Hilbert Space

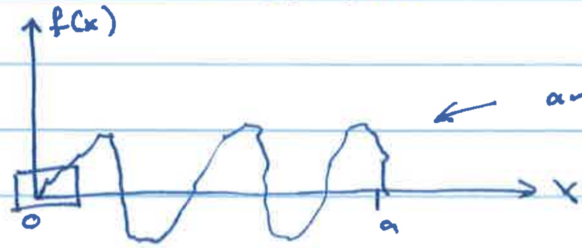
In cartesian coordinates, a vector is a set of components (v_x, v_y, v_z). Any vector can be written in terms of the 3 unit vectors or the basis set for this space:

$$\vec{V} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = v_x \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + v_y \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + v_z \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$= v_x \hat{i} + v_y \hat{j} + v_z \hat{k}$$

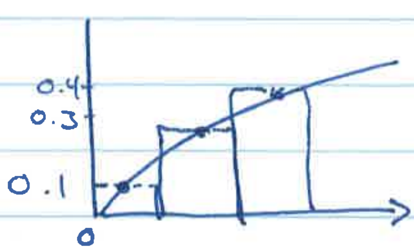
$\hat{i}, \hat{j}$, and $\hat{k}$ form a complete basis for 3D space. They span the space.

Now, we're going to expand our ideas about vectors. $\hat{i}\ \hat{j}\ \&\ \hat{k}$ were objects that we use to talk about a location in space. How might we describe a function? Consider



an arbitrary function f(x)

We could describe f(x) as a vector where each element was a small chunk of the line along x:



$$f(x) = 0.1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ \vdots \end{pmatrix} + 0.3 \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ \vdots \end{pmatrix} + 0.4 \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ \vdots \end{pmatrix} + \cdots$$

This isn't very efficient or sensible.

We would need to know Δx to describe the function, and if we change Δx (i.e. for a rapidly varying function) we have to change all of our coefficients

However, we could also write $f(x)$ in terms of other functions:

$$f(x) = 0.1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} + 0.2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} + 0.1 \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix} + \ldots$$

this represents $\sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}$ | represents $\sqrt{\frac{2}{a}} \sin \frac{2\pi x}{a}$ | represents $\sqrt{\frac{2}{a}} \sin \frac{3\pi x}{a}$

A <u>Hilbert space</u> is a function space where each function is treated as an <u>independent</u> <u>vector</u>.

$$f(x) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \leftarrow$$ expansion of $f(x)$ in the basis <u>functions</u>

$$= \sum_{n=1}^{\infty} c_n \, |n\rangle$$

c_n ← coefficients that describe $f(x)$ in this particular space

I picked $|n\rangle = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$ for a few reasons

- All of these functions $\rightarrow 0$ at $x = 0$ & $x = a$

$\therefore$ All $f(x)$ we can represent in this space also do this.

Now, vector spaces have dot products:

$$\vec{V} \cdot \vec{u} = V_x u_x + V_y u_y + V_z u_z = \sum_{i=x,y,z} V_i u_i$$

In a Hilbert space, we do something similar:

$$\int_0^a f^*(x) \cdot g(x)\, dx$$ ← doesn't look like a vector product...

$$f^*(x) = \sum_{n=1}^{\infty} c_n^* \langle n|$$ ← complex conjugate of basis function n

← complex conjugate of coefficients

$$g(x) = \sum_{m=1}^{\infty} g_m |m\rangle$$ ← g is a different function so the coefficients are different

$$\int_0^a f^*(x) \cdot g(x)\, dx = \int_0^a \left(\sum_{n=1}^{\infty} c_n^* \langle n|\right)\left(\sum_{m=1}^{\infty} g_m |m\rangle\right) dx$$

$$= \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} c_n^* g_m \int_0^a \langle n|m\rangle\, dx$$

The functions $\sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}$ & $\sqrt{\frac{2}{a}} \sin\frac{m\pi x}{a}$ have the neat property:

$$\int_0^a \langle n|m\rangle\, dx = \frac{2}{a} \int_0^a \sin\frac{n\pi x}{a} \sin\frac{m\pi x}{a}\, dx$$

$$= \begin{cases} 1 & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases}$$

$\therefore$

$$\int_0^a f^*(x)\, g(x)\, dx = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} c_n^* g_m \delta_{nm}$$

Kronecker $\delta_{nm} = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases}$

When the basis functions we use have this property, we call them orthogonal functions

$$\int f^*(x)\, g(x)\, dx = \sum_{n=1}^{\infty} c_n^* g_n$$

massively complicated integral

just like a dot product (and very simple)

Lot's of good examples of Hilbert spaces

$|n\rangle = e^{2\pi i n\theta}$ ← Fourier transform used in NMR, IR, Mass spectrometry

Orthogonal Polynomials

Consider the following set of functions:

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

$P_3(x) = \frac{1}{2}(5x^3 - 3x)$ $\quad$ $P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)$

Note a few things about them:

- In the range $-1 \le x \le 1$, each $P_n(x)$ function has exactly n zeros.

- When n is even, P_n has even symmetry around $x = 0$, and when n is <u>odd</u>, P_n has <u>odd</u> symmetry

- These functions are the first 5 in a series called <u>Legendre</u> Polynomials. They are orthogonal on the interval $-1 \le x \le 1$

$$\therefore \int_{-1}^{1} P_3(x) P_1(x)\,dx = \frac{1}{2}\int_{-1}^{1}(5x^3 - 3x)x\,dx$$

$$= \frac{1}{2}\left[\int_{-1}^{1} 5x^4\,dx - \int_{-1}^{1} 3x^2\,dx\right]$$

$$= \frac{1}{2}\left[x^5 - x^3\right]_{-1}^{1}$$

$$= \frac{1}{2}\left[1 - 1 - (-1 + 1)\right] = 0$$

In general:

$$\int_{-1}^{1} P_n(x) P_m(x)\,dx = 0 \quad \text{when } n \ne m$$

- They <u>aren't</u> normalized:

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

so:

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

Kronecker δ

- <u>Any</u> function on the interval $-1 \le x \le 1$ can be written in terms of these functions:

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

This is called a Fourier-Legendre series.

If we know $f(x)$, we can get the a_n values (or <u>vector components</u>) by doing integrals:

$$\int_{-1}^{1} f(x)\, P_m(x)\, dx = \int_{-1}^{1} \left(\sum_{n=0}^{\infty} a_n P_n(x) \right) P_m(x)\, dx$$

$$= \sum_{n=0}^{\infty} a_n \int_{-1}^{1} P_n(x)\, P_m(x)\, dx$$

$$= \sum_{n=0}^{\infty} a_n \frac{2}{2n+1}\, \delta_{nm}$$

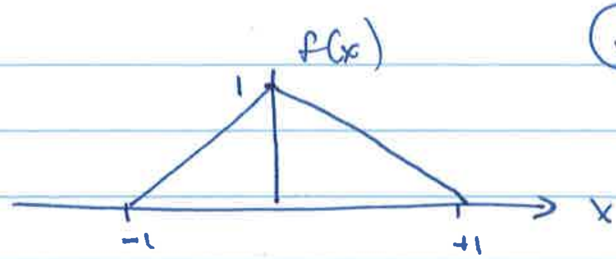
only 1 when $n=m$

$$= \frac{2a_m}{2m+1}$$

So, in general

$$a_m = \frac{2m+1}{2} \int_{-1}^{1} f(x)\, P_m(x)\, dx$$

Let's do an example:



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

So the 1st coefficient a_0:

$$a_0 = \frac{1}{2}\left[\int_{-1}^{0}(1+x)\,dx + \int_{0}^{+1}(1-x)\,dx\right] = \frac{1}{2}$$

Since $f(x)$ is an even function of x,

$$a_1 = a_3 = a_5 = a_7 = \int_{-1}^{1}(\text{even})(\text{odd})\,dx = 0$$

$$a_2 = -5/8$$

$$a_4 = 3/6$$

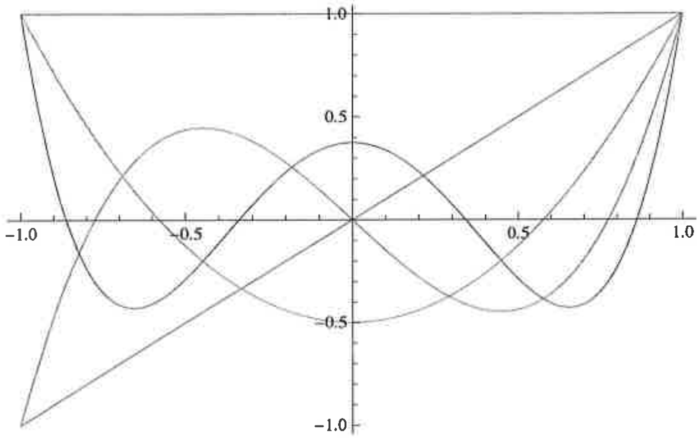
This is easiest to do in Mathematica:

In[48]:= **poly = {1, x, (3 x^2 - 1) / 2, (5 x^3 - 3 x) / 2, (35 x^4 - 30 x^2 + 3) / 8}**

Out[48]= $\left\{1,\ x,\ \frac{1}{2}\left(-1+3\,x^2\right),\ \frac{1}{2}\left(-3\,x+5\,x^3\right),\ \frac{1}{8}\left(3-30\,x^2+35\,x^4\right)\right\}$

In[49]:= **Plot[poly, {x, -1, 1}]**

Out[49]=



In[50]:= **Integrate[poly[[1]] * poly[[3]], {x, -1, 1}]**

Out[50]= 0

In[51]:= **Integrate[(1 + x) * poly, {x, -1, 0}] + Integrate[(1 - x) * poly, {x, 0, 1}]**

Out[51]= $\left\{1,\ 0,\ -\frac{1}{4},\ 0,\ \frac{1}{24}\right\}$

In[52]:= **a = {1 / 2, 0, -5 / 8, 0, 3 / 16}**

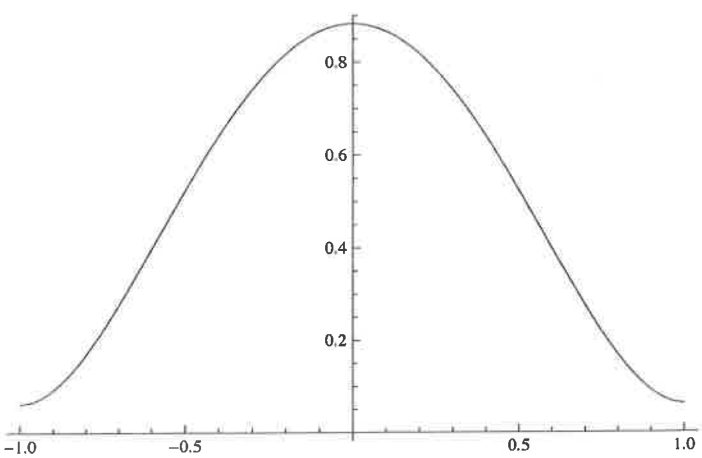
Out[52]= $\left\{\frac{1}{2},\ 0,\ -\frac{5}{8},\ 0,\ \frac{3}{16}\right\}$

In[53]:= **a.poly**

Out[53]= $\frac{1}{2}-\frac{5}{16}\left(-1+3\,x^2\right)+\frac{3}{128}\left(3-30\,x^2+35\,x^4\right)$

In[54]:= **Plot[a.poly, {x, -1, 1}]**

Out[54]=



In[55]:= **LegendreP[2, x]**

Out[55]= $\frac{1}{2}\left(-1+3\,x^2\right)$

In[56]:= `poly = Table[LegendreP[n, x], {n, 0, 6}]`

Out[56]= $\left\{1,\ x,\ \frac{1}{2}\left(-1+3x^2\right),\ \frac{1}{2}\left(-3x+5x^3\right),\ \frac{1}{8}\left(3-30x^2+35x^4\right),\ \frac{1}{8}\left(15x-70x^3+63x^5\right),\ \frac{1}{16}\left(-5+105x^2-315x^4+231x^6\right)\right\}$

In[57]:= `a = Table[(2 n + 1) / 2 * (Integrate[(1 + x) * LegendreP[n, x], {x, -1, 0}] + Integrate[(1 - x) * LegendreP[n, x], {x, 0, 1}]), {n, 0, 6}]`

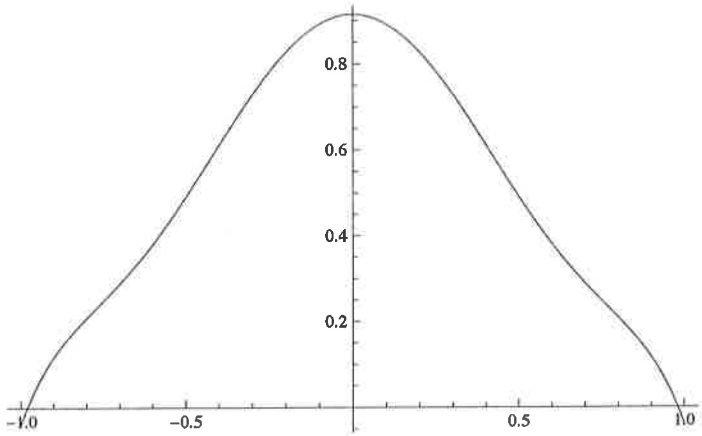
Out[57]= $\left\{\frac{1}{2},\ 0,\ -\frac{5}{8},\ 0,\ \frac{3}{16},\ 0,\ -\frac{13}{128}\right\}$

In[58]:= `a.poly`

Out[58]= $\frac{1}{2}-\frac{5}{16}\left(-1+3x^2\right)+\frac{3}{128}\left(3-30x^2+35x^4\right)-\frac{13\left(-5+105x^2-315x^4+231x^6\right)}{2048}$

In[59]:= `Plot[a.poly, {x, -1, 1}]`

Out[59]=



Orthogonal Polynomials over different ranges

$$\int_a^b \underbrace{r(x)}_{\text{weight function}} \phi_i(x)\, \phi_j(x)\, dx = 0 \quad \text{when } i \neq j$$

integration range

Families of orthogonal functions are defined with a range $a \leq x \leq b$ and a weight function $r(x)$

Family	Symbol	Interval	Weight	Relevance
Legendre	$P_n(x)$	$-1 \leq x \leq 1$	1	azimuthal electron motion $x = \cos\theta$ l quantum #
Laguerre	$L_n(x)$	$0 \leq x \leq \infty$	e^{-x}	radial electron motion
Associated Laguerre	$L_n^{\alpha}(x)$	$0 \leq x \leq \infty$	$x^{\alpha} e^{-x}$	radial electron motion n = principal QN $\alpha = l$
Hermite	$H_n(x)$	$-\infty \leq x \leq \infty$	e^{-x^2}	vibrational motion in bonds

There are lots of families that solve specific differential equations. (The Legendres solve:

$$(1-x^2)P''(x) - 2xP'(x) + n(n+1)P(x) = 0$$

These 4 are the most important in chemistry.

Fourier Series

One of the most useful set of function expansions is the Fourier series

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

over the interval $-\ell \le x \le \ell$

a_n & b_n are coefficients that describe the function $f(x)$ in terms of frequency functions.

Think of the fourier series as a set of orthogonal polynomials for a function that is explicitly periodic

Fourier Series

Last time, we talked about orthogonal polynomials:

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

where the $P_n(x)$ were a special set of functions on an interval

$$\int_a^b r(x)\, P_n(x)\, P_m(x)\, dx = 0 \quad \text{if } n \neq m$$

$a \le x \le b$ is the interval over which this is integrated

$r(x)$ is a weight function

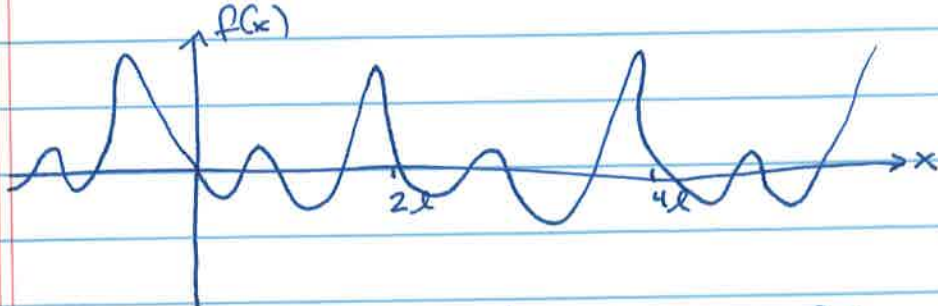
One very special version of this works for functions that are periodic in x over an interval

$$-\ell \le x \le \ell$$

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos \frac{n\pi x}{\ell} + b_n \sin \frac{n\pi x}{\ell} \right]$$

a_n & b_n are coefficients.

Consider an arbitrary periodic function:



(has a period $= 2\ell$) so

$$f(x+2\ell) = f(x)$$

$$f(x-\ell) = f(x+\ell)$$

The coefficients in the Fourier series are obtained just like they were for the orthogonal functions:

$$a_n = \frac{1}{\ell}\int_{-\ell}^{\ell} f(x)\cos\frac{n\pi x}{\ell}\,dx \qquad n = 0, 1, 2 \ldots$$

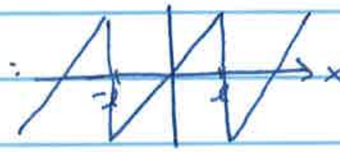
$$b_n = \frac{1}{\ell}\int_{-\ell}^{\ell} f(x)\sin\frac{n\pi x}{\ell}\,dx \qquad n = 1, 2, \ldots$$

These coefficients are called Fourier coefficients and they are obtained using orthogonality conditions

$$\int_{-\ell}^{\ell} \sin\frac{n\pi x}{\ell}\sin\frac{m\pi x}{\ell}\,dx = \int_{-\ell}^{\ell}\cos\frac{n\pi x}{\ell}\cos\frac{m\pi x}{\ell}\,dx = \ell\,\delta_{nm}$$

$$\int_{-\ell}^{\ell}\cos\frac{n\pi x}{\ell}\sin\frac{m\pi x}{\ell}\,dx = 0$$

Here's an example for a sawtooth function:



$$f(x) = x \qquad -\ell \le x \le \ell$$

$$= f(x + 2\ell) \quad \text{outside this interval}$$

$$a_n = \frac{1}{\ell}\int_{-\ell}^{\ell} x\cos\frac{n\pi x}{\ell}\,dx = 0 \quad \text{for all } n$$

because of symmetry

$$b_n = \frac{1}{\ell}\int_{-\ell}^{\ell} x\sin\frac{n\pi x}{\ell}\,dx$$

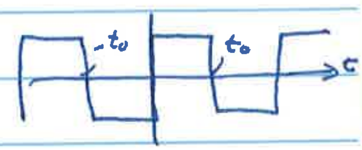
$$= \frac{2}{\ell}\left[\frac{\sin\frac{n\pi x}{\ell}}{n^2\pi^2/\ell^2} - \frac{x\cos\frac{n\pi x}{\ell}}{n\pi/\ell}\right]_0^{\ell}$$

$$b_n = (-1)^{n+1}\,2\ell/n\pi$$

So $$f(x) = \frac{2l}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sin \frac{n\pi x}{l}$$

Mathematica Demo 1

Another cool example is the square wave



$$f(t) = \begin{cases} -1 & -t_0 \leq t \leq 0 \\ +1 & 0 \leq t \leq t_0 \end{cases}$$

(Forier series work well for time-dependent phenomena)

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left(a_n \cos \frac{n\pi t}{t_0} + b_n \sin \frac{n\pi t}{t_0} \right)$$

Again the integrand is an odd function of t, so

$$a_n = \frac{1}{t_0} \int_{-t_0}^{t_0} f(t) \cos \frac{n\pi t}{t_0} \, dt = 0$$

$$b_n = \frac{1}{t_0} \int_{-t_0}^{t_0} f(t) \sin \frac{n\pi t}{t_0} \, dt = \frac{2}{n\pi} \left[1 - (-1)^n \right]$$

$$\therefore \quad f(t) = \sum_{n=1}^{\infty} \frac{2\left[1-(-1)^n\right]}{n\pi} \sin \frac{n\pi t}{t_0}$$

Mathematica Demo 2

Complex Fourier series :

$\omega_0 = \frac{\pi}{t_0}$

$$f(t) = \sum_{n=-\infty}^{\infty} c_n e^{in\omega_0 t}$$

In[1]:= `sines = Table[Sin[n Pi x / l], {n, 1, 10}]`

Out[1]= $\left\{\sin\left[\frac{\pi x}{l}\right], \sin\left[\frac{2\pi x}{l}\right], \sin\left[\frac{3\pi x}{l}\right], \sin\left[\frac{4\pi x}{l}\right], \sin\left[\frac{5\pi x}{l}\right], \sin\left[\frac{6\pi x}{l}\right], \sin\left[\frac{7\pi x}{l}\right], \sin\left[\frac{8\pi x}{l}\right], \sin\left[\frac{9\pi x}{l}\right], \sin\left[\frac{10\pi x}{l}\right]\right\}$

In[2]:= `cosines = Table[Cos[n Pi x / l], {n, 0, 10}]`

Out[2]= $\left\{1, \cos\left[\frac{\pi x}{l}\right], \cos\left[\frac{2\pi x}{l}\right], \cos\left[\frac{3\pi x}{l}\right], \cos\left[\frac{4\pi x}{l}\right], \cos\left[\frac{5\pi x}{l}\right], \cos\left[\frac{6\pi x}{l}\right], \cos\left[\frac{7\pi x}{l}\right], \cos\left[\frac{8\pi x}{l}\right], \cos\left[\frac{9\pi x}{l}\right], \cos\left[\frac{10\pi x}{l}\right]\right\}$

In[3]:= `bs = Table[(-1)^(n+1) 2 l / (n Pi), {n, 1, 10}]`

Out[3]= $\left\{\frac{2l}{\pi}, -\frac{l}{\pi}, \frac{2l}{3\pi}, -\frac{l}{2\pi}, \frac{2l}{5\pi}, -\frac{l}{3\pi}, \frac{2l}{7\pi}, -\frac{l}{4\pi}, \frac{2l}{9\pi}, -\frac{l}{5\pi}\right\}$

In[4]:= `bs . sines`

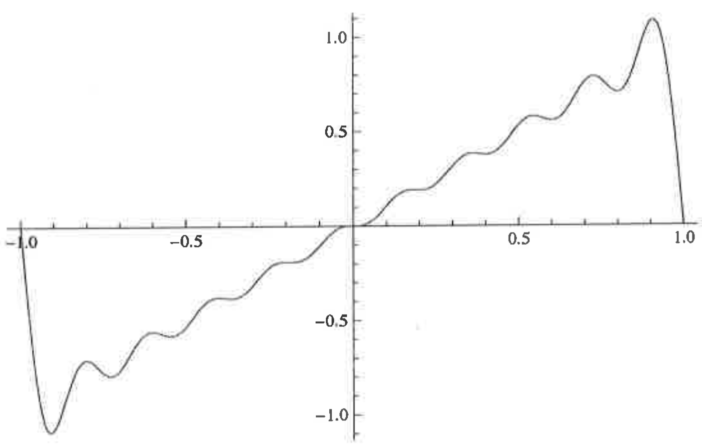
Out[4]= $\frac{2l\sin\left[\frac{\pi x}{l}\right]}{\pi} - \frac{l\sin\left[\frac{2\pi x}{l}\right]}{\pi} + \frac{2l\sin\left[\frac{3\pi x}{l}\right]}{3\pi} - \frac{l\sin\left[\frac{4\pi x}{l}\right]}{2\pi} + \frac{2l\sin\left[\frac{5\pi x}{l}\right]}{5\pi} - \frac{l\sin\left[\frac{6\pi x}{l}\right]}{3\pi} + \frac{2l\sin\left[\frac{7\pi x}{l}\right]}{7\pi} - \frac{l\sin\left[\frac{8\pi x}{l}\right]}{4\pi} + \frac{2l\sin\left[\frac{9\pi x}{l}\right]}{9\pi} - \frac{l\sin\left[\frac{10\pi x}{l}\right]}{5\pi}$

In[5]:= `l = 1`

Out[5]= 1

In[6]:= `Plot[bs.sines, {x, -1, 1}]`

Out[6]=

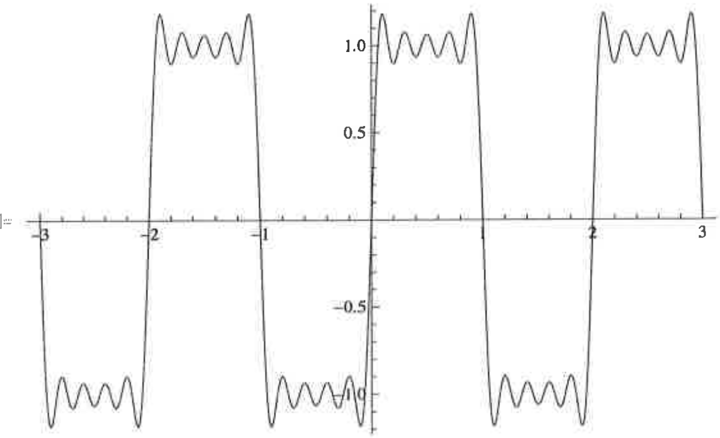


In[7]:= `bs = Table[2 (1 - (-1)^n) / (n Pi), {n, 1, 10}]`

Out[7]= $\left\{\frac{4}{\pi}, 0, \frac{4}{3\pi}, 0, \frac{4}{5\pi}, 0, \frac{4}{7\pi}, 0, \frac{4}{9\pi}, 0\right\}$

In[9]:= **Plot[bs.sines, {x, -3, 3}]**

Out[9]=



If we define $\tau = \frac{2\pi}{\omega_0}$

$$C_k = \frac{1}{\tau} \int_{-\tau/2}^{+\tau/2} f(t)\, e^{-i\omega_0 k_k t}\, dt$$

complex coefficient $\qquad c_k = \underset{\text{cosine}}{a_k} + i \underset{\text{sine}}{b_k}$

C_k gives us information about the contribution of signal $e^{i\omega_0 k t} = \cos \omega_0 k t + i \sin \omega_0 k t$ to $f(t)$

If we think of $\omega_0 k$ as a different frequency for each value of k

$$\omega = k\,\omega_0$$

we can obtain the Fourier transform

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

The contribution of a sine oscillation of frequency ω to a time function $f(t)$

$\hat{F}(\omega)$ is like the coefficients c_k but where the interval $-\tau/2 \rightarrow \tau/2$ has become infinitely long.

The inverse Fourier transform lets us recover the time signal from $\hat{F}(\omega)$

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

Fourier Transforms

$$\hat{F}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t)\, e^{-i\omega t}\, dt \quad \leftarrow \text{Fourier Transform}$$

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{F}(\omega)\, e^{i\omega t}\, d\omega \quad \leftarrow \text{Inverse Fourier Transform}$$

$\hat{F}(\omega)$ tells us about the contribution of signals with frequency ω make to a time signal $f(t)$

Lets practice a few:

$$f(t) = e^{-\alpha|t|} \qquad -\infty \leq t \leq \infty \quad \leftarrow \text{an exponentially decaying signal}$$

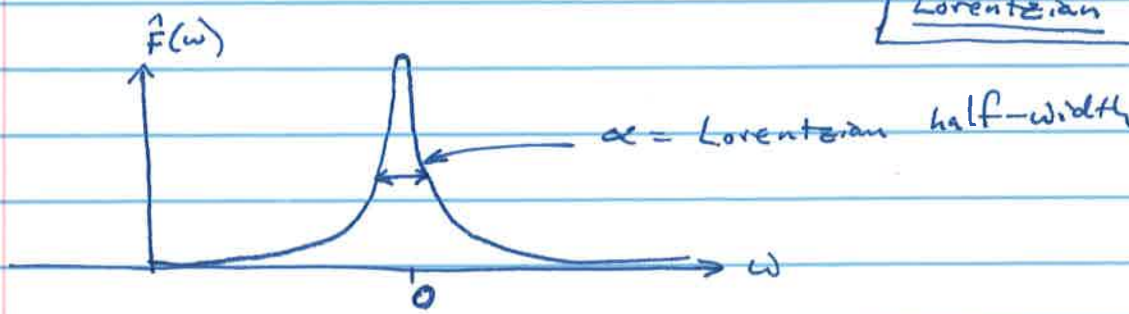
$$\hat{F}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\alpha|t|}\, e^{-i\omega t}\, dt$$

$$= \frac{1}{\sqrt{2\pi}} \left[\int_{-\infty}^{\infty} e^{-\alpha|t|} \cos\omega t\, dt - i \int_{-\infty}^{\infty} \underset{\text{even}}{e^{-\alpha|t|}}\, \underset{\text{odd}}{\sin\omega t}\, dt \right]$$

$\swarrow$ a "cosine" transform

$$\hat{F}(\omega) = \frac{2}{\sqrt{2\pi}} \int_{0}^{\infty} e^{-\alpha t} \cos\omega t\, dt = \sqrt{\frac{2}{\pi}}\, \frac{\alpha}{\omega^2 + \alpha^2}$$

This is called a Lorentzian function



$f(t) = e^{-\alpha|t|}$ $\hat{F}(\omega) = \frac{\sqrt{2}}{\sqrt{\pi}} \frac{\alpha}{\omega^2 + \alpha^2}$

Fourier transform pair

Inverse Fourier transform of $\hat{F}(\omega)$ recovers $f(t)$

Another important one:

$$f(t) = e^{i\omega_0 t} = \cos\omega_0 t + i\sin\omega_0 t$$

This is an oscillation at a fixed frequency.
What do you think $\hat{F}[\omega]$ will look like?

$$\hat{F}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega_0 t} e^{-i\omega t} dt$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i(\omega_0 - \omega)t} dt$$

$$= \frac{1}{\sqrt{2\pi}} \left[\int_{-\infty}^{\infty} \cos[(\omega_0 - \omega)t]\, dt + i \int_{-\infty}^{\infty} \sin[(\omega_0 - \omega)t]\, dt \right]$$

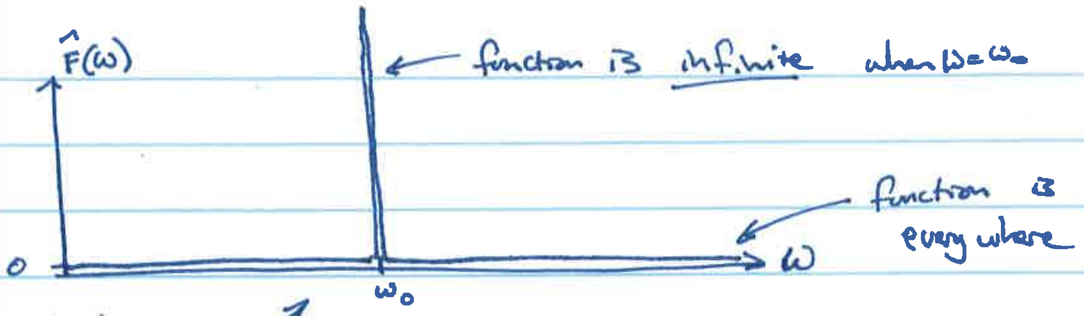
There are 2 cases here. If $\omega_0 \neq \omega$ these integrals are over an infinitely oscillating range of the function. For every $+$ region of $\cos[(\omega-\omega_0)t]$ there's an equivalent $-$ region.

That means that when $\omega \neq \omega_0$ the integrals are zero.

But if $\omega = \omega_0$

$$\hat{F}(\omega) = \frac{1}{\sqrt{2\pi}} \left[\int_{-\infty}^{\infty} \cos(0t)\, dt + i \int_{-\infty}^{\infty} \sin(0t)\, dt \right]$$

$$= \frac{1}{\sqrt{2\pi}} \left[\int_{-\infty}^{\infty} dt + 0 \right] = \infty$$



This is called the Dirac Delta function

$$\delta(\omega - \omega_0) = \begin{cases} 0 & \text{when } \omega \neq \omega_0 \\ \infty & \text{when } \omega = \omega_0 \end{cases}$$

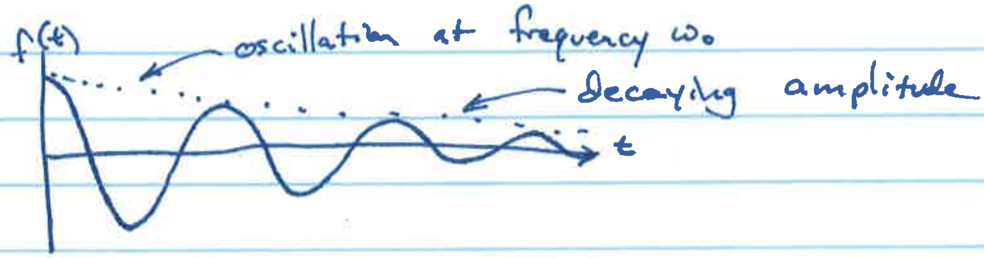
Note that it is very similar to the Kronecker Delta

$$\delta_{nm} = \begin{cases} 0 & \text{when } n \neq m \\ 1 & \text{when } n = m \end{cases}$$

Now lets put these together:

this is a very typical experimental signal

$$f(t) = e^{-\alpha t} \cos \omega_0 t \qquad t \geq 0$$



We can easily do the cosine transform

$$\hat{F}(\omega) = \frac{1}{\sqrt{\pi}} \int_0^\infty e^{-\alpha t} \cos \omega_0 t \ \cos \omega t \ dt$$

To do this, we'll dredge up:

$$\cos(a+b) = \cos a \ \cos b - \sin a \ \sin b$$
$$\cos(a-b) = \cos a \ \cos b + \sin a \ \sin b$$

$$\cos(a+b) + \cos(a-b) = 2 \cos(a) \cos(b)$$

$$\hat{F}(\omega) = \frac{1}{2\sqrt{2\pi}}\left[\int_0^\infty e^{-\alpha t}\cos[(\omega_0+\omega)t]\,dt + \int_0^\infty e^{-\alpha t}\cos[(\omega_0-\omega)t]\,dt\right]$$

Each of these integrals is exactly like the FT of $e^{-\alpha|t|}$ but at a shifted frequency

$$\frac{2}{\sqrt{2\pi}}\int_0^\infty e^{-\alpha t}\cos\omega t\,dt = \sqrt{\frac{2}{\pi}}\,\frac{\alpha}{\omega^2+\alpha^2}$$ ← we did this earlier!

So:

$$\hat{F}(\omega) = \underbrace{\sqrt{\frac{2}{\pi}}\,\frac{\alpha}{\alpha^2+(\omega+\omega_0)^2}}_{\text{usually very small for frequencies near } \omega_0} + \left(\frac{2}{\sqrt{\pi}}\right)^{1/2}\frac{\alpha}{\alpha^2+(\omega-\omega_0)^2}$$

$$\hat{F}(\omega) \cong \left(\frac{2}{\pi}\right)^{1/2}\frac{\alpha}{\alpha^2+(\omega-\omega_0)^2}$$ ← Lorentzian lineshape peaked at $\omega=\omega_0$, with a width α that tells us about the decay of the signal or the lifetime.

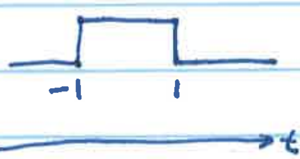
Most experimental spectra have Lorentzian lineshapes

NMR: α is very ~~large~~ small, ~~so peaks~~ so signals decay slowly, and lines are very narrow.

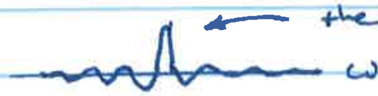
Vibrational spectra: α is large, so ~~the~~ signals decay quickly and lines are very broad.

Interesting Fourier pairs

	$f(t)$		$\hat{F}(\omega)$	
Oscillatory:	$e^{i\omega_0 t}$	$\longleftrightarrow$	$\frac{1}{\sqrt{2\pi}}\,\delta(\omega-\omega_0)$	: Delta Function
Exponential:	$e^{-\alpha\lvert t\rvert}$	$\longleftrightarrow$	$\left(\frac{2}{\pi}\right)^{1/2}\frac{\alpha}{\omega^2+\alpha^2}$	: Lorentzian
Gaussian	$e^{-\alpha^2 t^2}$	$\longleftrightarrow$	$\frac{1}{\sqrt{2\alpha^2}}\,e^{-\omega^2/4\alpha^2}$	: Gaussian

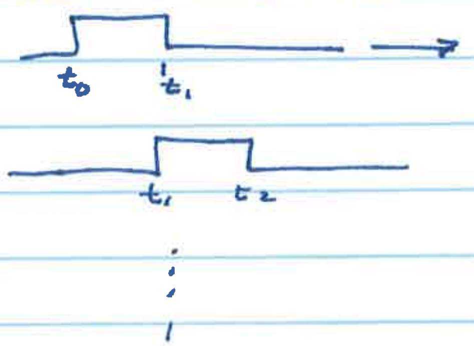
Block function: 

$\longleftrightarrow \quad \frac{1}{\sqrt{2\pi}}\;\frac{\sin\omega}{\omega}$



← the sinc function

Suppose we want to look at only a portion of $f(t)$



← these are window functions that can define a "wavelet" transform which is a time-resolved Fourier Transform

← wavelets are a lot like musical notation!

A close relative of the Fourier transform

$$\hat{F}(s) = \int_0^\infty e^{-st} f(t)\,dt \quad \leftarrow \text{The Laplace transform}$$

$$\hat{F}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} f(t)\,dt \quad \leftarrow \text{the Fourier transform}$$

$\hat{F}(\omega)$ tells us about oscillatory contributions to $f(t)$

$\hat{F}(s)$ tells us about <u>decay</u> contributions to $f(t)$ and can help us solve complicated differential equations

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The Laplace transform is a bit beyond the domain of this class, but I did want everyone to have seen it once. If you run into a <u>hard</u> diff EQ problem, you'll need to learn about Laplace transforms in some detail.