differently than vector under transformations since they remain unchanged under any coordinate transformation.

The behavior of linear operators is also different.

If a linear operator $\hat{A}$ is represented by some matrix A in a given coordinate system, then in a new (primed) coordinate system it is represented by the new matrix

$$A' = S^{-1}AS$$

We will now develop a formalism to describe all of these different types of objects and their transformation properties.

The generic name **tensor** will be introduced and scalars, vectors and linear operators will become tensors of zeroth, first and second **order** (the **order or rank** corresponding to the **number of subscripts** needed to specify a particular element of the tensor).

(3) Cartesian Tensors

We first confine our attention to rotations of Cartesian coordinate systems.

We assume that the origin remains fixed and we define the transformation in terms of the components of the position vector in the old $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$ and new $\{\hat{e}'_1, \hat{e}'_2, \hat{e}'_3\}$ bases.

We have

$$x'_i = L_{ij} x_j$$

In this case the transformation matrix L is orthogonal so that

$$L^{-1} = L^T$$

or

$$L^{-1} L = L^T L = L L^T$$

$$L_{ik} L_{jk} = \delta_{ij} = L_{ki} L_{kj}$$

This allows us to write

$$x_i = L_{ji} x'_j$$

since

$$\vec{x} = x_j \hat{e}_j = x'_j \hat{e}'_j$$

$$x'_j \hat{e}'_j \cdot \hat{e}'_i = x_j \hat{e}'_i \cdot \hat{e}_j$$

$$x'_j \delta_{ji} = (\hat{e}'_i \cdot \hat{e}_j) x_j$$

$$x'_i = (\hat{e}'_i \cdot \hat{e}_j) x_j$$

We then have the result

$$L_{ij} = \hat{e}'_i \cdot \hat{e}_j$$

We note that the product of two rotations is also a rotation.

For example, suppose

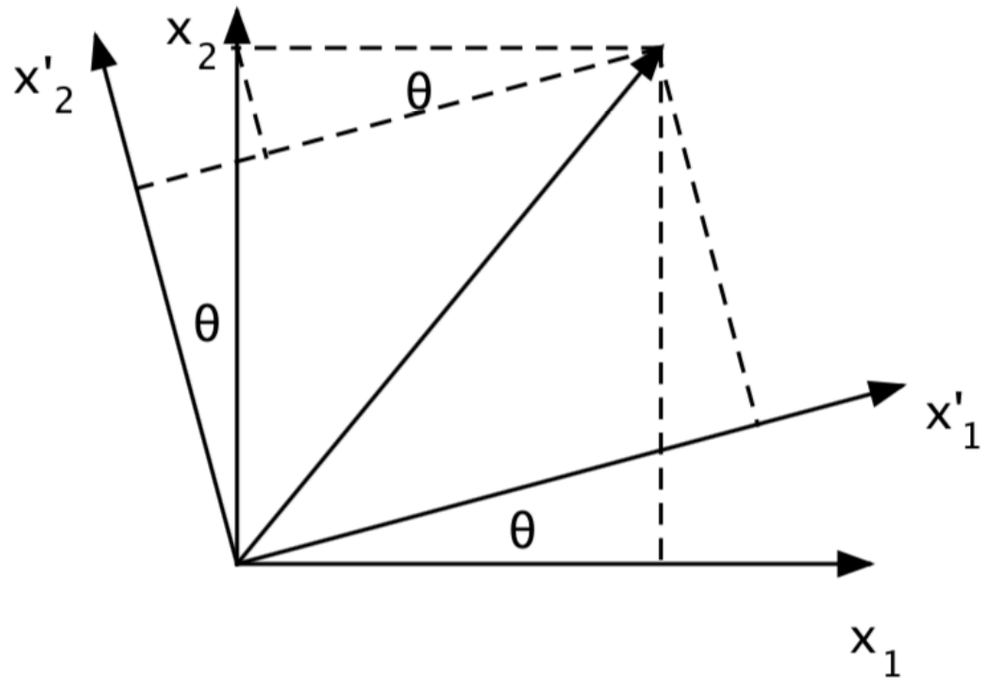
$$x'_i = L_{ij} x_j \quad \text{and} \quad x''_i = M_{ij} x'_j$$

$$x''_i = M_{ij} L_{jk} xk = (ML)_{ik} x_k$$

which implies that ML is also a rotation.

Example:

Let us consider a rotation of the coordinate axes through an angle θ about the $\hat{e}_3$-axis (or x_3-axis) as shown in figure below.



Let the vector be $\vec{x}$.

Looking at the dotted lines we have

$$x_1' = x_1 \cos\theta + x_2 \sin\theta$$

$$x_2' = -x_1 \sin\theta + x_2 \cos\theta$$

$$x_3' = x_3$$

Thus, we have (using $x'_i = L_{ij} x_j$)

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

The corresponding inverse relations are

$$x_1 = x'_1 \cos\theta - x'_2 \sin\theta$$

$$x_2 = x'_1 \sin\theta + x'_2 \cos\theta$$

$$x_3 = x'_3$$

(4) First- and Zero-Order Cartesian Tensors

We now assume that any set of (three) quantities v_i, which are explicitly or implicitly functions of the coordinates x_i, that transform according to

$$v_i = L_{ij} v_j$$

form the **components of a vector** or **first-rank Cartesian tensor**.

Clearly, the position coordinates are components of a first-rank tensor.

Examples:

Which of the following pairs of quantities are components of a first-rank Cartesian tensor in two dimensions?

(i) Suppose $(v_1, v_2) = (x_2, -x_1)$ are the components relative to the old axes.

We then have

$$v_1' = L_{11}v_1 + L_{12}v_2 = \cos\theta(x_2) + \sin\theta(-x_1) = x_2'$$

$$v_2' = L_{21}v_1 + L_{22}v_2 = -\sin\theta(x_2) + \cos\theta(-x_1) = -x_1'$$

Thus, $(v_1, v_2) = (x_2, -x_1)$ is a first-rank tensor.

(ii) Suppose $(v_1, v_2) = (x_2, x_1)$ are the components relative to the old axes.

We then have

$$v_1' = L_{11}v_1 + L_{12}v_2 = \cos\theta(x_2) + \sin\theta(x_1) \neq x_2'$$

$$v_2' = L_{21}v_1 + L_{22}v_2 = -\sin\theta(x_2) + \cos\theta(-x_1) \neq -x_1'$$

Thus, $(v_1, v_2) = (x_2, x_1)$ is not a first-rank tensor.

(iii) Suppose $(v_1, v_2) = (x_1^2, x_1^2)$ are the components relative to the old axes. We then have

$$v_1' = L_{11}v_1 + L_{12}v_2 = \cos\theta(x_1^2) + \sin\theta(x_2^2) \neq x_1'^2 = (\cos\theta(x_1) + \sin\theta(x_2))^2$$

$$\begin{aligned} v_2' = L_{21}v_1 + L_{22}v_2 &= -\sin\theta(x_1^2) + \cos\theta(x_2^2) \neq x_2'^2 \\ &= (-\sin\theta(x_1) + \cos\theta(x_2))^2 \end{aligned}$$

Thus, $(v_1, v_2) = (x_1^2, x_1^2)$ is not a first-rank tensor.

Examples of first-rank tensors (vectors) are position, velocity, momentum, acceleration and force.

We now consider quantities that are unchanged by a rotation of the axes.

They are called **scalars** or **tensors or rank zero**.

They contain only one element.

An example is the square of the distance of a point from the origin

$$r^2 = x_1^2 + x_2^2 + x_3^2$$

Under a transformation we get

$$r'^2 = x_1'^2 + x_2'^2 + x_3'^2 = r^2$$

so the it is an **invariant**.

We note that r^2 is a scalar product, i.e., $r^2 = \vec{x} \cdot \vec{x}$.

It is easy to show that any scalar product $\vec{A} \cdot \vec{B}$ is invariant under the transformation and is a tensor of rank zero.

$$\vec{A}' \cdot \vec{B}' = A'_i B'_i = L_{ij} A_j L_{ik} B_k = L^T_{ji} L_{ik} A_j B_k = (L^T L)_{jk} A_j B_k$$
$$= \delta_{jk} A_j B_k = A_j B_j = \vec{A} \cdot \vec{B}$$

We can use a scalar to generate a tensor of rank one.

Consider the new object (the **gradient**)

$$v_i = \frac{\partial \phi}{\partial x_i} \rightarrow \vec{v} = \nabla \phi$$

where ϕ is a scalar quantity. Under a rotation we get

$$v'_i = \left(\frac{\partial \phi}{\partial x_i} \right)' = \frac{\partial \phi'}{\partial x'_i} = \frac{\partial \phi}{\partial x'_i} = \frac{\partial x_j}{\partial x'_i} \frac{\partial \phi}{\partial x_j} = L_{ij} \frac{\partial \phi}{\partial x_j} = L_{ij} v_j$$

so we have constructed a first-rank tensor.

Now let us consider the quantity (the **divergence**)

$$s = \nabla \cdot \vec{v} = \frac{\partial v_i}{\partial x_i}$$

where $\vec{v}$ is a first-rank tensor.

Under a rotation we get

$$s' = \left(\frac{\partial v_i}{\partial x_i}\right)' = \frac{\partial v_i'}{\partial x_i'} = \frac{\partial x_j}{\partial x_i'}\frac{\partial v_i'}{\partial x_j} = \frac{\partial x_j}{\partial x_i'}\frac{\partial (L_{ij} v_k)}{\partial x_j} = L_{ij} L_{ik} \frac{\partial v_k}{\partial x_j}$$
$$= L_{ji}^T L_{ik} \frac{\partial v_k}{\partial x_j} = (L^T L)_{jk} \frac{\partial v_k}{\partial x_j} = \delta_{jk} \frac{\partial v_k}{\partial x_j} = \frac{\partial v_j}{\partial x_j} = s$$

so it is an invariant or zero rank tensor or scalar.

(5) Second- and Higher-Order Cartesian Tensors

We now define a **second-rank Cartesian tensor** as follows: the elements T_{ij} form the components of a second rank Cartesian tensor if

$$T'_{ij} = L_{ik} L_{jl} T_{kl} \quad \text{and} \quad T_{ij} = L_{ki} L_{lj} T'_{kl}$$

Generalizing, we say that the elements $T_{ij....k}$ form the components of an n^{th} rank Cartesian tensor (where $n =$ the number of indices) if

$$T'_{ij...k} = L_{ip} L_{jq} \ldots\ldots\ldots L_{kr} T_{pq...r} \quad \text{and} \quad T_{ij...k} = L_{pi} L_{qj} \ldots\ldots L_{rk} T'_{pq...r}$$

In 3 dimensions, an n^{th} rank Cartesian tensor has 3^n components.

Since a second-rank tensor has two indices, it is natural to display its components in **matrix** form.

The notation $[T_{ij}]$ is used, as well as $\overleftrightarrow{T}$, to denote the matrix having T_{ij} as the element in the i^{th} row and j^{th} column. We also denote the column matrix containing the elements v_i of a vector by $[v_i]$.

We can think of a second rank tensor $\overleftrightarrow{T}$ as a geometrical entity and the matrix containing its components as a representation of the tensor with respect to a particular coordinate system.

Let us look more closely at the transformation rule for second rank tensors using its matrix representation.

We have

$$T'_{ij} = L_{ik} K_{jl} T_{kl} = L_{ik} T_{kl} L_{jl} = L_{ik} T_{kl} (L^T)_{lj}$$

$$T' = LTL^T = LTL^{-1}$$

$$T_{ij} = L_{ki} T L_{lj} T'_{kl} = L_{ki} T'_{kl} L_{lj} = (L^T)_{ik} T'_{kl} L_{lj}$$

$$T = L^T T L = L^{-1} T L$$

Thus, the matrix representing a second rank tensor behaves in the same way under orthogonal transformations as the matrix representation of a linear operator.

Not all linear operators, however, are second rank tensors.

Examples

(i) The outer product of two vectors. Let u_i and v_i, $i = 1, 2, 3$ be the components of two vectors (first rank tensors) $\vec{u}$ and $\vec{v}$ and consider the set of quantities T_{ij} defined by

$$T_{ij} = u_i v_j$$

The set T_{ij} are called the components of the outer product of $\vec{u}$ and $\vec{v}$.

Under rotations the components of T_{ij} become

$$T'_{ij} = u'_i v'_j = L_{ik} u_k L_{jl} v_l = L_{ik} L_{jl} u_k v_l = L_{ik} L_{jl} T_{kl}$$

which shows that they do transform as the components of a second rank tensor.

We denote the outer product, without reference to a coordinate system, by the symbol

$$\overleftrightarrow{T} = \vec{u} \otimes \vec{v}$$

This tells us the basis to which the components T_{ij} of the second rank tensor refer.

Using

$$\vec{u} = u_i \hat{e}_i \quad \text{and} \quad \vec{v} = v_j \hat{e}_j$$

we have

$$\overleftrightarrow{T} = u_i \hat{e}_i \otimes v_j \hat{e}_j = u_i v_j \hat{e}_i \otimes \hat{e}_j = T_{ij} \hat{e}_i \otimes \hat{e}_j$$

Clearly, the quantities T'_{ij} are the components of the same tensor T but referred to a different coordinate system, i.e.,

$$\overleftrightarrow{T} = T_{ij} \hat{e}_i \otimes \hat{e}_j = T'_{ij} \hat{e}'_i \otimes \hat{e}'_j$$

(ii) The gradient of a vector. Suppose that v_i represents the components of a vector.

We consider the quantities generated by forming the derivatives of each v_i, $i = 1, 2, 3$, with respect to each x_j, $j = 1, 2, 3$, i.e.,

$$T_{ij} = \frac{\partial v_i}{\partial x_j}$$

We then have

$$T'_{ij} = \frac{\partial v'_i}{\partial x'_j} = \frac{\partial (L_{ik} v_k)}{\partial x'_j} = L_{ik} \frac{\partial v_k}{\partial x_l} \frac{\partial x_l}{\partial x'_j} = L_{ik} \frac{\partial v_k}{\partial x_l} L_{jl} = L_{ik} L_{jl} T_{kl}$$

which says that we have a second rank tensor $\overleftrightarrow{T} = \nabla \vec{v}$.

A test of whether any given set of quantities forms the components of a second rank tensor can always be made by direct substitution of the x'_i in terms of the x_i compared with using the transformation rule.

Example: Show that the elements T_{ij} given by

$$\overleftrightarrow{T} = [T_{ij}] = \begin{pmatrix} x_1^2 & -x_1 x_2 \\ -x_1 x_2 & x_1^2 \end{pmatrix}$$

are the components of a second rank tensor.

Let us consider a rotation by θ about the $\hat{e}_3$- axis.

The direct substitution using

$$x_1' = x_1 \cos\theta + x_2 \sin\theta$$

$$x_2' = -x_1 \sin\theta + x_2 \cos\theta$$

$$x'_3 = x_3$$

gives (using $c = \cos\theta$ and $s = \sin\theta$)

$$T'_{11} = x'^2_2 = (-sx_1 + cx_2)^2 = s^2x_1^2 - 2scx_1x_2 + c^2x_2^2$$

$$T'(12) = -x'_1x'_2 = -(cx_1+sx_2)(-sx_1+cx_2) = scx_1^2+(s^2-c^2)x_1x_2-scx_2^2$$

$$T'_{21} = -x'_1x'_2 = -(cx_1+sx_2)(-sx_1+cx_2) = scx_1^2+(s^2-c^2)x_1x_2-scx_2^2$$

$$T'_{22} = x'^2_1 = (cx_1 + sx_2)^2 = c^2x_1^2 + 2scx_1x_2 + c^2x_2^2$$

The transformation equations using

$$L = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

give

$$T'_{11} = L_{1k}L_{1l}T_{kl} = s^2x_1^2 - 2scx_1x_2 + c^2x_2^2$$

$$T'_(12) = L_{1k}L_{2l}T_{kl} = scx_1^2 + (s^2 - c^2)x_1x_2 - scx_2^2$$

$$T'_{21} = L_{2k}L_{1l}T_{kl} = scx_1^2 + (s^2 - c^2)x_1x_2 - scx_2^2$$

$$T'_{22} = L_{2k}L_{2l}T_{kl} = c^2x_1^2 + 2scx_1x_2 + c^2x_2^2$$

which are the same.

Thus, we have a second rank tensor.

The same result can be proved more easily by realizing that the T_{ij} are, in fact, the components of the outer product of the vector $\vec{v} = (x_2, -x_1)$ (we proved earlier that this is a vector or first rank tensor) with itself, i.e.,

$$\vec{v} \otimes \vec{v} = v_i v_j \hat{e}_i \otimes \hat{e}_j = T_{ij}\hat{e}_i \otimes \hat{e}_j$$

$$T_{ij} = v_i v_j$$

$$T_{11} = v_1 v_1 = x_2^2 \qquad T_{12} = v_1 v_2 = -x_1 x_2$$

$$T_{21} = v_2 V_1 = -x_1 x_2 \qquad T_{22} = v_2 v_2 = x_1^2$$

Another example of the transformation of tensors:

Consider a rotation through 45°.

The transformation array is given by

$$[a] = \begin{pmatrix} \cos 45^\circ & \sin 45^\circ \\ -\sin 45^\circ & \cos 45^\circ \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

Assume that we have a vector (tensor of rank 1)

$$[V] = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

then

$$[V'] = [a][V] \rightarrow V'_i = a_{ij} V_j$$

or

$$V'_1 = a_{11} V_1 + a_{12} V2 = 3\frac{\sqrt{2}}{2}$$

$$V'_2 = a_{21} V_1 + a_{22} V_2 = \frac{\sqrt{2}}{2}$$

$$[V'] = \frac{\sqrt{2}}{2}\begin{pmatrix} 3 \\ 1 \end{pmatrix}$$

Now consider the transformation of the rank 2 tensor

$$[T] = \begin{pmatrix} 4 & 6 \\ 3 & 1 \end{pmatrix}$$

We have

$$[T'] = [a][a][T] \rightarrow T'_{ij} = a_{ir} a_{js} T_{rs}$$

This is **NOT** matrix multiplication!

We can, however, cast the equation as a matrix multiplication by a rearrangement

$$T'_{ij} = a_{ir}\,a_{js}\,T_{rs} = a_{ir}\,T_{rs}\,a_{js} = a_{ir}\,T_{rs}(a_{sj})\,T = a_{ir}\,T_{rs}(a_{sj})^{-1}$$

$$[T'] = [a][T][a]^{-1}$$

This **IS** matrix multiplication!

We have

$$T'_{11} = T_{11}a_{11}a_{11} + T_{12}a_{11}a_{12} + T_{21}a_{12}a_{11} + T_{22}a_{12}a_{12} = 7$$

$$T'_{12} = T_{11}a_{11}a_{21} + T_{12}a_{11}a_{22} + T_{21}a_{12}a_{21} + T_{22}a_{12}a_{22} = 0$$

$$T'_{21} = T_{11}a_{21}a_{11} + T_{12}a_{21}a_{12} + T_{21}a_{22}a_{11} + T_{22}a_{22}a_{12} = -3$$

$$T'_{22} = T_{11}a_{21}a_{21} + T_{12}a_{21}a_{22} + T_{21}a_{22}a_{21} + T_{22}a_{22}a_{22} = -2$$

or

$$[T'] = \begin{pmatrix} 7 & 0 \\ -3 & -2 \end{pmatrix}$$

The matrix multiplication relation works also (but is not very useful), i.e.,

$$[T'] = [a][T][a]^T = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} 4 & 6 \\ 3 & 1 \end{pmatrix} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} 10 & 2 \\ 4 & -2 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 14 & 0 \\ -6 & -4 \end{pmatrix} = \begin{pmatrix} 7 & 0 \\ -3 & -2 \end{pmatrix}$$

as expected.

(6) The Algebra of Tensors

Addition and Subtraction

If two tensors have the **same** rank, then they can be added and subtracted using their components

$$S_{ij\ldots k} = V_{ij\ldots k} + W_{ij\ldots k}$$

$$D_{ij\ldots k} = V_{ij\ldots k} - W_{ij\ldots k}$$

The new objects are tensors of the same rank.

Switching Indices

If a pair of indices are switched the new object is a tensor of the same rank, i.e., if $V_{ij\ldots k}$ represents a tensor, then $V_{ji\ldots k}$ represents a tensor of the same rank.

If $V_{ji\ldots k} = V_{ij\ldots k}$ for all components, then $V_{ij\ldots k}$ is said to be **symmetric** with respect to that pair of indices (or simply symmetric for second rank tensors).

If $V_{ji\ldots k} = -V_{ij\ldots k}$ for all components, then $V_{ij\ldots k}$ is said to be **antisymmetric** with respect to that pair of indices (or simply antisymmetric for second rank tensors).

An arbitrary tensor is neither symmetric nor antisymmetric, but can always be written as the sum of a symmetric tensor $S_{ij\ldots k}$ and an antisymmetric tensor $A_{ij\ldots k}$, i.e.,

$$T_{ij\ldots k} = \frac{1}{2}(T_{ij\ldots k} + T_{ji\ldots k}) + \frac{1}{2}(T_{ij\ldots k} - T_{ji\ldots k}) = S_{ij\ldots k} + A_{ij\ldots k}$$

The outer product discussed earlier is an example of a kind of "**multiplication**" of two tensors producing a tensor of higher rank.

Our illustration had two first rank tensors producing a second rank tensor.

In general, the outer product of an n^{th} rank tensor with an m^{th} rank tensor produces an $(n+m)^{th}$ rank tensor.

We can produce a tensor of smaller rank from a tensor of larger rank using the **contraction** operation.

The contraction operation consists of making two indices equal (and thus summing over that index).

This reduces the number of indices (and hence the rank of the tensor) by two.

Example: Let $T_{ij..l..m..k}$ be the components of an n^{th} rank tensor.

This implies that

$$T'_{ij..l..m..k} = \underbrace{L_{ip}L_{jq}.....L_{lr}.....L_{ms}.....L_{kn}}_{n\,\text{factors}}\, T_{pq....r....s...n}$$

If we contract on the indices l and m (set them both equal to l) we get

$$\begin{aligned} T'_{ij...l...l...k} &= \underbrace{L_{ip}L_{jq}.....L_{lr}.....L_{ls}.....L_{kn}}_{n\,\text{factors}}\, T_{pq....r....s...n} \\ &= L_{ip}L_{jq}.....\delta_{rs}.....L_{kn}\, T_{pq....r....s...n} \\ &= \underbrace{L_{ip}L_{jq}.........L_{kn}}_{(n-2)\,\text{factors}}\, T_{pq....r....r...n} \end{aligned}$$

which says that $T_{ij\ldots l\ldots l\ldots k}$ are the components of a different Cartesian tensor of rank $(n-2)$.

For a second rank tensor, the process of contraction is the same as taking the trace of the corresponding matrix.

Therefore, the trace T_{ii} is a zero rank tensor (or scalar) and is invariant under rotations.

The scalar product or two vectors can be recast in tensor language as forming the outer product of two vectors (first rank tensors) $T_{ij} = u_i v_j$ and then contracting to form the scalar $T_{ii} = u_i v_i$ which is invariant under rotation as we found earlier.

Another familiar operation that is a special case of the contraction operation is the multiplication of a column vector $[u_i]$ by a matrix $[B_{ij}]$ to produce another column vector $[v_i]$, i.e.,

$$B_{ij} u_j = v_i$$

We can think of this as the contraction T_{ijj} of the third rank tensor T_{ijk} formed from the outer product of B_{ij} and u_j.

(7) The Quotient Law

If we know that $\overleftrightarrow{B}$ and $\overleftrightarrow{C}$ are tensors and also that

$$A_{pq\ldots k\ldots m}B_{ij\ldots k\ldots n} = C_{pq\ldots mij\ldots m}$$

does this imply that the $A_{pq\ldots k\ldots m}$ also form components of a tensor $\overleftrightarrow{A}$?

Here $\overleftrightarrow{A}$, $\overleftrightarrow{B}$ and $\overleftrightarrow{C}$ are respectively of m^{th}, n^{th} and $(m+n-2)^{th}$ rank.

The subscript k that has been contracted can be any of the subscripts in $\overleftrightarrow{A}$ and $\overleftrightarrow{B}$ independently.

The quotient law states that if the above component relation holds in all rotated coordinate systems, then the $A_{pq\ldots k\ldots m}$ do form the components of a tensor.

We will prove it for $m = n = 2$ only, but it should be clear that the principle of the proof holds for arbitrary m and n (just the algebra gets worse).

Suppose we start with

$$A_{pk}B_{ik} = C_{pi}$$

where B_{ik} and C_{pi} are arbitrary second rank tensors.

Under a rotation the set A_{pk} (whether they are a tensor or not) transforms to a new set A'_{pk} as follows

$$\begin{aligned} A'_{pk}B'_{ik} &= C'_{pi} \\ &= L_{pq}LL_{ij}C_{qj} = L_{pq}L_{ij}A_{ql}B_{jl} \\ &= L_{pq}L_{ij}A_{ql}L_{mj}L_{nl}B'_{mn} = L_{pq}L_{ij}L_{mj}L_{nl}A_{ql}B'_{mn} \\ &= L_{pq}\delta_{im}L_{nl}A_{ql}B'_{mn} = L_{pq}L_{nl}A_{ql}B'_{in} \end{aligned}$$

This can be rewritten (changing dummy index labels) as

$$(A'_{pk} - L_{pq}L_{kl}A_{ql})B'_{ik} = 0$$

Since B_{ik} and hence B'_{ik} is an arbitrary tensor, we must have

$$A'_{pk} = L_{pq}L_{kl}A_{ql}$$

which says that the A_{pk} are the components of a second rank tensor.

The same result holds if we start with

$$A_{pk}B_{ki} = C_{pi}$$

Using the quotient law to test whether a given set of quantities is a tensor is generally much more convenient than the direct substitution method we used earlier.

A particular way in which it is applied is by contracting the given set of quantities, having n subscripts, with some arbitrary n^{th} rank tensor and determining whether the result is a scalar.

Let us go back to an earlier example, namely,

$$T = [T_{ij}] = \begin{pmatrix} x_2^2 & -x_1x_2 \\ -x_1x_2 & x_1^2 \end{pmatrix}$$

The outer product $x_i x_j$ is a second rank tensor.

Contracting it with the T_{ij} we get

$$T_{ij}x_i x_j = x_2^2 x_1^2 - x_1x_2x_1x_2 - x_1x_2x_1x_2 + x_1^2x_2^2 = 0$$

which is clearly invariant.

Thus, by the quotient theorem T_{ij} must also be a tensor.

Very powerful!

The Tensors δ_{ij} and ϵ_{ijk}

Since

$$\delta'_{kl} = L_{ki}L_{lj}\delta_{ij} = L_{ki}L_{li} = \delta_{kl}$$

δ_{ij} is a second rank tensor.

Now consider the three-subscript **Levi-Civita symbol** ϵ_{ijk} where we have

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } i,j,k \text{ is an even permutation of } 1,2,3 \\ -1 & \text{if } i,j,k \text{ is an odd permutation of } 1,2,3 \\ 0 & \text{otherwise} \end{cases}$$

We then have

$$\epsilon'_{lmn} = L_{li} L_{mj} L_{nk} \epsilon_{ijk}$$

Before proceeding, we note that for a 3×3 matrix A, the determinant $|A|$ satisfies

$$|A| \epsilon_{lmn} = A_{li} A_{mj} A_{nk} \epsilon_{ijk}$$

Example: Evaluate the determinant of the matrix

$$A = \begin{pmatrix} 2 & 1 & -3 \\ 3 & 4 & 0 \\ 1 & -2 & 1 \end{pmatrix}$$

Setting $l = 1$, $m = 2$, and $n = 3$ we get

$$\begin{aligned} A\epsilon_{123} = |A| &= A_{1i}A_{2j}A_{3k}\epsilon_{ijk} \\ &= A_{11}A_{22}A_{33}\epsilon_{123} + A_{11}A_{23}A_{32}\epsilon_{132} + A_{12}A_{21}A_{33}\epsilon_{213} \\ &\quad + A_{13}A_{21}A_{32}\epsilon_{312} + A_{12}A_{23}A_{31}\epsilon_{231} + A_{13}A_{22}A_{31}\epsilon_{321} \\ &= (2)(4)(1) - (2)(0)(-2) - (1)(3)(1) + (-3)(3)(-2) \\ &\quad + (1)(0)(1) - (-3)(4)(1) = 35 \end{aligned}$$

Now, using the above relation, we get

$$\epsilon'_{lmn} = L_{li}L_{mj}L_{nk}\epsilon_{ijk} = |L|\epsilon_{lmn}$$

Since L is orthogonal, its determinant is 1 and thus we have

$$\epsilon'_{lmn} = \epsilon_{lmn}$$

Thus, we have a third rank tensor.

These two tensors also have **exactly the same components** in every coordinate system.

Many of the familiar expressions of vector calculus can be written as contracted tensors involving δ_{ij} and ϵ_{ijk}.

Examples:

(i)

$$\vec{a} = b \times \vec{c} \rightarrow a_i = \epsilon_{ijk} b_j c_k$$

so that the cross-product produces a vector.

(ii)

$$\vec{a} \cdot \vec{b} = a_i b_i = \delta_{ij} a_i b_j$$

(iii)

$$\nabla^2 \phi = \frac{\partial^2 \phi}{\partial x_i \partial x_i} = \delta_{ij} \frac{\partial^2 \phi}{\partial x_i \partial x_j}$$

(iv)

$$(\nabla \times \vec{v})_i = \epsilon_{ijk} \frac{\partial v_k}{\partial x_j}$$

(v)

$$[\nabla \cdot (\nabla \cdot \vec{v}]_i = \frac{\partial}{\partial x_i} \left(\frac{\partial v_j}{\partial x_j} \right) = \delta_{jk} \frac{\partial^2 v_j}{\partial x_i \partial x_k}$$

(vi)

$$[\nabla \times (\nabla \times \vec{v}]_i = \epsilon_{ijk} \frac{\partial}{\partial x_j} \left(\epsilon_{klm} \frac{\partial v_m}{\partial x_l} \right) = \epsilon_{ijk} \epsilon_{klm} \frac{\partial^2 v_m}{\partial x_j \partial x_l}$$

(vii)

$$(\vec{a} \times \vec{b}) \times \vec{c} = \delta_{ij} c_i \epsilon_{jkl} a_k b_l = \epsilon_{ikl} c_i a_k b_l$$

An important identity between the ϵ and δ tensors is

$$\epsilon_{ijk} \epsilon_{klm} = \delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}$$

This says that the two fourth rank tensors have identical components.

This allows us to find an alternative expression for

$$[\nabla \times (\nabla \times \vec{v}]_i = \epsilon_{ijk}\epsilon_{klm}\frac{\partial^2 v_m}{\partial x_j \partial x_l} = (\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl})\frac{\partial^2 v_m}{\partial x_j \partial x_l}$$

$$= \frac{\partial^2 v_j}{\partial x_i \partial x_j} - \frac{\partial^2 v_i}{\partial x_j \partial x_j} = [\nabla \cdot (\nabla \cdot \vec{v}]_i - \nabla^2 v_i$$

or

$$\nabla \times (\nabla \times \vec{v}) = \nabla \cdot (\nabla \cdot \vec{v}) - \nabla^2 \vec{v}$$

That would be very cumbersome to prove using standard methods! We can also show that

$$\epsilon_{ijk}\epsilon_{pqr} = \begin{vmatrix} \delta_{ip} & \delta_{iq} & \delta_{ir} \\ \delta_{jp} & \delta_{jq} & \delta_{jr} \\ \delta_{kp} & \delta_{kq} & \delta_{kr} \end{vmatrix}$$

The identity we derive above is then a special case where $(p, q, r) = (k, l, m)$.

If we contract the identity by setting $j = l$ and using $\delta_{kk} = 3$ we get

$$\epsilon_{ijk}\epsilon_{ijm} = 3\delta_{km} - \delta_{km} = 2\delta_{km}$$

and contracting once more by setting $k = m$ we get

$$\epsilon_{ijk}\epsilon_{ijk} = 2\delta_{kk} = 6$$

Improper Rotations and Pseudotensors

The kind of transformations we have been discussing are called **proper** rotations(where $|L| = 1$).

Another kind of transformation is called an **improper** rotation(where $|L| = -1$).

In general, we consider this kind of transformation as a proper rotation plus an **inversion** of the coordinate axes through the origin represented by the equations

$$x_i' = -x_i$$

An inversion changes a right-handed coordinate system into a left-handed coordinate system (proper rotations do not affect handedness).

The matrix corresponding to the inversion transformation is

$$L_{ij} = -\delta_{ij}$$

A vector is a geometrical operator whose direction and magnitude are not affected by describing it in different coordinate systems (only it components change relative to new basis vectors).

Therefore the components of a vector $\vec{v}$ transform according to

$$v_i' = L_{ij} v_j$$

under all proper and improper rotations.

Let us now define another type of object whose components can also be labelled with a single index but which transforms as

$$v_i' = L_{ij} v_j$$

under proper rotations and as

$$v_i' = -L_{ij} v_j$$

under improper rotations.

The new object is called a **pseudotensor** or **pseudovector**.

Pseudovectors should not be regarded as the same kind of geometrical object as a vector.

Their directions are reversed under a transformation such as inversion as shown below.

In a similar way we can define scalars and **pseudoscalars**, where pseudoscalars are invariant under proper rotations but change sign under inversion (or reflection).

We can extend this to tensors of rank greater than 1.

In general, we write

$$T'_{ij....k} = L_{il}L_{jm}.....L_{kn}T_{lm.....n} \quad \text{for tensors}$$

$$T'_{ij....k} = |L|L_{il}L_{jm}.....L_{kn}T_{lm.....n} \quad \text{for pseudotensors}$$

For example, earlier we found that

$$|L|\epsilon_{ijk} = L_{il}L_{jm}L_{kn}\epsilon_{lmn}$$

Since $|L| = \pm 1$ we can write this as

$$\epsilon_{ijk} = |L|L_{il}L_{jm}L_{kn}\epsilon_{lmn}$$

Therefore, ϵ_{ijk} is a third rank Cartesian pseudotensor.

Now consider the cross- or vector-product $\vec{a} = \vec{b} \times \vec{c}$ where $\vec{b}$ and $\vec{c}$ are vectors.

We then have

$$a_i = \epsilon_{ijk} b_j c_k$$

Under a transformation, we write

$$\begin{aligned} a'_i &= \epsilon'_{ijk} b'_j c'_k = |L| L_{il} L_{jm} L_{kn} \epsilon_{lmn} L_{jp} b_p L_{kq} c_q \\ &= |L| L_{il} L_{jm} L_{jp} L_{kn} L_{kq} \epsilon_{lmn} b_p c_q = |L| L_{il} \delta_{mp} \delta_{nq} \epsilon_{lmn} b_p c_q \\ &= |L| L_{il} \epsilon_{lmn} b_m c_n = |L| L_{il} a_i \end{aligned}$$

which says that the cross-product is a pseudovector (not a vector!).

Now the quantities $a_i = \epsilon_{ijk} b_j c_k$ are the components of the physical vector $\vec{a} = \vec{b} \times \vec{c}$ provided we are using a right-handed Cartesian coordinate system.

However, in a different coordinate system, which is left-handed, the quantities $a'_i = \epsilon'_{ijk} b'_j c'_k$ are not the components of the physical vector. $\vec{a} = \vec{b} \times \vec{c}$ which has, instead, the components $-a'_i$.

It is very important to note the handedness of a coordinate system before setting out to write in component form the vector relation $\vec{a} = \vec{b} \times \vec{c}$.

The kind of transformations we have been using are called **passive transformations**.

In passive transformations, the physical system is left unchanged and only the coordinate system used to describe it is changed.

In **active transformations**, the system itself is altered.

As an example, let us consider a particle of mass m that is located at a position $\vec{x}$ relative to the origin O and hence has a velocity $\dot{\vec{x}}$.

The angular momentum of the particle about O is thus

$$\vec{J} = m(\vec{x} \times \dot{\vec{x}})$$

If we merely invert the Cartesian coordinates used to describe the system through the origin O, neither the magnitude nor direction of the vectors will be changed since they may be considered simply as arrows in space that are independent of the coordinates used to describe them.

If we perform an active transformation such as inverting the position vector through O, then particle velocity is also reversed (it is the time derivative of the position vector).

The angular momentum vector, however, remains unaltered.

This suggests that vectors can be divided into two categories as follows: **polar vectors** (such as position and velocity), which reverse under an active inversion of the physical system through the origin O and **axial vectors** (such as angular momentum) that remain unchanged.

Note that we have specifically not introduced the concept of a pseudovector to describe a physical quantity.

(10) Dual Tensors

Consider a second rank pseudotensor A_{ij} (in three dimensions).

For every such object, we construct the object

$$p_i = \frac{1}{2}\epsilon_{ijk}A_{jk}$$

which is called the **dual** of A_{ij}.

It is a pseudovector.

If we denote the antisymmetric tensor by the matrix

$$[A_{ij}] = \begin{pmatrix} 0 & A_{12} & -A_{31} \\ -A_{12} & 0 & A_{23} \\ A_{31} & -A_{23} & 0 \end{pmatrix}$$

then the components of the dual pseudovector are

$$(p_1, p_2, p_3) = (A_{23}, A_{31}, A_{12})$$

We also have the result

$$\epsilon_{ijk} p_k = \frac{1}{2} \epsilon_{ijk} \epsilon_{klm} A_{lm} = \frac{1}{2} (\delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl}) A_{lm} = A_{ij}$$

(11) Physical Applications of Tensors

Mechanics Example

Consider a system of N rigidly connected point particles each characterized by a mass m and a position vector $\vec{r_i}$ with respect to an origin O.

We suppose that the system is rotating about an axis through O with angular velocity $\vec{\omega}$.

The angular momentum $\vec{J}$ about O of the system is given by

$$\vec{J} = \sum_{i=1}^{N} \vec{r_i} \times \vec{p_i}$$

where

$$\vec{p_i} = m_i \vec{v_i} \quad \text{and} \quad \vec{v_i} = \vec{\omega} \times \vec{r_i}$$

Substitution gives

$$
\begin{aligned}
J_i &= \sum_{i=1}^{N} m_i \epsilon_{lmn} x_{im} v_{in} = \sum_{i=1}^{N} m_i \epsilon_{lmn} x_{im} \epsilon_{npq} \omega_p x_{iq} \\
&= \sum_{i=1}^{N} m_i \epsilon_{lmn} \epsilon_{npq} x_{im} x_{iq} \omega_p = \sum_{i=1}^{N} m_i \left(\delta_{lp}\delta_{mq} - \delta_{lq}\delta_{mp}\right) x_{im} x_{iq} \omega_p \\
&= \sum_{i=1}^{N} m_i (x_{im} x_{im} \delta_{lp} - x_{ip} x_{il}) \omega_p = \sum_{i=1}^{N} m_i ((r_i^2)\delta_{lp} - x_{ip} x_{il}) \omega_p \\
&= I_{lp} \omega_p
\end{aligned}
$$

where I_{lp} is a symmetric second rank tensor(by the quotient rule since $\vec{J}$ and $\vec{\omega}$ are vectors) which depends only on the distribution of the masses in the system and not on any properties of $\vec{\omega}$.

It is called the **inertia tensor** of the system with respect to O.

For a continuous distribution of mass this becomes

$$I = [I_{ij}] = \begin{pmatrix} \int (y^2 + z^2)\rho dV & -\int xy\rho dV & -\int xz\rho dV \\ -\int xy\rho dV & \int (z^2 + x^2)\rho dV & -\int yz\rho dV \\ -\int xz\rho dV & -\int yz\rho dV & \int (x^2 + y^2)\rho dV \end{pmatrix}$$

where $\rho(x, y, z)$ is the mass density function and $dV = dxdydz$.

The diagonal elements are called the **moments of inertia** and the off-diagonal elements without the minus signs are called the **products of inertia**.

Similar algebra gives us an expression for the kinetic energy of the system.

$$
\begin{aligned}
T &= \frac{1}{2}\sum_{i=1}^{N} m_i v_{in} v_{in} = \sum_{i=1}^{N} m_i \epsilon_{njk}\omega_j x_{ik}\epsilon_{npq}\omega_p x_{iq} \\
&= \frac{1}{2}\sum_{i=1}^{N} m_i \epsilon_{njk}\epsilon_{npq} x_{ik} x_{iq}\omega_j\omega_p = \sum_{i=1}^{N} m_i\left(\delta_{jp}\delta_{kq} - \delta_{jq}\delta_{kp}\right)x_{ik}x_{iq}\omega_j\omega_p \\
&= \frac{1}{2}\sum_{i=1}^{N} m_i\left(x_{ik}x_{ik}\delta_{jp}\delta_{kq} - x_{ip}x_{ij}\right)\omega_j\omega_p = \sum_{i=1}^{N} m_i\left((r_i^2)\delta_{jp} - x_{ip}x_{ij}\right)\omega_j\omega_p \\
&= \frac{1}{2} I_{jp}\omega_j\omega_p \\
&= \frac{1}{2} J_\rho \omega_\rho
\end{aligned}
$$

This shows that the kinetic energy of the rotating body can be expressed as a scalar obtained by twice contracting $\vec{\omega}$ with the inertia tensor.

Since I is a real, symmetric second rank tensor representable by a real, symmetric 3×3 matrix(means it is always possible to diagonalize it), it possesses three mutually perpendicular eigenvectors (or principal axes) with respect to which the inertia tensor is diagonal, with diagonal entries equal to the eigenvalues of the matrix (one studies these tensors in in a second level mechanics course).

(12) Non-Cartesian Coordinates

The position of an arbitrary point P in space may be expressed in terms of the three curvilinear coordinates u^1, u^2, u^3.

If $\vec{r}(u^1, u^2, u^3)$ is the position vector of the point P, at every such point there exist **two sets** of basis vectors

$$\hat{e}_i = \frac{\partial \vec{r}}{\partial u^i} \quad \text{and} \quad \hat{e}^i = \nabla u^i$$

where the $\hat{e}_i$ (subscripts) are tangent to the coordinate curves (the axes) and the $\hat{e}^i$ (superscripts) are normal to the coordinate curves.

Thus, we can write a vector in two ways (we change our summation convention so that we now sum over repeated indices only if one is up and the other is down)

$$\vec{a} = a^i \hat{e}_i = a_i \hat{e}^i$$

The a^i are called the **contravariant** components of the vector $\vec{a}$ and the a_i are called the covariant components of the vector $\vec{a}$.

For cartesian coordinate systems there is no difference between these two sets of basis vectors, which is why we were able to only use lower indices.

The $\hat{e}_i$ are the covariant basis vectors and the $\hat{e}^i$ are the contravariant basis vectors.

In general, the vectors in each set are neither of unit length nor form an orthogonal basis.

The sets $\hat{e}_i$ and $\hat{e}^i$ are, however, dual systems of vectors, so that

$$\hat{e}_i \cdot \hat{e}^i = \delta_i^j$$

We thus have

$$\vec{a} \cdot \hat{e}^i = a^j \hat{e}_j \cdot \hat{e}^i = a^j \delta^i_j = a^i$$

$$\vec{a} \cdot \hat{e}_i = a_j \hat{e}^j \cdot \hat{e}_i = a_j \delta^j_i = a_i$$

If we consider the components of higher rank tensors in non-Cartesian coordinates, there are even more possibilities.

For example, consider a second rank tensor T.

Using the outer product notation we can write T in three different ways

$$T = T^{ij} \hat{e}_i \otimes \hat{e}_j = T^i_j \hat{e}_i \otimes \hat{e}^j = T_{ij} \hat{e}^i \otimes \hat{e}^j$$

where T^{ij}, T^i_j and T_{ij} are called the contravariant, **mixed** and covariant components of T respectively.

These three sets of quantities form the components of the same tensor T, but refer to different (tensor) bases made up from the basis vectors of the coordinate system.

In Cartesian coordinates, all three sets are identical.

(13) The Metric Tensor

Any particular curvilinear coordinate system is **completely** characterized (at each point in space) by the nine quantities

$$g_{ij} = \hat{e}_i \cdot \hat{e}_j$$

Since an infinitesimal vector displacement can be written as $d\vec{r} = du^i \hat{e}_i$ we have these results

$$(ds)^2 = d\vec{r} \cdot d\vec{r} = du^i \hat{e}_i \cdot du^j \hat{e}_j = du^i du^j \hat{e}_i \cdot \hat{e}_j = g_{ij} du^i du^j$$

Since $(ds)^2$ is a scalar and the du^i are components of a contravariant vector, the quotient law says that the g_{ij} are the covariant components of a tensor g called the **metric tensor**.

The scalar product can be written in four different ways in terms of the metric tensor

$$\begin{aligned}
\vec{a}\cdot\vec{b} &= a^i\hat{e}_i\cdot b^j\hat{e}_j = \hat{e}_i\cdot\hat{e}_j a^i b^j = g_{ij}a^i b^j \\
&= a_i\hat{e}^i\cdot b_j\hat{e}^j = \hat{e}^i\cdot\hat{e}^j a_i b_j = g^{ij}a_i b_j \\
&= a_i\hat{e}^i\cdot b^j\hat{e}_j = \hat{e}^i\cdot\hat{e}_j a_i b^j = \delta^i_j a_i b^j = a_i b^i \\
&= a^i\hat{e}_i\cdot b_j\hat{e}^j = \hat{e}_i\cdot\hat{e}^j a^i b_j = \delta^j_i a^i b_j = a^i b_i
\end{aligned}$$

These imply that

$$g^{ij}b_j = b^i \quad \text{and} \quad g_{ij}b^j = b_i$$

or that the covariant components of g can be used to lower in index and the contravariant components of g can be used to raise an index.

In a similar manner we can show that

$$\hat{e}^i = g^{ij}\hat{e}_j \quad \text{and} \quad \hat{e}_i = g_{ij}\hat{e}^j$$

Now since $\hat{e}^i$ and $\hat{e}_i$ are dual vectors, i.e.,

$$\hat{e}^i \cdot \hat{e}_j = \delta^j_i$$

we can always write

$$\hat{e}^i = \frac{\hat{e}_j \times \hat{e}_k}{\hat{e}_i \cdot (\hat{e}_j \times \hat{e}_k} \quad i,j,k = 1,2,3 \text{ and cyclic permutations}$$

$$\hat{e}_i = \frac{\hat{e}^j \times \hat{e}^k}{\hat{e}^i \cdot (\hat{e}^j \times \hat{e}^k)} \quad i,j,k = 1,2,3 \text{ and cyclic permutations}$$

We then have

$$\delta^i_k a^k = a^i = g^{ij} a_j = g^{ij} g_{jk} a^k$$

or

$$g^{ij} g_{jk} = \delta^i_k$$

In terms of matrix representations this says that

$$G = [g_{ij}], \bar{G} = [g^{ij}], I = [\delta^i_j] \rightarrow G\bar{G} = I \rightarrow \bar{G} = G^{-1}$$

or the matrix formed from the covariant components is the inverse of the matrix formed from the contravariant components.

The above relations also give the result

$$g^i_j = \hat{e}^i \cdot \hat{e}_j = \delta^i_j \rightarrow \text{ components are identical}$$

Finally, we have

$$g = |g| = \det[g_{ij}] = g_{1i} g_{2j} g_{3k} \epsilon_{ijk} = \hat{(e)}_1 \cdot (\hat{e}_2 \times \hat{e}_3)$$

and

$$dV = u^1 \hat{(e)}_1 \cdot (u^2 \hat{e}_2 \times u^3 \hat{e}_3) = \hat{(e)}_1 \cdot (\hat{e}_2 \times \hat{e}_3) du^1 du^2 du^3$$

or

$$dV = |g| du^1 du^2 du^3$$

(14) General Coordinate Transformations and Tensors

We now discuss the concept of general transformations from one coordinate system u^1, u^2, u^3 to another u'^1, u'^2, u'^3. We can describe the coordinate transformation using the three equations

$$u'^i = u'^i(u^1, u^2, u^3)$$

for $i = 1, 2, 3$ in which the new coordinates u'^i can be arbitrary

functions of the old ones u^i, rather than just represent linear orthogonal transformations (rotations) of the coordinate axes.

We shall also assume that the transformation can be inverted, so that we can write the old coordinates in terms of the new ones as

$$u^i = u^i(u'^1, u'^2, u'^3)$$

An example is the transformation from spherical polar to Cartesian coordinates given by

$$x = r \sin\theta \cos\phi$$

$$y = r \sin\theta \sin\phi$$

$$z = r \cos\theta$$

which is clearly not a linear transformation.

The two sets of basis vectors in the new coordinate system u'^1, u'^2, u'^3 are given by

$$\hat{e}'_i = \frac{\partial \vec{r}}{\partial u'^i} \quad \text{and} \quad \hat{e}'^i = \nabla u'^i$$

Considering the first set, we have from the chain rule that

$$\hat{e}_j = \frac{\partial \vec{r}}{\partial u^j} = \frac{\partial u'^i}{\partial u^j}\frac{\partial \vec{r}}{\partial u'^i} = \frac{\partial u'^i}{\partial u^j}\hat{e}'_i$$

so that the basis vectors in the old and new coordinate systems are related by

$$\hat{e}_j = \frac{\partial u'^i}{\partial u^j}\hat{e}'_i$$

Now, since we can write any arbitrary vector in terms of either basis as

$$\vec{a} = a'^i \hat{e}'_i = a^j \hat{e}_j = a^j \frac{\partial u'^i}{\partial u^j}\hat{e}'_j$$

it follows that the contravariant components of a vector must transform as

$$a'^i = \frac{\partial u'^i}{\partial u^j} a^j$$

In fact, we use this relation as the **defining property** that a set of quantities a^i must have if they are to form the contravariant components of a vector.

If we consider the second set of basis vectors, $\hat{e}'^i = \nabla u'^i$, we have from the chain rule that

$$\frac{\partial u^j}{\partial x} = \frac{\partial u^j}{\partial u'^i}\frac{\partial u'^i}{\partial x}$$

and similarly for $\partial u^j/\partial y$ and $\partial u^j/\partial z$.

So the basis vectors in the old and new coordinate systems are related by

$$\hat{e}^j = \frac{\partial u^j}{\partial u'^i}\hat{e}'^i$$

For any arbitrary vector $\vec{a}$,

$$\vec{a} = a'_i\hat{e}'^i = a_j\hat{e}^j = a_j\frac{\partial u^j}{\partial u'^i}\hat{e}'^i$$

and so the covariant components of a vector must transform as

$$a'_i = \frac{\partial u^j}{\partial u'^i} a_j$$

In a similar way to that used in the contravariant case, we take this result as the **defining property** that a set of quantities ai must have if they are to form the covariant components of a vector.

We may compare these two transformation laws with those for a first-order Cartesian tensor under a rigid rotation of axes.

Let us consider a rotation of the Cartesian axes x^i through an angle θ about the 3-axis to a new set $x'^i, i = 1, 2, 3$

$$x'_1 = x_1 \cos\theta + x_2 \sin\theta$$

$$x'_2 = -x_1 \sin\theta + x_2 \cos\theta$$

$$x'_3 = x_3$$

and the inverse transformation

$$x_1 = x_1' \cos\theta - x_2' \sin\theta$$

$$x_2 = x_1' \sin\theta + x_2' \cos\theta$$

$$x_3 = x_3'$$

It is then straightforward to show that

$$\frac{\partial x^j}{\partial x'^i} = \frac{\partial x'^i}{\partial x^j} = L_{ij}$$

where the elements jL_{ij} are given by

$$L = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Thus, the new relations agree with the earlier definitions in this special case of a rigid rotation of the Cartesian axes.

We now generalize these two laws for contravariant and covariant components of a vector to tensors of higher rank.

For example, the contravariant, mixed and covariant components, respectively, of a second-order tensor must transform as follows:

$$\text{contravariant components} \qquad T'^{ij} = \frac{\partial u'^i}{\partial u^k}\frac{\partial u'^j}{\partial u^l}T^{kl}$$

$$\text{mixed components} \qquad T'^i_j = \frac{\partial u'^i}{\partial u^k}\frac{\partial u^l}{\partial u'^j}T^k_l$$

$$\text{covariant components} \qquad T'_{ij} = \frac{\partial u^k}{\partial u'^i}\frac{\partial u^l}{\partial u'^j}T_{kl}$$

It is important to remember that these quantities form the components of the same tensor T but refer to different tensor bases made up from the basis vectors of the different coordinate systems.

For example, in terms of the contravariant components we may write

$$T = T^{ij}\,\hat{e}_i \otimes \hat{e}_j = T;^{ij}\,\hat{e}'_i \otimes \hat{e}'_j$$

We can clearly go on to define tensors of higher order, with arbitrary numbers of covariant (subscript) and contravariant (superscript) indices, by demanding that their components transform as follows:

$$T'^{ij\ldots k}_{lm\ldots.n} = \frac{\partial u'^i}{\partial u^a}\frac{\partial u'^j}{\partial u^b}\cdots\frac{\partial u'^k}{\partial u^c}\frac{\partial u^d}{\partial u'^l}\frac{\partial u^e}{\partial u'^m}\cdots\frac{\partial u^f}{\partial u'^n}\,T^{ab\ldots.c}_{de\ldots.f}$$

Using the revised summation convention (matched contravariant and covariant indices summed over), the algebra of general tensors is completely analogous to that of Cartesian tensors discussed earlier.

For example, as with Cartesian coordinates, the Kronecker delta is a tensor, provided it is written as a mixed tensor δ^i_j, since

$$\delta'^i_j = \frac{\partial u'^i}{\partial u^k}\frac{\partial u^l}{\partial u'^j}\delta^k_l = \frac{\partial u'^i}{\partial u^k}\frac{\partial u^k}{\partial u'^j} = \frac{\partial u'^i}{\partial u'^j} = \delta^i_j$$

where we have used the chain rule to prove the third equality.

Since we showed earlier that

$$g^i_j = \hat{e}^i \cdot \hat{e}_j = \delta^i_j$$

δ^i_j can be considered as the mixed components of the metric tensor g.

In the new (primed) coordinate system, we have

$$\frac{\partial u^k}{\partial u'^i}\frac{\partial u^l}{\partial u'^j}\hat{e}_k \cdot \hat{e}_l = \frac{\partial u^k}{\partial u'^i}\frac{\partial u^l}{\partial u'^j}g_{kl}$$

which shows that the g_{ij} are indeed the covariant components of a second-order tensor (the metric tensor g).

A similar argument shows that the quantities g^{ij} form the contravariant components of a second-order tensor, such that

$$g'^{ij} = \frac{\partial u'^i}{\partial u^k} \frac{\partial u'^j}{\partial u'^l} g^{kl}$$

Earlier we saw that the components g_{ij} and g^{ij} could be used to raise and lower indices in contravariant and covariant vectors.

This can be extended to tensors of arbitrary rank. In general, contraction of a tensor with g_{ij} will convert the contracted index from being contravariant(superscript) to covariant (subscript), i.e., it is lowered.

This can be repeated for as many indices as required.

For example,

$$T_{ij} = g_{ik} T^k_j = g_{ik} g_{jl} T^{kl}$$

Similarly, contraction with g^{ij} raises an index, i.e.,

$$T^{ij} = g^{ik} T^{j}_{k} - g^{ik} g^{jl} T_{kl}$$

That these two relations are mutually consistent, can be shown by using the relation

$$g^{ik} g_{kj} = \delta^{i}_{j}$$

(15) Derivatives of basis vectors and Christoffel symbols

In Cartesian coordinates, the basis vectors $\hat{e}_i$ are constant and so their derivatives with respect to the coordinates vanish.

In general coordinate systems, however, the basis vectors $\hat{e}_i$ and $\hat{e}^i$ are functions of the coordinates.

In order that we may differentiate general tensors, we must therefore first consider the derivatives of the basis vectors.

Let us consider the derivative

$$\frac{\partial \hat{e}_i}{\partial u^j}$$

Since this is itself a vector, it can be written as a linear combination of the basis vectors $\hat{e}_k$, $k = 1, 2, 3$.

If we introduce the symbol Γ_{ij}^k to denote the coefficients in this combination, we have

$$\frac{\partial \hat{e}_i}{\partial u^j} = \Gamma_{ij}^k \hat{e}_k$$

The coefficient Γ_{ij}^k is simply the k^{th} component of the vector $\frac{\partial \hat{e}_i}{\partial u^j}$.

Using the reciprocity relation $\hat{e}^i \cdot \hat{e}_j = \delta_j^i$, these 27 numbers are given (at each point in space) by

$$\hat{e}^k \cdot \frac{\partial \hat{e}_i}{\partial u^j} = \Gamma_{ij}^m \hat{e}^k \cdot \hat{e}_m = \Gamma_{ij}^m \delta_m^k = \Gamma_{ij}^k$$

$$\Gamma_{ij}^k = \hat{e}^k \cdot \frac{\partial \hat{e}_i}{\partial u^j}$$

Furthermore, we then have

$$\frac{\partial(\hat{e}^i \cdot \hat{e}_k)}{\partial u^j} = 0 = \hat{e}^i \cdot \frac{\partial \hat{e}_k}{\partial u^j} + \frac{\partial \hat{e}^i}{\partial u^j} \cdot \hat{e}_k$$

$$\frac{\partial \hat{e}^i}{\partial u^j} \cdot \hat{e}_k = -\hat{e}^i \cdot \frac{\partial \hat{e}_k}{\partial u^j} = -\Gamma^m_{kj} \hat{e}^i \cdot \hat{e}_m = -\Gamma^i_{kj}$$

$$\rightarrow \frac{\partial \hat{e}^i}{\partial u^j} = -\Gamma^i_{kj} \hat{e}^k$$

The symbol Γ^k_{ij} is called a **Christoffel symbol** (of the second kind), but despite appearances to the contrary, these quantities do not form the components of a third-order tensor.

In a new coordinate system

$$\Gamma'^k_{ij} = \hat{e}'^k \cdot \frac{\partial \hat{e}'_i}{\partial u'^j}$$

Using

$$\hat{e}'_i = \frac{\partial u^l}{\partial u'^i}\hat{e}_l \quad \text{and} \quad \hat{e}'^k = \frac{\partial u'^k}{\partial u^n}\hat{e}^n$$

we get

$$\begin{aligned}
\Gamma'^k_{ij} &= \hat{e}^n \cdot \frac{\partial}{\partial u'^j}\left(\frac{\partial u^l}{\partial u'^i}\hat{e}_l\right) \\
&= \frac{\partial u'^k}{\partial u^n}\hat{e}^n \cdot \left(\frac{\partial^2 u^l}{\partial u'^j \partial'^i}\hat{e}_l + \frac{\partial u^l}{\partial u'^i}\frac{\partial \hat{e}_l}{\partial u'^j}\right) \\
&= \frac{\partial u'^k}{\partial u^n}\frac{\partial^2 u^l}{\partial u'^j \partial u'^i}\hat{e}^n \cdot \hat{e}_l + \frac{\partial u'^k}{\partial u^n}\frac{\partial u^l}{\partial u'^i}\hat{e}^n \cdot \frac{\partial \hat{e}_l}{\partial u'^j} \\
&= \frac{\partial u'^k}{\partial u^n}\frac{\partial^2 u^l}{\partial u'^j \partial u'^i}\delta^n_l + \frac{\partial u'^k}{\partial u^n}\frac{\partial u^l}{\partial u'^i}\frac{\partial u^m}{\partial u'^j}\hat{e}^n \cdot \frac{\partial \hat{e}_l}{\partial u'^m} \\
&= \frac{\partial u'^k}{\partial u^l}\frac{\partial^2 u^l}{\partial u'^j \partial u'^i} + \frac{\partial u'^k}{\partial u^n}\frac{\partial u^l}{\partial u'^i}\frac{\partial u^m}{\partial u'^j}\Gamma^n_{lm}
\end{aligned}$$

This result shows that the Γ_{ij}^k **do not** form the components of a third-order tensor because of the presence of the first term on the right-hand side.

We note that in Cartesian coordinates it is clear from the relation

$$\Gamma_{ij}^k = \hat{e}^k \cdot \frac{\partial \hat{e}_i}{\partial u^j}$$

that $\Gamma_{ij}^k = 0$ for all values of the indices i, j and k.

In a given coordinate system we can, in principle, calculate the Γ_{ij}^k using the relation

$$\Gamma_{ij}^k = \hat{e}^k \cdot \frac{\partial \hat{e}_i}{\partial u^j}$$

In practice, however, it is often quicker to use an alternative expression, which we now derive, for the Christoffel symbol in terms of the metric tensor g_{ij} and its derivatives with respect to the coordinates.

First, we note that the Christoffel symbol Γ^k_{ij} is symmetric with respect to the interchange of its two subscripts i and j.

This is easily shown, since

$$\frac{\partial \hat{e}_i}{\partial u^j} = \frac{\partial^2 \vec{r}}{\partial u^j \partial u^i} \frac{\partial^2 \vec{r}}{\partial u^i \partial u^j} = \frac{\partial \hat{e}_j}{\partial u^i}$$

This gives

$$\frac{\partial \hat{e}_i}{\partial u^j} = \Gamma^k_{ij} \hat{e}_k = \Gamma^k_{ji} \hat{e}_k = \frac{\partial \hat{e}_j}{\partial u^i}$$
$$\Gamma^k_{ij} \hat{e}_k \cdot \hat{e}^l = \Gamma^k_{ji} \hat{e}_k \cdot \hat{e}^l$$
$$\Gamma^l_{ij} = \Gamma^l_{ji}$$

To obtain an expression for Γ^k_{ij} we then use $g_{ij} = \hat{e}_i \cdot \hat{e}_j$ and consider the derivative

$$\frac{\partial g_{ij}}{\partial u^k} = \frac{\partial \hat{e}_i}{\partial u^k} \cdot \hat{e}_j + \hat{e}_i \cdot \frac{\partial \hat{e}_j}{\partial u^k} = \Gamma^l_{ik} \hat{e}_l \cdot \hat{e}_j + \hat{e}_i \cdot \Gamma^l_{jk} \cdot \hat{e}_l$$
$$= \Gamma^l_{ik} g_{ij} + \Gamma^l_{jk} g_{il}$$

By cyclically permuting the free indices i,j,k in this relation we obtain two further equivalent relations

$$\frac{\partial g_{jk}}{\partial u^i} = \Gamma^l_{ji} g_{lk} + \Gamma^l_{ki} g_{jl}$$

$$\frac{\partial g_{ki}}{\partial u^j} = \Gamma^l_{kj} g_{li} + \Gamma^l_{ij} g_{kl}$$

where we have used the symmetry properties of both Γ^k_{ij} and g_{ij}.

Contracting both sides with g^{mk} leads to the required expression for the Christoffel symbol in terms of the metric tensor and its derivatives, namely

$$\Gamma^m_{ij} = \frac{1}{2} g^{mk} \left(\frac{\partial g_{jk}}{\partial u^i} + \frac{\partial g_{ki}}{\partial u^j} - \frac{\partial g_{jk}}{\partial u^i} \right)$$

Example: cylindrical polar coordinates

$$(u^1, u^2, u^3) = (\rho, \phi, z)$$

$$ds^2 = d\rho^2 + \rho^2 d\phi^2 + dz^2 = g_{ij} du^i du^j$$

$$\rightarrow g_{11} = 1, g_{22} = \rho^2, g_{33} = 1, \text{ all others } = 0$$

This implies that the only non-zero Christoffel symbols are $\Gamma^2_{12} = \Gamma^2_{21}$ and Γ^1_{22}.

These are given by

$$\Gamma^2_{12} = \Gamma^2_{21} = \frac{g^{22}}{2} \frac{\partial g_{22}}{\partial u^1} = \frac{1}{2g_{22}} \frac{\partial g_{22}}{\partial \rho} = \frac{1}{2\rho^2} \frac{\partial \rho^2}{\partial \rho} = \frac{1}{\rho}$$

$$\Gamma^1_{22} = -\frac{g^{11}}{2} \frac{\partial g_{22}}{\partial u^1} = -\frac{1}{2g_{11}} \frac{\partial g_{22}}{\partial \rho} = -\frac{1}{2} \frac{\partial \rho^2}{\partial \rho} = -\rho$$

Alternatively, we can use

$$\hat{e}_1 = \hat{e}_\rho = \cos\phi\hat{e}_x + \sin\phi\hat{e}_y$$

$$\hat{e}_2 = \hat{e}_\phi = -\sin\phi\hat{e}_x + \cos\phi\hat{e}_y$$

$$\hat{e}_3 = \hat{e}_z$$

$$\frac{\partial\hat{e}_\rho}{\partial\phi} = \frac{1}{\rho}\hat{e}_\phi \rightarrow \frac{\partial\hat{e}_1}{\partial u^2} = \frac{1}{u^1}\hat{e}_2 \rightarrow \Gamma^2_{12} = \frac{1}{u^1} = \frac{1}{\rho} = \Gamma^2_{21}$$

$$\frac{\partial\hat{e}_\phi}{\partial\phi} = -\rho\hat{e}_\rho \rightarrow \frac{\partial\hat{e}_2}{\partial u^2} = -u^1\hat{e}_1 \rightarrow \Gamma^1_{22} = -u^1 = -\rho$$

as expected.

(16) Covariant differentiation

For Cartesian tensors, we noted that the derivative of a scalar is a (covariant) vector.

This is also true for general tensors, as may be shown by considering the differential of a scalar

$$d\phi = \frac{\partial\phi}{\partial u^i}du^i$$

Since the du^i are the components of a contravariant vector, and $d\phi$ is a scalar, we have by the quotient rule that the quantities

$$\frac{\partial \phi}{\partial u^i}$$

must form the components of a covariant vector.

It is straightforward to show, however, that (unlike in Cartesian coordinates) the differentiation of the components of a general tensor, other than a scalar, with respect to the coordinates does not, in general, result in the components of another tensor.

For example, in Cartesian coordinates, if the v^i are the contravariant components of a vector, then the quantities

$$\frac{\partial v^i}{\partial x^j}$$

form the components of a second-order tensor.

In general coordinates, however, this is not the case.

We may show this directly by considering

$$\left(\frac{\partial v^i}{\partial u^j}\right)' = \frac{\partial v'^i}{\partial u'^j} = \frac{\partial u^k}{\partial u'^j}\frac{\partial v'^i}{\partial u^k} = \frac{\partial u^k}{\partial u'^j}\frac{\partial}{\partial u^k}\left(\frac{\partial u'^i}{\partial u^l}v^l\right)$$

$$= \frac{\partial u^k}{\partial u'^j}\frac{\partial u'^i}{\partial u^l}\frac{\partial v^l}{\partial u^k} + \frac{\partial u^k}{\partial u'^j}\frac{\partial^2 u'^i}{\partial u^k \partial u^l}v^l$$

The presence of the second term on the right-hand side shows that the

$$\frac{\partial v^i}{\partial u^j}$$

do not form the components of a second-order tensor.

This term arises because the "transformation matrix"

$$\left[\frac{\partial u'^i}{\partial u^j}\right]$$

changes with position in space.

This is not true in Cartesian coordinates, for which the second term vanishes, and

$$\frac{\partial v^i}{\partial x^j}$$

is a second-order tensor.

We can, however, use the Christoffel symbols to define a new **covariant** derivative of the components of a tensor, which does result in the components of another tensor.

Let us first consider the derivative of a vector $\vec{v}$ with respect to the coordinates.

Writing the vector in terms of its contravariant components $\vec{v} = v^i \hat{e}_i$, we find

$$\frac{\partial \vec{v}}{\partial u^j} = \frac{\partial v^i}{\partial u^j} \hat{e}_i + v^i \frac{\partial \hat{e}_i}{\partial u^j}$$

where the second term arises because, in general, the basis $\hat{e}_i$ are not constant (this term vanishes in Cartesian coordinates).

Using the definition of the Christoffel symbol we can write

$$\frac{\partial \vec{v}}{\partial u^j} = \frac{\partial v^i}{\partial u^j}\hat{e}_i + v^i \Gamma^k_{ij}\hat{e}_k$$

Since i and k are dummy indices in the last term on the right-hand side, we may interchange them to obtain

$$\frac{\partial \vec{v}}{\partial u^j} = \frac{\partial v^i}{\partial u^j}\hat{e}_i + v^k \Gamma^i_{kj}\hat{e}_i = \left(\frac{\partial v^i}{\partial u^j} + v^k \Gamma^i_{kj}\right)\hat{e}_i$$

The reason for interchanging the dummy indices is that we may then factor out $\hat{e}_i$.

The quantity in the bracket is called the **covariant derivative**, for which the standard notation is

$$v^i_{;j} = \frac{\partial v^i}{\partial u^j} + \Gamma^i_{kj} v^k$$

where the semicolon denotes covariant differentiation; a similar short-hand notation also exists for the simple partial derivative, in which a comma is used instead of a semicolon.

For example

$$v^i_{,j} = \frac{\partial v^i}{\partial u^j}$$

so that

$$v^i_{;j} = v^i_{,j} + \Gamma^i_{kj} v^k \rightarrow \frac{\partial \vec{v}}{\partial u^j} = v^i_{;j} \hat{e}_i = \nabla \vec{v}$$

Using the quotient rule, it is then clear that the $v^i_{;j}$ are the (mixed) components of a second-order tensor.

In Cartesian coordinates, all the Γ^k_{ij} are zero, and so the covariant derivative reduces to the simple partial derivative

$$\frac{\partial v^i}{\partial u^j}$$

Example: cylindrical polar coordinates

Contracting the definition of the covariant derivative we have

$$v^i_{;i} = v^i_{,i} + \Gamma^i_{ki} v^k = \frac{\partial v^i}{\partial u^i} + \Gamma^i_{ki} v^k$$

Using the Christoffel symbols we worked out earlier we find

$$\Gamma^i_{1i} = \Gamma^1_{11} + \Gamma^2_{12} + \Gamma^3_{13} = \frac{1}{\rho}$$

$$\Gamma^i_{2i} = \Gamma^1_{21} + \Gamma^2_{22} + \Gamma^3_{23} = 0$$

$$\Gamma^i_{3i} = \Gamma^1_{31} + \Gamma^2_{32} + \Gamma^3_{33} = 0$$

and

$$v^i_{;i} = \frac{\partial v^\rho}{\partial \rho} + \frac{\partial v^\phi}{\partial \phi} + \frac{\partial v^z}{\partial z} + \frac{1}{\rho} v^\rho = \frac{1}{\rho}\frac{\partial (\rho v^\rho)}{\partial \rho} + \frac{\partial v^\phi}{\partial \phi} + \frac{\partial v^z}{\partial z}$$

which is the standard expression for the divergence of a vector field in cylindrical polar coordinates.

So far we have considered only the covariant derivative of the contravariant components of a vector.

The corresponding result for the covariant components v_i may be found in a similar way, by considering the derivative of $\vec{v} = v_i \hat{e}^i$.

We obtain

$$v_{i;j} = \frac{\partial v_i}{\partial u^j} - \Gamma^k_{ij} v_k$$

Following a similar procedure we can obtain expressions for the covariant derivatives of higher-order tensors.

Expressing T in terms of its contravariant components, we have

$$\frac{\partial T}{\partial u^k} = \frac{\partial}{\partial u^k}\left(T^{ij}\hat{e}_i \otimes \hat{e}_j\right) = \frac{\partial T^{ij}}{\partial u^k}\hat{e}_i \otimes \hat{e}_j + T^{ij}\frac{\partial \hat{e}_i}{\partial u^k} \otimes \hat{e}_j + T^{ij}\hat{e}_i \otimes \frac{\partial \hat{e}_j}{\partial u^k}$$

Using the definition of the Christoffel symbols we can write

$$\frac{\partial T}{\partial u^k} = \frac{\partial T^{ij}}{\partial u^k}\hat{e}_i \otimes \hat{e}_j + T^{ij}\Gamma^l_{ik}\hat{e}_l \otimes \hat{e}_j + T^{ij}\hat{e}_i \otimes \Gamma^l_{jk}\hat{e}_l$$

Interchanging dummy indices i and l in the second term and j and l in the third term on the right-hand side this becomes

$$\frac{\partial T}{\partial u^k} = \left(\frac{\partial T^{ij}}{\partial u^k} + \Gamma^i_{lk}T^{lj} + \Gamma^j_{lk}T^{il}\right)\hat{e}_i \otimes \hat{e}_j$$

where the expression in brackets is the required covariant derivative

$$T^{ij}_{;k} = \frac{\partial T^{ij}}{\partial u^k} + \Gamma^i_{lk} T^{lj} + \Gamma^j_{lk} T^{il} = T^{ij}_{,k} + \Gamma^i_{lk} T^{lj} + \Gamma^j_{lk} T^{il}$$

In a similar way we can write the covariant derivative of the mixed and covariant components.

Summarizing we have

$$T^{ij}_{;k} = T^{ij}_{,k} + \Gamma^i_{lk} T^{lj} + \Gamma^j_{lk} T^{il}$$

$$T^{i}_{j;k} = T^{i}_{j,k} + \Gamma^i_{lk} T^{l}_{j} - \Gamma^l_{jk} T^{i}_{l}$$

$$T_{ij;k} = T_{ij,k} - \Gamma^l_{ik} T_{lj} - \Gamma^l_{jk} T^{il}$$

We note that the quantities $T^{ij}_{;k}$, $T^{i}_{j;k}$, $T_{ij;k}$ are the components of the same third-order tensor T with respect to different tensor bases, i.e.,

$$\nabla T = T^{ij}_{;k} \hat{e}_i \otimes \hat{e}_j \otimes \hat{e}^k = T^{i}_{j;k} \hat{e}_i \otimes \hat{e}^j \otimes \hat{e}^k = T_{ij;k} \hat{e}^i \otimes \hat{e}^j \otimes \hat{e}^k$$

We conclude by considering the covariant derivative of a scalar. The covariant derivative differs from the simple partial derivative with respect to the coordinates only because the basis vectors of the coordinate system change with position in space (hence for Cartesian coordinates there is no difference). However, a scalar function ϕ does not depend on the basis vectors at all, so its covariant derivative must be the same as its partial derivative, i.e.,

$$\phi_{;j} = \frac{\partial \phi}{\partial u^j} = \phi_{,j}$$

(17) Vector Operators in tensor form

We now use tensor methods to obtain expressions for the grad, div, curl and Laplacian that or valid in all coordinate systems.

Gradient. The gradient of a scalar ϕ is simply given by

$$\nabla \phi = \phi_{;i} \hat{e}^i = \frac{\partial \phi}{\partial u^i} \hat{e}^i$$

since the covariant derivative of a scalar is the same as its partial derivative.

Divergence. The divergence of a vector field $\vec{v}$ in a general coordinate system is given by

$$\nabla \vec{v} = v^i_{;i} = \frac{\partial v^i}{\partial u^i} + \Gamma^i_{ki} v^k$$

Using

$$\Gamma^i_{kl} = \frac{1}{2} g^{il} \left(\frac{\partial g_{il}}{\partial u^k} + \frac{\partial g_{kl}}{\partial u^i} - \frac{\partial g_{ki}}{\partial u^l} \right)$$

The last two terms cancel because

$$g^{il} \frac{\partial g_{kl}}{\partial u^i} = g^{li} \frac{\partial g_{ki}}{\partial u^l} = g^{il} \frac{\partial g_{ki}}{\partial u^l}$$

where in the first equality we have interchanged the dummy indices i and l, and in the second equality we have used the symmetry of the metric tensor.

We need one further result before we can simplify the divergence expression.

Suppose $A = [a_{ij}]$, $B = [b^{ij}]$ and that $B = A^{-1}$.

Let $a = |A| = \det A$.

If we denote the cofactor of the element a_{ij} by Δ^{ij}, then the elements of the inverse matrix are given by

$$b^{ij} = \frac{1}{a}\Delta^{ji}$$

in which we have fixed i and explicitly written the sum over j for clarity.

Partially differentiating both side with respect to a_{ij}, we then obtain

$$\frac{\partial a}{\partial a_{ij}} = \Delta^{ij}$$

since a_{ij} does not occur in any of the cofactors Δ^{ij}.

Now, if we suppose that the a_{ij} are function of the coordinates, then so also will the determinant a, and by the chain rule we have

$$\frac{\partial a}{\partial u^k} = \frac{\partial a}{\partial a_{ij}} \frac{\partial a_{ij}}{\partial u^k} = \Delta^{ij} \frac{\partial a_{ij}}{\partial u^k} = a b^{ji} \frac{\partial a_{ij}}{\partial u^k}$$

Applying this result to the determinant g of the metric tensor and using $g^{ij} g_{jk} = \delta^i_k$ and the fact that g^{ij} is symmetric we obtain

$$\frac{\partial g}{\partial u^k} = g g^{ij} \frac{\partial g_{ij}}{\partial u^k}$$

Finally, we get

$$\Gamma^i_{ki} = \frac{1}{2} g^{il} \frac{\partial g_{il}}{\partial u^k} = \frac{1}{2g} \frac{\partial g}{\partial u^k} = \frac{1}{\sqrt{g}} \frac{\partial \sqrt{g}}{\partial u^k}$$

which gives the result

$$\nabla \vec{v} = v^i_{;i} = \frac{\partial v^i}{\partial u^i} + \frac{1}{\sqrt{g}} \frac{\partial \sqrt{g}}{\partial u^k} v^k = \frac{1}{\sqrt{g}} \frac{\partial}{\partial u^k} (\sqrt{g} v^k)$$

Laplacian. If we replace $\vec{v}$ by $\nabla\phi$ in the above divergence result, we obtain the Laplacian $\nabla^2\phi$.

Now

$$\vec{v} = \nabla\phi = v_i\hat{e}^i = \frac{\partial\phi}{\partial u^i}\hat{e}^i \rightarrow v_i = \frac{\partial\phi}{\partial u^i} = \text{ covariantcomponents}$$

However, we need the contravariant components v^i.

These can be obtained by raising the index using the metric tensor, to give

$$v^j = g^{jk}v_k = g^{jk}\frac{\partial\phi}{\partial u^k}$$

We then obtain

$$\nabla^2\phi = \frac{1}{\sqrt{g}}\frac{\partial}{\partial u^j}\left(\sqrt{g}g^{jk}\frac{\partial\phi}{\partial u^k}\right)$$

For an orthogonal coordinate system (g diagonal since $\hat{e}_i \cdot \hat{e}_j = \delta_{ij}$), we have

$$\mathrm{g} = \begin{pmatrix} h_1^2 & 0 & 0 \\ 0 & h_2^2 & 0 \\ 0 & 0 & h_3^2 \end{pmatrix}$$

so that

$$ds^2 = \sum_i h_i^2 \, du^i \, du^i \quad \text{and} \quad v^i = \frac{v_i}{h_i} \quad (\text{no sum on } i)$$

Therefore, $\sqrt{g} = h_1 h_2 h_3$ and $g^{ij} = \frac{1}{h_i^2}\delta_{ij}$ and we get

$$\nabla^2 \phi = \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial u^i} \left(\frac{h_1 h_2 h_3}{h_j^2} \frac{\partial \phi}{\partial u^j} \right)$$

as expected.

Curl. The special vector form of the curl of a vector field exists only in three dimensions.

We therefore consider its more general form, which is also valid in higher-dimensional spaces.

In a general space the operation $curl\,\vec{v}$ is defined by

$$(curl\,\vec{v})_{ij} = v_{i;j} - v_{j;i}$$

which is an antisymmetric covariant tensor.

The difference of derivatives can be simplified since

$$v_{i;j} - v_{j;i} = v_{i,j} - \Gamma^{l}_{ij} v_l - v_{j,i} + \Gamma^{l}_{ji} v_l = v_{i,j} - v_{j,i}$$

using the symmetry properties of the Christoffel symbols.

Thus,

$$(curl\,\vec{v})_{ij} = v_{i,j} - v_{j,i}$$

(18) Absolute derivatives along curves

We now consider the problem of calculating the derivative of a tensor along a curve $\vec{r}(t)$ parameterized by some variable t.

Let us begin by considering the derivative of a vector $\vec{v}$ along the curve.

If we introduce an arbitrary coordinate system u^i with basis vectors $\hat{e}_i$, $i = 1, 2, 3$, then we can write $\vec{v} = v^i \hat{e}_i$, and we have

$$\frac{d\vec{v}}{dt} = \frac{dv^i}{dt}\hat{e}_i + v^i \frac{d\hat{e}_i}{dt} = \frac{dv^i}{dt}\hat{e}_i + v^i \frac{\partial \hat{e}_i}{\partial u^k}\frac{du^k}{dt}$$

where we have used the chain rule to rewrite the last term on the right-hand side.

Now, using the definition of the Christoffel symbols we obtain

$$\frac{d\vec{v}}{dt} = \frac{dv^i}{dt}\hat{e}_i + \Gamma^j_{ik} v^i \frac{du^k}{dt}\hat{e}_j$$

Interchanging the dummy indices i and j in the last term we get

$$\frac{d\vec{v}}{dt} = \left(\frac{dv^i}{dt} + \Gamma^i_{jk} v^j \frac{du^k}{dt} \right) \hat{e}_i$$

The expression in the brackets is called the **absolute** (or **intrinsic**) derivative of the components v^i along the curve $\vec{r}(t)$ and is usually denoted by

$$\frac{\delta v^i}{\delta t} \equiv \frac{dv^i}{dt} + \Gamma^i_{jk} v^j \frac{du^k}{dt} = \left(\frac{\partial v^i}{\partial u^k} + \Gamma^i_{jk} v^j \right) \frac{du^k}{dt} = v^i_{;k} \frac{du^k}{dt}$$

so that

$$\frac{d\vec{v}}{dt} = \frac{\delta v^i}{\delta t} \hat{e}_i = v^i_{;k} \frac{du^k}{dt} \hat{e}_i$$

Similarly, we can show that the absolute derivative of the covariant components v_i of a vector is given by

$$\frac{\delta v_i}{\delta t} \equiv v_{i;k} \frac{du^k}{dt}$$

and the absolute derivatives of the contravariant, mixed and covariant components of a second-order tensor T are

$$\frac{\delta T^{ij}}{\delta t} \equiv T^{ij}_{;k} \frac{du^k}{dt}$$

$$\frac{\delta T^{i}_{j}}{\delta t} \equiv T^{i}_{j;k} \frac{du^k}{dt}$$

$$\frac{\delta T_{ij}}{\delta t} \equiv T_{ij;k} \frac{du^k}{dt}$$

The derivative of T along the curve $\vec{r}(t)$ may then be written in terms of, for example, its contravariant components as

$$\frac{dT}{dt} = \frac{\delta T^{ij}}{\delta t} \hat{e}_i \otimes \hat{e}_j = T^{ij}_{;k} \frac{du^k}{dt} \hat{e}_i \otimes \hat{e}_j$$

(19) Geodesics

As an example of the use of the absolute derivative, we conclude our discussion of tensors with a short discussion of geodesics.

A geodesic in real three-dimensional space is a straight line, which has two equivalent defining properties.

First, it is the curve of shortest length between two points and, second, its tangent vector always points along the same direction (along the line).

Although we have explicitly considered only the familiar three dimensional space in our discussions, much of the mathematical formalism developed can easily be generalized to more abstract spaces of higher dimensionality in which the familiar ideas of Euclidean geometry are no longer valid.

It is often of interest to find geodesic curves in such spaces by using the properties of straight lines in Euclidean space that define a geodesic.

Consideration of these more complicated space is studied in a general relativity course.

Instead, we will derive the equation that a geodesic in Euclidean three dimensional space(i.e., a straight line) must satisfy, in a sufficiently general way that it may be applied with little modification, to find the equations satisfied by geodesics in more abstract spaces.

Let us consider a curve $\vec{r}(s)$, parameterized by the arc length s from some point on the curve, and choose as our defining property for a geodesic that its tangent vector

$$\vec{t} = \frac{d\vec{r}}{ds}$$

always points in the same direction everywhere on the curve, i.e.,

$$\frac{d\vec{t}}{ds} = 0$$

This is called **parallel transport** of the tangent vector, i.e., the vector is always moved parallel to itself along the curve, which is the same as its direction not changing for a straight line.

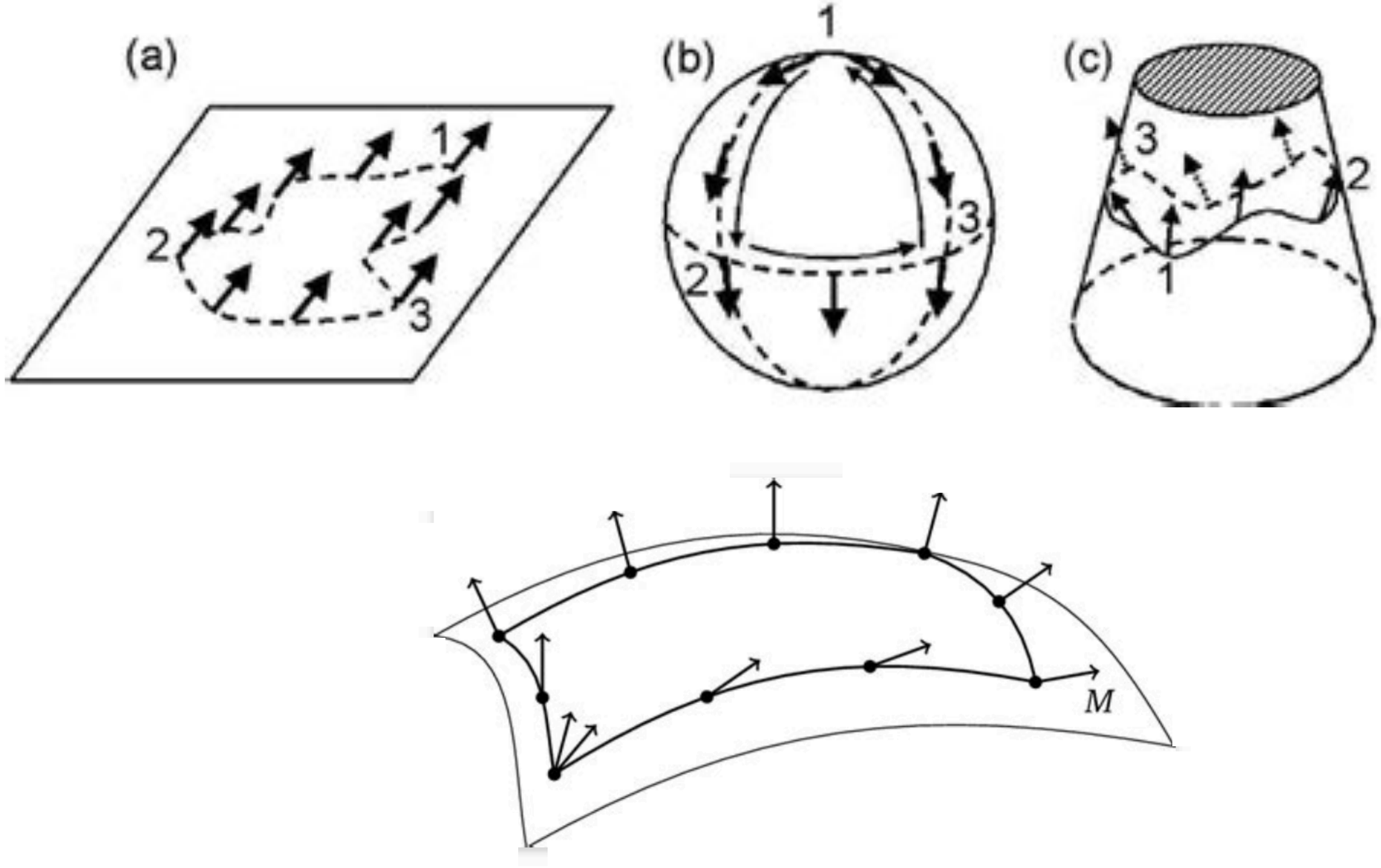
see next slide for illustrations

If we now introduce an arbitrary coordinate system u^i with basis vectors $\hat{e}_i$, $i = 1, 2, 3$, then we can write $\vec{t} = t^i \hat{e}_i$, and we have

$$\frac{d\vec{r}}{ds} = t^i_{;k} \frac{du^k}{ds} \hat{e}_i = 0$$

Writing out the covariant derivative, we obtain

$$\left(\frac{dt^i}{ds} + \Gamma^i_{jk} t^j \frac{du^k}{ds} \right) \hat{e}_i = 0$$


(a)
1
2
3
(b)
1
2
3
(c)
3
1
2
1

M

N
A
B

But since

$$t^j = \frac{du^j}{ds}$$

we find that the equation satisfied by a geodesic is

$$\frac{d^2u^i}{ds^2} + \Gamma^i_{jk}\frac{du^j}{ds}\frac{du^k}{ds} = 0$$

Example: Cartesian coordinates

All Christoffel symbols are zero.

Therefore, the equations of a geodesic are

$$\frac{d^2x}{ds^2} = 0 \ , \quad \frac{d^2y}{ds^2} = 0 \ , \quad \frac{d^2z}{ds^2} = 0$$

which correspond to a straight line.

Example: cylindrical polar coordinates

The only non-zero Christoffel symbols are

$$\Gamma^1_{22} = -\rho \quad \text{and} \quad \Gamma^2_{12} = \Gamma^2_{21} = \frac{1}{\rho}$$

The geodesic equations are then

$$\frac{d^2u^1}{ds^2} + \Gamma^1_{22}\frac{du^2}{ds}\frac{du^2}{ds} = 0 \rightarrow \frac{d^2\rho}{ds^2} - \rho\left(\frac{d\phi}{ds}\right)^2 = 0$$

$$frac d^2u^2 ds^2 + 2\Gamma^2_{12}\frac{du^1}{ds}\frac{du^2}{ds} = 0 \rightarrow \frac{d^2\phi}{ds^2} + \frac{2}{\rho}\frac{d\rho}{ds}\frac{d\phi}{ds} = 0$$

$$\frac{d^2u^3}{ds^2} = 0 \rightarrow \frac{d^2z}{ds^2} = 0$$

On the surface of a cylinder given by $\rho =$ constant we have

$$\frac{d^2\rho}{ds^2} = 0 \ , \quad \frac{d^2\phi}{ds^2} = 0 \ , \quad \frac{d^2z}{ds^2} = 0$$

which also corresponds to a straight line.

Think if unrolling the cylinder. It is then just a plane!

Example: spherical polar coordinates

The metric tensor is

$$\mathrm{g} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -r^2 & 0 \\ 0 & 0 & -r^2 \sin\theta \end{pmatrix}$$

The non-zero Christoffel symbols are

$$\Gamma^1_{22} = -r \;\;,\;\; \Gamma^1_{33} = -r\sin^2\theta \;\;,\;\; \Gamma^2_{33} = -\sin\theta\cos\theta$$

$$\Gamma^2_{12} = \Gamma^2_{21} = \frac{1}{r} \;\;,\;\; \Gamma^3_{13} = \Gamma^3_{31} = \frac{1}{r} \;\;,\;\; \Gamma^3_{23} = \Gamma^3_{32} = \cot\theta$$

The corresponding geodesic equations on the surface of the sphere $r =$ constant are

$$\frac{d^2r}{ds^2} = 0$$

$$\frac{d^2\theta}{ds^2} - \sin\theta\cos\theta\left(\frac{d\phi}{ds}\right) = 0$$

$$\frac{d^2\phi}{ds^2} + 2\cot\theta\frac{d\phi}{ds}\frac{d\theta}{ds}$$

which correspond to the equations of a great circle!

Parallel Transport and the Riemann Tensor

If a vector is parallel transported along a curve, the geodesic equations tells us how the vector components change during the transport.

$$\frac{d^2u^i}{ds^2} + \Gamma^i_{jk}\frac{du^j}{ds}\frac{du^k}{ds} = 0$$

It also can be shown that for a covariant vector field A_β we have this result

$$A_{\beta;\mu;\nu} - A_{\beta;\nu;\mu} = R^\alpha_{\beta\mu\nu}A_\alpha$$

that is, in a general curved spacetime the covariant derivatives do not commute (order is important).

In a Cartesian or flat space the difference would be zero.

Thus the fourth-rank tensor $R^\alpha_{\beta\mu\nu}$, which is called the Riemann curvature tensor is a measure of the curvature of spacetime.

It is given by

$$R^{\alpha}_{\beta\mu\nu} = -\Gamma^{\alpha}_{\beta\mu,\nu} + \Gamma^{\alpha}_{\beta\nu,\mu} - \Gamma^{\sigma}_{\beta\nu}\Gamma^{\alpha}_{\sigma\mu} - \Gamma^{\sigma}_{\beta\mu}\Gamma^{\alpha}_{\sigma\nu}$$

If a vector field is parallel transported around a closed path in a curved spacetime, the vector components do not return to the same values at the end (as they would do in flat space).

In fact, parallel transport around a parallelogram gives the result

$$\Delta A^{\alpha} = R^{\alpha}_{\beta\mu\nu} A^{\beta} d\xi^{\nu} d\xi^{\mu}$$

where the $d\xi^{\mu}$ represent the sides of the parallelogram.

Thus, once again the Riemann tensor serves as a measure of the curvature of spacetime.

The second-rank Ricci tensor is defined by a contraction over the first and last indices of the Riemann tensor

$$R_{\beta\mu} = R^{\alpha}_{\beta\mu\alpha}$$

In addition we define the curvature scalar R by

$$R = R^{\beta}_{\beta} = R^{\alpha\beta}_{\beta\alpha}$$

Einstein Field Equations for Metric Coefficients

The gravitational field equations developed by Einstein are

$$R_{\mu\nu} = \frac{1}{2} g_{\mu\nu} R = -\frac{8\pi G}{c^4} T_{\mu\nu}$$

where the inclusion of the Riemann scalar term is necessary for energy-momentum conservation, and where $T_{\mu\nu}$ is a second-rank tensor that gives the energy-momentum content of spacetime.

This equation represents 16 coupled differential equations for the metric coefficients $g_{\mu\nu}$.

An alternative form of these field equations originally proposed by Einstein but later discarded by him (he described this action as his worst mistake), is now coming back into favor.

It contains the so-called cosmological constant Λ.

$$R_{\mu\nu} = \frac{1}{2} g_{\mu\nu} R + \Lambda g_{\mu\nu} = -\frac{8\pi G}{c^4} T_{\mu\nu}$$

It predicts the existence of a repulsive gravitational force on a cosmological scale and is of interest now that data seems to indicated that the universal expansion is accelerating.

Schwarzschild Solution

For a spherically symmetric point mass at the origin, the field equations are given by (for $r > 0$)

$$R_{\mu\nu} = \frac{1}{2} g_{\mu\nu} R = 0$$

Schwarzschild solved these equations in 1915.

His solution written as the square of the spacetime interval(which involves the metric coefficients) looks like

$$ds^2 = \left(1 - \frac{2GM}{r}\right) c^2 dt^2 - \frac{dr^2}{\left(1 - \frac{2GM}{r}\right)} - r^2(d\theta^2 + \sin^2\theta d\phi^2)$$

where M is the central mass.

This solution accounts for bending of light around the sun, the advance of the perihelion of mercury, gravitational redshift, radar time delays from signals bounced off of planets, the precession of spinning satellites in earth orbit and black holes, where the radius $r = 2GM$ is the radius of the event horizon or the boundary where nothing can escape the mass, even light.

Probability and Statistics — A Quick Introduction

The understanding of many physical phenomena depends on statistical and probabilistic concepts. **Statistical mechanics** is the physics of systems composed of many parts - gases, liquids, solids, etc. 1 mole of anything contains 6×10^{23} particles(Avogadro's number).

It is impossible to keep track of all 6×10^{23} particles even with the fastest computer imaginable.

Therefore, we must resort to learning about groups or clusters of particles.

Probabilistic ideas dominate the theory.

Quantum Mechanics is the physics of atoms and all other micro-physical phenomena.

Quantum phenomena are inherently probabilistic.

The **understanding/interpretation of experimental data** depends on statistical and probabilistic concepts to answer these questions

- How do we extract the best value of a quantity from a set of measurements?
- How do we decide if our experiment is consistent/inconsistent with a given theory?
- How do we decide if our experiment is internally consistent?
- How do we decide if our experiment is consistent with other experiments?

Definition of Probability

Suppose we have N trials and a specified event E occurs r times.

For example, rolling a dice and the event could be rolling a 6.

We define the probability P of an event E occurring as:

$$P(E) = \frac{r}{N} \quad \text{when} \quad N \to \infty$$

Examples:

1. six side dice: $P(6) = 1/6$
2. coin toss: $P(\mathit{heads}) = 0.5$

We note our expectation that $P(\mathit{heads})$ should approach 0.5 the more times you toss the coin and that for a single coin toss we never get $P(\mathit{heads}) = 0.5 \rightarrow$we have $P(\mathit{heads}) = 1$ if we get heads and $P(\mathit{heads}) = 0$ if we get tails; that is all that can happen in a single toss.

By definition probability is a non-negative number bounded by

$$0 \leq P \leq 1$$

Some properties:

(1) If $P = 0$, then the event **never** occurs.

(2) If $P = 1$, then the event **always** occurs.

(3) The sum (or integral) of all probabilities of **mutually exclusive** (see (6) below) events $= 1$.

(4) Two events are mutually exclusive or disjoint if they cannot occur at the same time.

(5) The probability that Events A and B both occur is the probability of the intersection of A and B. The probability of the intersection of Events A and B is denoted by $P(A \cap B)$.

(6) Events are **mutually exclusive** (disjoint) if

$$P(A \cup B) = 0 \text{ or } P(A \cup B) = P(A) + P(B)$$

(7) The probability that Events A or B occur is the probability of the union of A and B. The probability of the union of Events A and B is denoted by $P(A \cup B)$.

(8) Events are **independent** if

$$P(A \cap B) = P(A)P(B)$$

(9) Events are **mutually exclusive** (disjoint) if

$$P(A \cup B) = 0 \text{ or } P(A \cup B) = P(A) + P(B)$$

Probability can be a discrete or a continuous variable.

Discrete probability: P can have certain values only.

Examples:

1. Tossing a 6-sided dice:

   $P(x_i) = P_i$ where $x_1 = 1, 2, 3, 4, 5, 6$ and $P_i = 1/6$ for all x_1.

2. Tossing a coin:

   $P(x_i) = P_i$ where $x_1 =$ heads or tails and $P_i = 1/2$ for all x_1.

For both of the above discrete examples (and in general) when we sum over all mutually exclusive possibilities we have

$$\sum_i P_i = 1$$

Continuous probability: P can be any number between 0 and 1.

We define a "probability density function", **pdf**, $f(x)$ such that

$$f(x)dx = P(x \leq \alpha \leq x + dx)$$

with α a continuous variable.

Then the probability for x to be in the range $a \leq x \leq b$ is given by

$$P(a \leq x \leq b) = \int_a^b f(x)dx$$

Just like the discrete case, the sum of all probabilities satisfy

$$P(-\infty \leq x \leq \infty) = \int_{-\infty}^{\infty} f(x)dx = 1$$

that is, $f(x)$ is **normalized** to 1.

We note that the probability for x to be exactly some number is zero since:

$$P(a \leq x \leq a) = P(x = a) = \int_{a}^{a} f(x)dx = 0$$

Examples of some common $P(x)$'s and $f(x)$'s:

Discrete $= P(x)$	Continuous $= f(x)$
binomial	uniform, i.e., constant
Poisson	Gaussian
	exponential
	chi square

Formal Theory

Probability Concepts

We will be interested in understanding the quantity

$$P(A|B) = \text{ probability of event } A \text{ given that event } B \text{ is true}$$

In essence, event B sets up the conditions or an environment and then we ask about the (conditional) probability of event A given that those conditions exist. All probabilities are conditional in this sense.

In other words, we set up an experimental apparatus, which is expressed by properties B and do a measurement with that apparatus, which is expressed by properties A.

We generate numbers (measurements) which we use to give a value to the quantity $P(A|B)$.

We start with a mathematical formalism based on axioms.

We define these events

$A =$ occurrence of A

$\sim A =$ NOT $A =$ nonoccurrence of A

$A \cap B = A$ AND $B =$ occurrence of both A and B

$A \cup B = A$ OR $B =$ occurrence of at least one of the events A and B

and set up a theory of probability with these axioms:

(1) $P(A|A) = 1$

This is the probability of the occurrence A given the occurrence of A. This represents a **certainty** and, thus, the probability must $= 1$. This is clearly an obvious assumption that we must make if our probability ideas are to make any sense at all.

In other words, if I set the experimental apparatus such that the meter reads A, then it reads A with probability $= 1$.

(2) $0 \leq P(A|B) \leq P(B|B) = 1$

This just expresses the sensible idea that no probability is greater than the probability of a certainty and it make no sense to have the probability be less than 0.

(3) $P(A|B) + P(\sim A|B) = 1$ or $P(\sim A|B) = 1 - P(A|B)$

This just expresses the fact that the probability of something (anything) happening (A or $\sim A$) given B is a certainty ($= 1$), that is, since the set A or $\sim A$ includes everything that can happen, the total probability that one or the other occurs must be the probability of a certainty and be equal to one.

(4) $P(A \cap B|C) = P(A|C)P(B|A \cap C)$

This says that the probability that 2 events A, B both occur given that C occurs equals the probability of A given C multiplied by the probability of B given $(A \cap C)$, which makes sense if you think of them happening in sequence.

All other probability relationships can be derived from these axioms.

The nonoccurrence of A given that A occurs must have probability $= 0$.

This is expressed by

$$P(\sim A|A) = 0$$

This result clearly follows from the axioms since

$$P(A|B) + P(\sim A|B) = 1$$

$$P(A|A) + P(\sim A|A) = 1$$

$$P(\sim A|A) = 1 - P(A|A) = 1 - 1 = 0$$

Example: Let us evaluate $P(X \cap Y|C) + P(X \cap \sim Y|C)$. We use axiom (4) in the 1st term with $A = X$, $B = Y$ and $C = C$ and in the 2nd term with $A = X$, $B = \sim Y$ and $C = C$ to get

$$
\begin{aligned}
P(X \cap Y|C) + P(X \cap \sim Y|C) & \\
&= P(X|C)P(Y|X \cap C) + P(X|C)P(\sim Y|X \cap C) \\
&= P(X|C)\left[P(Y|X \cap C) + P(\sim Y|X \cap C)\right] \\
&= P(X|C)[1] \quad \text{using axiom (3)}
\end{aligned}
$$

and finally

$$P(X \cap Y|C) + P(X \cap \sim Y|C) = P(X|C)$$

Now let us use this result with $X = \sim A$, $Y = \sim B$. This gives

$$
\begin{aligned}
P(\sim A \cap \sim B|C) &= P(\sim A|C) - P(\sim A \cap B|C) \\
&= 1 - P(A|C) - P(\sim A \cap B|C)
\end{aligned}
$$

Expanding the last term using $X = B$, $Y = A$ we then have

$$P(B \cap \sim A|C) + P(B \cap A|C) = P(B|C)$$

or

$$P(\sim A \cap B|C) = P(B|C) - P(B \cap A|C)$$

which gives

$$P(\sim A \cap \sim B|C) = 1 - P(A|C) - P(B|C) + P(A \cap B|C)$$

Now

$$P(A \cup B|C) = 1 - P(\sim (A \cup B)|C = 1 - P(\sim A \cap \sim B|C)$$

and since

$$(\sim (A \cup B)) = (\sim A \cap \sim B)$$

i.e.,

A	B	$(\sim(A \cup B))$	$(\sim A \cap \sim B)$
1	1	0	0
1	0	0	0
0	1	0	0
0	0	1	1

which is called a "truth table" and clearly shows the equality, we finally get

$$P(A \cup B|C) = P(A|C) + P(B|C) - P(A \cap B|C)$$

This is a very important and useful result.

If we have $P(A \cap B|C) = 0$, then events A and B are said to be **mutually exclusive** given that C is true and the relation then reduces to

$$P(A \cup B|C) = P(A|C) + P(B|C)$$

This is the rule of **addition of probabilities for exclusive events.**

Some other important results are:

If $A \cap B = B \cap A$, then $P(A|C)P(B|A \cap C) = P(B|C)P(A|B \cap C)$

If $P(A|C) \neq 0$, then $P(B|A \cap C) = P(A|B \cap C)\dfrac{P(B|C)}{P(A|C)}$

which is **Baye's theorem**.

It relates the probability of B given A to the probability of A given B.

This rule, which relates $prob(A|B \cap C)$ to $prob(B|A \cap C)$, allows us to turn things around with respect to the conditioning symbol, which leads to a reorientation of our thinking about probability.

The fundamental importance of this property to data analysis becomes apparent if we replace A and B by **hypothesis** and **data**:

$$prob(A|B \cap C) \propto prob(B|A \cap C) \times prob(A|C)$$

$$prob(hypothesis|data \cap I) \propto prob(data|hypothesis \cap I) \times prob(hypothesis|I)$$

Note that the equality has been replaced with a proportionality because the term $prob(data|I) =$ **evidence** has been omitted.

The proportionality constant is found from the normalization requirement that the sum of the probabilities for something happening must equal 1.

The power of Bayes' theorem lies in the fact that it relates the quantity of interest, the probability that the hypothesis is true given the data, to the term that we have a better chance of being able to assign, the probability that we would have obtained the measured data if the hypothesis was true.

The various terms in Bayes' theorem have formal names.

The term $prob(hypothesis|I)$ = **prior** probability represents our state of knowledge(or ignorance) about the truth of the hypothesis before we have analyzed the current data.

This is modified by the experimental measurements through the term

$$prob(data|hypothesis\,\&I) = \textbf{likelihood function}.$$

This product gives $prob(hypothesis|data\,\&I)$ = **posterior** probability representing our state of knowledge about the truth of the hypothesis in the light of the data(after measurements).

In some sense, Bayes' theorem encapsulates **the process of learning**.

When we say that B is **independent** of A, we will mean

$$P(B|A \cap C) = P(B|C)$$

or the occurrence of A has **NO influence** on the probability of B given C.

Using axiom (4) we then have the result:

If A and B are independent given C, then $P(A \cap B|C) = P(A|C)P(B|C)$

This is called **statistical** or **stochastic** independence.

The result generalizes to a set of events $\{A_i\,, i = 1, 2, ..., n\}$.

All these events are independent if and only if

$$P(A_1 \cap A_2 \cap .... \cap A_m|C) = P(A_1|C)P(A_2|C).....P(A_m|C)$$

for all $m < n$.

How do we describe a probability distribution?

The main variables are the **mean, mode, median and the variance**.

For a **continuous distribution**, these quantities are defined by:

$$\text{mean} \;=\; \text{average} \;= \mu = \int_{-\infty}^{\infty} xf(x)dx$$

$$\text{mode} \;=\; \text{most probable} \;=\; \left.\frac{\partial f(x)}{\partial x}\right|_{x=a} = 0$$

$$\text{median} \;=\; 50\%\ \text{point} \;= 0.5 = \int_{-\infty}^{a} x f(x)\,dx$$

$$\text{variance} \;=\; \text{width of distribution} \;= \sigma^2 = \int_{-\infty}^{\infty} f(x)(x-\mu)^2\,dx$$

For a discrete distribution the mean and variance are defined by:

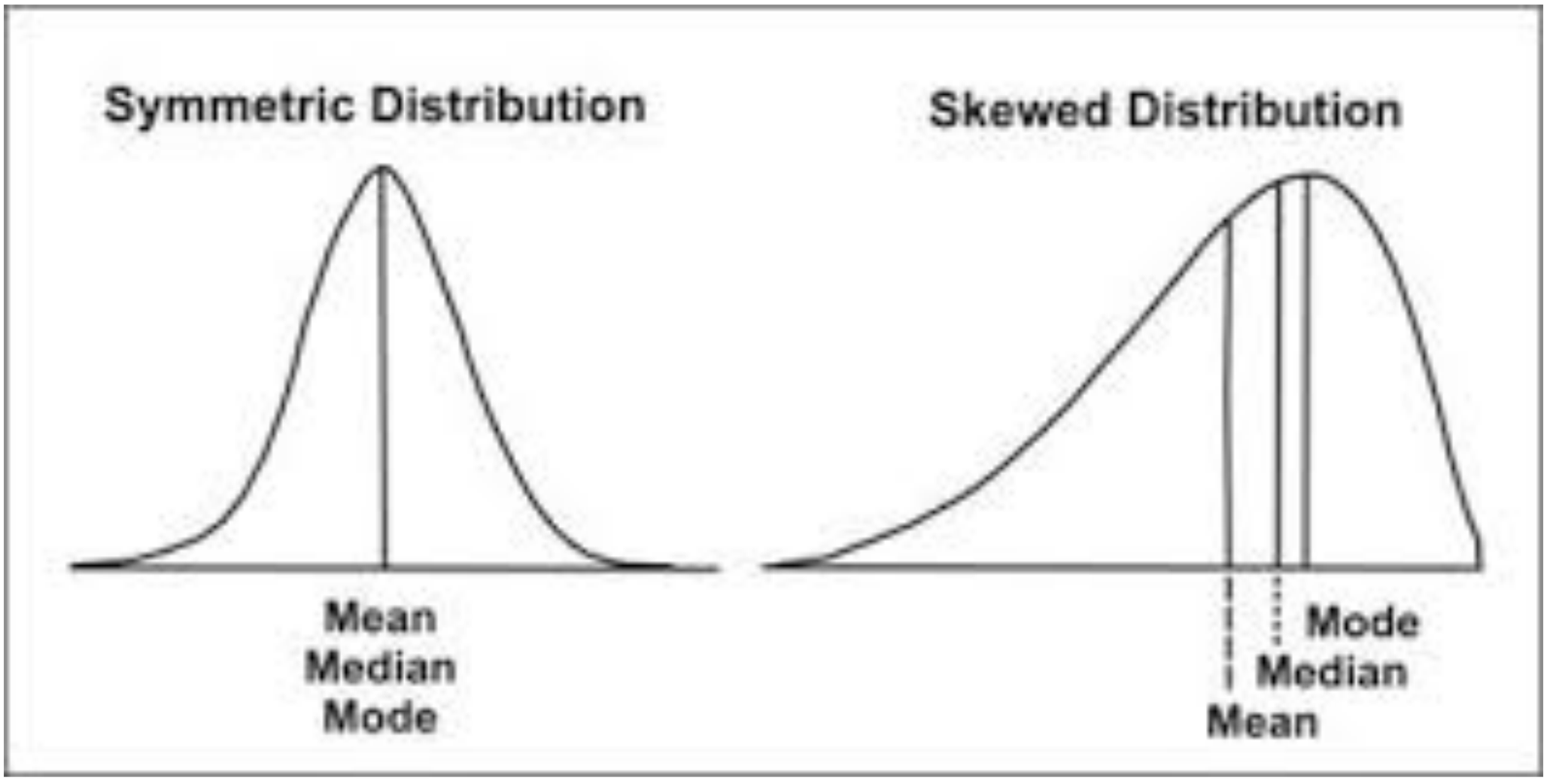
$$\text{mean} \;= \mu = \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$\text{variance} \;= \sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i-\mu)^2$$

Some continuous **pdf**:

symmetric distribution (gaussian): in this case the mean, mode and median are all at the same x. See figure below.

asymmetric distribution: in this (and most) cases the mean, mode, and median are at different x-values.



Calculation of mean and variance:

Example: Given a discrete data set containing the three numbers

$$x_i = \{1, 2, 3\}$$

the average μ is

$$\mu = \frac{1}{n}\sum_{i=1}^{n} x_i = \frac{1}{3}(1 + 2 + 3) = 2$$

A complication arises if some measurements are more precise than others, that is, if each measurement x_i has a weight w_i associated with it then we calculate the average using

$$\mu = \frac{1}{\sum_{i=1}^{n} w_i}\sum_{i=1}^{n} w_i x_i$$

which is called a "weighted average".

So if the three data points are such that the value 3 is 10 times more precise than the values 1 and 2 we have

$$w_i = \{1, 1, 10\}$$

and

$$\mu = \frac{1}{12}(1 + 2 + 30) = \frac{33}{12} = 2.75$$

The variance σ^2 (σ = standard deviation) or squared average deviation from the mean is

$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2$$

It describes the width of the **pdf**. Expanding the summations we can rewrite this expression in a more useful form:

$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}[x_i^2 - 2]mux_i + \mu^2] = \frac{1}{n}\sum_{i=1}^{n}x_i^2 - 2\mu\frac{1}{n}\sum_{i=1}^{n}x_i + \mu^2\frac{1}{n}\sum_{i=1}^{n}1$$

$$(x_i^2)_{average} - 2\mu(x_i)_{average} + \frac{1}{n}\mu^2(n)$$

$$\langle x^2\rangle - 2\mu(\mu) + \mu^2 = \langle x^2\rangle - \mu^2$$

$$\langle x^2\rangle - \langle x\rangle^2 \qquad where \langle\cdots\rangle = \text{ average}$$

For our sample data set we have

$$\sigma^2 = \frac{1}{3}(1+4+9) - (2)^2 = 4.67 - 4 = 0.67$$

and in the case of different weights for the data values we have

$$\sigma^2 = \frac{1}{\sum_{i=1}^{n} w_i} \sum_{i=1}^{n} w_i (x_i - \mu)^2 = \frac{1}{\sum_{i=1}^{n} w_i} \sum_{i=1}^{n} w_i x_i^2 - \mu^2$$

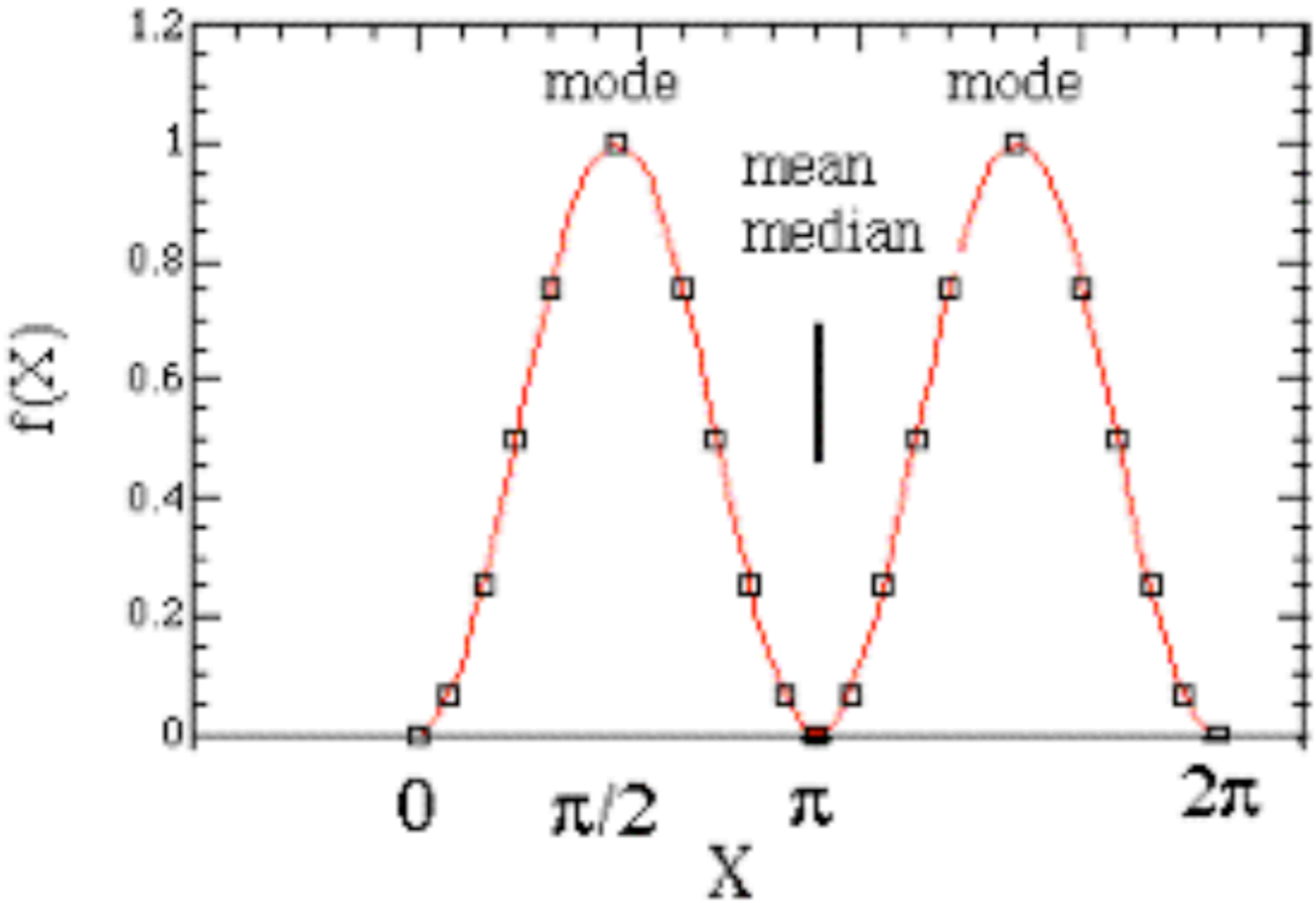
$$= \frac{95}{12} - (2.75)^2 = 7/92 - 7.56 = 0.36$$

Example: a continuous probability distribution

$$f(x) = \sin^2 x \quad , \quad 0 \leq x \leq 2\pi$$

This distribution has two modes.

The mean and median are equal, but different from the mode as shown below



First, we note that $f(x)$ is not properly normalized, i.e.,

$$\int_0^{2\pi} f(x)dx = \int_0^{2\pi} \sin^2 x dx = \pi \neq 1$$

Therefore, the normalized pdf is given by

$$f(x) = \frac{\sin^2 x}{\int_0^{2\pi} f(x)dx} = \frac{1}{\pi}\sin^2 x$$

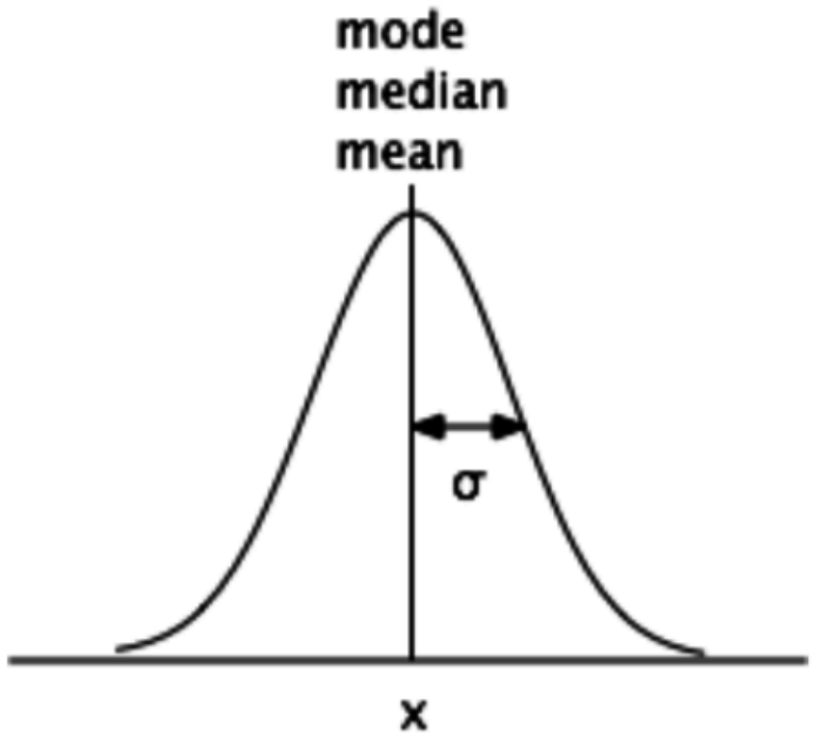
The actual values for this distribution are

$$\mu = \frac{1}{\pi}\int_0^{2\pi} x \sin^2 x dx = \pi$$

$$\frac{\partial}{\partial x}\sin^2 x = 0 \rightarrow x = \frac{\pi}{2}, \frac{3\pi}{2} = \text{ modes}$$

$$\frac{1}{\pi}\int_0^{\alpha} x \sin^2 x dx = 0.5 \rightarrow \alpha = \pi = \text{ median}$$

Another continuous distribution example: a **Gaussian**: we have (see figure below)



where

$$f(x) = \frac{1}{\sigma\sqrt{2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

and $\sigma =$ standard deviation and $x =$ mean $=$ mode $=$ median $= \pi$.

We note that 68% of the area under the curve lies within $\pm\sigma$.

Accuracy and Precision

The **accuracy** of an experiment refers to how close the experimental measurement is to the "true" value of the quantity being measured.

The **precision** refers to how well the experimental result has been determined, without regard to the true value of the quantity being measured. Remember, just because an experiment is precise, it does not mean it is accurate!

Measurement Errors (Uncertainties)

The most common quality indicator is the **relative precision** defined by:

$$\text{relative precision} = \frac{\text{[uncertainty in measurement]}}{\text{measurement}}$$

where the [uncertainty in measurement] is the square root of the variance or the the standard deviation σ.

This is usually calculated using "propagation of errors".

Statistics and Systematic Errors

Results from experiment are often presented as:

$$N \pm XX \pm YY$$

where

N = value of quantity measured (or determined) by experiment
XX = statistical error (usually assumed to be from a Gaussian distribution).

With the assumption of Gaussian statistics we can say (calculate) something about how well our experiment agrees with other experiments and/or theories.

We are saying that we expect a 68% chance that the true value is between $N - XX$ and $N + XX$.
YY = systematic error; very hard to estimate since the distribution of such errors is generally not know.

What is the difference between statistical and systematic errors?

Statistical errors are "random" in the sense that if we repeat the measurement enough times $XX \to 0$ in the sense described earlier.

Systematic errors do not $\to 0$ with repetition.

An example of a systematic error might be a poorly calibrated voltmeter.

Because of systematic errors an experiment can be precise, but not accurate!

How do we combine systematic and statistical errors to get one estimate of precision?

This is always a big problem.

We have two choices:

$$\sigma_{total} = XX + YY \quad \text{add them linearly}$$

or

$$\sigma_{total} = (XX^2 + YY^2)^{1/2} \quad \text{add them in quadrature.}$$

Now let us now look in more detail at some discrete probability distributions.

Binomial Probability Distribution

Consider a situation where there are only two possible outcomes (a so-called **Bernoulli** trial), for example, flipping a coin (head or tail) or rolling a dice (6 or not 6).

Label the possible outcomes by the variable k; we want to determine the probability $P(k)$ for event k to occur.

Since k can take on only 2 values we define those values as

$$k = 0 \quad \text{or} \quad k = 1$$

Let $P(k = 0) = q$ (remember $0 \leq q \leq 1$).

Now something must happen (one of our postulates) so that we must have

$$P(k = 0) + P(k = 1) = 1$$

$$P(k = 1) = p = 1 - P(k = 0) = 1 - q$$

We can write the probability distribution $P(k)$ as

$$P(k) = p^k q^{1-k} \quad \text{(Bernoulli distribution)}$$

For the coin toss case, if we define the probability for a head as $P(1)$, then

$$P(1) = P(0) = 0.5$$

For the dice roll case, if we define the probability for a 6 to be rolled as $P(1)$, then

$$P(1) = 1/6 \; ; \; P(0) = 5/6 = P(\textit{not a}\, 6) = p(1,2,3,4,5)$$

What is the mean μ of $P(k)$?

$$\mu = \frac{\sum_{k=0}^{1} kP(k)}{\sum_{k=0}^{1} P(k)} = \frac{0 \times q + 1 \times p}{q + p} = \frac{p}{1} = p$$

What is the variance σ^2 of P(k)?

$$\sigma^2 = \langle k^2 \rangle - \langle k \rangle^2 = \frac{\sum_{k=0}^{1} k^2 P(k)}{\sum_{k=0}^{1} P(k)} - \mu^2 = \frac{0 \times q + 1 \times p}{q + p} - p^2$$
$$= p - p^2 = p(1-p) = pq$$

Suppose we have N trials (e.g. we flip a coin N times).

What is the probability of m successes (= heads). Clearly $m \leq N$.

Consider tossing the coin twice.

The possible outcomes are

$$\text{no heads}: \; P(m=0) = q^2$$

$$\text{one head}: \; P(m=1) = qp + pq = 2pq \quad (\text{tail/head} + \text{head/tail})$$

$$\text{two heads}: \; P(m=2) = p^2$$

Therefore, $P(0) + P(1) + P(2) = q^2 + 2pq + p^2 = (q+p)^2 = 1$ as expected.

We want the probability distribution function $P(m, N, p)$ where

$$m = \text{ number of successes (number of heads)}$$

$$N = \text{ number of trials (number of coin tosses)}$$

$$p = \text{ probability of success (0.5 for head)}$$

If we look at these three choices for the coin flip example, each term is of the form:

$$C_m p^m q^{N-m}$$

with $m = 0, 1, ..., N$.

Now $N = 2$ for our example and $q = 1 - p$ always. The coefficient C_m takes into account the number of ways an outcome can occur regardless of order.

For $m = 0$ or $m = 2$, there is only one way for the outcome (both tosses give heads or tails) so that $C_0 = C_2 = 1$. For $m = 1$ (one head in two tosses) there are two ways that this can occur so that $C_1 = 2$.

The so-called Binomial coefficients (introduced earlier) tell us the number of ways of taking N things m at a time, that is,

$$C_{N,m} = \binom{N}{m} = \frac{N!}{m!(N-m)!}$$

Note that we are assuming that order of things is not important so that head followed by tail counts the same as tail followed by head. Unordered groups such as this example are called **combinations**.

Ordered arrangements are called **permutations**.

For N distinguishable objects, if we want to group them m at a time, the number of permutations is

$$P_{N,m} = \frac{N!}{(N-m)!}$$

Examples:

(1) If we tossed a coin twice ($N = 2$), there are two ways to get one head ($m = 1$).

(2) Suppose we have 3 balls, one white, one red and one blue. The number of possible pairs we could have(keeping track of the order) is 6 (rw, wr, rb, br, wb, bw) and

$$P_{3,2} = \frac{3!}{(3-2)!} = 6$$

If order is not important (rw = wr), then the binomial formula gives

$$C_{3,2} = \binom{3}{2} = \frac{3!}{2!(3-2)!} = 3$$

namely, (wr, bw, rb).

The binomial distribution in general: the probability of m successes out of N trials is

$$P(m, N, p) = C_{N,m} p^m q^{N-m} = \binom{N}{m} p^m q^{N-m} = \frac{N!}{m!(N-m)!} p^m q^{N-m}$$

Now consider a game where a player bats 4 times and

$$p = \text{ probability of a hit } = 1/3$$

$$q = 1 - p = \text{ probability of not hit } = 2/3$$

We then have (for hits)

$$\text{probability of } 0/4 = [4!/(4!0!)](1/3)^0(2/3)^4 = 19.75\%$$

$$\text{probability of } 1/4 = [4!/(1!3!)](1/3)^1(2/3)^3 = 39.51\%$$

$$\text{probability of } 2/4 = [4!/(2!2!)](1/3)^2(2/3)^2 = 29.63\%$$

$$\text{probability of } 3/4 = [4!/(3!1!)](1/3)^3(2/3)^1 = 9.88\%$$

$$\text{probability of } 4/4 = [4!/(4!0!)](1/3)^4(2/3)^0 = 1.23\%$$

Clearly the probability of getting at least one hit is

$$1 - P(0) = 80.25\%$$

Now in general

$$\begin{aligned}
\langle n \rangle &= \text{ average or expectation value(for hits)} \\
&= \text{ sum over [possible values times probability of that value]} \\
&= \sum_{m=0}^{N} mP(m,N,p) = \sum_{m=0}^{N} m\frac{N!}{m!(N-m)!}p^m q^{N-m}
\end{aligned}$$

We now use a clever mathematical trick to evaluate this sum.

For the moment consider p and q to be two arbitrary independent variables.

At the end of the calculation we will let $q = 1 - p$ as is appropriate for a real physical system.

From the Binomial expansion formula, we have, in general,

$$\sum_{m=0}^{N} P(m, N, p) = \sum_{m=0}^{N} m \frac{N!}{m!(N-m)!} p^m q^{N-m} = (p+q)^N$$

Since $p + q = 1$, the says the the probability distribution $P(m, N, P)$ is properly normalized.

We then have

$$p \frac{\partial}{\partial p} \sum_{m=0}^{N} \frac{N!}{m!(N-m)!} p^m q^{N-m} = p \frac{\partial}{\partial p} (p+q)^N$$

or

$$\sum_{m=0}^{N} m \frac{N!}{m!(N-m)!} p^m q^{N-m} = Np(p+q)^{N-1}$$

or

$$\sum_{m=0}^{N} mP(m,N,p) = Np(p+q)^{n-1}$$

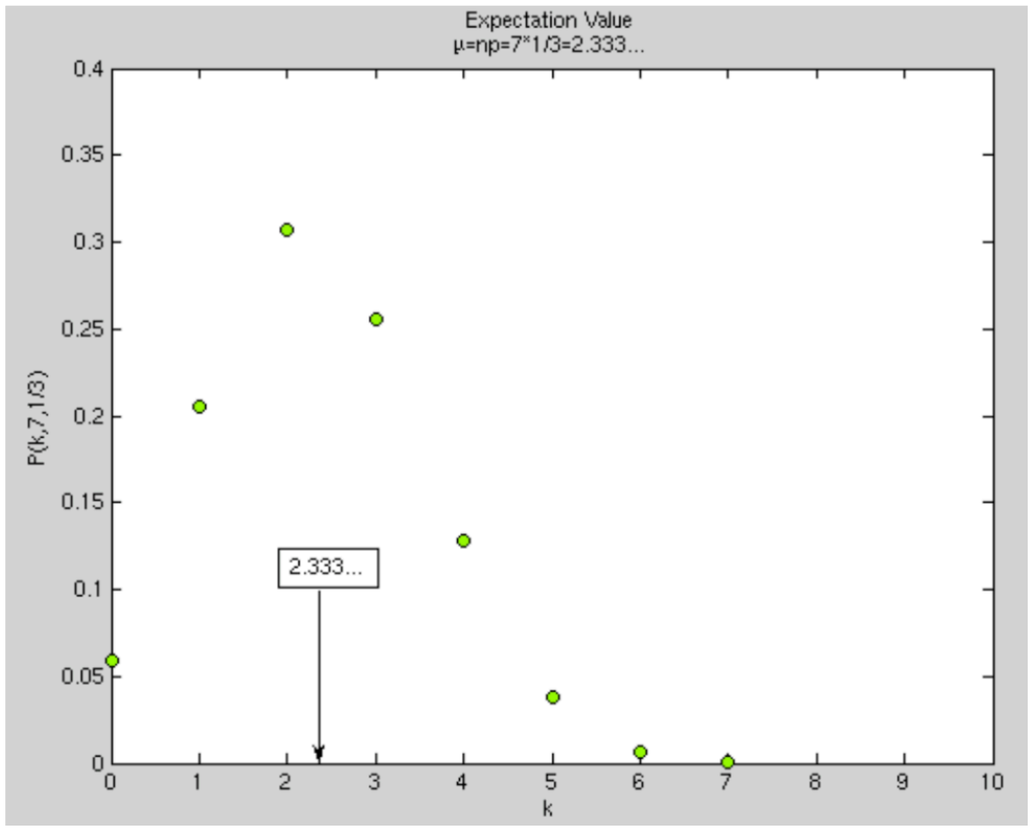
Thus,

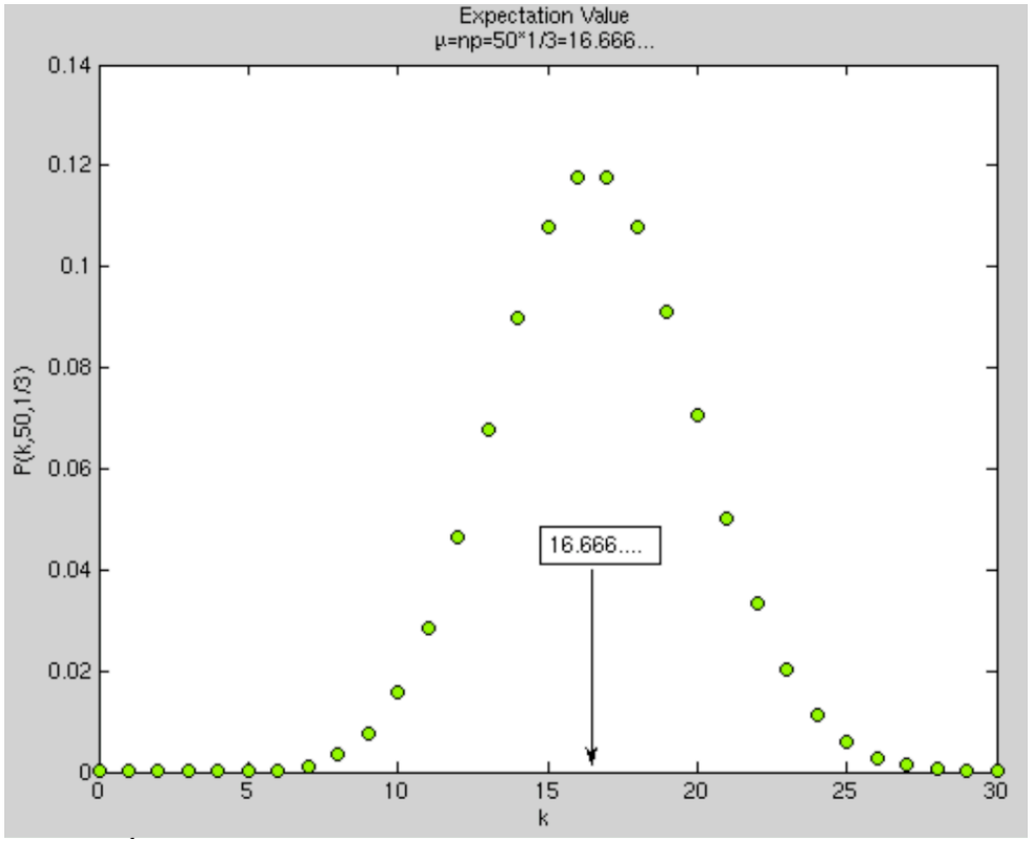
$$\langle n \rangle = Np(p+q)^{N-1}$$

In a real physical system, we must have $p + q = 1$, so that we end up with the result

$$\langle n \rangle = Np$$

Some results for $N = 7$ and $N = 50$ are shown below.





The variance can be calculated in a similar ways and we het

$$\sigma^2 = \frac{\sum_{n=0}^{N}(m-\mu)^2 P(m,N,p)}{\sum_{n=0}^{N} 2P(m,N,p)} = Npq$$

Example: Suppose you observed m special events (success) in a sample of N events.

The measured probability for a special event to occur is then

$$\epsilon = \frac{m}{N}$$

The error of the probability is

$$\sigma_\epsilon = \frac{\sigma_m}{N} = \frac{\sqrt{N\epsilon(1-\epsilon)}}{N} = \sqrt{\frac{\epsilon(1-\epsilon)}{N}}$$

which implies that the sample (N) should be as large as possible to reduce the uncertainty in the probability.

Example: Suppose a baseball player's batting average is 1/3 (1 for 3 on average).

Consider the case where the player either gets a hit or makes an out (forget about walks here!).

Then

$$p = \text{ probability for a hit } = p = 1/3$$

$$q = 1 - p = \text{ probability for “no hit” } = q = 1 - p = 2/3$$

On average how many hits does the player get in 100 at bats?

$$\mu = Np = 100(1/3) = 33.33$$

What is the standard deviation for the number of hits in 100 at bats?

$$\sigma = (Npq)^{1/2} = (200/9)^{1/2} = 4.71$$

therefore, we expect 33 ± 5 hits in 100 at bats.

The Poisson Probability Distribution

This is a very widely used discrete probability distribution.

Consider the following conditions:

1. p is very small and approaches 0

   example: a 100 sided dice instead of a 6 sided dice
   $\rightarrow p = 1/100$ instead of $1/6$

   example: a 1000 side dice with $p = 1/1000$
2. N is very large and approaches ∞

   example: throwing 100 or 1000 dice instead of 2 dice
3. the product Np is finite

Example: radioactive decay

Suppose we have 25 mg of an element; this corresponds to a very large number of atoms, $N \approx 10^{20}$.

Suppose the lifetime of this element is

$$\lambda = 10^{12} \text{ years } \approx 5 \times 10^{19} \text{ seconds}$$

These numbers imply that the probability of a given nucleus to decay in one second is very small

$$p = \frac{1}{\lambda} = 2 \times 10^{-20} \text{ sec}^{-1}$$

Note that $Np = 2 \text{ sec}^{-1}$ which clearly is finite!

It then turns out that the number of counts in a time interval is a **Poisson process** (governed by the Poisson probability distribution).

The Poisson distribution can be derived by taking the appropriate limits of the binomial distribution

$$P(m,N,p) = \frac{N!}{m!(N-m)!}p^m q^{N-m}$$

We have these limits

$$\frac{N!}{(N-m)!} = \frac{N(N-1)....(N-m+1)(N-m)!}{(N-m)!} \approx N^m$$

and

$$q^{N-m} = (1-p)^{N-m} = 1 - p(N-m) + \frac{p^2(N-m)(N-m-1)}{2!} + ...$$

$$\approx 1 - PN + \frac{(pN)^2}{2!} + ... \approx e^{-pN}$$

so that

$$P(m,N,p) = \frac{N^m}{m!}p^m e^{-pN}$$

Now let $\mu = Np$ and we have

$$P(m, \mu) = \frac{e^{-\mu}\mu^m}{m!}$$

This is properly normalized since we have

$$\sum_{m=0}^{\infty} P(m, \mu) = \sum_{m=0}^{\infty} \frac{e^{-\mu}\mu^m}{m!} = e^{-\mu} \sum_{m=0}^{\infty} \frac{\mu^m}{m!} = e^{-\mu} e^{\mu} = 1$$

We note that m is always an integer $\neq 0$, but μ does not have to be an integer.

It is straightforward to show that

$$\mu = Np = \text{ mean of Poisson distribution}$$

$$\sigma^2 = Np = \mu = \text{ variance of the Poisson distribution}$$

The mean and variance are the same!

Returning to the radioactivity example we have $\mu = Np = 2$ decays/sec . What is the probability of zero decays in one second?

$$P(0,2) = \frac{e^{-2}2^0}{0!} = 0.135 \rightarrow 13.5\%$$

What is the probability of more than one decay in one second?

$$P(>1,2) = 1 - P(0,2) - P(1,2) = 1 - \frac{e^{-2}2^0}{0!} - \frac{e^{-2}2^1}{1!} = 0.594 \rightarrow 59.4\%$$

Another example:

The number of false fire alarms in a suburb of Houston averages 2.1 per day. Assuming a Poisson distribution is appropriate, the probability that 4 false alarms will occur on a given day is given by

$$P(4,2.1) = \frac{e^{-2.1}2.1^4}{4!} = 0.0992 \rightarrow 9.92\%$$

Some other processes governed by a Poisson distribution are

1. The number of phone calls received by a telephone operator in a 10-minute period.
2. The number of flaws in a bolt of fabric.
3. The number of typos per page made by anyone entering text.

Probability Interpretation

As we have said, in the standard way of thinking about probability in relation to experiments, measured results are related to probabilities using the concept of a **limit frequency**.

The limit frequency is linked to probability by this definition:

> *If C can lead to either A or $\sim A$ and if in n repetitions, A occurs m times, then*

$$P(A|C) = \lim_{n\to\infty}\left(\frac{m}{n}\right)$$

We must now connect the mathematical formalism with this limit frequency concept so that we can use the formalism to make predictions for experiments in real physical systems.

This approach depends on whether we can prove that the limit makes sense for real physical systems.

Let us see how we can understand the real meaning of the above interpretation of probability and thus learn how to use it in quantum mechanics, where probability will be the dominant property.

Suppose that we have an experimental measurement, M, that can yield either A or $\sim A$ as results, with a probability for result A given by

$$P(A|M) = p$$

In general, we let any sequence of n independent measurements be labeled as event M^n and we define n_A as the number of times A occurs, where $0 \leq n_A \leq n$.

We repeat the earlier, but so very important derivation.

Now imagine we carry out a sequence of n independent measurements and we find that A occurs r times.

The probability for a sequence of results that includes result A r times and $\sim A$ $(n-r)$ times (independent of their order in the sequence) is given by

$$p^r q^{(n-r)} \qquad\qquad p^r q^{(n-r)}$$

where

$$q = P(\sim A|M) = 1 - P(A|M) = 1 - p$$

The different sequence orderings are mutually exclusive events and thus we have

$$P(n_A = r|M^n) = \sum_{\substack{\textit{all possible} \\ \textit{orderings}}} p^r q^{(n-r)}$$

The sum

$$\sum_{\substack{\textit{all possible} \\ \textit{orderings}}}$$

just counts the number of ways to distribute r A's and $(n-r)$ $\sim A$'s, where all the terms contain the common factor $p^r q^{(n-r)}$.

This result is given by the Binomial probability distribution (more about this later) as

$$\frac{n!}{r!(n-r)!}$$

so that

$$P(n_A = r|M^n) = \frac{n!}{r!(n-r)!}\, p^r q^{(n-r)}$$

Now to get to the heart of the problem.

The frequency of A in M^n is given by

$$f_n = \frac{n_A}{n}$$

This is **not necessarily** $= p$ in any set of measurements.

What is the relationship between them?

Consider the following:

$$\begin{aligned}\langle n_A \,|\, r \rangle &= \text{average or expectation value} \\ &= \text{sum over [possible values times probability of that value]} \\ &= \sum_{r=0}^{n} r P(n_A = r | M^n) = \sum_{r=0}^{n} r \frac{n!}{r!(n-r)!}\, p^r q^{(n-r)}\end{aligned}$$

We now use the same clever mathematical trick as used earlier to evaluate this sum.

For the moment consider p and q to be two arbitrary independent variables.

At the end of the calculation we will let $q = 1 - p$ as is appropriate for a real physical system.

From the Binomial expansion formula, we have, in general,

$$\sum_{r=0}^{n} \frac{n!}{r!(n-r)!} p^r q^{(n-r)} = (p+q)^n$$

We then have

$$p\frac{\partial}{\partial p} \sum_{r=0}^{n} \frac{n!}{r!(n-r)!} p^r q^{(n-r)} = p\frac{\partial}{\partial p}(p+q)^n$$

or

$$\sum_{r=0}^{n} r\frac{n!}{r!(n-r)!} p^r q^{(n-r)} = np(p+q)^{n-1}$$

or

$$\sum_{r=0}^{n} P(n_A = r|M^n) = np(p+q)^{n-1}$$

and thus

$$\langle n_A \rangle = np(p+q)^{n-1}$$

In a real physical system, we must have $p + q = 1$, so that we end up with the result

$$\langle n_A \rangle = np$$

and

$$\langle f_n \rangle = \frac{\langle n_A \rangle}{n} = p$$

This says that $p =$ the average frequency.

This **does not** say, however, that f_n is close to p.

Now consider a more general experiment where the outcome of a measurement is the value of some continuous variable Q, with probability density (for its continuous spectrum) given by

$$P(q < Q < q + dq|M) = h(q)dq$$

If we let $h(q)$ contain delta-functions, then this derivation is also valid for the discrete part of the spectrum.

We can now derive the following useful result.

If Q is a nonnegative variable, which means that $h(q) = 0$ for $q < 0$, then for any $\epsilon > 0$

$$\langle Q \rangle = \int_0^\infty h(q) q dq \geq \int_\epsilon^\infty h(q) q dq \geq \epsilon \int_\epsilon^\infty h(q) dq = \epsilon P(Q \geq \epsilon | M)$$

This implies that

$$P(Q \geq \epsilon | M) \leq \frac{\langle Q \rangle}{\epsilon}$$

Now we apply this result to the nonnegative variable $|Q - c|^\alpha$ where $\alpha > 0$ and $c =$ number, to obtain

$$P(|Q - c| \geq \epsilon | M) = P(|Q - c|^\alpha \geq \epsilon^\alpha | M) \leq \frac{\langle |Q - c|^\alpha \rangle}{\epsilon^\alpha}$$

which is called **Chebyshev's inequality**.

In the special case where

$$\alpha = 2 \ , \ \ c = \langle Q \rangle = \text{ mean of distribution}$$

$$\langle |Q-c|^2 \rangle = \langle |Q-\langle Q \rangle|^2 \rangle = \langle Q^2 \rangle = \langle Q \rangle^2 = \sigma^2 = \text{ variance} \ , \ \epsilon = k\sigma$$

we have

$$P(|Q - \langle Q \rangle| \geq k\sigma|M) \leq \frac{1}{k^2}$$

or, the probability of Q being k or more standard deviations from the mean is no greater than $1/k^2$ (independent of the form of the probability distribution).

It can also be shown that

$$P(|f_n - p| \geq \delta|M) \leq \frac{1}{n\delta^2}$$

which implies that the probability of f_n (the relative frequency of A in n independent repetitions of M) being more than δ away from p converges to 0 as $n \to \infty$.

This is an example of the **law of large numbers** in action.

This **DOES NOT** say $f_n = p$ at any time or that f_n remains close to p as $n \to \infty$.

It **DOES** say that the deviation of f_n from p becomes more and more improbable or that the probability of any deviation approaches 0 as $n \to \infty$.

It is in this sense that one uses the limit frequency from experiment to compare with theoretical probability predictions in physics.

From probability theory one derives only statements of probability, not of necessity.

First hints of "subversive" or “Bayesian” thinking.....

How do we reason in situations where it is not possible to argue with certainty?

In other words, is there a way to use techniques of deductive logic to study the inference problem arising when using inductive logic?

No matter what scientists say, this is what they are actually doing most of the time.

The answer to this last question resides in the Bayes' rule.

To Bayes (along with Bernoulli and Laplace), a probability represented a "degree-of-belief" or "plausibility", that is, how much one thinks that something is true, **based** on the **evidence on hand**.

The developers of standard probability theory (Fisher, Neyman and Pearson) thought this seemed too vague and subjective a set of ideas to be the basis of a "rigorous" mathematical theory.

Therefore, they **defined** probability as the long-run relative frequency with which an event occurred, given **infinitely many repeated** experimental trials.

Since such probabilities can be measured, probability was then thought to be an objective tool for dealing with random phenomena.

This frequency definition certainly **seems** to be more objective, but it turns out that its **range of validity** is far more limited.

In this view, probability represents a **state of knowledge**.

The conditional probabilities represent **logical** connections rather than **causal** ones.

Example: Consider an urn that contains 5 red balls and 7 green balls.

If a ball is selected at "random", then we would all agree that the probability of picking a red ball would be 5/12 and of picking a green ball would be 7/12.

If the ball is not returned to the urn, then it seems reasonable that the probability of picking a red or green ball must depend on the outcome of the first pick (because there will be one less red or green ball in the urn).

Now suppose that we are not told the outcome of the first pick, but are given the result of the second pick.

Does the probability of the first pick being red or green change with the knowledge of the second pick?

Initially, many observers would probably say "no", that is, at the time of the first draw, there were still 5 red balls and 7 green balls in the urn, so the probabilities for picking red and green should still be 5/12 and 7/12 independent of the outcome of the second pick.

The error in this argument becomes clear if we consider the extreme example of an urn containing only 1 red and 1 green ball.

Although, the second pick cannot affect the first pick in a physical sense, a knowledge of the second result does influence what we can infer about the outcome of the first pick, that is, if the second ball was green, then the first ball must have been red, and vice versa.

We can calculate the result as shown below:

$Y = pick\ is\ GREEN(2nd\ pick)$

$X = pick\ is\ RED(1st\ pick)$

$I =$ initial number of RED/GREEN balls=$\{n,m\}$

A Bayesian would say:

$$prob(X \mid Y\ \&\ I) = \frac{prob(Y \mid X\ \&\ I) \times prob(X \mid I)}{prob(Y \mid I)}$$

$$prob(X \mid Y\ \&\ \{n,m\}) = \frac{prob(Y \mid X\ \&\ \{n,m\}) \times \frac{n}{n+m}}{\frac{n}{n+m}\frac{m}{n+m-1} + \frac{m}{n+m}\frac{m-1}{n+m-1}} = \frac{\frac{m}{(n+m-1)} \times n}{\frac{nm}{n+m-1} + \frac{m(m-1)}{n+m-1}} = \frac{n}{n+m-1}$$

$$n = m = 1 \Rightarrow prob(X \mid Y\ \&\ \{1,1\}) = \frac{n}{(n+m-1)} = 1$$

$$n = 5\,,\ m = 7 \Rightarrow prob(X \mid Y\ \&\ \{5,7\}) = \frac{5}{11} = 0.456$$

Non – Bayesian says:

$$prob(X \mid \{5,7\}) = \frac{5}{12} = 0.417$$

Clearly, the Bayesian and Non-Bayesian disagree.

However, the Non-Bayesian is just **assuming** that the calculated result 0.417 is correct, whereas, the Bayesian is using the rules of probability (Bayes' Rule) to infer the result 0.456 correctly.

The concerns about the subjectivity of the Bayesian view of probability are understandable.

I think that the presumed shortcomings of the Bayesian approach merely reflect a confusion between subjectivity and the difficult technical question of how probabilities(especially prior probabilities) should be assigned.

The popular argument is that if a probability represents a degree-of-belief, then it must be subjective, because my belief could be different from yours.

The Bayesian view is that a probability does indeed represent how much we believe that something is true, but that this belief should be based on all the relevant information available(all prior probabilities).

While this makes the assignment of probabilities an open-ended question, because the information available to me may not be the same as that available to you, it is not the same as subjectivity.

It simply means that probabilities are **always conditional**, and this conditioning must be stated **explicitly**.

Objectivity demands only that two people having the same information should assign the same probability.

Gaussian Probability Distribution

The Gaussian probability distribution is perhaps the most used distribution in all of science.

It is sometimes called the "bell-shaped curve" or normal distribution.

Unlike the binomial or Poisson distributions, the Gaussian is a continuous distribution given by

$$\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(y-\mu)^2}{2\sigma^2}}$$

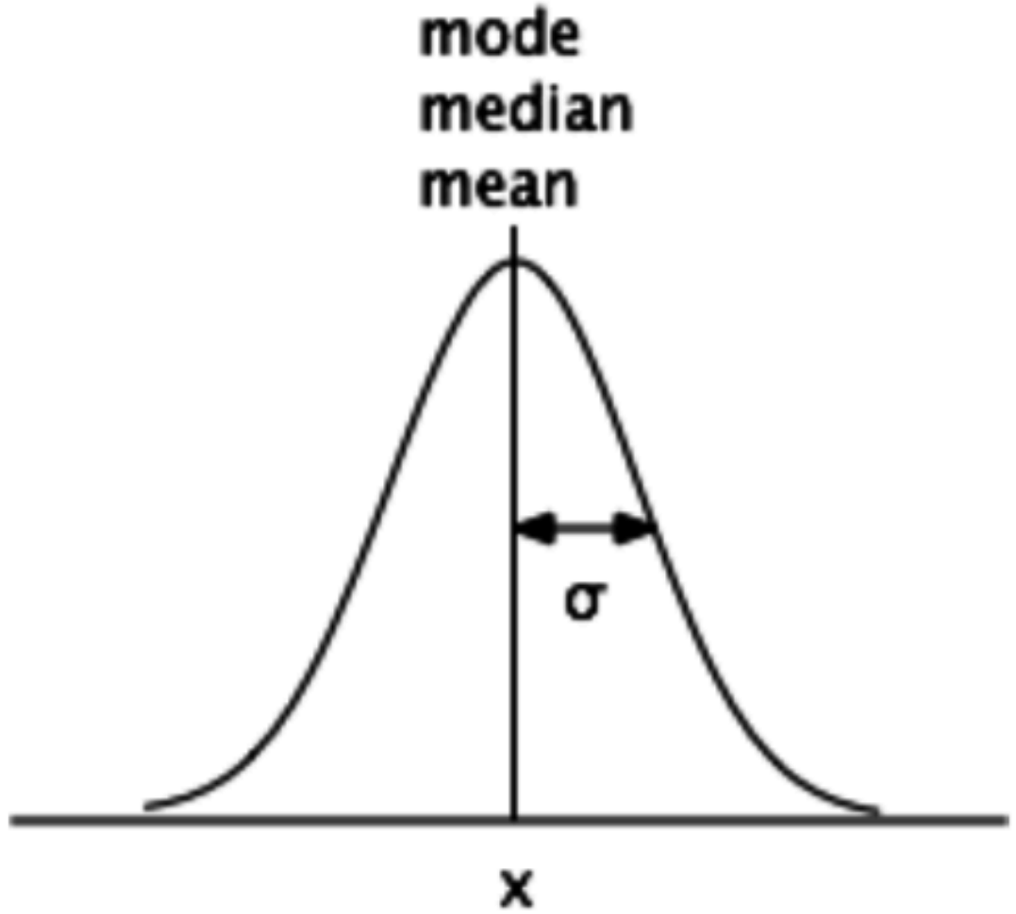
where

$$\mu = \text{ mean(=mode=median) of distribution}$$

$$\sigma^2 = \text{ variance of the distribution}$$

$$y = \text{ continuous variable } \quad -\infty \leq y \leq \infty$$

See figure below.



The probability of y being in the range $[a, b]$ is given by an integral

$$P(a < y < b) = \frac{1}{\sigma\sqrt{2\pi}} \int_a^b e^{-\frac{(y-\mu)^2}{2\sigma^2}} dy$$

which cannot be evaluated analytically.

The probability distribution is properly normalized to 1 since

$$P(-\infty < y < \infty) = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{(y-\mu)^2}{2\sigma^2}} dy = 1$$

One often hears statements about a measurement being a certain number of standard deviations (σ) away from the mean (μ) of the Gaussian.

We can associate a probability for a measurement to be $|\mu - n\sigma|$ from the mean just by calculating the area **outside** of this region.

n	Prob. of exceeding $\pm n\sigma$
0.67	0.5
1	0.32
2	0.05
3	0.003
4	0.00006

which shows that it is very unlikely ($< 0.3\%$) that a measurement taken at random from a gaussian pdf will be more than $\pm 3\sigma$ from the true mean of the distribution.

Relationship between Gaussian and Binomial Distributions

The Gaussian distribution can be derived from the binomial(or Poisson) distribution assuming:

1. p is finite
2. N is very large
3. We have a continuous rather than a discrete variable

An example illustrating the small difference between the two distributions (remember one is continuous and the other is discrete) under the above conditions is:

Consider an experiment of tossing a coin many times where

$$P(heads) = 0.5 \quad , \quad N = 10000$$

For the **binomial distribution**:

$$\text{mean number of heads } = \mu = Np = 5000$$

$$\text{standard deviation } = \sigma = [Np(1-p)]^{1/2} = 50$$

The probability to be within $\pm\sigma$ is

$$P(\pm\sigma) = \sum_{m=5000-50}^{m=5000+50} \frac{10^4!}{(10^4-m)!m!} 0.5^m 0.5^{10^4-m} = 0.69$$

For the Gaussian distribution:

$$P(\mu-\sigma < y < \mu+\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \int_{\mu-\sigma}^{\mu+\sigma} e^{-\frac{(y-\mu)^2}{2\sigma^2}}\, dy = 0.68$$

so that both distributions give about the same probability under these conditions.

Central Limit Theorem

The Gaussian distribution is important because of the Central Limit Theorem.

A crude statement of the Central Limit Theorem is

> *Things that are the result of the addition of lots of small effects tend to become Gaussian.*

A more exact statement goes as follows:

Let $Y_1, Y_2, ..., Y_n$ be an infinite sequence of independent random variables each with the same probability distribution (the Y's actually can be from different pdf's).

Suppose that the mean (μ) and the variance (σ^2) of this distribution are both finite.

For any numbers a and b:

$$\lim_{n\to\infty} P\left[a < \frac{Y_1 + Y_2 + ... + Y_n - n\mu}{\sigma\sqrt{n}} < b\right] = \frac{1}{\sqrt{2\pi}} \int_a^b e^{-\frac{1}{2}y^2} dy$$

The CLT tells us that under a wide range of circumstances the probability distribution that describes the sum of random variables tends towards a Gaussian distribution as the number of terms in the sum $\rightarrow \infty$.

Alternatively we have the statement

$$\lim_{n\to\infty} P\left[a < \frac{\bar{Y}-\mu}{\sigma/\sqrt{n}} < b\right] = \lim_{n\to\infty} P\left[a < \frac{\bar{Y}-\mu}{\sigma_m} < b\right] = \frac{1}{\sqrt{2\pi}}\int_a^b e^{-\frac{1}{2}y^2}dy$$

where σ_m is sometimes called the "error in the mean".

For the CLT to be valid: μ and σ must be finite and no one term in the sum should dominate the sum.

We note that a random variable is not the same as a random number.

A random variable is a rule which associates a number with each outcome in a set of possible outcomes S.

We note that if y is described by a gaussian pdf with $\mu = 0$ and $\sigma = 1$ then the probability that $a < y < b$ is given by

$$\frac{1}{\sqrt{2\pi}} \int_a^b e^{-\frac{1}{2}y^2} dy$$

which is the RHS of the CLT.

Example: A watch makes an error of at most $\pm 1/2$ minute per day. After one year, what is the probability that the watch is accurate to within ± 25 minutes? Assume that the daily errors are uniform in $[-1/2, 1/2]$.

For each day, the average error is zero and the standard deviation $1/\sqrt{12}$ minute, that is, $P(y) = 1.0$, $\mu = 0$ so that

$$\sigma^2 = \frac{\int_{-1/2}^{1/2} (y-\mu)^2 P(y) dy}{\int_{-1/2}^{1/2} P(y) dy} = \int_{-1/2}^{1/2} y^2 dy = \frac{1}{12} \rightarrow \sigma = \frac{1}{\sqrt{12}}$$

The error over the course of a year is just the addition of the daily error.

Since the daily errors come from a uniform distribution with a well defined mean and variance, the CLT is applicable.

Thus,

$$\lim_{n\to\infty} P\left[a < \frac{Y_1 + Y_2 + ... + Y_n - n\mu}{\sigma\sqrt{n}} < b\right] = \frac{1}{\sqrt{2\pi}}\int_a^b e^{-\frac{1}{2}y^2}dy$$

The upper limit corresponds to +25 minutes, i.e.,

$$b = \frac{Y_1 + Y_2 + ... + Y_n - n\mu}{\sigma\sqrt{n}} = \frac{+25 - (365)(0)}{(1/\sqrt{12})\sqrt{365}} = 4.5$$

and the lower limit corresponds to -25 minutes, i.e.,

$$a = \frac{Y_1 + Y_2 + ... + Y_n - n\mu}{\sigma\sqrt{n}} = \frac{-25 - (365)(0)}{(1/\sqrt{12})\sqrt{365}} = -4.5$$

Therefore, the probability to be within ± 25 minutes is

$$P = \frac{1}{\sqrt{2\pi}}\int_{-4.5}^{4.5} e^{-\frac{1}{2}y^2}dy = 0.999997 = 1 - 3\times 10^{-6}$$

that is, **less than three in a million chance** that the watch will be off by more than 25 minutes after a year.

Example: Generate a Gaussian distribution using random numbers.

We have a random number generator which gives numbers distributed uniformly in the interval $[0, 1]$ so that $\mu = 1/2$ and $\sigma = 1/12$.

Procedure:

1. Take $n = 12$ numbers (r_i) from the random number generator
2. Add them together
3. Subtract $n\mu = 6$

This should generate a number that looks like it is from a Gaussian pdf, that is,

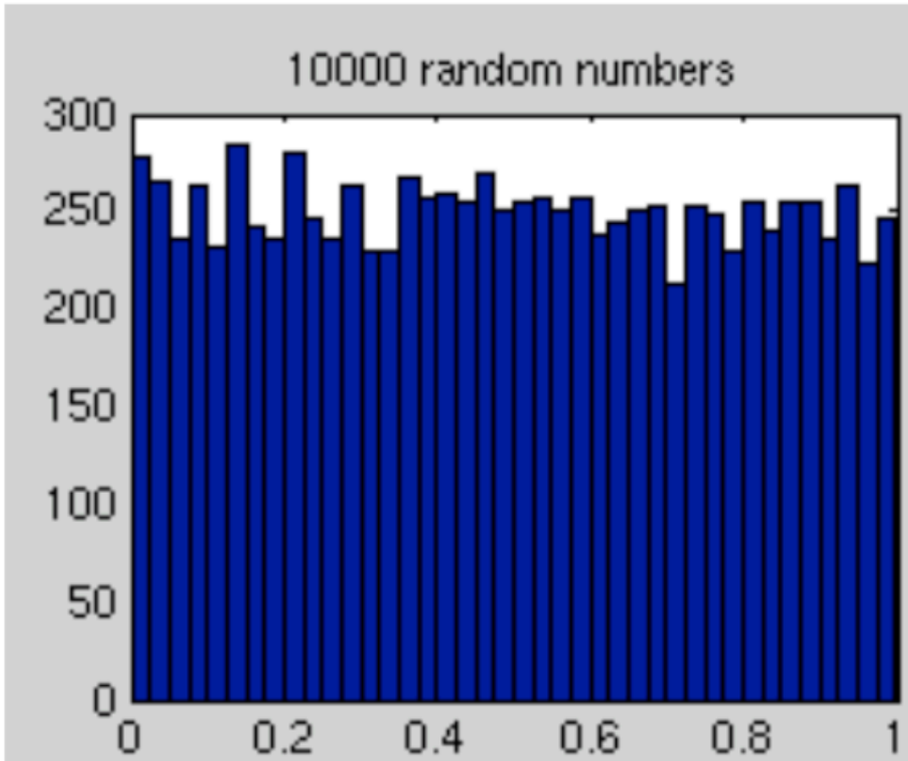
$$P\left[a < \frac{Y_1 + Y_2 + ... + Y_n - n\mu}{\sigma\sqrt{n}} < b\right] = P\left[a < \frac{r_1 + r_2 + ... + r_{12} - 12(1/2)}{(1/\sqrt{12})\sqrt{12}} < b\right]$$

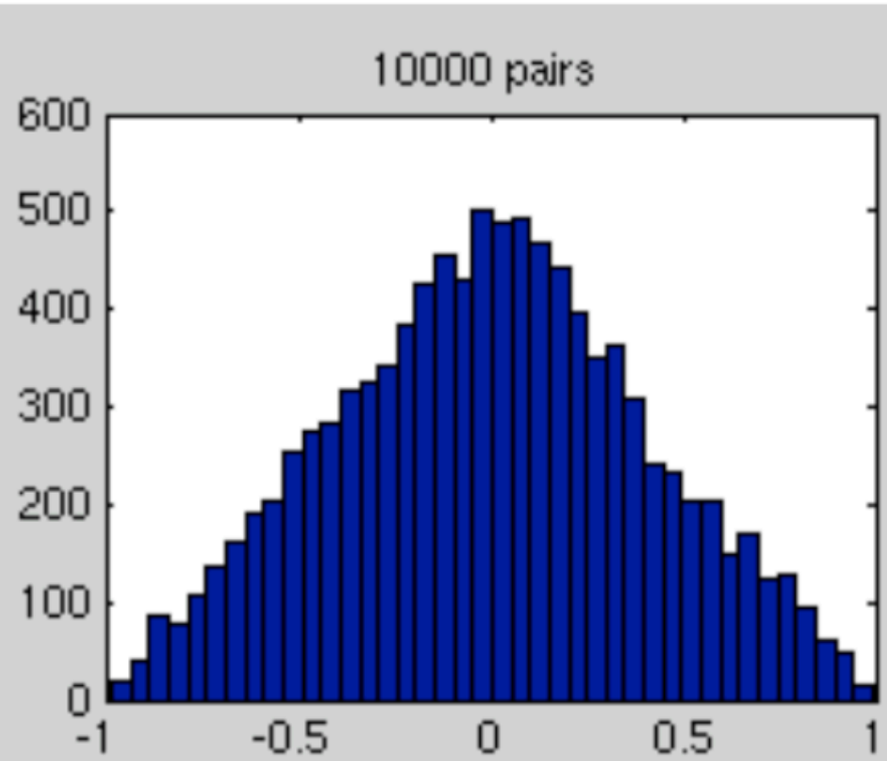
$$= P[-6 < (r_1 + r_2 + ... + r_{12} - 6) < 6] = \frac{1}{\sqrt{2\pi}} \int_{-4.5}^{4.5} e^{-\frac{1}{2}y^2} dy$$

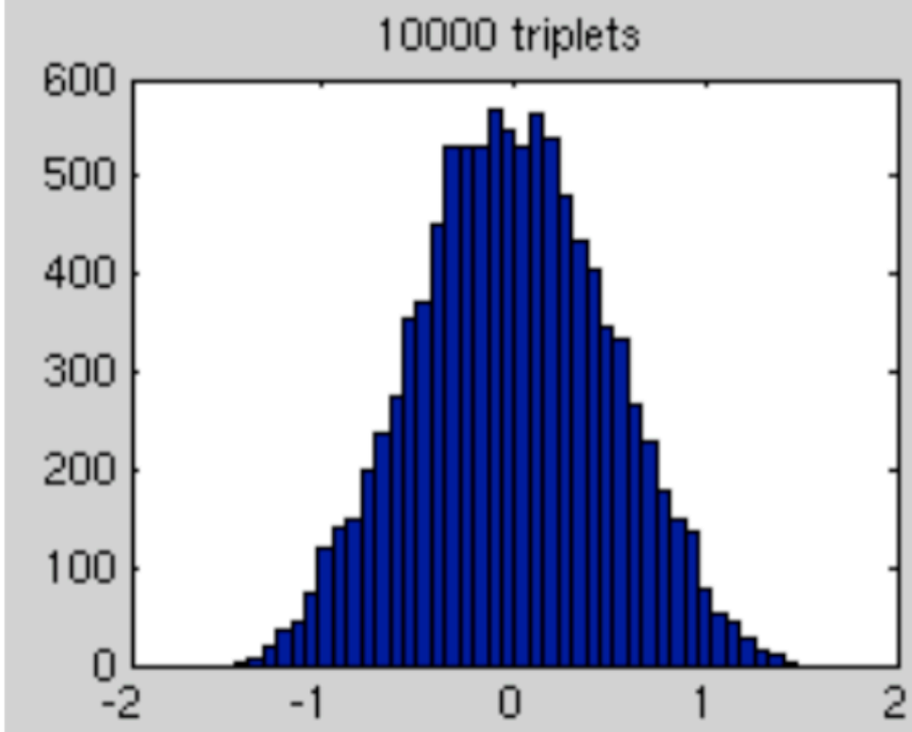
where the value of a arises from all $r_i = 0$ and the value of b arises from all $r_i = 1$.

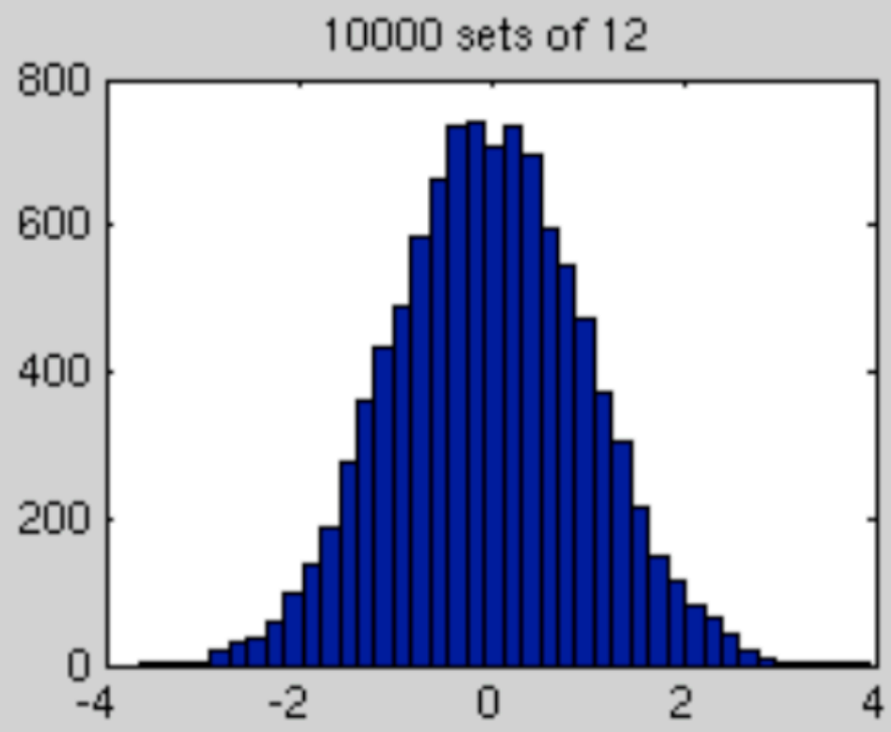
OCTAVE code: cent-lim.m

```
m=10000;
k=40;
r1=rand(1,m);
mu=0.5;
sig=1/sqrt(12);
val=rand(2,m);
r2=val(1,:)+val(2,:)-1;
val=rand(3,m);
r3=val(1,:)+val(2,:)+val(3,:)-1.5;
val=rand(12,m);
r12=val(1,:)+val(2,:)+val(3,:)+val(4,:)+val(5,:)+val(6,:)+val(7,:)+val(8,:)+val(9,:)+val(10,:)+val(11,:)+val(12,:)-6;
subplot(2,2,1)
hist(r1,k);
title('10000 random numbers');
subplot(2,2,2)
hist(r2,k);
title('10000 pairs');
subplot(2,2,3)
hist(r3,k);
title('10000 triplets');
subplot(2,2,4)
hist(r12,k);
title('10000 sets of 12');
```


10000 random numbers
300
250
200
150
100
50
0
0
0.2
0.4
0.6
0.8
1


10000 pairs
600
500
400
300
200
100
0
-1
-0.5
0
0.5
1


10000 triplets
600
500
400
300
200
100
0
-2
-1
0
1
2


10000 sets of 12
800
600
400
200
0
-4
-2
0
2
4

Example: The daily income of a "card shark" has a uniform distribution in the interval $[-\$40, \$50]$.

What is the probability that she wins more than \$500 in 60 days?

Let us use the CLT to estimate this probability

$$\lim_{n\to\infty} P\left[a < \frac{Y_1 + Y_2 + ... + Y_n - n\mu}{\sigma\sqrt{n}} < b\right] = \frac{1}{\sqrt{2\pi}} \int_a^b e^{-\frac{1}{2}y^2} dy$$

The probability distribution of daily income is uniform, $P(y) = 1$.

Thus, we have

$$\mu = \frac{\int_{-40}^{50} yP(y)dy}{\int_{-40}^{50} P(y)dy} = \frac{\frac{1}{2}(50^2 - 40^2)}{50 - (-40)} = 5$$

$$\sigma^2 = \frac{\int_{-40}^{50} y^2P(y)dy}{\int_{-40}^{50} P(y)dy} - \mu^2 = \frac{\frac{1}{3}(50^3 - 40^3)}{50 - (-40)} - 25 = 675$$

The lower value a is

The lower value a is

$$a = \frac{Y_1 + Y_2 + ... + Y_n - n\mu}{\sigma\sqrt{n}} = \frac{500 - (60)(5)}{\sqrt{675}\sqrt{60}} = 1$$

The upper value b is the maximum the shark could win ($50/day for 60 days)

$$b = \frac{Y_1 + Y_2 + ... + Y_n - n\mu}{\sigma\sqrt{n}} = \frac{3000 - (60)(5)}{\sqrt{675}\sqrt{60}} = 13.4$$

Thus,

$$P = \frac{1}{\sqrt{2\pi}} \int_1^{13.4} e^{-\frac{1}{2}y^2} dy \approx \frac{1}{\sqrt{2\pi}} \int_1^{\infty} e^{-\frac{1}{2}y^2} dy = 0.16$$

or a 16% chance to win $>$ \$500 in 60 days.

Propagation of Errors

Example: we measure the current(I) and the resistance (R) of a resistor.

Ohm's law is $V = IR$.

If we know the uncertainties (e.g. standard deviations) in I and R, what is the uncertainty in V?

Given a functional relationship between several variables (x, y, z), say $Q = f(x, y, z)$ we ask:

What is the uncertainty in Q if the uncertainties in x, y, and z are known? Usually when we talk about uncertainties in a measured variable such as x, we assume:

1. the value of x represents the mean of a Gaussian distribution
2. the uncertainty in x is the standard deviation of the Gaussian distribution

Remember, however, that not all measurements can be represented by Gaussian distributions and that can cause difficulties.

Propagation of Error Formula

Suppose $Q = f(x, y)$.

To calculate the variance in Q as a function of the variances in x and y we use the following:

$$\sigma_Q^2 = \sigma_x^2 \left(\frac{\partial Q}{\partial x}\right)^2 + \sigma_y^2 \left(\frac{\partial Q}{\partial y}\right)^2 + 2\sigma_{xy} \left(\frac{\partial Q}{\partial x}\right) \left(\frac{\partial Q}{\partial y}\right)$$

If the variables are uncorrelated ($\sigma_{xy} = 0$), the last term is zero.

Assume that we have several measurements of the quantities x, say $x_1, x_2, ..., x_N$ and y, say, $y_1, y_2, ..., y_N$.

The average of x and y are

$$\mu_x = \frac{1}{N}\sum_{i=1}^{N} x_i \quad , \quad \mu_y = \frac{1}{N}\sum_{i=1}^{N} y_i$$

We define

$$Q_i = f(x_i, y_i)$$

$$Q = f(\mu_x, \mu_y) \quad \text{evaluated at the average values}$$

If we expand Q_i about the average values (neglecting 2^n-order or higher terms) we get

$$Q_i - Q = (x_i - \mu_x)\left(\frac{\partial Q}{\partial x}\right)\Big|_{\mu_x} + (y_i - \mu_y)\left(\frac{\partial Q}{\partial y}\right)\Big|_{\mu_y}$$

so that

$$\sigma_Q^2 = \frac{1}{N}\sum_{i=1}^{N}(Q_i - Q)^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu_x)^2 \left(\frac{\partial Q}{\partial x}\right)^2_{\mu_x}$$

$$+ \frac{1}{N}\sum_{i=1}^{N}(y_i - \mu_y)^2 \left(\frac{\partial Q}{\partial y}\right)^2_{\mu_y}$$

$$+ \frac{2}{N}\sum_{i=1}^{N}(x_i - \mu_x)(y_i - \mu_y) \left(\frac{\partial Q}{\partial x}\right)_{\mu_x} \left(\frac{\partial Q}{\partial y}\right)_{\mu_y}$$

$$= \sigma_x^2 \left(\frac{\partial Q}{\partial x}\right)^2_{\mu_x} + \sigma_y^2 \left(\frac{\partial Q}{\partial y}\right)^2_{\mu_y}$$

$$+ 2\left(\frac{\partial Q}{\partial x}\right)_{\mu_x} \left(\frac{\partial Q}{\partial y}\right)_{\mu_y} \sum_{i=1}^{N}(x_i - \mu_x)(y_i - \mu_y)$$

If the measurements are uncorrelated (uncorrelated errors)

$$\sigma_Q^2 = \sigma_x^2 \left(\frac{\partial Q}{\partial x}\right)^2_{\mu_x} + \sigma_y^2 \left(\frac{\partial Q}{\partial y}\right)^2_{\mu_y}$$

When x and y are correlated, define

$$\sigma_{xy} = \sum_{i=1}^{N}(x_i - \mu_x)(y_i - \mu_y)$$

so that for correlated errors

$$\sigma_Q^2 = \sigma_x^2 \left(\frac{\partial Q}{\partial x}\right)^2_{\mu_x} + \sigma_y^2 \left(\frac{\partial Q}{\partial y}\right)^2_{\mu_y} + 2\sigma_{xy} \left(\frac{\partial Q}{\partial x}\right)_{\mu_x} \left(\frac{\partial Q}{\partial y}\right)_{\mu_y}$$

Example: Power in an electric circuit - $P = I^2R/$

Let $I = 1.0 \pm 0.1$ amp and $R = 10 \pm 1\,\Omega$ so that $P = 10$ watts. We calculate the variance in the power using propagation of errors

$$\sigma_P^2 = \sigma_I^2 \left(\frac{\partial P}{\partial I}\right)^2_{I=1} + \sigma_R^2 \left(\frac{\partial P}{\partial R}\right)^2_{R=10} = \sigma_I^2 \left(2IR\right)^2_{I=1} + \sigma_R^2 \left(I^2\right)^2_{R=10} = 5 \text{ watts}^2$$

so that

$$P = 10 \pm 2 \text{ watts}$$

This means that if the true value of the power was 10 W and we measured it many times with an uncertainty σ of ± 2 W and Gaussian statistics apply, then 68% of the measurements would lie in the range $[8, 12]$ W. Sometimes it is convenient to put the above calculation in terms of relative errors.

$$\frac{\sigma_P^2}{P^2} = \frac{\sigma_I^2}{P^2}\left(\frac{\partial P}{\partial I}\right)^2_{I=1} + \frac{\sigma_R^2}{P^2}\left(\frac{\partial P}{\partial R}\right)^2_{R=10} = \frac{4\sigma_I^2}{I^2} + \frac{\sigma_R^2}{R^2} = 4\left(\frac{0.1}{1}\right)^2 + \left(\frac{1}{10}\right)^2 = 0.05 = 5 \text{ watts}^2$$

Clearly, the uncertainty in the current dominates (80%) the uncertainty in the power, which mean that current must be measured more precisely to greatly reduce the uncertainty in the power.

Example: The error in the average

The average of several measurements each with the same uncertainty (σ) is given by

$$\mu = \frac{1}{n}(x_1 + x_2 + ... + x_n)$$

and the variance of the mean is

$$\sigma_\mu^2 = \sigma_{x_1}^2 \left(\frac{\partial \mu}{\partial x_1}\right)^2 + \sigma_{x_2}^2 \left(\frac{\partial \mu}{\partial x_2}\right)^2 + ... + \sigma_{x_n}^2 \left(\frac{\partial \mu}{\partial x_n}\right)^2 = n\sigma^2 \left(\frac{1}{n}\right)^2$$

or

$$\sigma_\mu = \frac{\sigma}{\sqrt{n}}$$

is the "error in the mean".

Clearly, we can determine the mean better by combining measurements and the precision increases (gets better) as the square root of the number of measurements.

Do not confuse σ_μ with σ.

σ is related to the width of the pdf (e.g. Gaussian) that the measurements come from.

σ does not get smaller as we combine measurements.

Maximum Likelihood Method

Suppose that we are trying to measure the true value of some quantity (x_T) .

We make repeated measurements of this quantity $(x_1, x_2, ..., x_n)$.

The standard way to estimate x_T from our measurements is to calculate the mean value:

$$\mu_x = \frac{1}{n} \sum_{i=1}^{n} x_i$$

and then set $x_T = \mu_x$.

Does this procedure make sense?

To answer this question we investigate the maximum likelihood method(MLM), which is a general method for estimating parameters of interest from data.

Statement of the Maximum Likelihood Method

Assume we have made n measurements of x $(x_1, x_2, ..., x_n)$.

Assume we know the probability distribution function that describes x, namely, $f(x, \alpha)$.

Assume that we want to determine the parameter α.

MLM: pick α to maximize the probability of getting the measurements (the x_i's) that we did!

How do we use the MLM?

(1) Let $f(x, \alpha)$ be given by a Gaussian distribution

(2) Let $\alpha = \mu$ be the mean of the Poisson distribution

(3) We want to estimate α from our set of n measurements

(4) Assume that σ is the same for each measurement. Thus,

$$f(x_i, \alpha) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\alpha)^2}{2\sigma^2}}$$

(5) The likelihood function for this problem is

$$L = \prod_{i=1}^{n} f(x_i, \alpha) = \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\alpha)^2}{2\sigma^2}} = \left[\frac{1}{\sigma\sqrt{2\pi}}\right]^n e^{-\frac{(x_1-\alpha)^2}{2\sigma^2}} \ldots e^{-\frac{(x_n-\alpha)^2}{2\sigma^2}}$$

$$= \left[\frac{1}{\sigma\sqrt{2\pi}}\right]^n e^{-\sum_{i=1}^{n} \frac{(x_i-\alpha)^2}{2\sigma^2}}$$

(6) Find α that maximizes the log(likelihood function):

$$\frac{\partial \ln L}{\partial \alpha} = \frac{\partial}{\partial \alpha}\left[n \ln\left(\frac{1}{\sigma\sqrt{2\pi}}\right) - \sum_{i=1}^{n} - \sum_{i=1}^{n} \frac{(x_i-\alpha)^2}{2\sigma^2}\right] = 0$$

$$\frac{\partial}{\partial \alpha} \sum_{i=1}^{n} \frac{(x_i-\alpha)^2}{2\sigma^2} = 0 \rightarrow \sum_{i=1}^{n} (x_i - \alpha) = 0$$

$$\sum_{i=1}^{n} x_i = n\alpha \rightarrow \alpha = \frac{1}{n} \sum_{i=1}^{n} x_i$$

which is just the average value as expected.

If σ is different for each data point, then α is just the weighted average

$$\alpha = \frac{\sum_{i=1}^{n} \frac{x_i}{\sigma_i^2}}{\sum_{i=1}^{n} \frac{1}{\sigma_i^2}}$$

Example:

(1) Let $f(x, \alpha)$ be given by a Poisson distribution

(2) Let $\alpha = \mu$ be the mean of the Gaussian

(3) We want to estimate α from our set of n measurements

(4) The likelihood function for this problem is

$$L = \prod_{i=1}^{n} f(x_i, \alpha) = \prod_{i=1}^{n} \frac{e^{\alpha}\alpha^{x_i}}{x_i!} = \frac{e^{\alpha}\alpha^{x_2}}{x_2!}\frac{e^{\alpha}\alpha^{x_1}}{x_1!}.....\frac{e^{\alpha}\alpha^{x_n}}{x_n!}$$

$$= \frac{e^{n\alpha}\alpha^{\sum_{i=1}^{n} x_i}}{x_1!x_2!....x_n!}$$

(5) Find α that maximizes the log(likelihood function):

$$\frac{\partial \ln L}{\partial \alpha} = \frac{\partial}{\partial \alpha}\left[-n\alpha - \ln \alpha \sum_{i=1}^{n} x_i - \ln x_1!x_2!....x_n!\right] = 0$$

$$-n + \frac{1}{\alpha}\sum_{i=1}^{n} x_i = 0 \rightarrow \alpha = \frac{1}{n}\sum_{i=1}^{n} x_i$$

which is just the average value as expected.

General Properties of the MLM

1. For large data sets (large n) the likelihood function L approaches a Gaussian.
2. For large n estimates converge to the true value of the parameters.
3. MLM estimates are unbiased, efficient, sufficient and has smallest variance. Solution is unique.
4. **BAD NEWS:** we must know the correct probability distribution for the problem under consideration!

Maximum Likelihood Fit of Data to a Function

Suppose we have a set of n measurements:

$$x_1, y_1 \pm \sigma_1$$

$$x_2, y_2 \pm \sigma_2$$

$$\ldots$$

$$x_n, y_n \pm \sigma_n$$

Assume each measurement error(σ) is a standard deviation from a Gaussian pdf.

Assume that for each measured value y, there is an x which is known exactly.

Suppose we know the functional relationship between the y's and the x's:

$$y = q(x, \alpha, \beta, ...)$$

where $\alpha, \beta, ...$ are parameters.

MLM gives us a method to determine $\alpha, \beta, ...$ from the data.

Example: Fitting data points to a straight line:

$$y = q(x, \alpha, \beta, ...) = \alpha + \beta x$$

$$L = \prod_{i=1}^{n} f(x_i, \alpha, \beta) = \prod_{i=1}^{n} \frac{1}{\sigma_i \sqrt{2\pi}} e^{\frac{(y_i - q(x_i, \alpha, \beta ....))^2}{2\sigma_i^2}} -$$

We find α and β by maximizing the likelihood function L :

$$\frac{\partial \ln L}{\partial \alpha} = \frac{\partial}{\partial \alpha} \sum_{i=1}^{n} \left[\ln \left(\frac{1}{\sigma_i \sqrt{2\pi}} \right) - \frac{(y_i - \alpha - \beta x_i)^2}{2\sigma_i^2} \right]$$

$$= \sum_{i=1}^{n} \left[- \frac{(y_i - \alpha - \beta x_i)^2}{2\sigma_i^2} \right] = 0$$

$$\frac{\partial \ln L}{\partial \beta} = \frac{\partial}{\partial \beta} \sum_{i=1}^{n} \left[\ln \left(\frac{1}{\sigma_i \sqrt{2\pi}} \right) - \frac{(y_i - \alpha - \beta x_i)^2}{2\sigma_i^2} \right]$$

$$= \sum_{i=1}^{n} \left[\frac{(y_i - \alpha - \beta x_i)^2}{2\sigma_i^2} \right] = 0$$

which is two linear equations with two unknowns.

Assuming all of the σ's are the same for simplicity:

$$\sum_{i=1}^{n} y_i - \sum_{i=1}^{n} \alpha - \sum_{i=1}^{n} \beta x_i = 0 = \sum_{i=1}^{n} y_i - n\alpha - \beta \sum_{i=1}^{n} x_i$$

$$\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} \alpha x_i - \sum_{i=1}^{n} \beta x_i^2 = 0 = \sum_{i=1}^{n} x_i y_i - \alpha \sum_{i=1}^{n} x_i - \beta \sum_{i=1}^{n} x_i^2$$

The solutions are

$$\alpha = \frac{\sum_{i=1}^{n} y_i \sum_{i=1}^{n} x_i^2 - \sum_{i=1}^{n} x_i y_i \sum_{i=1}^{n} x_i}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$\beta = \frac{n \sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} y_i \sum_{i=1}^{n} x_i}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

These results = “least squares” idea.

The fitted line best represents the data.

Not all the data points will be on the line.

The line minimizes the sum of squares of the deviations between the line and the data

$$\delta = \sum_{i=1}^{n} [data_i - \ prediction_i]^2 = \sum_{i=1}^{n} [y_i - \alpha = \beta x_i]^2$$

And now for something completely different.....

Testable Information: The Principle of Maximum Entropy

Let us move on to a situation where we do not have total ignorance.

Suppose that a die, with the usual six faces, was rolled a very large number of times and we are only told that the average result was 4.5.

What probability should we assign for the various outcomes $\{X_i\}$ that the face on top had i dots?

The information or conditions provided by the experiment is written as a simple constraint equation

$$\sum_{i=1}^{6} i\, prob(X_i|I) = 4.5$$

If we had assumed a uniform pdf, then we would have predicted a different average

$$\sum_{i=1}^{6} i\, prob(X_i|I) = \frac{1}{6}\sum_{i=1}^{6} i = \frac{1}{6}(21) = 3.5$$

which means the uniform pdf is not a valid assignment.

There are many pdfs that are consistent with the experimental results.

Which one is the best?

The constraint equation above is called **testable information**.

With such a condition, we can either accept or reject any proposed pdf.

Jaynes proposed that, in this situation, we should make the assignment by using the principle of maximum entropy (**MaxEnt**), that is, we should choose that pdf which has the most entropy S while satisfying the available constraints.

Explicitly, for case if the die experiment above, we need to maximize

$$S = -\sum_{i=1}^{6} p_i \log_e (p_i)$$

where $p_i = prob(X_i|I)$ subject to the conditions

1. normalization constraint

$$\sum_{i-1}^{6} p_i = 1$$

and

2. testable information constraint

$$\sum_{i=1}^{6} ip_i = 4.5$$

Such a constrained optimization is done using the method of **Lagrange multipliers** as shown below:

Define the functions

$$f(p_i) = \sum_{i-1}^{6} p_i - 1 = 0 \rightarrow \frac{\partial f}{\partial p_j} \equiv 0$$

$$g(p_i) = \sum_{i=1}^{6} ip_i - 4.5 = 0 \rightarrow \frac{\partial g}{\partial p_j} \equiv 0$$

The maximization problem can then be written

$$\frac{\partial S}{\partial p_j} + \lambda_f \frac{\partial f}{\partial p_j} + \lambda_g \frac{\partial g}{\partial p_j} = 0 \quad j = 1, 2, 3, 4, 5, 6$$

where the constants λ_f, λ_g are called undetermined multipliers.

We get the equations

$$-\log_e(p_j) - 1 + \lambda_f + j\lambda_g = 0 \quad j = 1, 2, 3, 4, 5, 6$$

We then obtain

$$-\log_e(p_{j+1}) - 1 + \lambda_f + (j+1)\lambda_g = -\log_e(p_j) - 1 + \lambda_f + j\lambda_g$$

$$\rightarrow \log_e \frac{p_{j+1}}{p_j} = \lambda_g \rightarrow \frac{p_{j+1}}{p_j} = \beta = \text{ constant}$$

and

$$-\log_e(p_1) - 1 + \lambda_f + \log_e(\beta) = 0$$

$$\lambda_f = 1 + \log_e \frac{p_1}{\beta}$$

Therefore,

$$\sum_{i-1}^{6} p_i = 1 = p_1(1 + \beta + \beta^2 + \beta^3 + \beta^4 + \beta^5)$$

$$\sum_{i=1}^{6} ip_i = 4.5 = p_1(1 + 2\beta + 3\beta^2 + 4\beta^3 + 5\beta^4 + 6\beta^5)$$

or

$$\frac{1 + 2\beta + 3\beta^2 + 4\beta^3 + 5\beta^4 + 6\beta^5}{1 + \beta + \beta^2 + \beta^3 + \beta^4 + \beta^5} = 4.5$$

$$1.5\beta^5 + 0.5\beta^4 - 0.5\beta^3 - 1.5\beta^2 - 2.5\beta - 3.5 = 0$$

Solving for β we get 1.449255 so that

$$p_1 = \frac{1}{1+\beta+\beta^2+\beta^3+\beta^4+\beta^5} = 0.05435$$

$$p_2 = \beta p_1 = 0.07877$$

$$p_3 = \beta p_2 = 0.11416$$

$$p_4 = \beta p_3 = 0.16545$$

$$p_5 = \beta p_4 = 0.23977$$

$$p_6 = \beta p_5 = 0.34749$$

is the MaxEnt assignment for the pdf for the outcomes of the die roll, given only that it has the usual six faces and yields an average result of 4.5.

Why should the entropy function

$$S = -\sum_{i=1}^{6} p_i \log_e (p_i)$$

specified above be the choice for a selection criterion?

Let us look at two examples that suggest this criterion is highly desirable and probably correct.

Kangeroo Problem(Gull and Skilling) The kangeroo problem is as follows:

Information: 1/3 of all kangeroos have blue eyes and 1/3 of all kangeroos are left-handed

Question: On the basis of this information alone, what proportion of kangeroos are both blue-eyed and left-handed?

For any particular kangeroo, there are four distinct possibilities, namely, that it is

1. blue-eyed and left-handed
2. blue-eyed and right-handed
3. not blue-eyed but left-handed
4. not blue-eyed but right-handed

Bernoulli's law of large numbers says that the expected values of the fraction of kangeroos with characteristics (1)-(4) will be equal to the probabilities (p_1, p_2, p_3, p_4) we assign to each of these propositions. This is represented by a 2×2 **truth or contingency table** as shown below:

	Left-Handed True	**Left-handed False**
Blue-Eyed True	p_1	p_2
Blue-Eyed False	p_3	p_4

Although there are four possible combinations of eye-color and handedness to be considered, the related probabilities are not completely independent of each other.

We have the standard normalization requirement

$$\sum_{i=1}^{4} p_i = 1$$

In addition, we also have two conditions on the so-called **marginal** probabilities

$$p_1 + p_2 = prob(blue \,\&\, left|I) + prob(blue \,\&\, right|I) - prob(blue|I) = 1/3$$

$$p_1 + p_3 = prob(blue \,\&\, left|I) + prob(not-blue \,\&\, left|I) - prob(left|I) = 1/3$$

Since any $p_i \geq 0$, these imply that $0 \leq p_1 \leq 1/3$.

Using this result we can characterize the contingency table by a single variable $x = p_1$ as in the table below:

	Left-Handed True	**Left-handed False**
Blue-Eyed True	$0 \leq x \leq 1/3$	$1/3 - x$
Blue-Eyed False	$1/3 - x$	$2/3 + x$

where we have used

$$x = p_1$$

$$p_1 + p_2 = \frac{1}{3} \rightarrow p_2 = \frac{1}{3} - p_1$$

$$p_1 + p_3 = \frac{1}{3} \rightarrow p_3 = \frac{1}{3} - p_1$$

$$p_1 + p_2 + p_3 + p_4 = 1 \rightarrow p_4 = \frac{2}{3} + x$$

All such solutions, where $0 \leq x \leq 1/3$, satisfy the constraints of the testable information that is available.

Which one is best?

Common sense leads us towards the assignment based on independence of these two traits, that is, any other assignment would indicate a knowledge of kangeroo eye-color told us something about its handedness.

Since we have no information to determine even the sign of any potential correlation, let alone its magnitude, any choice other than independence is not justified.

The independence choice says that

$$x = p_1 = \ prob(blue\ \&\ left|I) = prob(blue|I)prob(left|I) = \frac{1}{9}$$

In this particular example it was straightforward to decide the most sensible pdf assignment in the face of the inadequate information.

We now ask whether there is some function of the $\{p_i\}$ which, when maximized subject to the known constraints, yields the "independence" solution.

The importance of finding an answer to this question is that it would become a good candidate for a general **variational principle** that could be used in situations that were too complicated for our common sense.

Skilling has shown that the only function which gives $x = 1/9$ is the entropy S as specified above or

$$S = -\sum_{i=1}^{4} p_i \log_e (p_i) = -x \log_e (x) - 2\left(\frac{1}{3} - x\right) \log_e \left(\frac{1}{3} - x\right)$$
$$- \left(\frac{1}{3} + x\right) \log_e \left(\frac{1}{3} + x\right)$$

The results of Skilling's investigations, including three proposed alternatives,

$$S1 = -\sum_{i=1}^{4} p_i \log_e (p_i) \rightarrow \textbf{MaxEnt}$$

$$S2 = -\sum_{i=1}^{4} p_i^2 \quad / \quad S3 = -\sum_{i=1}^{4} \log_e (p_i)$$

$$S4 = -\sum_{i=1}^{4} \sqrt{p_i}$$

are shown in the table below:

Function	Optimal x	Implied Correlation
S1	0.1111	None
S2	0.0833	Negative
S3	0.1301	Positive
S4	0.1218	Positive

Clearly, only the MaxEnt assumption leads to an optimal value with no correlations as expected.

Let us look at another example that lends further support to the MaxEnt principle.

The Team of Monkeys

Suppose there are M distinct possibilities $\{X_i\}$ to be considered. How can we assign truth tables ($prob(X_i|I) = p_i$) to these possibilities given some testable information I (experimental results).

What is the most honest and fair procedure?

Imagine playing the following game.

The various propositions are represented by different boxes all of the same size into which pennies are thrown at random.

The tossing job is often assigned to a team of monkeys under the assumption that this will not introduce any underlying bias into the process.

After a very large number of coins have been distributed into the boxes, the fraction found in each of the boxes gives a possible assignment of the probability for the corresponding $\{X_i\}$.

The resulting pdf may not be consistent with the constraints of I, of course, in which case it must be rejected as a potential candidate.

If it is in agreement, then it is a viable option.

The process is then repeated by the monkeys many times.

After many such trials, some distributions will be found to come up more often than others.

The one that occurs most frequently (and satisfies I) would be a sensible choice for $(prob(X_i|I)$.

This is so because the team of monkeys has no axe to grind (no underlying bias) and thus the most frequent solution can be regarded as the one that best represents our state of knowledge.

It agrees with all the testable information available while being as indifferent as possible to everything else.

Does this correspond to the pdf with the greatest value of

$$S = -\sum_i p_i \log_e (p_i) \, ?$$

After the monkeys have tossed all the pennies given to them, suppose that we find n_1 in the first box, n_2 in the second box, and so on.

We then have

$$N = \sum_{i=1}^{M} n_i = \text{ total number of coins}$$

which will be assumed to be very large and also much greater than the number of boxes M.

This distribution gives rise to the candidate pdf $\{p_i\}$ for the possibilities $\{X_i\}$:

$$p_i = \frac{n_i}{M} \quad , \quad i = 1, 2, ..., M$$

Since every penny can land in any of the boxes there are M^N number of different ways of tossing the coins among the boxes.

Each way, by assumption of randomness and no underlying bias by the monkeys, is equally likely to occur.

All of the basic sequences, however, are not distinct, since many yield the same distribution $\{n_i\}$.

The expected frequency F with which a set $\{p_i\}$ will arise, is given by

$$F(\{p_i\}) = \frac{\text{number of ways of obtaining}\{n_i\}}{M^n}$$

The numerator is just the number of ways to distribute N coins in a distribution $\{n_i\}$ which is given by

$$\text{number of ways of obtaining}\{n_i\} = \frac{N!}{n_1!n_2!....n_M!}$$

Putting everything together we have

$$F(\{p_i\}) = \frac{\frac{N!}{n_1!n_2!....n_M!}}{M^n}$$

$$\log F) = -N\log(M) + \log(N!) - \sum_{i=1}^{M} \log(n_i!)$$

Using Stirling's approximation $\log(n!) \approx n\log(n) - n$ for large n, we find

$$\log F) = -N\log(M) + N\log(N) - \sum_{i=1}^{M} n_i \log(n_i) - N + \sum_{i=1}^{M} n_i$$

$$= -N\log(M) + N\log(N) - \sum_{i=1}^{M} n_i \log(n_i)$$

and thus

$$
\begin{aligned}
\log F) &= -N \log(M) + N \log(N) - \sum_{i=1}^{M} p_i N \log(p_i N) \\
&= -N \log(M) + N \log(N) - \sum_{i=1}^{M} p_i N (\log(p_i) + \log(N)) \\
&= -N \log(M) + N \log(N) - N \sum_{i=1}^{M} p_i \log(p_i) + N \log(N) \sum_{i=1}^{M} p_i \\
&= -N \log(M) + N \log(N) - N \sum_{i=1}^{M} p_i \log(p_i) + N \log(N) \\
&= -N \log(M) - N \sum_{i=1}^{M} p_i \log(p_i)
\end{aligned}
$$

Maximizing $\log(F)$ is equivalent to maximizing F, which is the expected frequency with which the monkeys will come up with the candidate pdf $\{p_i\}$, that is, that is, maximizing $\log(F)$ will give us the assignment $prob(\{X_i\}|I)$ which best represents our state of knowledge consistent with the testable information I.

Since M and N are constants, this is equivalent to the constrained maximization of the entropy function

$$S = -\sum_i p_i \log_e(p_i)$$

and so we recover the MaxEnt procedure once again.

Group Theory and Elementary Particles

Introduction to Group Theory

The theory of finite groups and continuous groups is a very useful tool for studying symmetry and invariance.

In order to use group theory we need to introduce some definitions and concepts.

A **group** G is defined as a set of objects or operations (called **elements**) that may be combined or **multiplied** to form a well-defined product and that satisfy the following four conditions.

If we label the elements $a, b, c, \ldots\ldots\ldots$, then the conditions are:

1. If a and b are any two elements, then the product ab is an element.
2. The defined multiplication is associative, $(ab)c = (a(bc)$
3. There is a unit element I, with $Ia = aI = a$ for all elements a.
4. Each element has an inverse $b = a^{-1}$, with $a^{-1} = a^{-1}a = I$ for all elements a.

In physics, these abstract conditions will take on direct physical meaning in terms of transformations of vectors and tensors.

As a very simple, but not trivial, example of a group, consider the set $\{I, a, b, c\}$ that combine according to the group multiplication table below.

	I	**a**	**b**	**c**
I	I	a	b	c
a	a	b	c	I
b	b	c	I	a
c	c	I	a	b

Clearly, the four conditions of the definition of group are satisfied.

The elements $\{I, a, b, c\}$ are abstract mathematical entities, completely unrestricted except for the above multiplication table.

A **representation** of the group is a set of particular objects $\{I, a, b, c\}$ that satisfy the multiplication table.

Some examples are:

$$\{I = 1, a = i, b = -1, c = -i\}$$

where the combination rules=ordinary multiplication.

This group representation is labelled C_4.

Since multiplication of the group elements is "commutative", i.e., $ab = ba$ for any pair of elements, the group is labelled "commutative or abelian".

This group is also a "cyclic" group, since all of the elements can be written as successive powers of one element. In this case,

$$\{I = i^4, a = i, b = i^2, c = i^3\}$$

Another representation is given by the successive 90° rotations in a plane.

Remember the matrix that represents a rotation through angle ϕ in 2-dimensions is given by

$$R = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}$$

With $\phi = 0, \pi/2, \pi, 3\pi/2$, we have

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \quad a = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad , \quad b = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad c = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

Thus, we have seen two explicit representations.

One with numbers(complex) using ordinary multiplication and the other with matrices using matrix multiplication.

There maybe a correspondence between the elements of two groups.

The correspondence can be one-to-one , two-to-one or, many-to-one.

If the correspondence satisfies the same group multiplication table, then it is said to be **homomorphic**.

If it is also one-to-one, then it is said to be **isomorphic**.

The two representations that we discussed above are one-to-one and preserve the multiplication table and hence, are **isomorphic**.

The representation of group elements by matrices is a very powerful technique and has been almost universally adopted among physicists.

It can be proven that all the elements of finite groups and continuous groups of the type important in physics can be represented by unitary matrices.

For unitary matrices we have

$$A^\dagger = A^{-1}$$

or, in words, the **complex conjugate/transposed** is equal to the **inverse**.

If there exists a transformation that will transform our original representation matrices into diagonal or block-diagonal form, for example,

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{44} & A_{44} \end{pmatrix} \Rightarrow \begin{pmatrix} P_{11} & P_{12} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & Q_{11} & Q_{12} \\ 0 & 0 & Q_{21} & Q_{22} \end{pmatrix}$$

such that the smaller portions or submatrices are no longer coupled together, then the original representation is said to be **reducible**.

Equivalently, we have

$$R = SAS^{-1} = \begin{pmatrix} P & 0 \\ 0 & Q \end{pmatrix}$$

which is a "similarity" transformation.

We write

$$R = P \oplus Q$$

and say that R has been **decomposed** into the representations P and Q.

The **irreducible** representations play a role in group theory that is roughly analogous to the unit vectors of vector analysis.

They are the simplest representations → all others may be built up from them.

If a group element x is transformed into another group element y by means of a similarity transformation involving a third group element g_i

$$g_i x g_i^{-1} = y$$

then y is said to be **conjugate** to x.

A **class** is a set of mutually conjugate group elements.

A class is generally not a group.

The **trace** of each group element (each matrix of our representation) is invariant under unitary transformations. We define

$$\mathrm{Tr}(A) = \sum_{i=1}^{n} A_{ii} = \mathrm{Trace}(A)$$

Then we have

$$\begin{aligned}
\mathrm{Tr}(SAS^{-1}) &= \sum_{i=1}^{n}(SAS^{-1})_{ii} = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} s_{ik}a_{kj}s_{ji}^{-1} \\
&= \sum_{j=1}^{n}\sum_{k=1}^{n} a_{kj}\sum_{i=1}^{n} s_{ji}^{-1}s_{ik} = \sum_{j=1}^{n}\sum_{k=1}^{n} a_{kj}(S^{-1}S)_{jk} \\
&= \sum_{j=1}^{n}\sum_{k=1}^{n} a_{kj}(I)_{jk} = \sum_{j=1}^{n}\sum_{k=1}^{n} a_{kj}\delta_{jk} \\
&= \sum_{j=1}^{n} a_{jj} = \mathrm{Tr}(A)
\end{aligned}$$

We now relabel the trace as the **character**.

Then we have that all members of a given class (in a given representation) have the same character.

This follows directly from the invariance of the trace under similarity or unitary transformations.

If a subset of the group elements (including the identity element I) satisfies the four group requirements (means that the subset is a group also), then we call the subset a **subgroup**.

Every group has two trivial subgroups: the identity element alone and the group itself.

The group C_4 we discussed earlier has a nontrivial subgroup comprised of the elements $\{I, b\}$.

The **order** of a group is equal to the number of group elements.

Consider a subgroup H with elements $\{h_i\}$ and a group element x not in H.

Then xh_i and h_ix are not in the subgroup H.

The sets generated by

$$xh_i \ , \ i = 1, 2, ... \ \text{ and } \ h_i x \ , \ 1 = 1, 2....$$

are called the left and right **cosets**, respectively, of the subgroup H with respect to x.

The coset of a subgroup has the same number of distinct elements as the subgroup.

This means that the original group G can be written as the sum of H and its cosets:

$$G = H + x_1 H + x_2 H + ...$$

Since H and all of its cosets have the same order(same number of elements), the order(number of elements) of any subgroup is a divisor of the order(number of elements) of the group.

The similarity transformation of a subgroup H by a fixed group element x **not** in H

$$xHx^{-1}$$

yields a subgroup.

If this subgroup is identical to H for all x, i.e., if

$$xHx^{-1} = H$$

then H is called an **invariant, normal or self-conjugate** subgroup.

In physics, groups usually appear as a set of operations that leave a system unchanged or invariant.

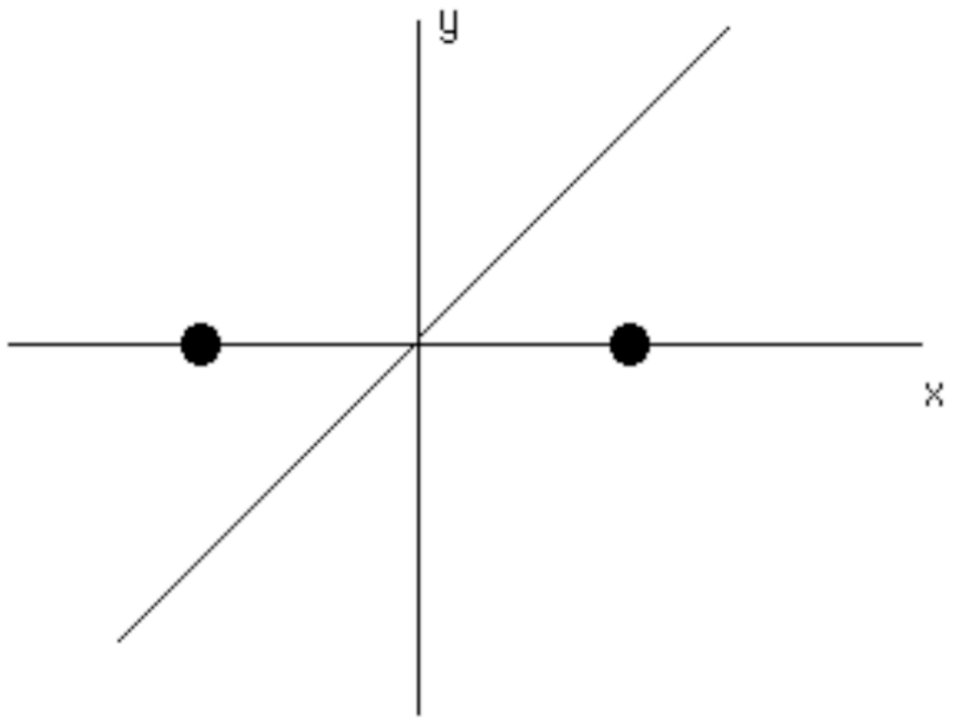
This is an expression of symmetry.

A symmetry is usually defined as the invariance of the Hamiltonian of a system under a group of transformations.

We now investigate the symmetry properties of sets of objects such as the atoms in a molecule or a crystal.

Two Objects - Twofold Symmetry Axis

Consider first the two-dimensional system of two identical atoms in the xy-plane located at $(1, 0)$ and $(-1, 0)$ as shown below.



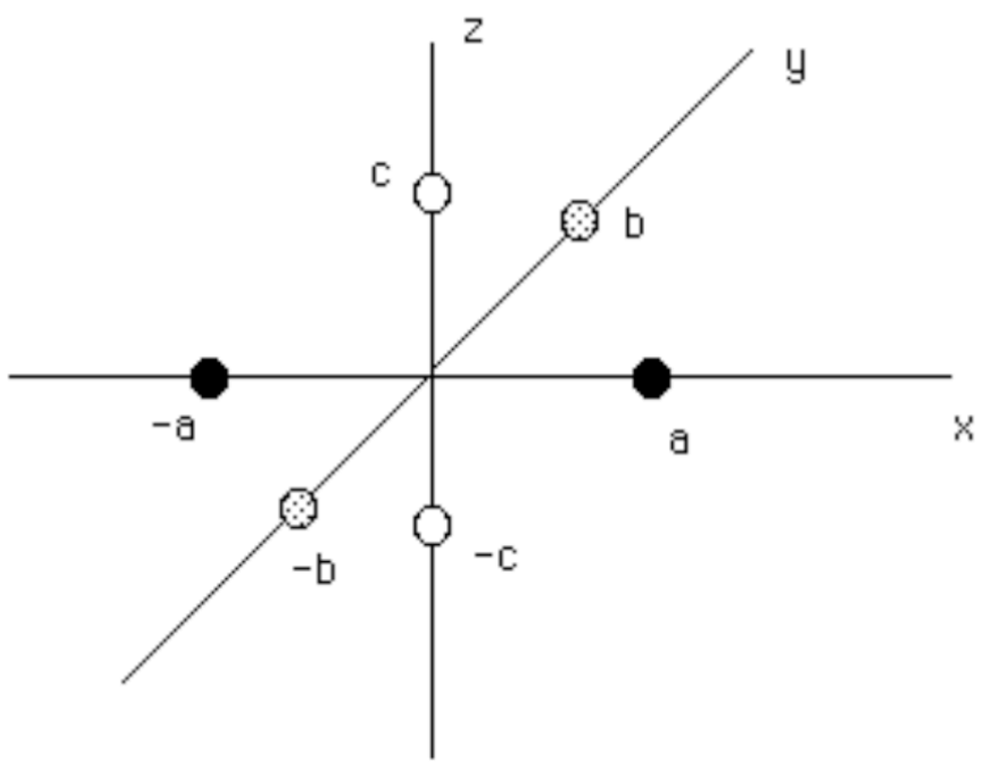
What rotations can be carried out (keeping both atoms in the xy-plane) that will leave the system invariant?

The only ones are I (always works) and a rotation by π about the z-axis.

So we have a rather uninteresting group of two elements.

The z-axis is labelled a **twofold** symmetry axis, corresponding to the two rotation angles 0 and π that leave the system invariant.

Our system becomes more interesting in 3-dimensions. Now imagine a molecule (or part of a crystal) with atoms of element X at $\pm a$ on the x-axis, atoms of element Y at $\pm b$ on the y-axis, and atoms of element Z at $\pm c$ on the z-axis as shown below:



Clearly, each axis is now a twofold symmetry axis.

The matrix representation of the corresponding rotations are:

$$R_x(\pi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, R_y(\pi) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$R_z(\pi) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

These four elements $\{I, R_x(\pi), R_y(\pi), R_z(\pi)\}$ form an abelian group with a group multiplication table:

	I	R_x	R_y	R_z
I	I	R_x	R_y	R_z
R_x	R_x	I	R_z	R_y
R_y	R_y	R_z	I	R_x
R_z	R_z	R_y	R_x	I

The products in this table can be obtained in either of two distinct ways:

(1) We may analyze the operations themselves - a rotation of π about the x-axis followed by a rotation of π about the y-axis is equivalent to a rotation of π about the z-axis

$$R_y(\pi)R_x(\pi) = R_z(\pi)$$

and so on.

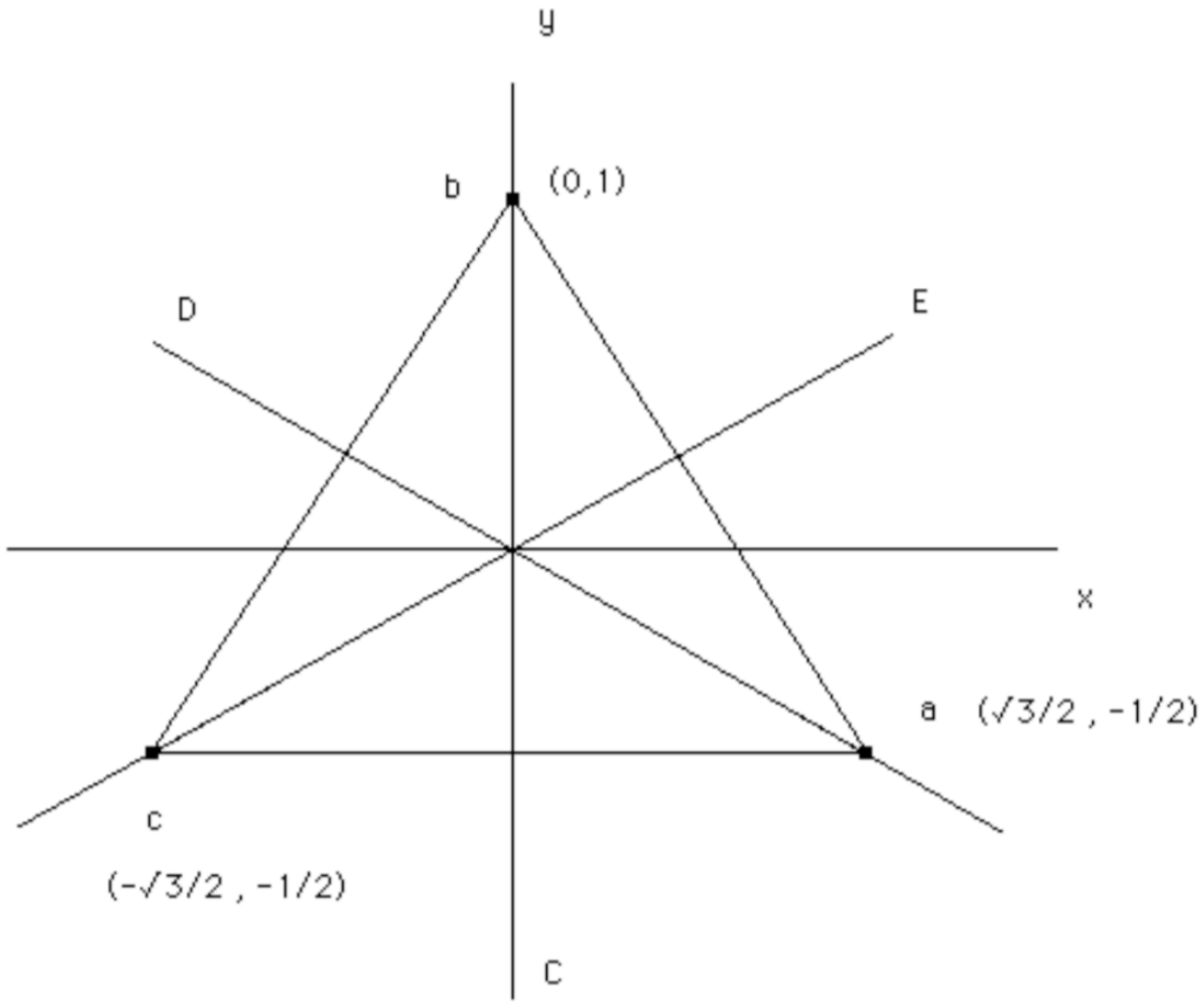
(2) Alternatively, once the matrix representation is established, we can obtain the products by direct matrix multiplication.

This latter method is especially important when the system is too complex for direct physical interpretation.

This symmetry group is often labelled D_2, where the D signifies a **dihedral** group and the subscript 2 signifies a twofold symmetry axis (and that no higher symmetry axis exists).

Three Objects – Threefold Symmetry Axis

Consider now three identical atoms at the vertices of an equilateral triangle as shown below:



Rotations (in this case we assume counterclockwise) of the triangle of $0, 2\pi/3, and 4\pi/3$ leave the triangle invariant.

In matrix form, we have

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$A = R_z(2\pi/3) = \begin{pmatrix} \cos(2\pi/3) & -\sin(2\pi/3) \\ \sin(2\pi/3) & \cos(2\pi/3) \end{pmatrix} = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$$

$$B = R_z(4\pi/3) = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$$

The z-axis is a threefold symmetry axis.

$\{I, A, B\}$ form a cyclic group, which is a subgroup of the complete 6-element group that we now discuss.

In the $x - y$ plane there are three additional axes of symmetry - each atom (vertex) and the origin define the twofold symmetry axes C, D, and E.

We note that twofold rotation axes can also be described via reflections through a plane containing the twofold axis.

In this case, we have for rotation of π about the C-axis.

$$C = R_C(\pi) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

The rotation of π about the D-axis can be replaced by a rotation of $4\pi/3$ about the z-axis followed by a reflection in the $y - z$ plane $(x \to -x)$ or

$$D = R_D(\pi) = CB = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix} = \begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$$

Similarly the rotation of π about the E-axis can be replaced by a rotation of $2\pi/3$ about the z-axis followed by a reflection in the $y - z$ plane $(x \to -x)$ or

$$E = R_E(\pi) = CA = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$$

The complete group multiplication table is:

	I	**A**	**B**	**C**	**D**	**E**
I	I	A	B	C	D	E
A	A	B	I	D	E	C
B	B	I	A	E	C	D
C	C	E	D	I	B	A
D	D	C	E	A	I	B
E	E	D	C	B	A	I

Notice that each element of the group appears only once in each row and in each column.It is clear from the multiplication table that the group is not abelian.

We have explicitly constructed a 6-element group and a 2×2 irreducible matrix representation of it.

The only other distinct 6-element group is the cyclic group $\{I, R, R^2, R^3, R^4, R^5\}$ with

$$R = \begin{pmatrix} \cos(\pi/3) & -\sin(\pi/3) \\ \sin(\pi/3) & \cos(\pi/3) \end{pmatrix} = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$$

The group $\{I, A < B, C, D, E\}$ is labeled D_3 in crystallography, the dihedral group with a threefold axis of symmetry.

The three axes (C, D, E) in the $x - y$ plane are twofold symmetry axes and, as a result, (I, C), (I, D), and (I, E) all form two-element subgroups.

None of these two-element subgroups are invariant.

There are two other irreducible representations of the symmetry group of the equilateral triangle.

They are

1. the trivial $\{1, 1, 1, 1, 1, 1\}$
2. the almost as trivial $\{1, 1, 1, -1, -1, -1\}$

Both of these representations are homomorphic to D_3.

A general and most important result for finite groups of h elements is that

$$\sum_i n_i^2 = h$$

where n_i is the dimension of the matrices of the i^{th} irreducible representation. equality is called the **dimensionality theorem** and is very useful in establishing the irreducible representations of a group. Here for D_3 we have

$$1^2 + 1^1 + 2^2 = 6$$

for our three representations.

This means that no other representations of the symmetry group of three objects exists.

We note from the examples above that for the transformations involving rotations and reflections, the transformations involving only pure rotations have determinant $= 1$ and the those involving a rotation and a reflection have determinant $= -1$.

Continuous Groups

The groups that we have been discussing all have a finite number of elements.

If we have a group element that contains one or more parameters that vary continuously over some range, then variation of the parameter will produce a continuum of group elements (an infinite number).

These groups are called continuous groups.

If continuous group has a rule for determining combination of elements or the transformation of an element or elements into a different element which is an analytic function of the parameters, where analytic means having derivatives of all orders, then it is called a **Lie** group.

For example, suppose we have the transformation rule

$$x_i' = f_i(x_1, x_2, x_3, \theta)$$

then for this transformation group to be a Lie group the functions f_i must be analytic functions of the parameter θ.

This analytic property will allow us to define infinitesimal transformations thereby reducing the study of the whole group to a study of the group elements when they are only slightly different than the identity element I.

Orthogonal Groups

We begin our study by looking at the orthogonal group O_3.

In particular, we consider the set of $n \times n$ real, orthogonal matrices with determinant $= +1$ (no reflections).

The defining property of a real orthogonal matrix is

$$A^T = A^{-1}$$

where T represents the **transpose** operation.

In terms of matrix elements this gives

$$\sum_i (A^T)_{ji} A_{ik} - \sum_i (A^{-1})_{ji} A_{ik} = I_{jk} - \delta_{jk} = 0 \,.$$

The ordinary rotation matrices are an example of real 3×3 orthogonal matrices:

$$R_x(\phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & \sin\phi \\ 0 & -\sin\phi & \cos\phi \end{pmatrix} \,, \; R_y(\theta) = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix}$$

$$R_z(\gamma) = \begin{pmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

These matrices follow the convention that the rotation is a counterclockwise rotation of the coordinate system to a new orientation.

Each $n \times n$ real orthogonal matrix with determinant $= +1$ has $n(n-1)/2$ independent parameters.

For example, 2-dimensional rotations are described by 2×2 real orthogonal matrices and they need only one independent parameter $(2(2-1)/2 = 1)$, namely the rotation angle.

On the other hand, 3-dimensional rotations require three independent angles $(3(3-1)/2 = 3)$.

Let us see this explicitly for the 2×2 case: Suppose we have the general 2×2 matrix

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

where all the elements are real.

Imposing the condition determinant $= +1$ gives

$$ad - bc = 1$$

Imposing the condition that the transpose is the inverse gives

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} a & c \\ b & d \end{pmatrix} = \begin{pmatrix} a^2 + b^2 & ac + bd \\ ac + bd & c^2 + d^2 \end{pmatrix} = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

These equations imply the solution

$$\begin{pmatrix} a & \sqrt{1-a^2} \\ -\sqrt{1-a^2} & a \end{pmatrix}$$

which shows that there is only one independent parameter.

Special Unitary Groups, $SU(2)$

The set of complex $n \times n$ unitary matrices also forms a group.

This group is labeled $U(n)$.

If we impose an additional restriction that the determinant of the matrices be $+1$, then we get the special unitary group, labeled $SU(n)$.

The defining relation for complex unitary matrices is

$$A^\dagger = A^{-1}$$

where $\dagger$ represents the complex-conjugate-transpose or adjoint operation.

In this case we have $n^2 - 1$ independent parameters.

This can be seen explicitly below: Suppose we have the general 2×2 matrix representing the transformation U

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

where all the elements are complex.

Imposing the condition determinant $= +1$ gives

$$ad - bc = 1$$

Imposing the condition that the adjoint is the inverse gives

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix} = \begin{pmatrix} |a|^2 + |b|^2 & ac^* + bd^* \\ a^*c + b^*d & |c|^2 + |d|^2 \end{pmatrix} = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

These equations imply the solution

$$\begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}$$

where

$$|a|^2 + |b|^2 = aa^* + bb^* = 1$$

Since each complex number has two independent components, this shows that there are three $(2^2 - 1)$ independent parameters.

For $n = 3$, there will be eight $(3^2 - 1)$ independent parameters.

This will become the famous **eightfold way** of elementary particle physics(later).

An alternative general form is for the 2×2 case is

$$U(\xi, \eta, \zeta) = \begin{pmatrix} e^{i\xi} \cos\eta & e^{i\zeta} \sin\eta \\ e^{-i\zeta} \sin\eta & e^{-i\xi} \cos\eta \end{pmatrix}$$

Now we will determine the irreducible representations of $SU(2)$.

Since the transformations are 2×2 matrices, the objects being transformed (the vectors or states) will be a two-component complex column vector (called a spinor):

$$\begin{pmatrix} u' \\ v' \end{pmatrix} = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}$$

or

$$u' = au + bv \quad , \quad v' = -b^* u + a^* v$$

From the form of this result, if we were to start with a homogeneous polynomial of the n^{th} degree in u and v and carry out the unitary transformation given by the last two equations, we would still have a homogeneous n^{th} degree polynomial.

To illustrate what happens we use the function (due to Wigner):

$$f_m(u,v) = \frac{u^{j+m}v^{j-m}}{\sqrt{(j+m)!(j-m)!}}$$

The index m will range from $-j$ to j, covering all terms of the form $u^p v^q$ with $p+q=2j$.

The denominator makes sure that our representation will be unitary.

Now we can show that

$$Uf_m(u,v) = f_m(u',v')$$

which becomes

$$Uf_m(u,v) = f_m(au+bv, -b^*u+a^*v') = \frac{(au+bv)^{j+m}(-b^*u+a^*v)^{j-m}}{\sqrt{(j+m)!(j-m)!}}$$

We now express this last equation as a linear combination of terms of the form $f_m(u, v)$.

The coefficients in the linear combination will give the matrix representation in the standard way.

We expand the two binomials using the binomial theorem:

$$(au + bv)^{j+m} = \sum_{k=0}^{j+m} \frac{(j+m)!}{k!(j+m-k)!} a^{j+m-k} u^{j+m-k} b^k v^k$$

$$(-b^* u + a^* v)^{j-m} = \sum_{n=0}^{j-m} (-1)^{j-m-n} \frac{(j-m)!}{n!(j-m-n)!} b^{*(j-m-n)} u^{j-m-n} a^{*n} v^n$$

Upon rearranging and changing some dummy indices we get

$$U f_m(u, v) = f_m(u', v') = \sum_{m'=-j}^{j} U_{mm'} f_{m'}(u, v)$$

where the matrix element $U_{mm'}$ is given by

$$U_{mm'}$$
$$= \sum_{k=0}^{j+m} (-1)^{m'-m+k} \frac{\sqrt{((j+m)!)^2((j-m)!)^2}}{k!\sqrt{(j-m'-k)!(j+m-k)!(m'-m+k)!}} a^{j+m-k} a^{*(j-m'-k)} b^k b^{*(m'-m+k)}$$

The index k starts with zero and runs up to $j+m$, but the factorials in the denominator guarantee that the coefficient will vanish if any exponent goes negative (since $(-n)! = \pm\infty$ for $n = 1, 2, 3, ...$).

Since m and m' each range from $-j$ to j in unit steps, the matrices $U_{mm'}$ representing $SU(2)$ have dimensions $(2j+1) \times (2j+1)$.

If $j = 1/2$, then we get

$$U = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} = \begin{pmatrix} U_{m=1/2,m'=1/2} & U_{m=1/2,m'=-1/2} \\ U_{m=-1/2,m'=1/2} & U_{m=-1/2,m'=-1/2} \end{pmatrix}$$

which is identical to the earlier equation.

$SU(2) - O_3$ Homomorphism (for the mathematically inclined)

The operation of $SU(2)$ on a matrix is given by a unitary transformation

$$M' = UMU^\dagger$$

Now any 2×2 matrix M can be written in terms of I and the three Pauli matrices

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \ , \ \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \ , \ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

that is, these four matrices span the 2×2 world; they are a basis.

Let M be a zero-trace matrix(then I does not contribute) so that in general

$$M = x\sigma_1 + y\sigma_2 + z\sigma_3 = \begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix}$$

Since the trace is invariant under a unitary transformation, M' must have the same form

$$M = x'\sigma_1 + y'\sigma_2 + z'\sigma_3 = \begin{pmatrix} z' & x' - iy' \\ x' + iy' & -z' \end{pmatrix}$$

The determinant is also invariant under a unitary transformation.

Therefore

$$-(x^2 + y^2 + z^2) = -(x'^2 + y'^2 + z'^2)$$

or $x^2 + y^2 + z^2$ is invariant under this operation of $SU(2)$ (same as with O_3, the rotation group). $SU(2)$ must, therefore, describe some kind of rotation.

In fact, it is easy to check that the square of the length of a spinor (2-element column vector)

$$s^\dagger s = \begin{pmatrix} u^* & v^* \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = u * u + v^* v$$

is invariant under the transformation U.

This suggests that $SU(2)$ and O_3 may be isomorphic or homomorphic.

We can figure out what rotation $SU(2)$ describes by considering some special cases.

Consider

$$U_z(\alpha/2) = \begin{pmatrix} e^{i\alpha/2} & 0 \\ 0 & e^{-i\alpha/2} \end{pmatrix}$$

Now we carry out the transformation of each of the three Pauli matrices.

For example,

$$U_z \sigma_1 U_z^\dagger = \begin{pmatrix} e^{i\alpha/2} & 0 \\ 0 & e^{-i\alpha/2} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{-i\alpha/2} & 0 \\ 0 & e^{i\alpha/2} \end{pmatrix} = \begin{pmatrix} 0 & e^{i\alpha} \\ e^{-i\alpha} & 0 \end{pmatrix}$$

or

$$U_z x\sigma_1 U_z^\dagger = (x\cos\alpha)\sigma_1 - (x\sin\alpha)\sigma_2$$

Similarly,

$$U_z x\sigma_2 U_z^\dagger = (y\sin\alpha)\sigma_1 + (y\cos\alpha)\sigma_2$$

$$U_z x\sigma_3 U_z^\dagger = (z)\sigma_3$$

Our earlier expression for M' then gives

$$x' = x\cos\alpha + y\sin\alpha$$

$$y' = -x\sin\alpha + y\cos\alpha$$

$$z' = z$$

Thus, the 2×2 unitary transformation using $U_z(\alpha/2)$ is equivalent to the rotation operator $R_z(\alpha)$.

The same correspondence can be shown for

$$U_y(\beta/2) = \begin{pmatrix} \cos(\beta/2) & \sin(\beta/2) \\ -\sin(\beta/2) & \cos(\beta/2) \end{pmatrix}$$

$$U_x(\phi/2) = \begin{pmatrix} \cos(\phi/2) & i\sin(\phi/2) \\ i\sin(\phi/2) & \cos(\phi/2) \end{pmatrix}$$

In general, we have

$$U_k(\gamma/2) = I\cos(\gamma/2) + i\sigma_k \sin(\gamma/2)$$

The correspondence

$$U_z(\alpha/2) = \begin{pmatrix} e^{i\alpha/2} & 0 \\ 0 & e^{-i\alpha/2} \end{pmatrix} \Leftrightarrow R_z(\alpha) = \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha 0 & \\ 0 & 0 & 1 \end{pmatrix}$$

is not a simple one-to-one correspondence.

Specifically, as α in $R_z(\alpha)$ ranges from 0 to 2π the parameter in $U_z(\alpha/2)$, $\alpha/2$, goes from 0 to π.

We find

$$R_z(\alpha + 2\pi) = R_z(\alpha)$$

$$U_z(\alpha/ + \pi) = \begin{pmatrix} -e^{i\alpha/2} & 0 \\ 0 & -e^{-i\alpha/2} \end{pmatrix} = -U_z(\alpha/2)$$

Therefore both $U_z(\alpha/2)$ and $U_z(\alpha/ + \pi) = -U_z(\alpha/2)$ correspond to $R_z(\alpha)$.

The correspondence is 2 to 1, or $SU(2)$ and O_3 are homomorphic.

The establishment of the correspondence between representations of $SU(2)$ and those of O_3 means that the known representations of $SU(2)$ automatically provide us with representations of O_3.

Combining the various rotations, we find that a unitary transformation using

$$U(\alpha, \beta, \gamma) = U_z(\gamma/2)U_y(\beta/2)U_z(\alpha/2)$$

corresponds to the general Euler rotation $R_z(\alpha)R_y(\beta)R_z((\gamma)$ (studied Advanced Mechanics and Quantum Mechanics courses) .

By direct multiplication we get

$$U(\alpha, \beta, \gamma) = U_z(\gamma/2)U_y(\beta/2)U_z(\alpha/2)$$

From our alternative original definition of U, using

$$\xi = (\gamma + \alpha)/2 \ , \ \eta = \beta/2 \ , \ \psi = (\gamma - \alpha)/2$$

we identify the parameters a and b as

$$a = e^{i(\gamma+\alpha)/2} \cos(\beta/2) \quad , \quad b = e^{i(\gamma-\alpha)/2} \sin(\beta/2)$$

Finally the $SU(2)$ representation of $U_{mm'}$ becomes

$$U_{mm'}(\alpha,\beta,\gamma)$$

$$= \sum_{k=0}^{j+m}(-1)^k \frac{\sqrt{((j+m)!)^2((j-m)!)^2}}{k!\sqrt{(j-m'-k)!(j+m-k)!(m'-m+k)!}}$$

$$\times e^{im\gamma}(\cos(\beta/2)^{2j+m-m'-2k}(-\sin(\beta/2)^{m-m'+2k}e^{im'\alpha}$$

Here the irreducible representations are in terms of the Euler angles.

This result allows us to calculate the $(2j+1)\times(2j+1)$ irreducible representations of S$U(2)$ for all j ($j = 0, 1/2, 1, 3/2, ...$) and the irreducible representations of $)_3$ for integral orbital angular momentum j ($j = 0, 1, 2, 3, ...$) (in Quantum Mechanics course).

Generators

In all cases, rotations about a **common axis** combine as

$$R_z(\phi_2)R_z(\phi_1) = R_z(\phi_1 + \phi_2)$$

that is, multiplication of these matrices is equivalent to addition of the arguments.

This suggests that we look for an **exponential** representation of the rotations, i.e.,

$$\exp(\phi_2)\exp(\phi_1) = \exp(\phi_1 + \phi_2)$$

Suppose we define the exponential function of a matrix by the following relation:

$$U = e^{iaH} = I + iaH + \frac{(iaH)^2}{2!} + ...$$

where a is a real parameter independent of matrix(operator) H.

It is easy to prove that if H is Hermitian, then U is unitary and if U is unitary, the H is Hermitian.

In group theory, H is labeled a **generator**, the generator of U.

The following matrix describes a finite rotation of the coordinates through an angle ϕ counterclockwise about the z-axis:

$$R_z(\phi) = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi 0 & \\ 0 & 0 & 1 \end{pmatrix}$$

Now letR_z be an infinitesimal rotation through an angle $\delta\phi$.

We can then write

$$R_z(\delta\phi) = I + i\delta\phi M_z$$

where

$$M_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Similarly, we find

$$M_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad , \quad M_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

A finite rotation ϕ can be compounded out of successive infinitesimal rotations $\delta\phi$

$$R_z(\delta\phi_2 + \delta\phi_1) = (I + i\delta\phi_2 M_z)(I + i\delta\phi_1 M_z)$$

Letting $\delta\phi = \phi/N$ for N rotations, with $N \to \infty$, we get

$$R_z(\phi) = \lim_{N\to\infty} (I + (i\phi/N)M_z))^N = \exp(i\phi M_z)$$

This implies that M_z is the generator of the group $R_z(\phi)$, a subgroup of O_3.

Before proving this result, we note:

(a) M_z is Hermitian and thus, $R_z(\phi)$ is unitary

(b) $\mathrm{Tr}(M_z) = 0$ and $\det(R_z(\phi)) = +1$

In direct analogy with M_z, M_x may be identified as the generator of R_x, the subgroup of rotations about the x-axis, and M_y as the generator of R_y .

$$R_z(\phi) = \exp(i\phi M_z) = I + i\phi M_z + \frac{(i\phi M_z)^2}{2!} + \frac{(i\phi M_z)^3}{3!} + \ldots\ldots$$

$$= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$+ i\phi M_z + \frac{(i\phi)^2}{2!} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{(i\phi)^3}{3!} M_z + \ldots..$$

$$= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} (1 - \frac{\phi^2}{2!} + ...) + i(\phi - \frac{\phi^3}{3!} + ...)M_z + ...$$

$$= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \cos\phi + i \sin\phi M_z + ...$$

$$= \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

where we have used the relations

$$M_z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad , \quad M_z^3 = M_z \quad , \ , \quad \text{etc}$$

and we recognized the two series as $\cos\phi$ and $\sin\phi$.

Thus, we get the same matrix $R_z(\phi)$ as earlier.

Other relations we can write are:

1. all infinitesimal rotations commute

$$[R_i(\delta\phi_i), R_j(\delta\phi_j)] = 0$$

2. an infinitesimal rotation about an axis defined by unit vector $\hat{n}$ is

$$R(\delta\phi) = I + i\delta\phi\ \hat{n}M$$

3. the generators satisfy the commutation rules

$$[M_i, M_j] = \sum_k i\epsilon_{ijk}M_k$$

This will turn out to be the commutation relations for angular momentum operators in quantum mechanics.

In a similar way the elements (U_1, U_2, U_3) of the two-dimensional unitary group, $SU(2)$, may be generated by

$$\exp(a\sigma_1/2) \quad , \quad \exp(a\sigma_2/2) \quad , \quad \exp(a\sigma_3/2)$$

where $\sigma_1, \sigma_2, \sigma_3$ are the Pauli spin matrices and a, b, and c are real parameters.

We note that the σ's are Hermitian and have zero trace and thus, the elements of $SU(2)$ are unitary and have determinant $= +1$.

We also note that the generators in diagonal form such as σ_3 will lead to conserved quantum numbers.

Finally, if we define $s_i = \frac{1}{2}\sigma_i$ then we have

$$[s_i, s_j] = \sum_k i\epsilon_{ijk} s_k$$

which are the angular momentum commutation rules implying that the $s_i$are angular momentum operators.(Quantum mechanics course)

SU(3) and the Eightfold Way of Elementary Particles

The basic elements of a group are unitary operators (matrices of determinant $= +1$ or unimodular matrices) that transform the basis vectors $|q_i\rangle$ (we switch to Dirac notation which you learned in Quantum class for convenience) among themselves as

$$\left|q_j'\right\rangle = \sum_{i=1}^{n} u_{ji} \left|q_i\right\rangle$$

We **assume** that the **observed** elementary particle states or vectors, as linear combinations (or composites) of these basis vectors also transform into one another under the unitary operations of the group. It is most convenient to work with infinitesimal unitary transformations where

$$U = \exp\left(\frac{i}{2}\sum_j \epsilon_j \lambda_j\right) = I + \frac{i}{2}\sum_j \epsilon_j \lambda_j$$

where the ϵ_j are infinitesimal.

Now

$$\det(U) = 1 = \det\left(I + \frac{i}{2}\sum_j \epsilon_j \lambda_j\right) = \det(I) + \frac{i}{2}\sum_j \epsilon_j \mathrm{Tr}(\lambda_j) + O(\epsilon^2)$$

Therefore we have, in the general case,

$$\sum_j \epsilon_j \mathrm{Tr}(\lambda_j) = 0$$

We can satisfy this condition by choosing matrices λ_j such that

$$\mathrm{Tr}(\lambda_j) = 0$$

for all j.

For $n \times n$ matrices, there are $n^2 - 1$ linearly independent traceless matrices.

Since these matrices now have all of the properties of the generators of a group as discussed in the earlier parts of these notes, we will make that designation. The λ_j,$j = 1, 2, 3, ..., n^2 - 1$ are the generators of the group.

We need, therefore, only study the commutation relations among the generators in order to understand all of the group properties.

To see how this all works and to connect it to earlier ideas we will now use $SU(2)$ as an illustration.

As we stated earlier, the algebra is defined by the commutation relations among a certain group of operators(the generators).

In order to find

1. all the operators, and
2. the defining commutation relations of the algebra we start with the simplest physical realization of this algebra.

We assume the existence some entity with 2 states (we end up with the 2-dimensional representation) and represent it by a 2-element column vector, i.e.,

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \text{amount of ``upness''} \\ \text{amount of ``downness''} \end{pmatrix}$$

The example we will use is a quantity called **isospin** (I_1, I_2, I_3) and the "upness" and "downness" will refer to the values of $I_3 = I_z$, i.e.,

$$|proton\rangle = |p\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |neutron\rangle = |n\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The operator (2×2 matrix) which converts a neutron into a proton (a **raising** operator) is given by

$$\tau_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

where

$$\tau_+ |n\rangle = |p\rangle \quad , \quad \tau_= |p\rangle = 0$$

Similarly, its Hermitian adjoint (a **lowering** operator) is

$$\tau_- = \tau_+^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

where

$$\tau_- |p\rangle = |n\rangle \quad , \quad \tau_- |n\rangle = 0$$

Note that τ_+ "annihilates" protons and τ_- "annihilates" neutrons.

Forming their commutator we find that

$$[\tau_+, \tau_-] = \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and

$$\tau_3 |p\rangle = |p\rangle \quad , \quad \tau_3 |n\rangle = -|n\rangle$$

We also find that

$$[\tau_3, \tau_\pm] = \pm 2\tau_\pm$$

We then set

$$\mathsf{I} \to (I_1, I_2, I_3) \to \text{ Isospin}$$

$$\boldsymbol{\tau} \to (\tau_1, \tau_2, \tau_3)$$

and then define

$$\mathsf{I} = \frac{1}{2}\boldsymbol{\tau} \Rightarrow (I_1, I_2, I_3) = \frac{1}{2}(\tau_1, \tau_2, \tau_3)$$

so that the "upness" values are given by $\pm\frac{1}{2}$. i.e.,

$$I_3 \left|p\right\rangle = \frac{1}{2}\left|p\right\rangle \quad , \quad I_3 \left|n\right\rangle = -\frac{1}{2}\left|n\right\rangle$$

That completes the discussion of the 2-dimensional representation.

The same commutation relations are also used to derive higher order representations.

Note that these three commutators only involve the same three operators.

This means that these three commutators complete the commutation relations (all further commutators can be expressed in terms of these three operators or we have a **closed commutator algebra**).

The three operators τ_+, τ_-, τ_3 are the basic set for $SU(2)$.

An equivalent set is

$$\tau_1 = i(\tau_+ - \tau_-) \ , \ \tau_2 = i(\tau_- + \tau_+) \ , \ \tau_3$$

This also correlates with the earlier statements that we would have $n^2 - 1 = 3$ generators for $SU(2)$.

To obtain the other representations of the $SU(2)$ algebra, we must only use these defining commutation relations.

It is clear from the commutators that only one of the Hermitian operators τ_1, τ_2, τ_3 can be diagonalized in a given representation of the space(using a given set of basis vectors).

We will choose a representation in which τ_3 is diagonal (this was the choice in the 2-dimensional representation above also).

Remember that these diagonal elements are the eigenvalues of τ_3.

We label the state by the eigenvalue m of τ_3, i.e.,

$$\tau_3 |m\rangle = m |m\rangle$$

Now let us use the commutation relations.

$$\tau_3\tau_+ |m\rangle = (\tau_+\tau_3 + 2\tau_+) |m\rangle = (m+2)\tau_+ |m\rangle$$

This implies that

$$\tau_+ |m\rangle = c |m+2\rangle$$

In a similar manner, we can show that

$$\tau_- |m\rangle = c' |m-2\rangle$$

Now, if we start with any state in a given representation, we can generate states with higher eigenvalues, until we reach the state with maximum eigenvalue M (which we assume exists).

Since we cannot go any higher, this state must have the property that

$$\tau_+ |M\rangle = 0$$

This was the case for the 2-dimensional representation where

$$\tau_+ |p\rangle = 0$$

We now start with this highest weight state, which it turns out is unique for an irreducible representation.

We then have

$$\tau_- |M\rangle = \lambda_1 |M-2\rangle$$

which implies that (assuming λ_1 is real)

$$\langle M|\,\tau_+ = \lambda_1\,\langle M-2|$$

You can make sense of this by thinking in terms of matrices.

As usual, we choose to normalize our basis states to 1, i.e.,
$\langle m\,|\,m\rangle = 1$ and we then obtain

$$\begin{aligned}\langle M|\,\tau_+\tau_-\,|M\rangle &= \langle M-2|\,\lambda_1\lambda_1\,|M-2\rangle = \lambda_1^2\,\langle M-2\,|\,M-2\rangle = \lambda_1^2\\ &= \langle M|\,([\tau_+,\tau_-]+\tau_-\tau_+)\,|M\rangle\\ &= \langle M|\,[\tau_+,\tau_-]\,|M\rangle + \langle M|\,\tau_-\tau_+\,|M\rangle\\ &= \langle M|\,\tau_3\,|M\rangle = M\end{aligned}$$

where we have used

$$\tau_+\,|M\rangle = 0\ \ ,\ \ [\tau_+,\tau_-] = \tau_3\ \ ,\ \ \tau_3\,|M\rangle = M\,|M\rangle$$

So we get

$$\lambda_1^2 = M$$

We also note that

$$\langle M-2|\,\tau_-\,|M\rangle = \lambda_1 = \langle M|\,\tau_+\,|M-2\rangle$$

which implies that

$$\tau_+\,|M-2\rangle = \lambda_1\,|M\rangle$$

Now consider

$$\tau_-\,|M-2\rangle = \lambda^2\,|M-4\rangle$$

which gives (same algebra as before)

$$\begin{aligned}
\lambda_2^2 &= \langle M-2|\,\tau_+\tau_-\,|M-2\rangle = \langle M-2|\,([\tau_+,\tau_-]+\tau_-\tau_+)\,|M-2\rangle \\
&= \langle M-2|\,[\tau_+,\tau_-]\,|M-2\rangle + \langle M-2|\,\tau_-\tau_+\,|M-2\rangle \\
&= \langle M-2|\,\tau_3\,|M-2\rangle + \langle M|\,\lambda_1^2\,|M\rangle = \lambda_1^2 + M - 2
\end{aligned}$$

In general, we can state..... if

$$\tau_- \left|M - 2(p-1)\right\rangle = \lambda_p \left|M - 2p\right\rangle$$

we get

$$\lambda_p^2 = \lambda_{p-1}^2 + M - 2(p-1)$$

Now $\lambda_0^2 = 0$ (from definition of maximum eigenvalue and also see below).

Thus, we have

$$\lambda_1^2 = \lambda_0^2 + 1(M - 1 + 1) = M \quad \text{as before!}$$
$$\lambda_2^2 = \lambda_1^2 + m - 2(2-1) = \lambda_1^2 + M - 2 = 2(M - 2 + 1)$$
$$\lambda_3^2 = \lambda_2^2 + M - 2(3-1) = 3(M - 3 + 1)$$

or generalizing

$$\lambda_p^2 = p(M - p + 1)$$

When $\lambda_p^2 = 0\,(p \neq 0)$ we reach the minimum eigenvalue.

This gives

$$p = M + 1$$

which implies the minimum eigenvalue is $-M$, that is,

$$\tau_- \left|M - 2(p-1)\right\rangle = \tau_- \left|M - 2(M+1-1)\right\rangle$$

$$= \tau_- \left|-M\right\rangle = 0 \quad (\lambda_{M+1} = 0)$$

$$\rightarrow \tau_- \left|-M\right\rangle = 0$$

The total number of states contained in this set is

$$p = M + 1 = \quad \text{multiplicity}$$

Let us represent the states by a linear array

The operators $\tau_{\pm}$ represent steps between equally spaced points.

There is only **one** state for a given value of m and only **one** set of states (an irreducible representation) is generated from a given maximum state $|M\rangle$.

This result implies that there exists one independent operator that can be constructed from $\tau_\pm$ and τ_3 which commutes with $\tau_\pm$ and τ_3 (has simultaneous eigenstates with τ_3 and thus can simultaneously label the states) and which serves to distinguish representations.

We consider the operator (the square of the isospin)

$$\Gamma = \frac{1}{2}(\tau_+\tau_- + \tau_-\tau_+) + \frac{1}{4}\tau_3^2 = \frac{1}{4}(\tau_1^2 + \tau_2^2 + \tau_3^2) = \frac{1}{4}\tau^2$$

We have

$$[\Gamma, \tau_i] = 0$$

which implies that

$$\Gamma\,|m\rangle = c\,|m\rangle \quad \text{for all} \quad m$$

or

$$\langle m|\,\Gamma\,|m\rangle = \langle M|\,\Gamma\,|M\rangle = c$$

Using the commutation relations we have

$$\Gamma = \frac{1}{4}\tau_3^2 + \frac{1}{2}\tau_3 + \tau_-\tau_+$$

which gives

$$c = \langle M| \Gamma |M\rangle = \frac{1}{4}M^2 + \frac{1}{2}M = \frac{M}{2}\left(\frac{M}{2} + 1\right)$$

If we let $t = M/2$ then we have $c = t(t+1)$.

This means that

$$p = M + 1 = 2t + 1 = \quad \text{multiplicity}$$

where $2t + 1$ is an integer.

We note the connection to ordinary Isospin I:

$$I_3 = \frac{1}{2}\tau_3 \quad , \quad I^2 = \Gamma = \frac{1}{4}\tau^2$$

Now to delineate the representations.

First, the 2-dimensional representation (so that we can see the general stuff give back the specific case that we started with).

This is the smallest or lowest representation.

We choose $M = 1$ corresponding to

$$t = 1 \quad \text{and } p = \quad \text{multiplicity } = 2$$

We are most interested in finding the basis states or the simultaneous eigenvectors of I^2 and I_3 since these will turn out to represent elementary particles.

We have (as before)

$$|proton\rangle = |p\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |neutron\rangle = |n\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$I = \frac{1}{2}$$

$$I_3|p\rangle = \frac{1}{2}|p\rangle \quad , \quad I_3|n\rangle = -\frac{1}{2}|n\rangle$$

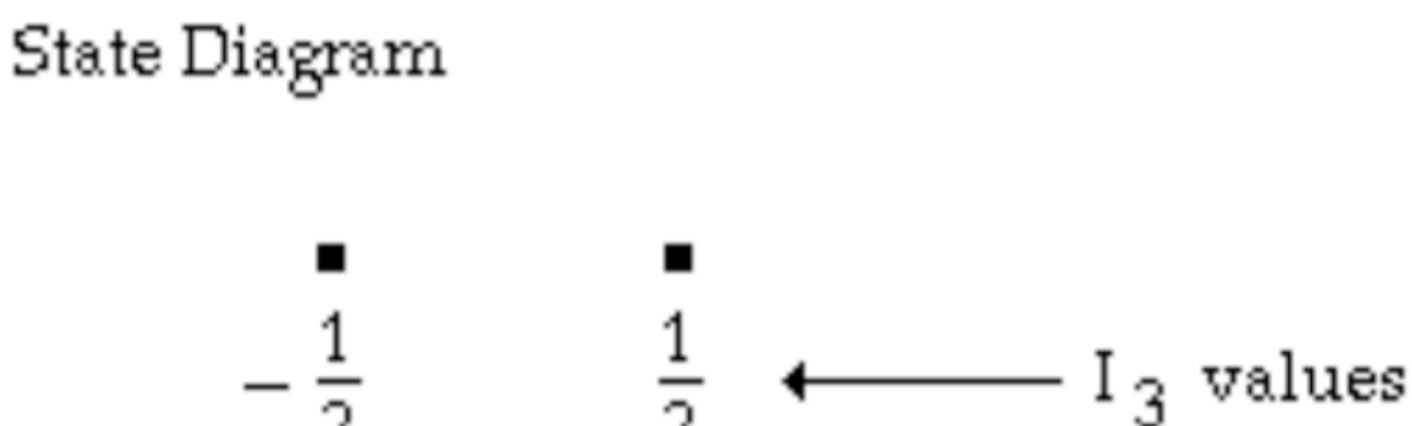
$$I^2|p\rangle = \frac{1}{2}\left(\frac{1}{2}+1\right)|p\rangle = \frac{3}{4}|p\rangle \quad , \quad I^2|n\rangle = \frac{1}{2}\left(\frac{1}{2}+1\right)|n\rangle = \frac{3}{4}|n\rangle$$

$$I_+|n\rangle = |p\rangle \quad , \quad I_-|p\rangle = |n\rangle$$

where we have used

$$I_3 = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix} \quad , \quad I_+ = \begin{pmatrix} 0 & 1 \\ 0 & -0 \end{pmatrix} \quad , \quad I_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

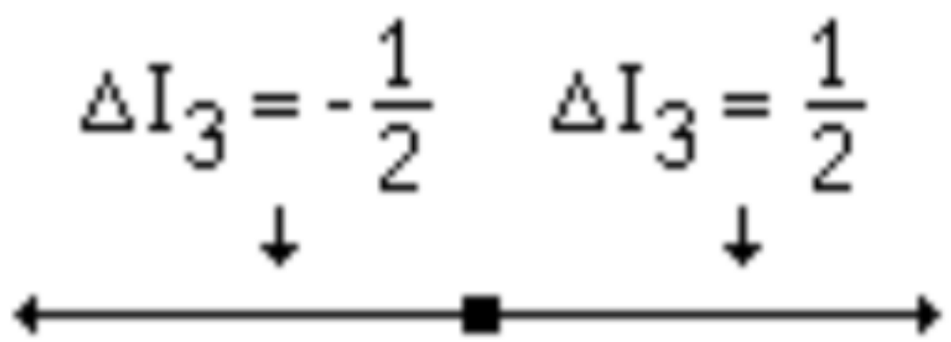
Therefore the state diagram for the $\frac{1}{2}$-representation (representations are labeled by I value) is given by



where

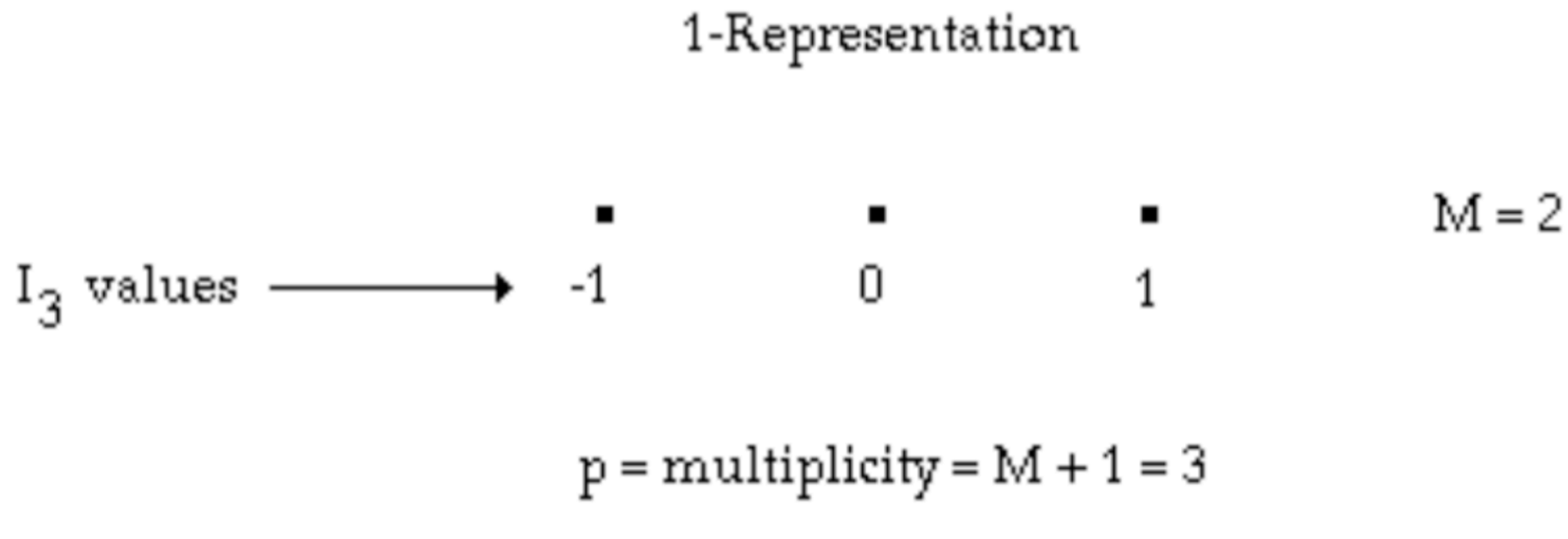
$$M = 2I_3(\text{maximum}) = 1 \quad , \quad p = \quad \text{multiplicity} \quad M + 1 = 2$$

We now define a weight diagram for SU(2) by the following symbol:



SU(2) Weight Diagram

Generating the 1-representation is just as easy and leads to a general graphical method for generating higher representations via the weight diagrams.



Generalizing, the I-representation ($M = 2I$) has a multiplicity $2I + 1$ or $2I + 1$ equally spaced points ($\Delta I_3 = \text{constant}$) representing states in the representation.

We now consider the higher representation generated by combining two $\frac{1}{2}$-representations.

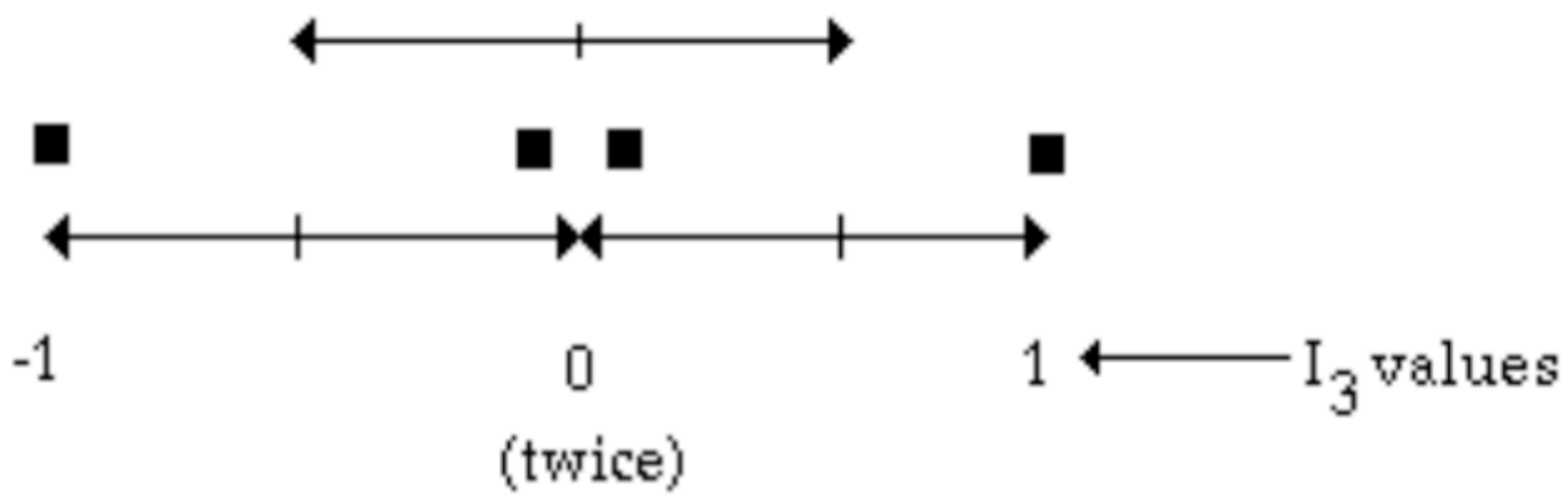
The formal name for this product is a **direct product** and it is written

$$\frac{1}{2} \otimes \frac{1}{2}$$

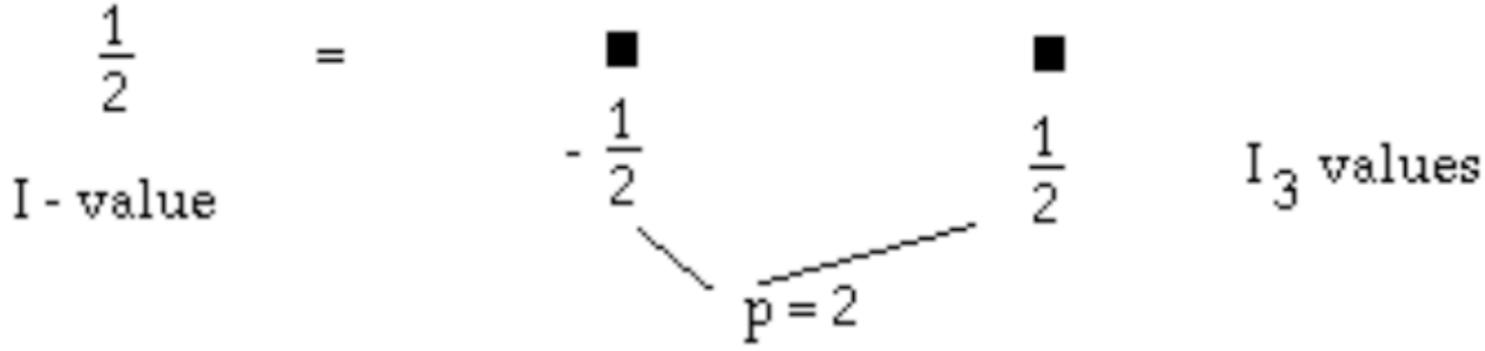
The **rules** for using the weight diagrams are as follows:

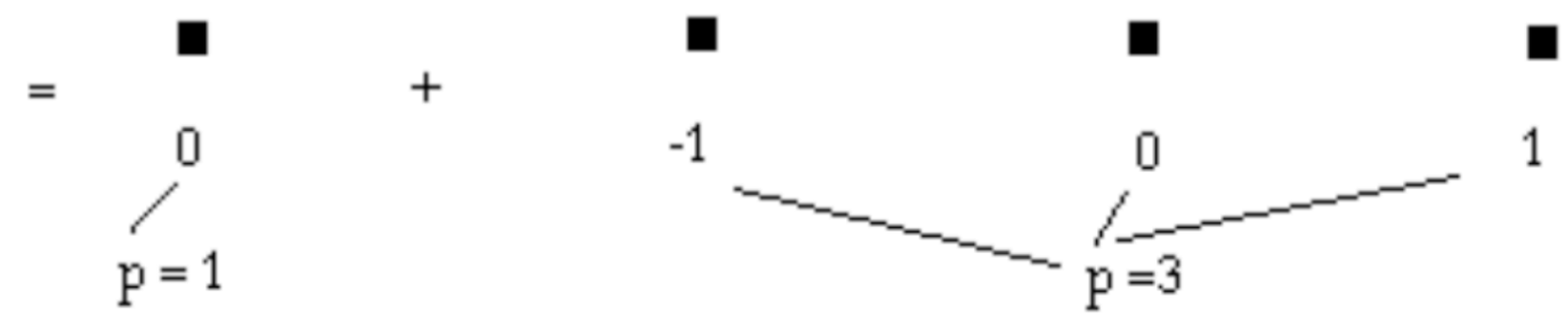
1. **draw** the first weight diagram
2. **superpose** a set of weight diagrams **centered** at the arrow tips of the first weight diagram
3. **allowed** states are at the **final** arrow tips

For the case we are considering this looks like:



We observe that



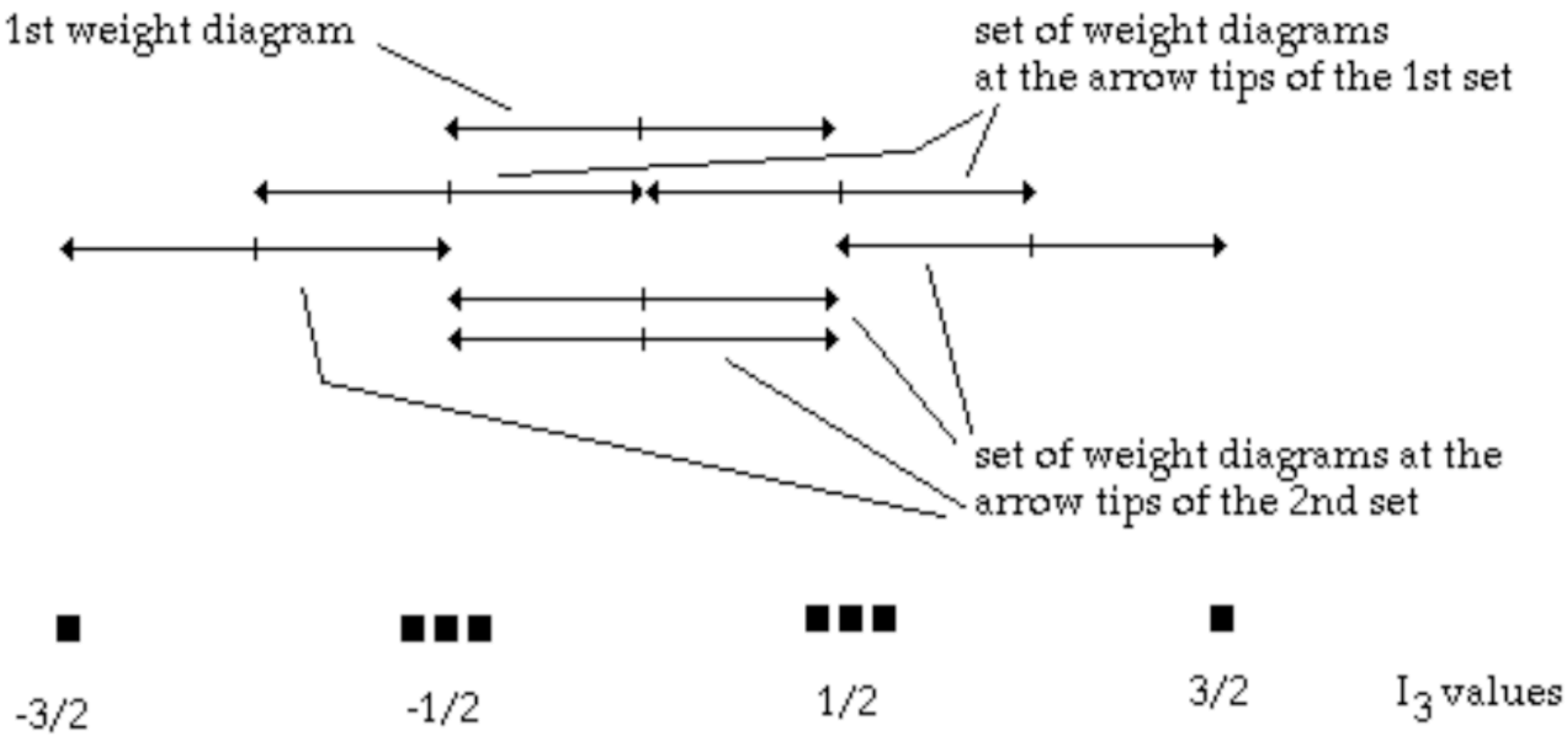


= 0 ⊕ 1

I - values of new representations

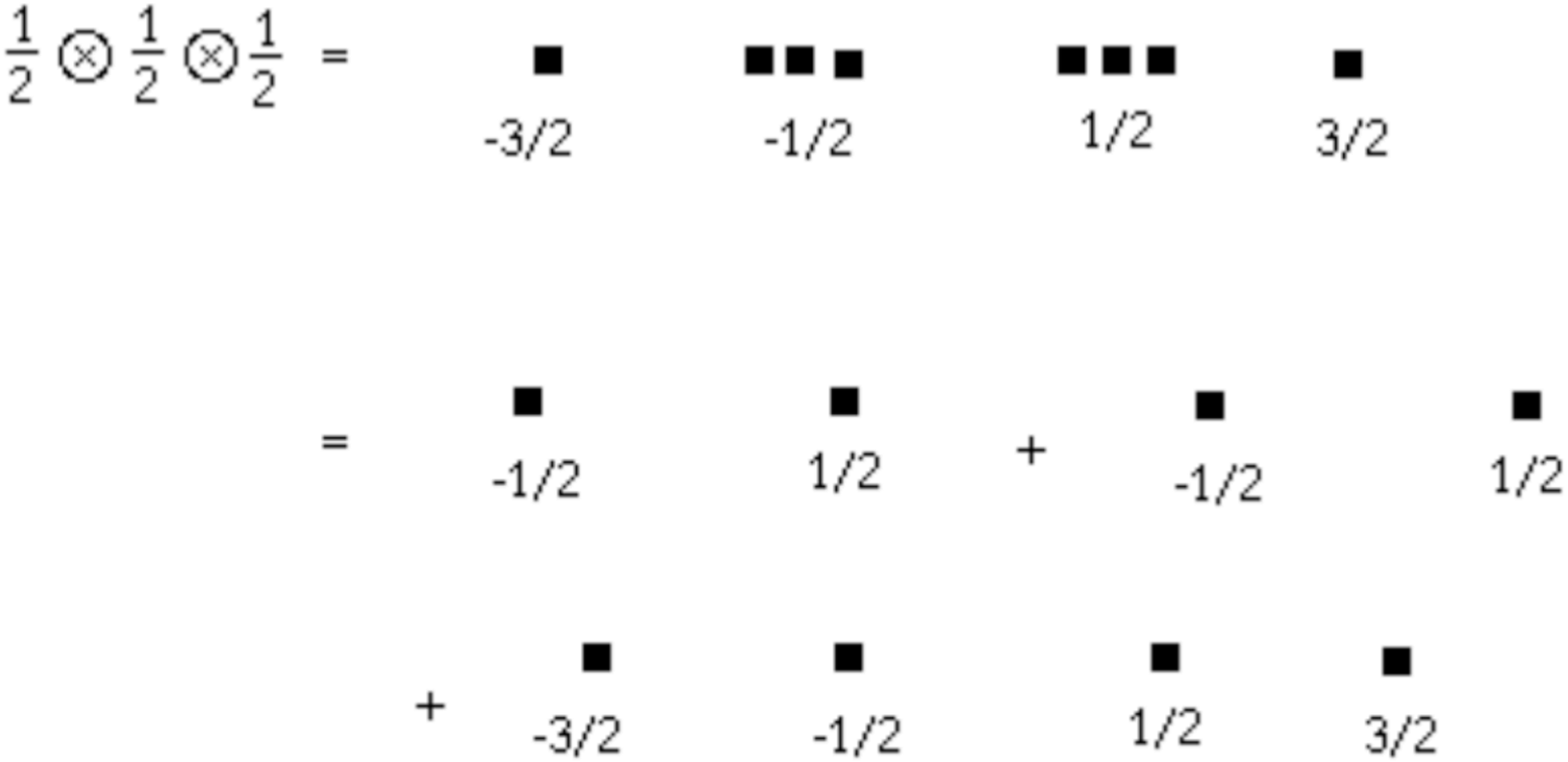
The superposed weight diagram picture looks like:

$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2}$



Note how multiple arrow tips require multiple weight diagrams in the next stage and multiple arrow tips at the end imply multiple states with that value of I_3.

Rearranging we have



which gives the result

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{3}{2}$$

Another way to think about it is to write

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = (0 \oplus 1) \otimes \frac{1}{2} = 0 \otimes \frac{1}{2} \oplus 1 \otimes \frac{1}{2}$$

$$0 \otimes \frac{1}{2} = \frac{1}{2} \quad , \quad 1 \otimes \frac{1}{2} = \frac{1}{2} \oplus \frac{3}{2}$$

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{3}{2}$$

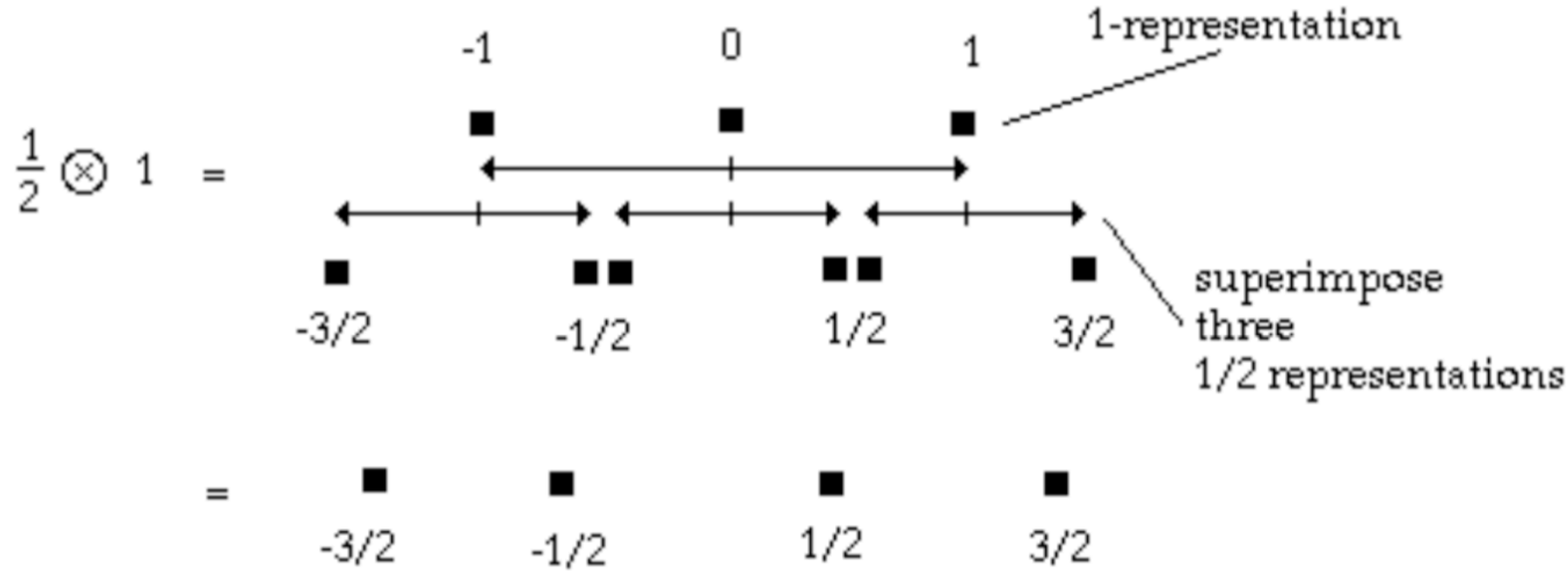
where we have used the fact that the 0-representation represents no additional states

$$0 \otimes \frac{1}{2} = \frac{1}{2}$$

and

$$1 \otimes \frac{1}{2} = \frac{1}{2} \oplus \frac{3}{2}$$

as can be seen from the weight diagrams below:



This will all reappear in a Quantum mechanics course because it is exactly the same as the angular momentum coupling rule (remember the homomorphism).

We have the general rule:

$$I_1 \otimes I_2 = |I_1 - I_2| \oplus |I_1 - I_2| + 1 \oplus ..... \oplus I_1 + I_2$$

Now if $SU(2)$ were the correct group for describing the real world, then all possible states (all known particles) should be generated from the $\frac{1}{2}$-representation (most fundamental building block), i.e., from $|p\rangle$ and $|n\rangle$ as the fundamental building blocks.

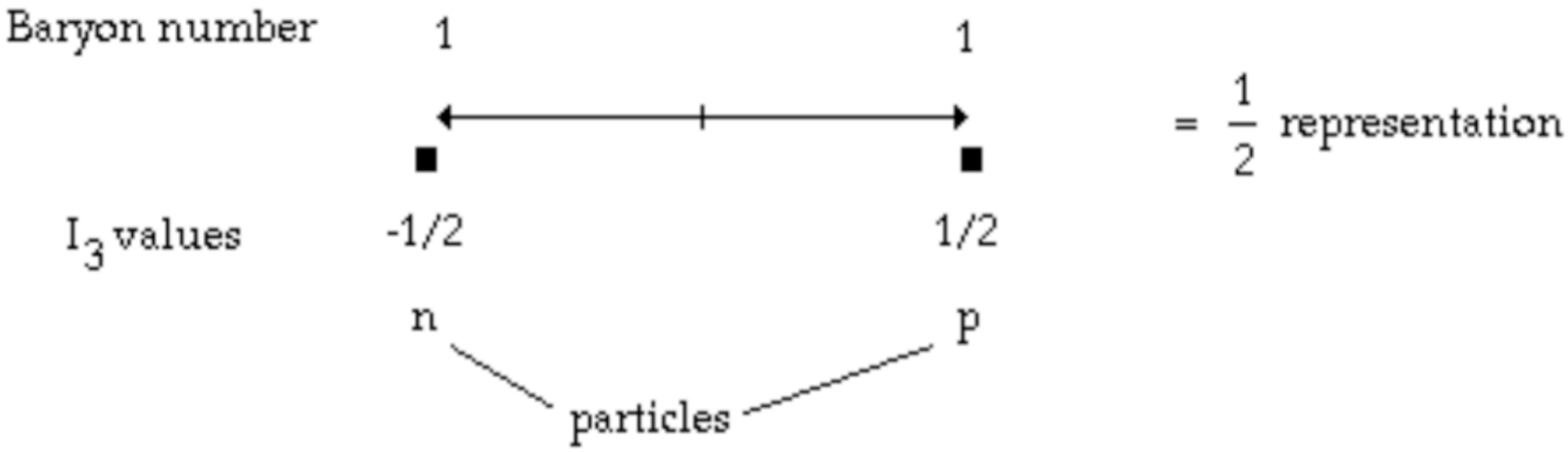
We know this is not possible, however, because:

1. we have not included any anti-baryons, which implies that we cannot have any states (particles) with baryon number $B = 0$.
2. we have not introduced strangeness (or hypercharge) so our states cannot represent the **real** world

Let us correct (1) first, within the context of $SU(2)$, and then attack (2), which will require that we look at $SU(3)$.

Let us now add particle labels to our weight diagrams.

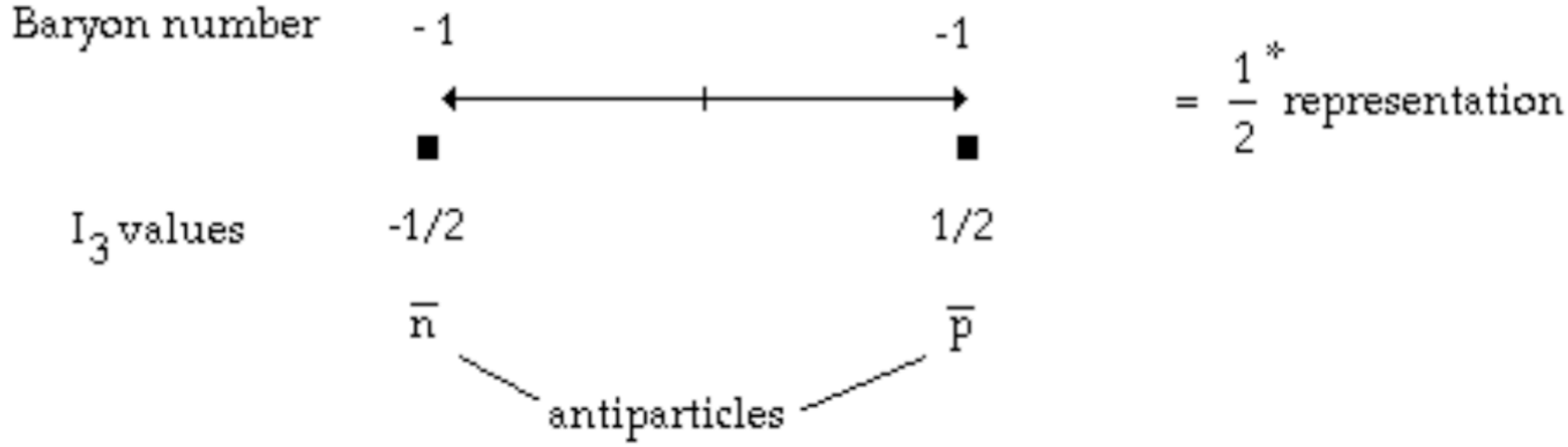
The weight diagram for the $\frac{1}{2}$-representation or as we now rename it, the **pn weight diagram** is given by



where we assumed Baryon number $= B = 1$ for each particle.

We also assume that Baryon number is additive.

We then define the $\frac{1}{2}^*$-representation by the weight diagram



where we assumed Baryon number $= B = -1$ for each antiparticle.

Now let us see the effect of this assumption on higher representations.

Remember

$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$$

Now we would have

$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1 = \blacksquare + \blacksquare \blacksquare \blacksquare$$

I_3	=	0	-1	0	1
B	=	2	2	2	2
state	=	| np-pn >	| nn >	| np+pn >	| pp >

Now consider

$$\frac{1}{2}^{*} \otimes \frac{1}{2} = 0 \oplus 1 =$$

I_3	=	0		-1	0	1
B	=	0		0	0	0
state	=	$\lvert p\bar{p}+n\bar{n}\rangle$		$\lvert n\bar{p}\rangle$	$\lvert p\bar{p}-n\bar{n}\rangle$	$\lvert p\bar{n}\rangle$

The isospin structure is the same as

$$\frac{1}{2} \otimes \frac{1}{2}$$

but $B = 0$ (these could be mesons!).

The original identifications were a "triplet" of mesons (π^+, π^0, π^-) and a "singlet" meson η^0.

The mesons would somehow be bound states made from the baryon-antibaryon pairs! It was the correct idea but the wrong baryons!

In order to include hypercharge Y or strangeness S into our structure, we must start with three basic states (no identification with any known particles will be attempted at this point).

We choose:

$$|q_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad , \quad |q_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad , \quad |q_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Since we will be working with vectors containing three elements and our operators will be 3×3 matrices, there will be $3^2 - 1 = 8$ independent matrices representing the generators of the transformations (this is the group $SU(3)$).

These 8 operators will :

(1) represent I_3

(2) represent Y

where we will want $[I_3, Y] = 0$ so that our states can be simultaneous eigenstates of both operators and hence our particles can be characterized by values of both quantum numbers.

(3) represent $|q_1\rangle \rightarrow |q_2\rangle$

(4) represent $|q_1\rangle \rightarrow |q_3\rangle$

(5) represent $|q_2\rangle \rightarrow |q_1\rangle$

(6) represent $|q_2\rangle \rightarrow |q_3\rangle$

(7) represent $|q_3\rangle \rightarrow |q_1\rangle$

(8) represent $|q_3\rangle \rightarrow |q_2\rangle$

which correspond to raising and lowering operators. I will now write down(just straightforward algebra) the shift operators, the isospin and hypercharge operators and a whole mess of commutators and state equations.

After that we will discuss their meanings.

Shift Operators

$$E_1 = \frac{1}{\sqrt{6}}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = E^+_{-1} \qquad E_2 = \frac{1}{\sqrt{6}}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = E^+_{-2} \qquad E_3 = \frac{1}{\sqrt{6}}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = E^+_{-3}$$

where

$$E_1|q_2\rangle = |q_1\rangle \quad , \quad E_2|q_3\rangle = |q_1\rangle \quad , \quad E_3|q_3\rangle = |q_2\rangle$$
$$E_{-1}|q_1\rangle = |q_2\rangle \quad , \quad E_{-2}|q_1\rangle = |q_3\rangle \quad , \quad E_{-3}|q_2\rangle = |q_3\rangle$$

Commutation Relations

$$[E_1, E_2] = [E_1, E_{-3}] = [E_2, E_3] = [E_{-1}, E_{-2}] = [E_{-1}, E_{-3}] = [E_{-2}, E_{-3}] = \mathbf{0}$$

$$[E_1, E_{-2}] = -\frac{1}{\sqrt{6}} E_{-3} \quad , \quad [E_1, E_3] = \frac{1}{\sqrt{6}} E_2 \quad , \quad [E_2, E_{-3}] = \frac{1}{\sqrt{6}} E_1$$

$$[E_{-1}, E_2] = \frac{1}{\sqrt{6}} E_3 \quad , \quad [E_{-1}, E_{-3}] = -\frac{1}{\sqrt{6}} E_{-2} \quad , \quad [E_{-2}, E_3] = -\frac{1}{\sqrt{6}} E_{-1}$$

and

$$[E_1, E_{-1}] = \frac{1}{\sqrt{3}} H_1 \quad , \quad [E_2, E_{-2}] = \frac{1}{2\sqrt{3}} H_1 + \frac{1}{2} H_2$$

$$[E_3, E_{-3}] = -\frac{1}{2\sqrt{3}} H_1 + \frac{1}{2} H_2$$

where

$$H_1 = \frac{1}{2\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad , \quad H_2 = \frac{1}{6}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

and finally

$$[H_1, E_1] = \frac{1}{\sqrt{3}} E_1 \quad , \quad [H_1, E_2] = \frac{1}{2\sqrt{3}} E_2 \quad , \quad [H_1, E_3] = -\frac{1}{2\sqrt{3}} E_3$$

$$[H_2, E_1] = 0 \quad , \quad [H_2, E_2] = \frac{1}{2} E_2 \quad , \quad [H_2, E_3] = \frac{1}{2} E_3 \quad , \quad [H_1, H_2] = 0$$

It is clear from the commutators that we have a closed algebra, i.e., all of the commutators among the 8 operators only involve the same 8 operators.

We note that $|q_1\rangle, |q_2\rangle, |q_3\rangle$ are eigenstates of both H_1 and H_2 simultaneously, which suggests that we will be able to use H_1 and H_2 to represent I_3 and Y.

Now we have

$$H_1 |q_1\rangle = \frac{1}{2\sqrt{3}} |q_1\rangle \ , \ H_1 |q_2\rangle = -\frac{1}{2\sqrt{3}} |q_2\rangle \ , \ H_1 |q_3\rangle = 0$$

$$H_2 |q_1\rangle = \frac{1}{6} |q_1\rangle \ , \ H_2 |q_2\rangle = \frac{1}{6} |q_2\rangle \ , \ H_2 |q_3\rangle = -\frac{1}{3} |q_3\rangle$$

Thus, if we define $I_3 = \sqrt{3} H_1$, $Y = 2H_2$ we get

	I_3	Y
q_1	1/2	1/3
q_2	-1/2	1/3
q_3	0	-2/3

Construction of Representations

We define eigenstates $|m_1, m_2\rangle$ where we assume

$$H_1 |m_1, m_2\rangle = m_1 |m_1, m_2\rangle \quad , \quad H_2 |m_1, m_2\rangle = m_2 |m_1, m_2\rangle$$

Now $\sqrt{6}E_1, \sqrt{6}E_{-1}, 2\sqrt{3}H_1$ obey the same commutation relations as τ_+, τ_-, τ_3 – in fact, they form a sub-algebra of the closed algebra of the 8 operators.

Therefore, we construct the operator

$$I^2 = 3(E_1 E_{-1} + E_{-1} E_1) + 3H_1^2$$

in analogy to

$$\Gamma = \frac{1}{2}(\tau_+ \tau_- + \tau_- \tau_+) + \frac{1}{4}\tau_3^2$$

Since $[I^2, H_1] = [I^2, H_2] = 0$ the states $|m_1, m_2\rangle$ are also eigenstates of I^2 or

$$I^2 |m_1, m_2, i\rangle = i(i+1) |m_1, m_2, i\rangle$$

We note that

$$[I^2, E_{\pm 1}] = 0$$

but

$$[I^2, E_{\pm 2}] \neq 0 \ , \ [I^2, E_{\pm 3}] \neq 0$$

Which implies that I^2 is **not** an **invariant** operator or that **it can change** within a representation.

This suggests the following possible picture:

where each line is the same as in our earlier discussion ($I^2 =$ constant), but there are many different lines (values of I^2) in the representation.

It is not difficult to deduce the following table:

operator/effect	Δm_1	Δm_2
E_1	$1/\sqrt{3}$	0
E_{-1}	$-1/\sqrt{3}$	0
E_2	$1/2\sqrt{3}$	1/2
E_{-2}	$-1/2\sqrt{3}$	-1/2
E_3	$-1/2\sqrt{3}$	1/2
E_{-3}	$1/2\sqrt{3}$	-1/2

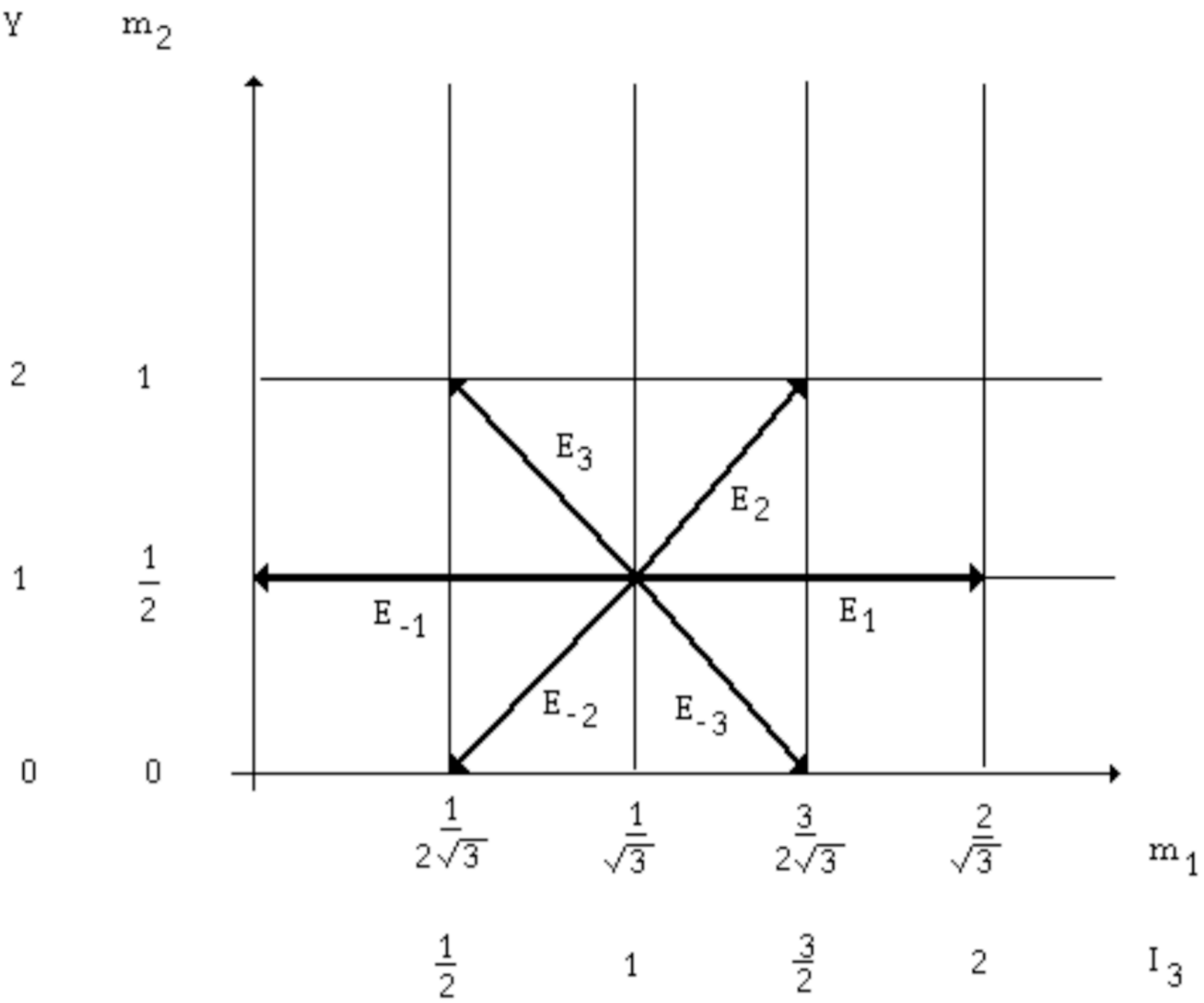
This table implies relation like:

$$H_1 E_1 \left|m_1, m_2\right\rangle = E_1 \left(H_1 + \frac{1}{\sqrt{3}}\right) \left|m_1, m_2\right\rangle = \left(m_1 + \frac{1}{\sqrt{3}}\right) E_1 \left|m_1, m_2\right\rangle$$

or

$$E_1 \left|m_1, m_2\right\rangle = \text{constant} \left|m_1 + \frac{1}{\sqrt{3}}, m_2\right\rangle$$

Graphically, this table is represented by the diagram below.

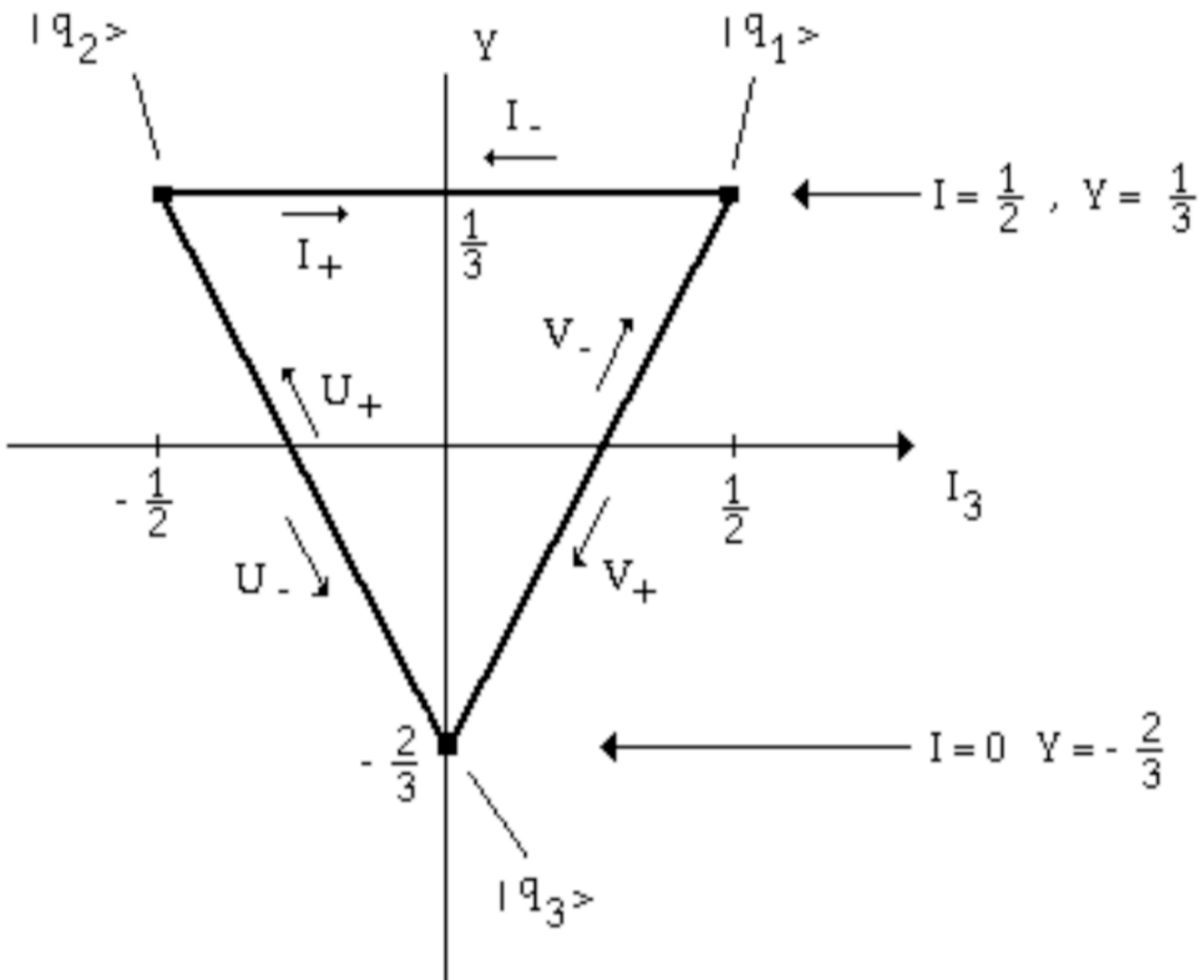


Let us now represent our states on a $Y - I_3$ diagram and indicate the effect of the operators

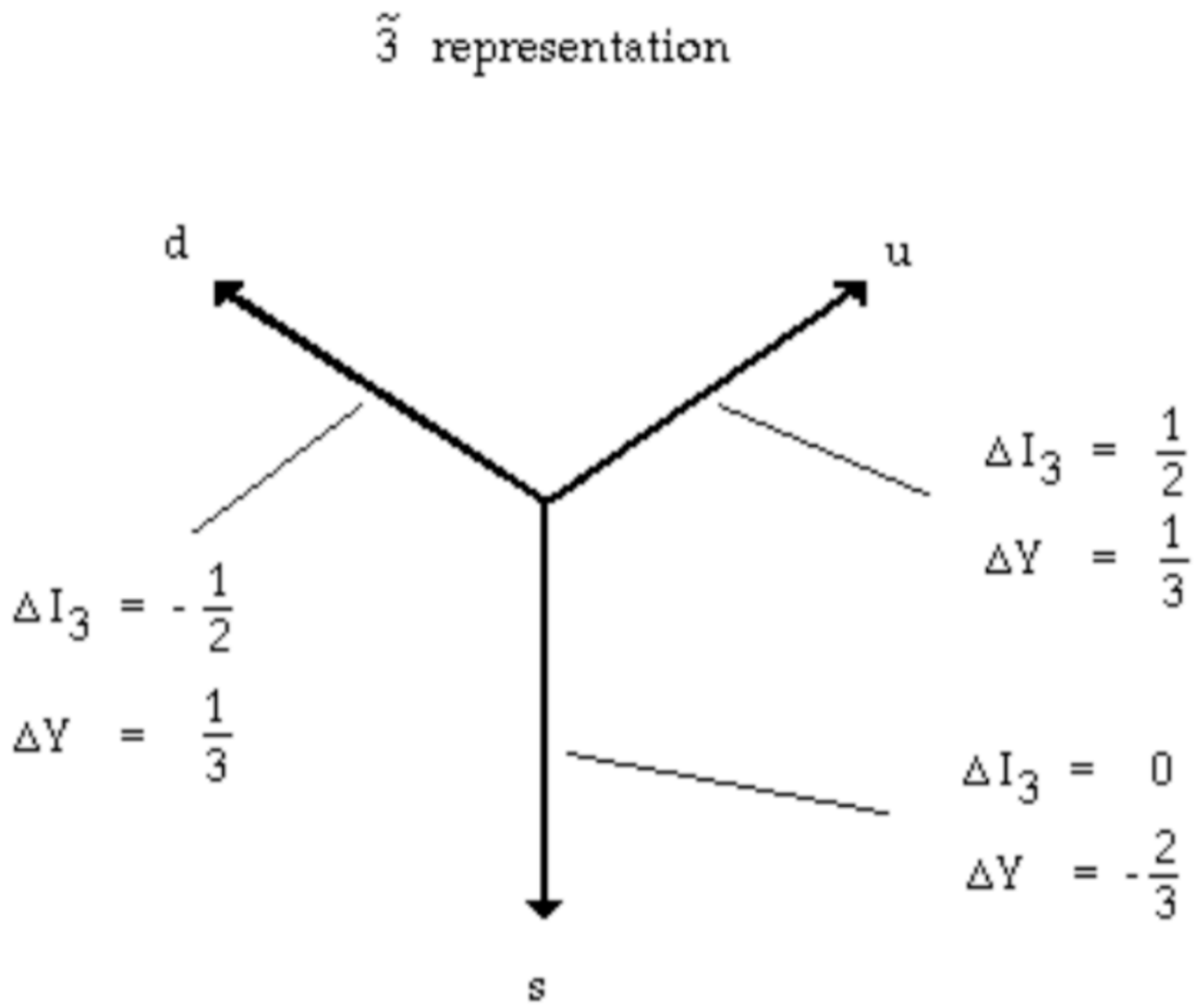
$$I_\pm = E_{\pm 1} \qquad (\Delta I_3 = \pm 1, \Delta Y = 0)$$
$$V_\pm = E_{\pm 2} \qquad (\Delta I_3 = \pm 1/2, \Delta Y = \pm 1)$$
$$U_\pm = E_{\pm 3} \qquad (\Delta I_3 = \pm 1/2, \Delta Y = \pm 1)$$

Remember that $I_3 = \sqrt{3} H_1$ and $Y = 2 H_2$.

This gives the simplest representation of SU(3):



and suggests a weight diagram as shown below:



We have other related quantum numbers:

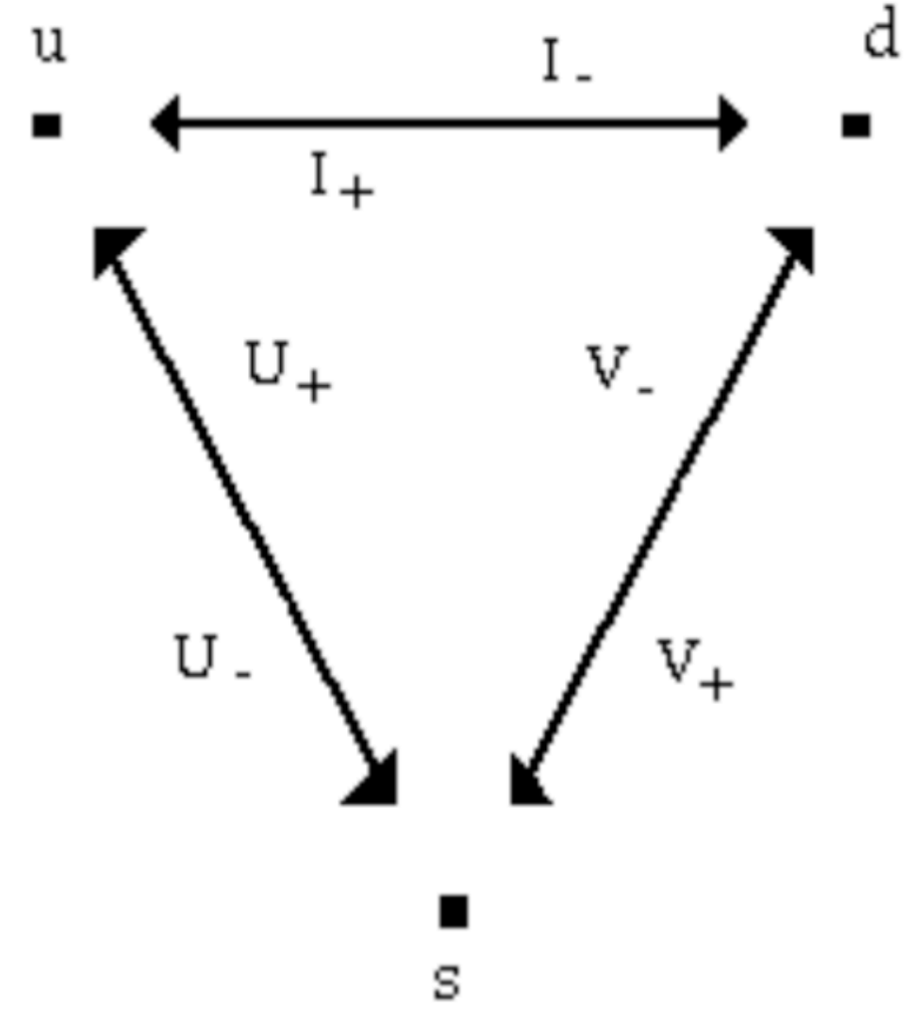
$$Q(\text{charge}) = I_3 + \frac{Y}{2} \quad , \quad Y = B + S$$

This leads to the table below:

Quark	I	I_3	Y	Q	B	S
u	1/2	1/2	1/3	2/3	1/3	0
d	1/2	-1/2	1/3	-1/3	1/3	0
s	0	0	-2/3	-1/3	1/3	-1

The baryon number of each of these states or particles is $B = 1/3$ and they represent the original three quarks.....**up, down and strange**.

Another way of visualizing the shifts (shift operators) is the diagram below:

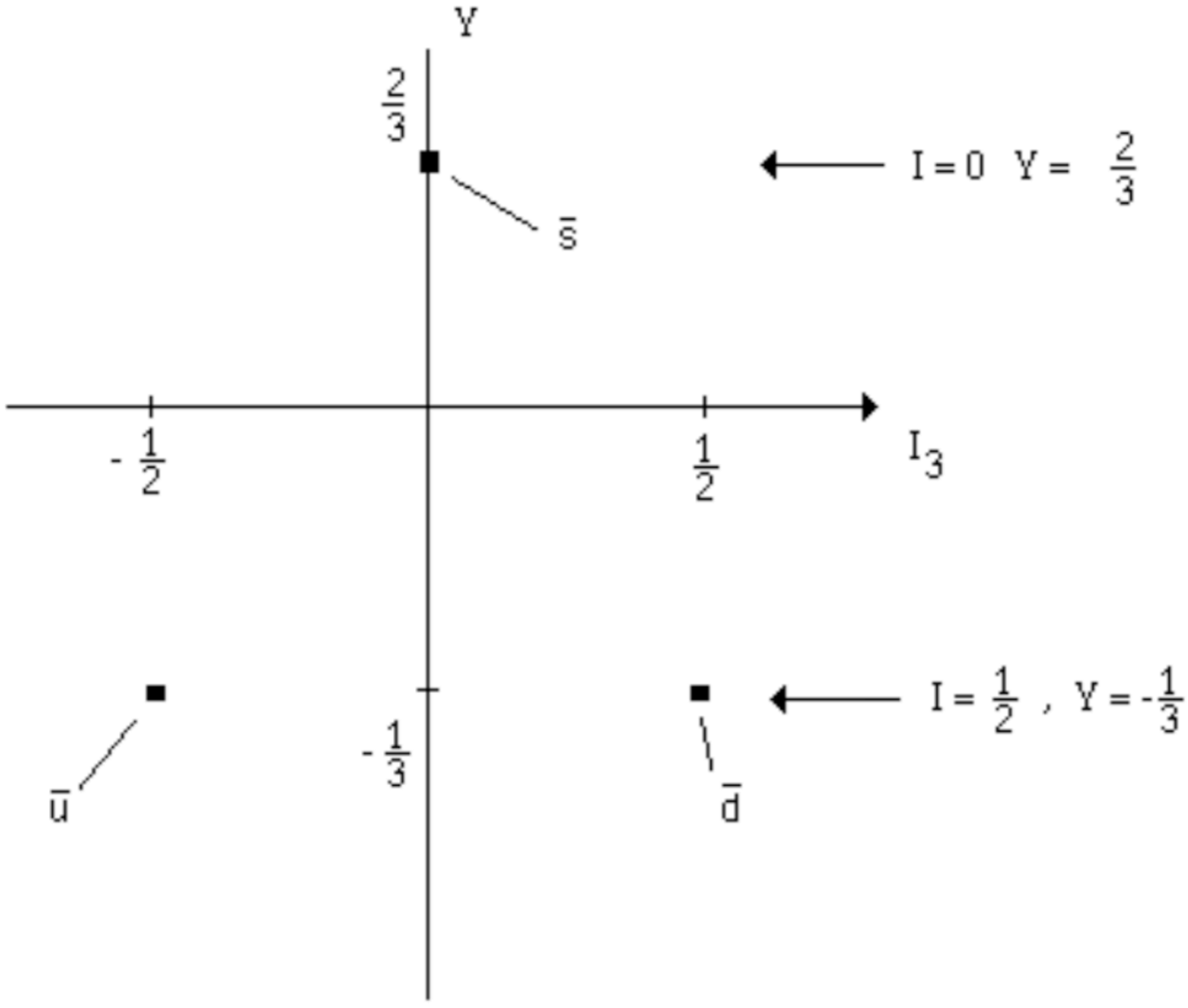


These shift operator transform quarks into each other.

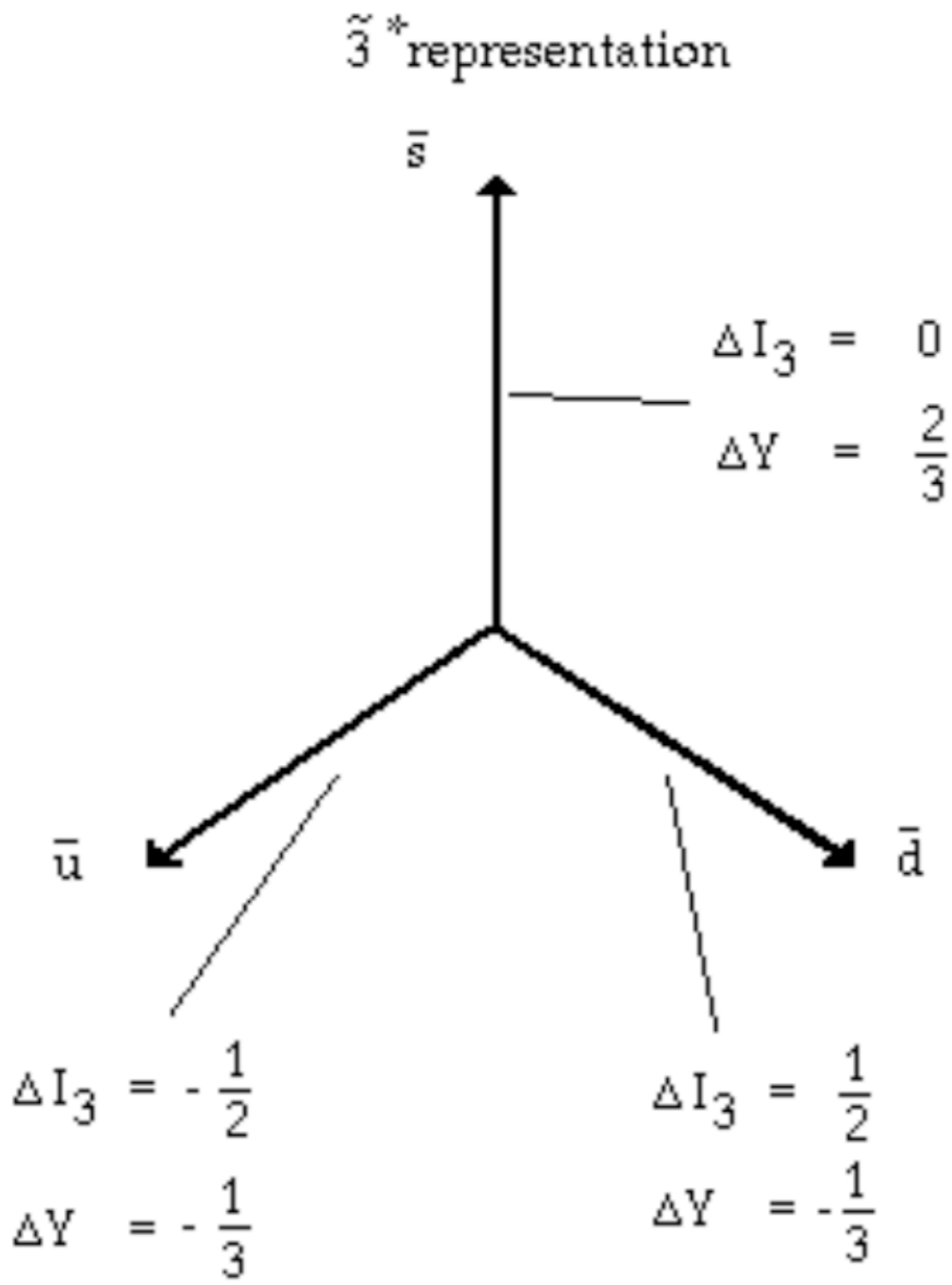
They will turn out to represent **gluons** later on.

It turns out that there exists an equivalent simple representation.

It is shown below:



It corresponds to the weight diagram below:



It is the $\tilde{3}^*$ representation and the particles or states are the anti-quarks.

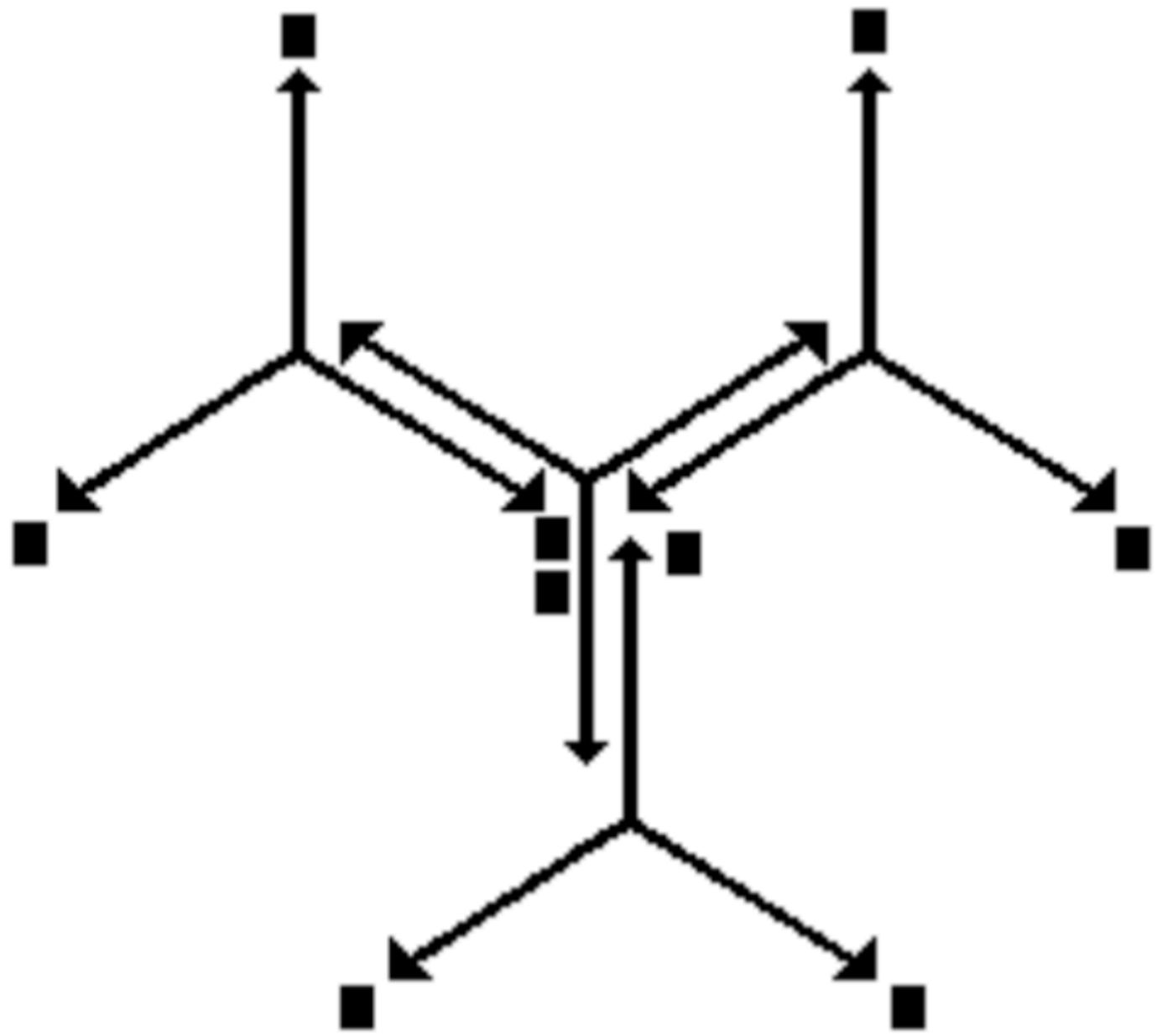
The corresponding table looks like:

Quark	I	I_3	Y	Q	B	S
anti-u=ū	1/2	-1/2	-1/3	-2/3	-1/3	0
anti-d=đ	1/2	1/2	-1/3	1/3	-1/3	0
anti- s=ŝ	0	0	2/3	1/3	-1/3	1

We now use these simplest representations or simplest weight diagrams to build higher representations.

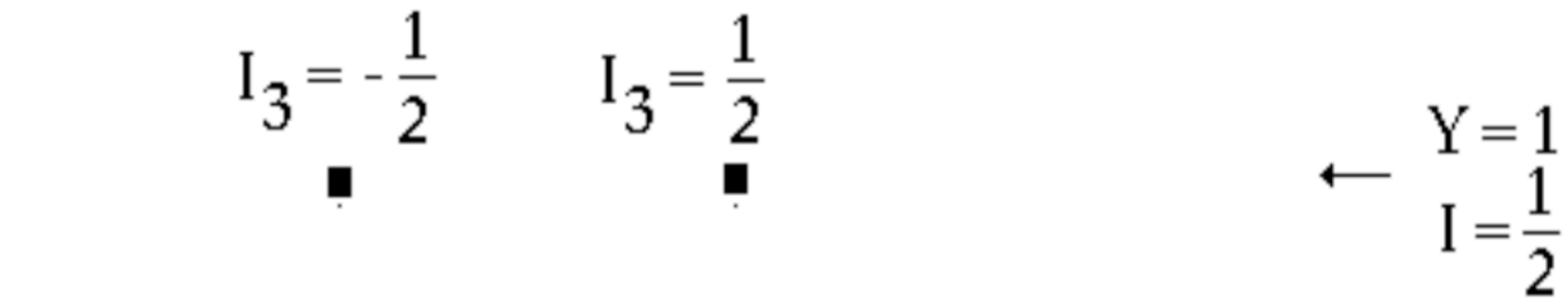
We note that $\tilde{3} \otimes \tilde{3}^*$ will have $B = 0$ (quark + anti-quark) and should represent **mesons** and $\tilde{3} \otimes \tilde{3} \otimes \tilde{3}$ will have $B = 1$ and should represent **baryons**.

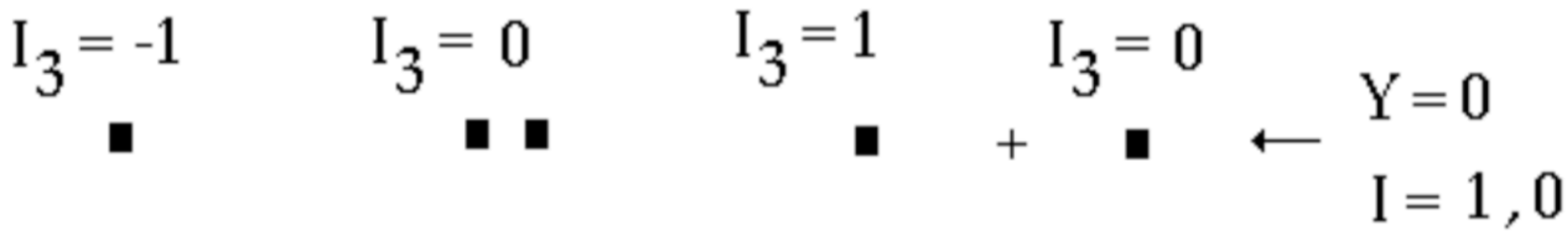
So we now consider $\tilde{3} \otimes \tilde{3}^*$ using the weight diagrams as shown below:

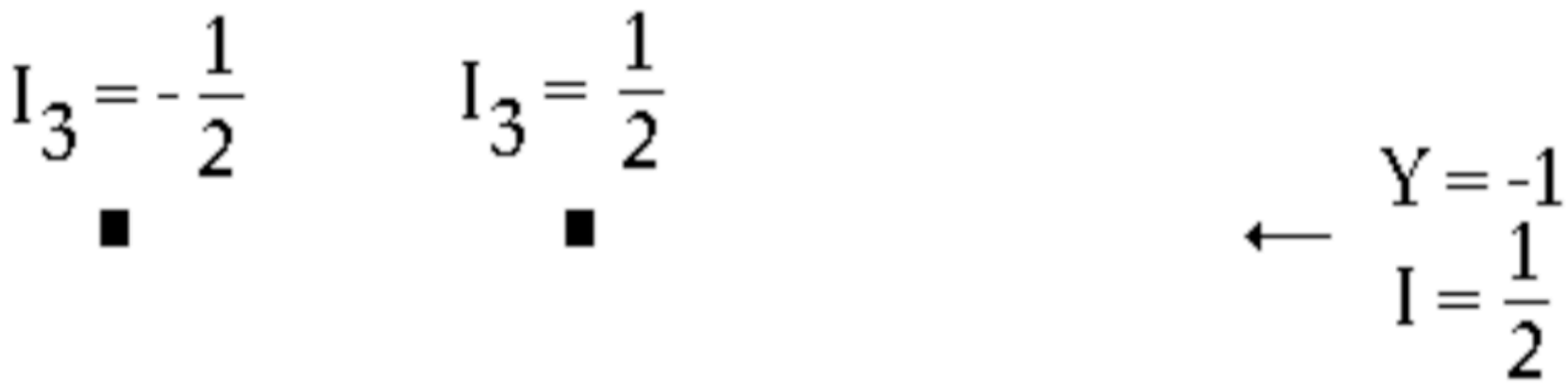


where the black dots represent the final states of the new (higher) representations.

Looking only the states we have







The I-values associated with a line are determined by the multiplicity of a line (remember each line is a different I-value).

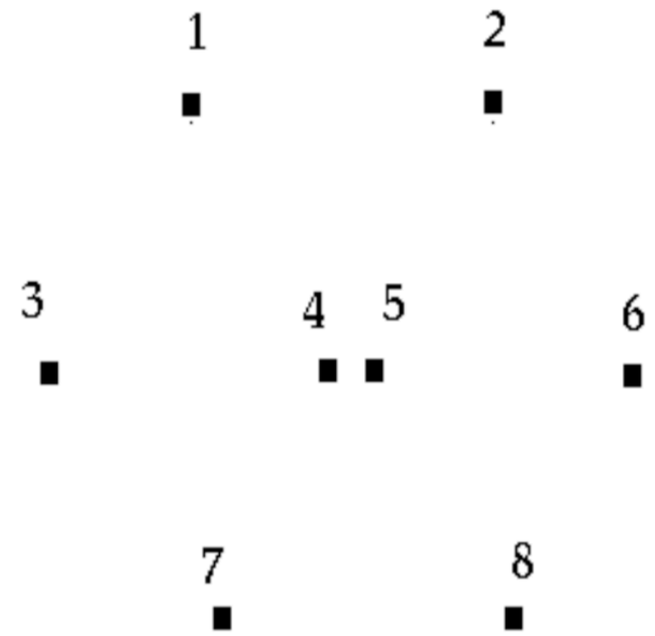
Note that there were three(3) final states at the same point.

Symbolically we have

$$\tilde{3} \otimes \tilde{3}^* = \tilde{8} \oplus \tilde{1} = \quad \text{octet} + \text{singlet}$$

We now look more carefully at the OCTET representation.

If we label the states as



We get the table

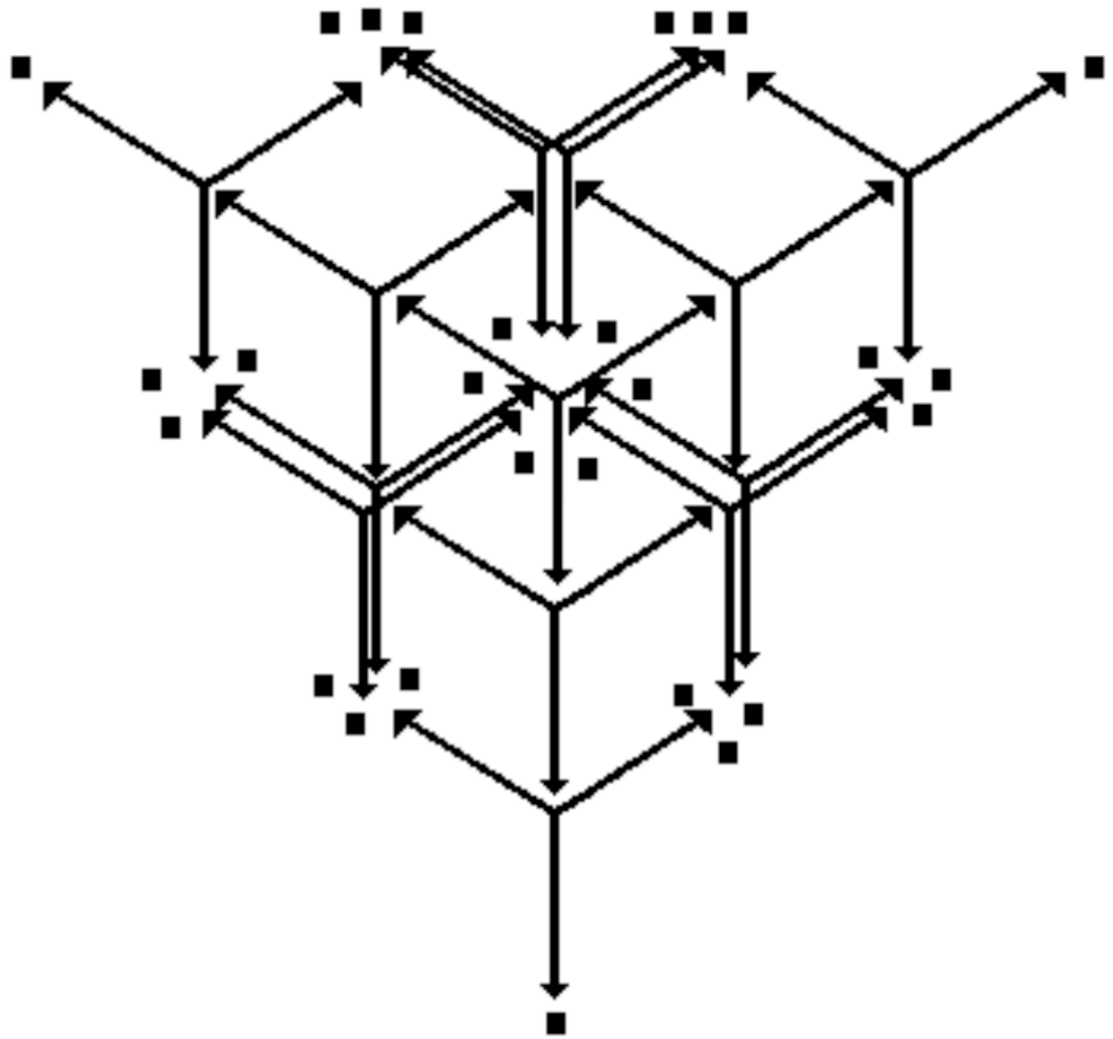
#	quarks	I	I3	Y	Q	B	S	meson
1	dŝ	1/2	-1/2	1	0	0	1	K^0
2	uŝ	1/2	1/2	1	1	0	1	K^+
3	dū	1	-1	0	-1	0	0	π^-
4	d**đ**-uū	1	0	0	0	0	0	π^0
5	d**đ**+uū-2sŝ	0	0	0	0	0	0	η^0
6	-u**đ**	1	1	0	1	0	0	π^+
7	sū	1/2	-1/2	-1	-1	0	-1	K^-
8	s**đ**	1/2	1/2	-1	0	0	-1	K^0-bar

Our $SU(3)$ scheme has produced the known mesons (including the strange particles) as linear combination of quarks and anti-quarks.

Let us push it even further and consider the baryon states.

This means we look at the $\tilde{3} \otimes \tilde{3} \otimes \tilde{3}$ representation.

Using weight diagrams we get



These states separate as follows:

The particle identifications are given in the table below (only partly filled in):

#	States	I	I3	Y	Q	B	S	Particle
1	ddd	3/2	-3/2	1	-1	1	0	Δ^-
2	udd+dud+ddu	3/2	-1/2	1	0	1	0	Δ^0
3	duu+udu+uud	3/2	1/2	1	1	1	0	Δ^+
4	uuu	3/2	3/2	1	2	1	0	Δ^{++}
5	sdd+dsd+dds	1	-1	0	-1	1	-1	Σ^{*-}
6	sdu+dsu+dus +sud+usd+uds	1	0	0	0	1	-1	Σ^{*0}
7	suu+usu+uus	1	1	0	1	1	-1	Σ^{*+}
8	dss_sds+ssd	1/2	-1/2	-1	-1	1	-2	Ξ^{*-}
9	uss+sus+ssu	1/2	1/2	-1	0	1	-2	Ξ^{*0}
10	sss	0	0	-2	-1	1	-3	Ω^-
11	d[ud]	----	----	----	----	----	----	----
12	u[ud]	----	----	----	----	----	----	----
13	d[ds]	----	----	----	----	----	----	----
14	u[ds]+d[su]-2s[ud]	----	----	----	----	----	----	----
15	u[ds]-d[su]	----	----	----	----	----	----	----
16	u[su]	----	----	----	----	----	----	----
17	s[ds]	----	----	----	----	----	----	----
18	s[su]	----	----	----	----	----	----	----
19	----	----	----	----	----	----	----	----
20	uud+udu-2duu	----	----	----	----	----	----	----
----	----	----	----	----	----	----	----	----
27	u[ds]+d[su]+s[ud]	----	----	----	----	----	----	----

Consider the DECUPLET representation.

All of the particles had been previously observed except for the Ω^-, which we will discuss further later.

We end up with two OCTET representations.The first is antisymmetric in the second and third quarks and the second is symmetric in the second and third quarks. They are completely equivalent representations within $SU(3)$ and represent the same physical particles.

The Mass Formula

We will simply state and discuss the mass formula here. The most general form for the mass formula is given by (from group theory arguments):

$$M = A + BY + C\left(I(I+1) - \frac{1}{4}Y^2\right) + DI_3$$

where the A, B, and C terms represent the average mass (within a row) and the D term represents electromagnetic splittings.

Some OCTET experimental data implies that:

$$M_8 = 1109.80 - 189.83Y + 41.49\left(I(I+1) - \frac{1}{4}Y^2\right) + DI_3$$

which gave the following table(decades ago - it is even better agreement now) :

particle	experiment	formula
n	939.5	943.2
p	938.2	938.3
Λ^0	1115.4	1109.8
Σ^-	1189.4	1190.3
Σ^0	1193.2	1192.8
Σ^+	1197.6	1195.2
Ξ^-	1316	1317.9
Ξ^0	1321	1322.8

This is an average error of only 0.19%.

The experimental data in the table below was also available.

particle	experiment
Δ	1238
Σ^*	1385
Ξ^*	1530

As we said above, the Ω^- particle had not yet been discovered.

This data gives the DECUPLET mass formula below:

$$M_{10} = 1501.8 - 58.5Y - 58.4\left(I(I+1) - \frac{1}{4}Y^2\right)$$

The mass formula then allows us to predict the mass of the Ω^- particle ($SU(3)$ also predicts all of the other quantum numbers). The prediction is $M_{\Omega^-} = 1677$ (1685 was observed or about a 0.5% error (even better agreement now)).

Introduction of Color We now know there are 6 quarks.

u(up),d(down),s(strange),c(charm),b(bottom),t(top)

Let me discuss a few of the reasons why the other quarks had to exist.

A basic problem with the quark model of hadrons is with the wave function antisymmetry.

Consider the Ω^- state.

It is strangeness $S = -3$ baryon with isospin $I = 3/2$.

In the 3 quark model we have been discussing

$$\left|\Omega^-\right\rangle = |s\rangle\,|s\rangle\,|s\rangle$$

Each of these quarks has the following states

$$|s\rangle = \left|\frac{1}{2},\frac{1}{2}\right\rangle_{spin}\left|\frac{1}{2},\frac{1}{2}\right\rangle_{isospin}\left|B=\frac{1}{3},S=-1\right\rangle$$

and, thus, the final state is **symmetric** in all of its quantum numbers (the orbital angular momentum states are also symmetric when one solves the bound state problems), which violates the Pauli Principle for fermions - they must have **antisymmetric** states.

The solution to the problem was to generalize the definition of the quarks such that each quarks can have one of three colors (**r=red, b=blue, g=green**) or

$$\begin{pmatrix} u \\ d \\ s \end{pmatrix} = \begin{pmatrix} u_r & u_b & u_g \\ d_r & d_b & d_g \\ s_r & s_b & s_g \end{pmatrix}$$

The associated observable is called **flavor**.

Quarks now are assumed to come in three flavors, namely, red, blue and green.

The problem with the Ω^- state is fixed by assuming that it is completely antisymmetric in the flavor space or we write it as

$$\left|\Omega^{-}\right\rangle = |s_r\rangle\,|s_b\rangle\,|s_g\rangle - |s_r\rangle\,|s_g\rangle\,|s_b\rangle - |s_b\rangle\,|s_r\rangle\,|s_g\rangle + |s_b\rangle\,|s_g\rangle\,|s_r\rangle$$
$$+\,|s_g\rangle\,|s_r\rangle\,|s_b\rangle - |s_g\rangle\,|s_b\rangle\,|s_r\rangle$$

It is equal parts red, green and blue!

Another type of problem was that certain reactions were not occurring when SU(3) said they were allowed. This usually signals that an extra (new) quantum number is needed to prevent the reaction.

The new quantum number would have a new conservation law that would be violated if the reaction occurred and hence it is disallowed.

The new quantum number introduced was **charm**. In the quark model this is treated as the appearance of a new quark.

I will delineate only the starting point of this discussion below. It leads to the formalism of $SU(4)$ if we carried out the same steps as we did with $SU(3)$.

Quark states:

$$|u\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad , \quad |d\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad , \quad |s\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad , \quad |c\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

We now have

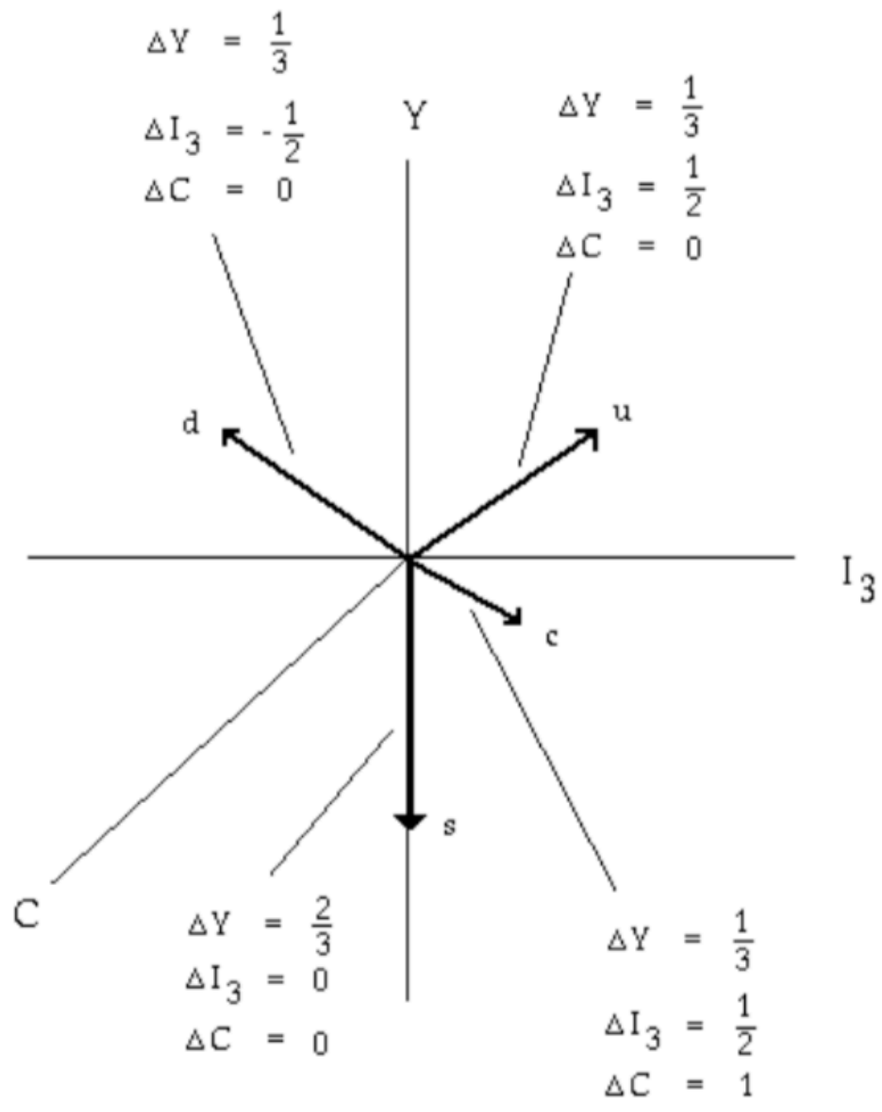
$$Q = I_3 + \frac{B + S + C}{2} \quad , \quad C = \text{ charm}$$

The four quarks then have quantum numbers

Quark	Y	Q	B	S	C
u	1/3	2/3	1/3	0	0
d	1/3	-1/3	1/3	0	0
s	-2/3	-1/3	1/3	-1	0
c	1/3	2/3	1/3	0	1

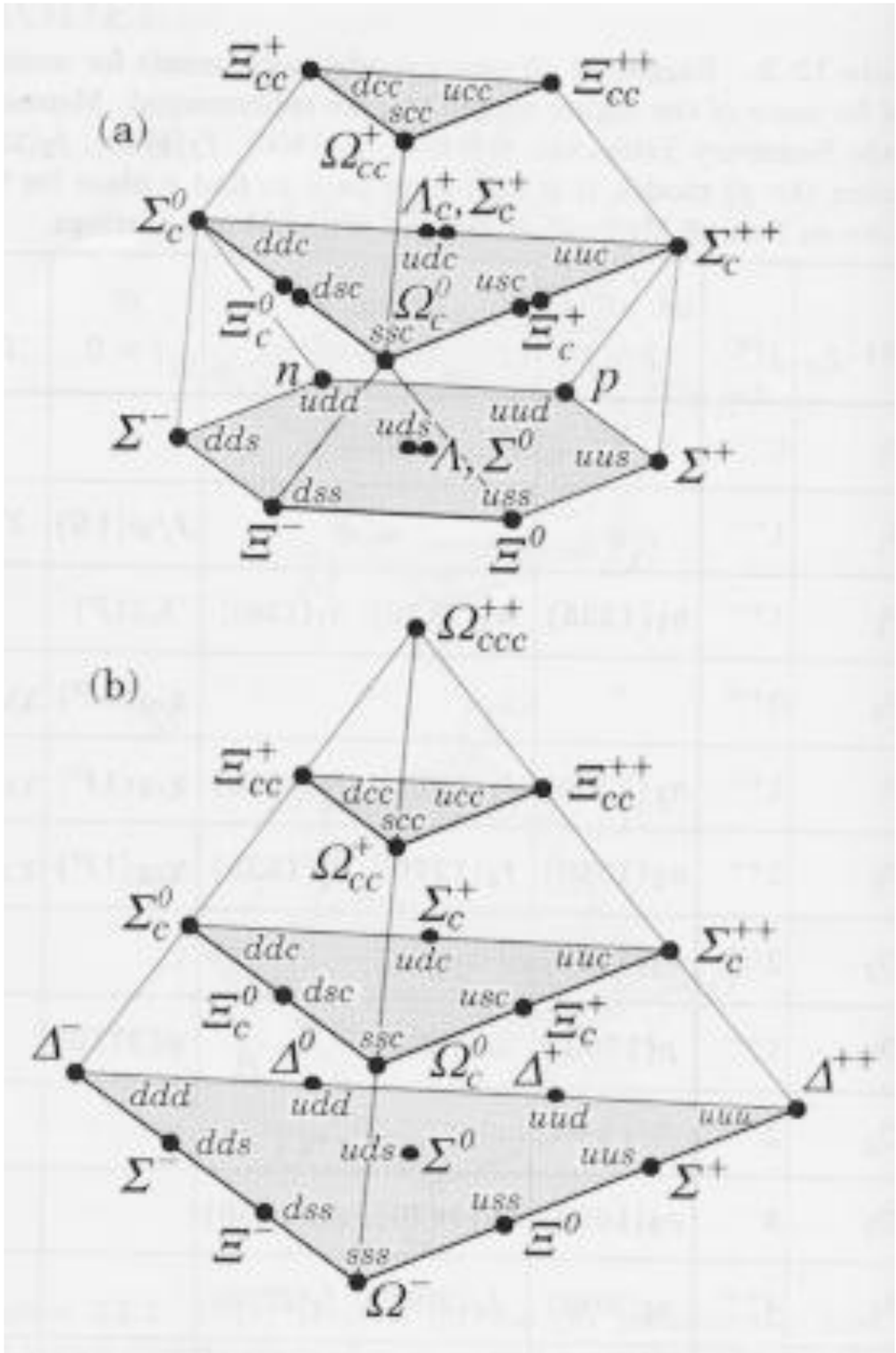
The charm quark is the same as the up quark except for the charm value.

The corresponding lowest representation weight diagram is



This is the $\tilde{4}$ representation.

The typical particle diagrams (now in 3 dimensions) look like



That concludes the discussion of the Eightfold Way and we end the course.