Fourier Series

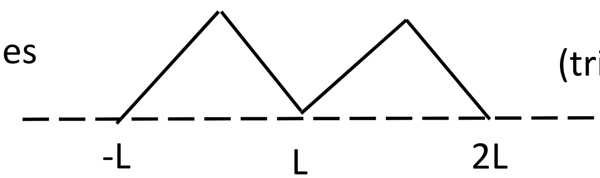
March. 14, 2018

Any function with period 2L can be represented with a Fourier series

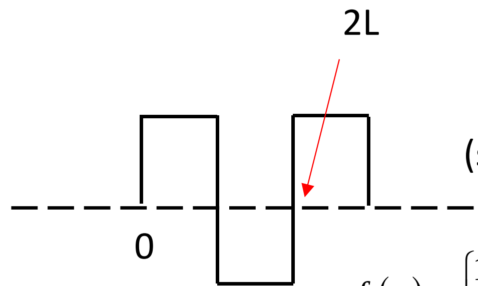
$$f(x) = a_0 + \sum_{n=1} a_n \cos\left(\frac{n\pi x}{L}\right) + \sum_{n=1} b_n \sin\left(\frac{n\pi x}{L}\right)$$

periodic with period 2L

Examples



(triangle wave)



(square wave)

$$f(x) = \begin{cases} 1, 0 < x < L \\ -1, -L < x < 0 \end{cases}$$

In other words, sin(nπx/L), and cos(nπx/L) form a basis set in terms of which other functions can be expanded

The basis functions are orthogonal to one another

$$\int_{-L}^{L} \cos\left(\frac{m\pi x}{L}\right)\cos\left(\frac{n\pi x}{L}\right)dx = L\delta_{m,n}, \qquad m,n \neq 0$$

$$\int_{-L}^{L} \sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)dx = L\delta_{m,n}$$

$$\int_{-L}^{L} (1)\sin\left(\frac{n\pi x}{L}\right)dx = \int_{=L}^{L} (1)\cos\left(\frac{n\pi x}{L}\right)dx = 0$$

$$\int_{-L}^{L} \cos\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)dx = 0$$

The leading term, the constant a_0, is orthogonal to the sin and cos terms.

How does one determine the coefficients?

$$f(x) = a_0 + \sum a_n \cos\left(\frac{n\pi x}{L}\right) + \sum b_n \sin\left(\frac{n\pi x}{L}\right)$$

$\int_{-L}^{L} f(x) \bullet 1 dx = a_0 \int_{-L}^{L} dx = a_0 2L$ | multiply both sides of eq. by 1 and $\int$

$\int_{-L}^{L} f(x) \cos\left(\frac{n\pi x}{a}\right) dx = a_n L$ | multiply both sides of eq. by $\cos\left(\frac{n\pi x}{a}\right)$ and $\int$

$\int_{-L}^{L} f(x) \sin\left(\frac{n\pi x}{a}\right) dx = b_n L$ | multiply both sides of eq. by $\sin\left(\frac{n\pi x}{a}\right)$ and $\int$

$$a_0 = \frac{1}{2L} \int_{-L}^{L} f(x) dx$$

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

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

The coefficients in the expansion are given by the projection of *f(x)* onto the basis functions | projection $\equiv$ overlap

Even if the function is not periodic, we can represent it on (-L, L) with a Fourier series

Even function: all $b_n = 0$
Odd function: all $a_n = 0$

Example

$f(x) = x$ for –L < x < L (Sawtooth function)

Because this is an odd function only the sin(nπx/L) terms contribute to the expansion

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

$$= \frac{2}{L}\int_{0}^{L} x\sin\left(\frac{n\pi x}{L}\right)dx = \frac{2L}{n\pi}(-1)^{n-1}$$

$$f(x) = \frac{2L}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n}\sin\left(\frac{n\pi x}{L}\right)$$

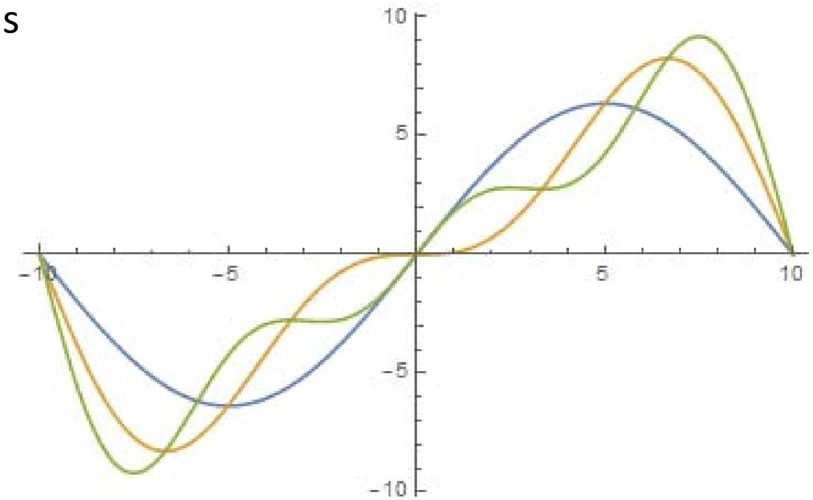
$$= \frac{2L}{\pi}\left[\sin\left(\frac{\pi x}{L}\right) - \frac{1}{2}\sin\left(\frac{2\pi x}{L}\right) + \frac{1}{3}\sin\left(\frac{3\pi x}{L}\right) - \frac{1}{4}\sin\left(\frac{4\pi x}{L}\right) + \ldots\right]$$

Note, that in the text an integration symbol (Ex 11.1) is missing)

Note this expression → 0, at x = -L and L
But the actual sawtooth function is discontinuous at those points

Mathematica code to plot the Fourier series of the sawtooth function approximated with one, two, three terms

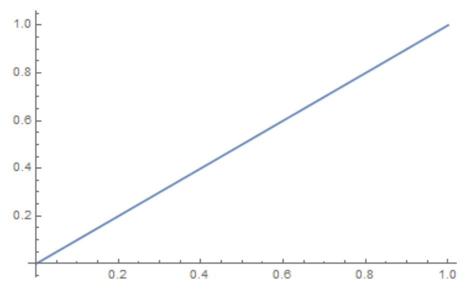
```
L = 10
a=2*L/Pi
one=a*Sin[Pi x/L]
two=one-(a/2)*Sin[2 Pi x/L]
three=two + (a/3)*Sin[3 Pi x/L]
Plot[{one, two, three},{x,-L,L}]
```



In practice, one would employ more than three terms.

Also, Mathematica has built-in functions for functions like the sawtooth function and for evaluating Fourier series

```
Plot[SawtoothWave[x],{x,0,1}]
```



Can shift to -1 to 1 with

```
F[y_]:=2*(SawtoothWave[0.5y+0.5])-1.0
```

If we only want to represent a function on (0, L), we can use either the sine or cosine series

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An alternative representation

Euler relations

$$\cos(\alpha) = \frac{1}{2}\left[e^{i\alpha} + e^{-i\alpha}\right]$$

$$\sin(\alpha) = \frac{1}{2i}\left[e^{i\alpha} - e^{-i\alpha}\right]$$

So we can also use

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/L}$$

for a real function, a_n, b_n real, c_n complex

$$\int_{-L}^{L}\left[\exp\left(\frac{im\pi x}{L}\right)\right]^*\left[\exp\left(\frac{in\pi x}{L}\right)\right]dx = 2L\delta_{nm}$$

$$c_m = \frac{1}{2L}\int_{-L}^{L}\exp\left(\frac{im\pi x}{L}\right)f(x)\,dx$$

Many other classes of orthogonal functions

The orthogonal functions form a basis set in which other functions can be expanded

$$f = \sum_n c_n \psi_n$$

ψ_n ← a set of orthogonal functions that obey the same boundary conditions as *f*

again $c_n = \int_a^b f\psi \, d\tau$, where *a*, *b* are the relevant integration limits, and $d\tau$ represents the variable(s) integrated over

scalar product of two functions

$$\int_a^b f^*(x) g(x)\, dx$$

assuming 1D
readily generalized to 2D or 3D

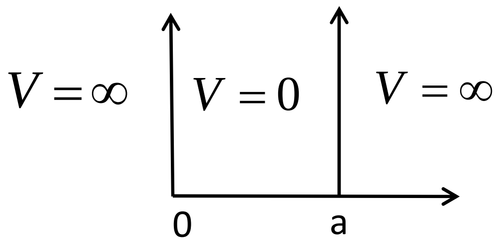
If the functions are also normalized

$$\int_a^b \psi_n^* \psi_m \, dx = \delta_{nm}$$

QM particle-in-box

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = E\psi$$

$$E = \frac{\hbar^2 n^2 \pi^2}{2ma^2} = \frac{\hbar^2 n^2}{8ma^2}$$



eigenfunctions $\psi_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$

Expand $f(x) = x^2 - ax$ for 0 ≤ x ≤ a

in terms of the eigen functions

$$\frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

$$c_1 = \sqrt{\frac{2}{a}}\int_0^a \left(x^2 - ax\right)\sin\left(\frac{\pi x}{a}\right)dx = \sqrt{\frac{2}{a}}\int_0^a x^2 \sin\left(\frac{\pi x}{a}\right)dx - \sqrt{\frac{2}{a}}\int_0^a (ax)\sin\left(\frac{n\pi x}{a}\right)dx$$

$$= -\frac{4\sqrt{2}a^{5/2}}{\pi^3} = -0.182442a^{5/2}$$

$$f = x^2 - ax \approx -\frac{8a^2}{\pi^3}\sin\left(\frac{\pi x}{a}\right)$$

leading term of
a Fourier series

Fourier transform

As $L \to \infty$ the sum in the Fourier series goes over to an integral (all wavelengths become possible)

Let $k = \frac{n\pi}{L}$, k continuous as $L \to \infty$

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

↑ this replaces c_n in the sum

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

we can work in x or k space

Note, there are several slightly different definitions of FT's. In one common on one has 1/(2π) for the FT, and 1 for the inverse FT.

The 2π can also be folded into the exponent

One often encounters FT's between frequency and time.

But two definitions of frequency: ω=2πν

The Fourier transform converges if

$$\int_{-\infty}^{\infty} \left| f(x) \right|^2 dx < \infty$$

In that case, *f(x)* is said to be "square integrable"

This requires $f(x) \to 0$ as $|x| \to \infty$

Consider:

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$$

Gaussian function with μ = the mean of x, and σ is the standard deviation

Evaluate the Fourier transform of $f(x) = e^{-ax^2}$

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

$$= \frac{1}{\sqrt{2\pi}} \left[\int_{-\infty}^{\infty} e^{-ax^2} \cos(kx)\, dx - \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ax^2} \sin(kx)\, dx \right]$$

$$= \frac{1}{\sqrt{2a}} e^{-k^2/4a}$$

even odd

so integral is zero

Note: $\int_{-\infty}^{\infty} \exp(-ax^2) dx = \sqrt{\pi / a}$

The Fourier transform can be done by "completing the square"

The FT of a Gaussian is a Gaussian

Now consider $a = \frac{1}{2\sigma^2}$

$$e^{-\frac{x^2}{2\sigma^2}} \rightarrow e^{-\sigma^2 k^2/2}$$

$\sigma \rightarrow 0:$ $e^{-x^2/2\sigma^2}$ very spread out; $e^{-\sigma^2 k^2/2}$ very narrow

opposite behavior as $\sigma \rightarrow$ very large

Note: You will see in P. Chem. that $k \propto p$
This illustrates the "uncertainty principle" between *x* and *p*. We can also use Fourier transforms to go between the frequency and time domains

FTs are also very using in going from frequency to time

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

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

circular frequency
$\omega = 2\pi\nu$

FTIR and NMR measure signals as a function of time
and use FT to get spectrum in the frequency domain

Actually, one measures the signal at discrete values of *t* and uses an algorithm called "fast Fourier Transform (FFT)"

Example: generate the sine transform of $e^{-at}\sin(bt)$

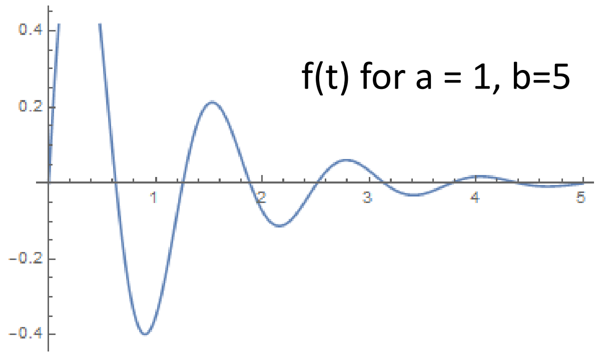
typical of a signal from an NMR measurement

$$F(\omega) = \frac{\sqrt{2}}{\sqrt{\pi}} \int_0^{\infty} e^{-at} \sin(bt) \sin(\omega t)\, dt$$

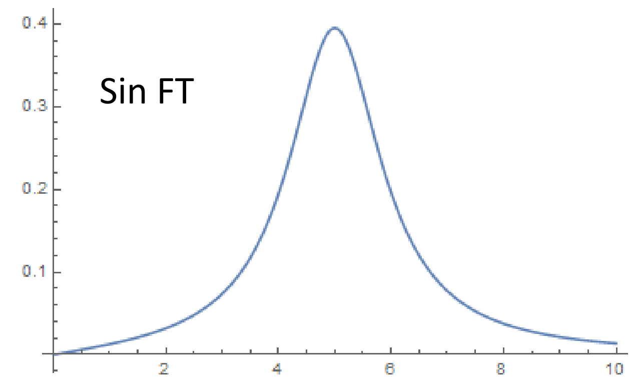
$$= \frac{\sqrt{2}}{\sqrt{\pi}} \frac{2ab\omega}{\left[a^2 + (b-\omega)^2\right]\left[a^2 + (b+\omega)^2\right]}$$

if $f(t) = e^{-at}\sin(bt) + e^{-at}\sin(ct)$

get two peaks in the spectrum



f(t) for a = 1, b=5



Sin FT

Note, some texts/web pages use non-symmetrical definition of FTs. E.g.,

$$F(\omega) = \int_{-\infty}^{\infty} e^{-i\omega t} f(t)\, dt$$

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

Some interesting cases

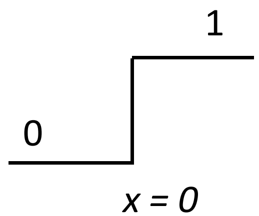
$$f(t) = \sin(at)$$

$$F(\omega) = -\sqrt{\frac{\pi}{2}}\, i \left[\delta(\omega - a) - \delta(\omega + a) \right]$$

sin(*at*) goes on forever in time
gives a delta function in the frequency domain

$$f(t) = \delta(t)$$ delta function in time

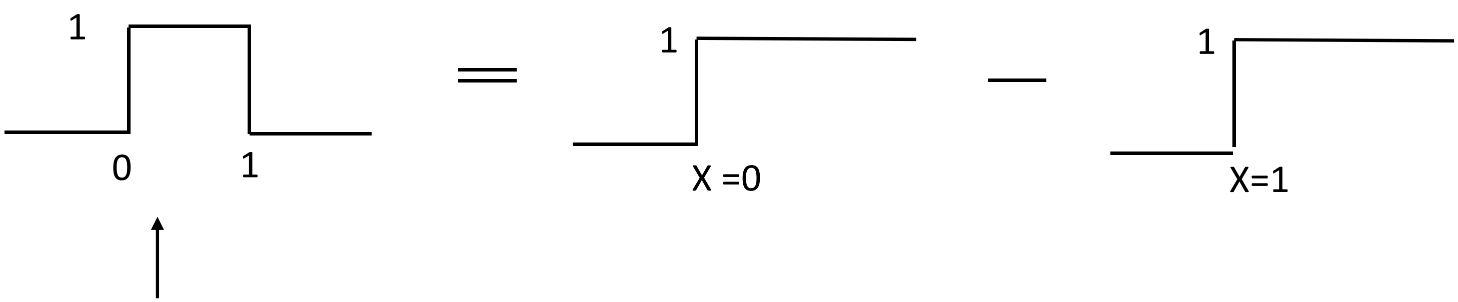
$$F(\omega) = \frac{1}{\sqrt{2\pi}}$$ all frequencies equally probable



$$F(\omega) = \frac{1}{\sqrt{2\pi}}\left[\frac{1}{i\omega} + \pi\delta(\omega)\right]$$

Heaviside step function

Note that the derivative of the Heaviside function is the delta function



This is a sum of two Heaviside functions

Some useful links

http://www.falstad.com/fourier/

https://www.projectrhea.org/rhea/index.php/Fourier_analysis_in_Music

https://na01.safelinks.protection.outlook.com/?url=https%3A%2F%2Fphysics.info%2Fmusic%2F&data=01%7C01%7Cjordan%40pitt.edu%7Ca403e6449d1b441a33cf08d585e46842%7C9ef9f489e0a04eeb87cc3a526112fd0d%7C1&sdata=66QeijFhhqooj%2FW8rRX6KvrhNothVaoo1LA22uz8FY0%3D&reserved=0

https://soundphysics.ius.edu/?page_id=949

https://www.youtube.com/watch?v=YsZKvLnf7wU

Laplace transform

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

in general, *s* is real

$$F(s) = \mathcal{L}\left[f(t) \right]$$

$$f(t) = \mathcal{L}^{-1}\left[F(s) \right]$$

$\mathcal{L}$ denotes the Laplace transform

$F(s)$	$f(t)$
$\frac{1}{s}$	1
$\frac{1}{s^2}$	t
$\frac{1}{s-a}$	$e^{at} \left(s > a\right)$
$\frac{s}{s^2+a^2}$	$\cos(at)$
$\frac{a}{s^2+a^2}$	$\sin(at)$

$$\int_0^\infty e^{-st} dt = \left. \frac{-e^{-st}}{s} \right|_0^\infty = \frac{1}{s}$$

$$\mathcal{L}[t] = \int_0^\infty t e^{-st} dt = -\frac{d}{ds} \int_0^\infty e^{-st} dt = \frac{1}{s^2}$$

Can use this "trick" repeatedly to evaluate $\mathcal{L}\left[t^n \right]$

$$\int_0^\infty \cos(at) e^{-st} dt = \frac{1}{2} \int_0^\infty (e^{iat} + e^{-iat}) e^{-st} dt = \frac{1}{2} \int_0^\infty (e^{(ia-s)t} + e^{-(ia+s)t}) dt$$

Shifting theorem $\mathcal{L}\left[e^{at} f(t)\right] = F(s-a)$

$$\int_0^\infty e^{-st} e^{at} f(t)dt = \int_0^\infty e^{-(s-a)t} f(t)dt = \int_0^\infty e^{-ut} f(t)dt, \text{ where } u = s-a$$

Derivative theorem $\mathcal{L}\left[\frac{df}{dt}\right] = \mathcal{L}\left[f'(t)\right] = s\mathcal{L}\{f(t)\} - f(0)$

$\mathcal{L}[f''] = s^2\mathcal{L}[f] - sf(0) - f'(0),$ etc.

Example: from above $\int_0^\infty te^{-st}dt = \frac{1}{s^2}$, where $f(t) = t$, $f'(t) = 1$

Recall, $\int_0^\infty e^{-st}dt = \frac{1}{s}$

$s\mathcal{L}[f(t)] - f(0) = \frac{s}{s^2} - 0 = \frac{1}{s}$

Integral theorem $\mathcal{L}\left\{\int_0^t f(u)du\right\} = \frac{1}{s}\mathcal{L}\left[f(t)\right]$

Integral Theorem $\mathcal{L}\left\{\int_0^t f(u)\,du\right\} = \frac{1}{s}\mathcal{L}\left[f(t)\right]$

Example: $f(u)=\exp(au)$

$$\int_0^t e^{au}du = \frac{e^{at}}{a} - \frac{1}{a} = \frac{1}{a}(e^{at}-1)$$

$$\mathcal{L}\left[\int_0^t e^{au}du\right] = \frac{1}{a}\left(\frac{1}{s-a} - \frac{1}{s}\right) = \frac{1}{a}\frac{a}{s(s-a)} = \frac{1}{s(s-a)}$$

$$\mathcal{L}\left[\int_0^t e^{au}du\right] = \frac{1}{s}\mathcal{L}\left[e^{at}\right] = \frac{1}{s}\frac{1}{s-a}$$

Example: $\mathcal{L}^{-1}\left[\left(\frac{1}{s}\right)\left(\frac{1}{s^2+k^2}\right)\right] = \int_0^t \frac{1}{k}\sin(ku)du = \frac{-1}{k}\frac{\cos(ku)}{k}\Big|_0^t = -\frac{1}{k^2}\left[\cos(kt)-1\right]$

Using information in the table, we see that $-\mathcal{L}\left[\frac{1}{k^2}(\cos kt - 1)\right] = \frac{1}{s}\frac{1}{s^2+k^2}$

$$\mathcal{L}\left[\cos(kt)\right] = \frac{s}{k^2+s^2}$$

$$\mathcal{L}\left[1\right] = \frac{1}{s}$$

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