~~Delta Functions~~

Introduction

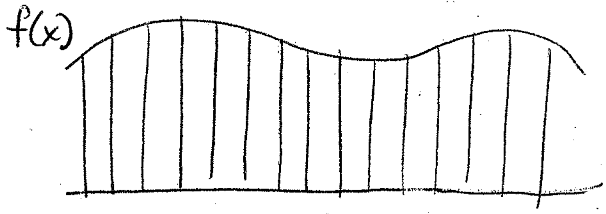
So far we have been talk about discrete particles so far.

Exs
- MD
- bead on a wire
- Plan~~ets~~s → each planet is particle
- grains of sand

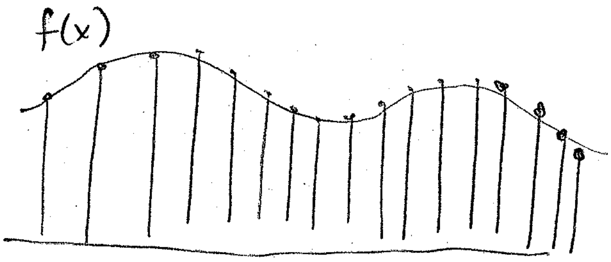
Now we are going to start talking about modeling cts materials w/ particle methods.

Exs
- Fluids (ie a wave, cup of water, flow behind an airplane)
- wire
- any material that is cts.
- Solids

* In this case must first approximate the continuous material w/ discrete particles.



cts in 1D



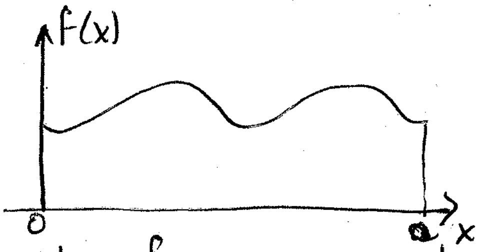
approximation w/ particles

point particles using delta fncs

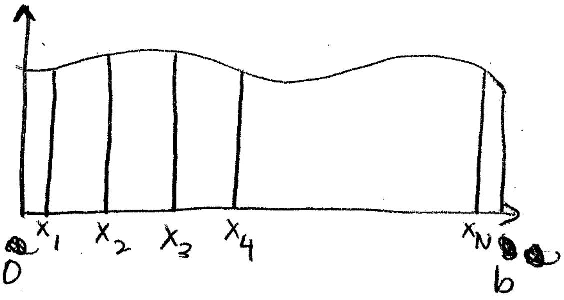
Today
- Point particles using δ-functions
- δ - functions
- ~~Smooth Approximations~~ ~~using~~ ~~of~~ ~~δ-functions~~

Point Particle Approximations

(Work in 1D for now)



cts fnc we want to approximate using particles!



$$f(x) \approx f_h(x) = \sum_p f(x_p)\, h\, \delta(x - x_p)$$

$$x_p = ph - \frac{h}{2} \qquad p = 1, \ldots N$$

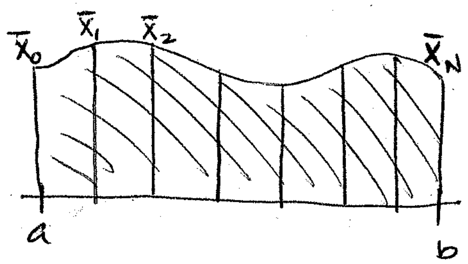
$\delta(x - x_p) \rightarrow$ delta function

Now we are going to talk about where this comes from and some basics about the delta function.

First, Midpoint Rule for Integration

$$\int_a^b g(x)\,dx = \sum_{p=0}^{N-1} \int_{\bar{x}_p}^{\bar{x}_{p+1}} g(x)\,dx$$

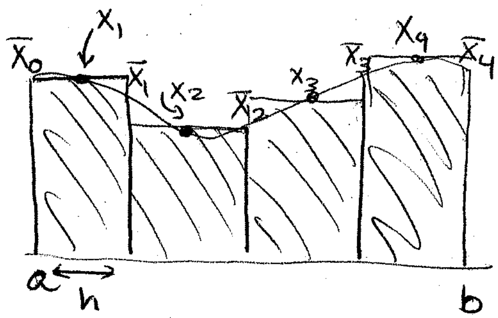
(above $a = 0$)



$(\bar{x}_p = x_p + \frac{1}{2}h)$

$$\approx \sum_{p=0}^{N-1} g\left(\frac{\bar{x}_p + \bar{x}_{p+1}}{2}\right) h$$

$$= \sum_{p=1}^{N} g(x_p)\, h$$



Now the delta function is defined such that

$$f(x) = \int_a^b f(y)\,\delta(x-y)\,dy$$

* convolution btn f and delta function

$\Rightarrow$ if use midpoint rule

$$f(x) = \int_a^b f(y)\,\delta(x-y)\,dy$$

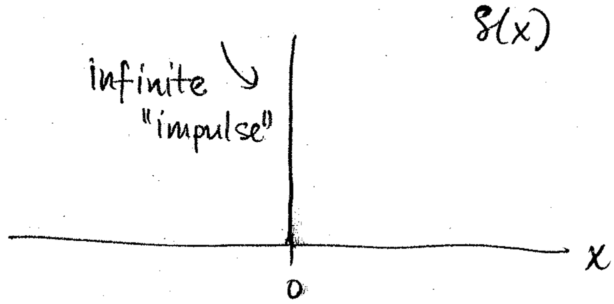
$$\approx \sum_{p=1}^{N} f(x_p)\,\delta(x-x_p)\,h$$

Delta fncs (Dirac Delta function)

Definition is given above: (convolution)

$$f(x) = \int_a^b f(y)\,\delta(x-y)\,dy$$

"function": $\delta(x)$ is infinite at 0 and 0 everywhere else



st $\displaystyle\int_{-\infty}^{\infty} \delta(x)\,dx = 1$

* not really a function (in the strict sense) since it is nonzero only at one pt and the integral is nonzero!

$$\left(\text{ie } f(x) = \begin{cases} 1 & x=0 \\ 0 & x \neq 0 \end{cases} \Rightarrow \int_{\mathbb{R}} f(x)\,dx = 0 \right)$$

moments

~~$\int_{-\infty}^{\infty} x \delta(x) \delta x$~~

Note:

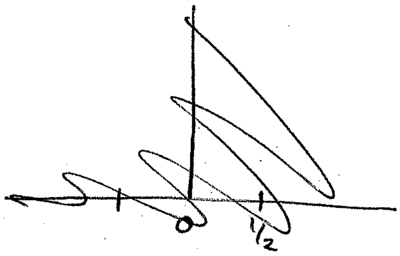
nth moment:
$$\int_{-\infty}^{\infty} x^n \delta(x)\,dx = 0 \qquad \text{for } n \neq 0$$

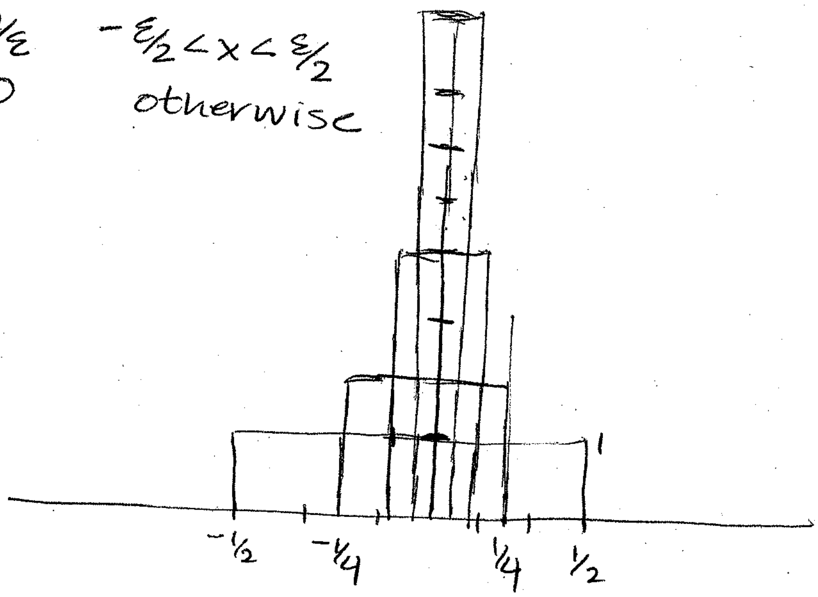
OR
$$\int_{-\infty}^{\infty} (x-y)^n \delta(x)\,dx = 0 \qquad \text{for } n \neq 0$$

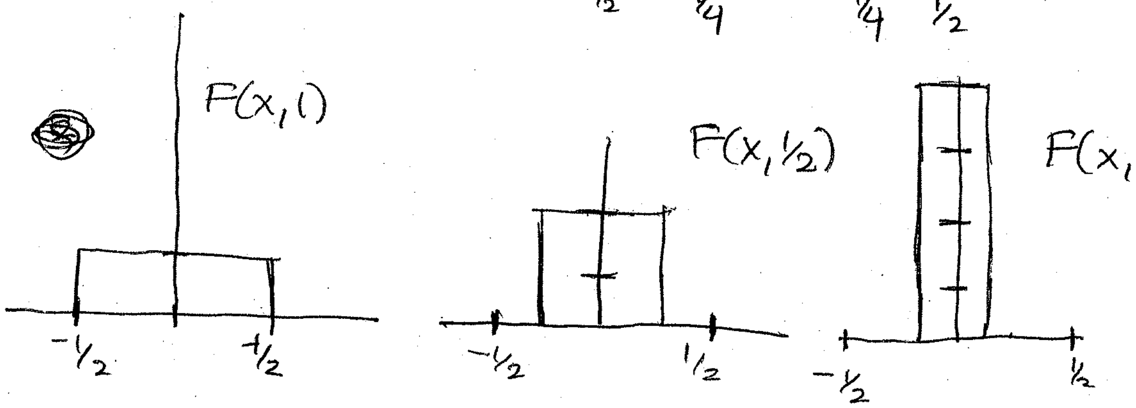
Often thought of as a limit of as a sequence of functions:

~~Examples~~
$$\delta(x) = \lim_{\varepsilon \to 0} F(x, \varepsilon)$$

Exs ① $F(x,\varepsilon) = \begin{cases} 1/\varepsilon & -\varepsilon/2 < x < \varepsilon/2 \\ 0 & \text{otherwise} \end{cases}$

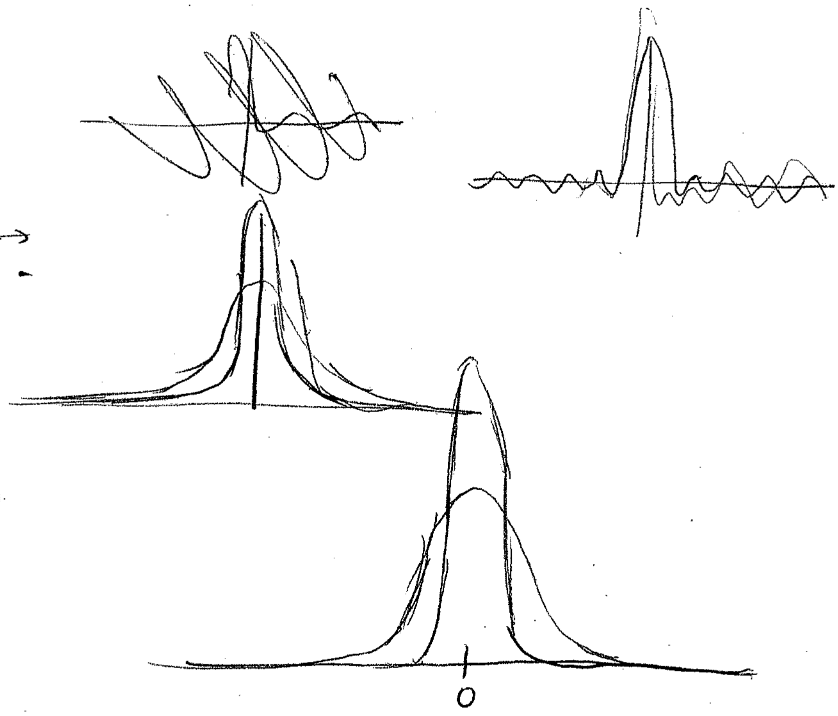






so on . . .

② $F(x,\varepsilon) = \dfrac{\sin(x/\varepsilon)}{\pi x}$



③ $F(x,\varepsilon) = \dfrac{\varepsilon/\pi}{x^2+\varepsilon^2}$ $\longrightarrow$

④ $F(x,\varepsilon) = \dfrac{1}{2\varepsilon} e^{-(x^2/\varepsilon^2)}$
(Gaussian) ~~covariance~~

(all of these fncs are symmetric but does not have to be).

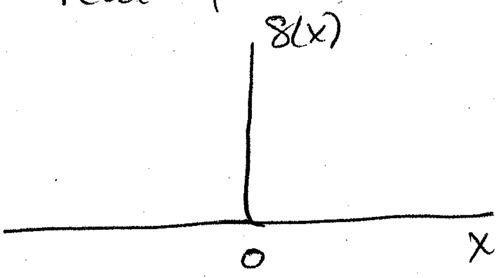
Fourier Transform

$$\hat{\delta}(k) = \int_{-\infty}^{\infty} e^{-2\pi i x k}\, \delta(x)\, dx = e^{-2\pi i (0) k} = 1$$

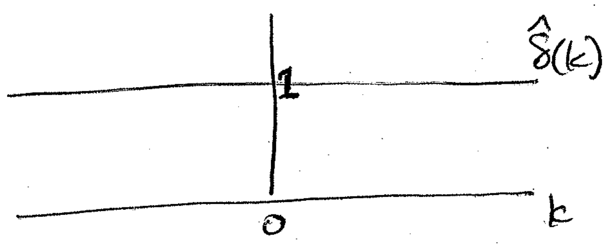
or more generally

$$\hat{\delta}_{x_0}(k) = \int_{-\infty}^{\infty} e^{-2\pi i x k}\, \delta(x-x_0)\, dx = e^{-2\pi i x_0 k}$$

real space



Fourier space (frequency domain)



constant across all wave #s

Fourier Series (FS)

Idea: write a function (periodic) in terms of sins and coss

$$f(x) = \sum_{k=-\infty}^{\infty} a_k e^{ikx} \quad \text{where} \quad a_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x) e^{-ikx}\,dx$$

$\Rightarrow$ If want FS representation of $\delta(x)$:

Let $f(x) = \delta(x)$ $\quad \Rightarrow a_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} \delta(x) e^{ikx}\,dx = \frac{1}{2\pi}$

$$\Rightarrow \delta(x) = \sum_{k=-\infty}^{\infty} \frac{1}{2\pi} e^{ikx}$$

$$= \lim_{N\to\infty} \sum_{k=-N}^{N} \frac{1}{2\pi} e^{ikx}$$

$$= \lim_{N\to\infty} \left(1 + e^{ix} + e^{-ix} + \dots + e^{iNx} + e^{-iNx}\right)\frac{1}{2\pi}$$

$$= \lim_{N\to\infty} \frac{1}{2\pi}\left(1 + e^{ix} + e^{i2x} + \dots + e^{i2Nx}\right) e^{-iNx}$$

$$= \lim_{N\to\infty} \frac{1}{2\pi} e^{-iNx}\left[\frac{1 - e^{ix(2N+1)}}{1 - e^{ix}}\right] \cdot \frac{e^{-i\frac{1}{2}x}}{e^{-i\frac{1}{2}x}}$$

$$= \lim_{N\to\infty} \frac{1}{2\pi} \frac{e^{-i(N+\frac{1}{2})x} - e^{i(N+\frac{1}{2})x}}{e^{-i\frac{1}{2}x} - e^{i\frac{1}{2}x}}$$

$$= \lim_{N\to\infty} \frac{1}{2\pi} \frac{\sin((N+\frac{1}{2})x)}{\sin(\frac{1}{2}x)}$$

* just another sequence of fncs leading to δ-fnc.

(if $x = 0 \Rightarrow \lim_{N\to\infty} \frac{1}{2\pi}(2N+1)$)

* Also, if $\delta(x-x_0)$ $\Rightarrow a_k = \frac{1}{2\pi} e^{-ikx_0}$

and $\delta(x-x_0) = \sum_{k=-\infty}^{\infty} \frac{1}{2\pi} e^{ik(x-x_0)}$

Higher dimensions:

$\delta(\vec{x}) = \delta(x_1)\delta(x_2)\dots\delta(x_n)$ if $\vec{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$

Green's functions and ODEs

A Green's function of a linear differential operator is defined:

$L[G(x,s)] = \delta(x-s)$ where L is a linear differential operator (in terms of x)

ex) $L = -\frac{d^2}{dx^2} + a^2$ $\Rightarrow L[G(x,s)] = -\frac{d^2 G(x,s)}{dx^2} + a^2 G(x,s) = \delta(x-s)$

Having the Green's function allows us to solve equations of the type:

$L[u(x)] = f(x)$

since $\int_{-\infty}^{\infty} L[G(x,s)]\, f(s)\,ds = \int_{-\infty}^{\infty} \delta(x-s) f(s)\,ds = f(x)$

$\Rightarrow L[u(x)] = \int_{-\infty}^{\infty} L[G(x,s)] f(s)\,ds$

$= L\left[\int_{-\infty}^{\infty} G(x,s) f(s)\,ds\right]$

so $u(x) = \int_{-\infty}^{\infty} G(x,s) f(s)\,ds$

So in our example:

need to solve for $G(x,s)$

$$-\frac{d^2G(x,s)}{dx^2} + a^2 G(x,s) = \delta(x-s)$$

~~take FT (in x)~~ $\cancel{-(ik)^2\hat{G}(k,s) + a^2\hat{G}(k,s) = \hat{\delta}}$

take FT (in x)

$$-(ik)^2\hat{G}(k,s) + a^2\hat{G}(k,s) = \hat{\delta}_s(k) = e^{-2\pi isk}$$

$$\hat{G}(k,s)\left(-(ik)^2 + a^2\right) = e^{-2\pi isk}$$

$$\hat{G}(k,s) = \frac{e^{-2\pi isk}}{-(ik)^2 + a^2}$$

$\Rightarrow$ just take inverse FT to get $G(x,s)$

$\Rightarrow$ can solve $\cancel{-\frac{d^2G(x,s)}{dx^2} + a^2G(x,s) = f(x)}$

$$\frac{d^2u(x)}{dx^2} + a^2u(x) = f(x)$$

as $u(x) = \int_{-\infty}^{\infty} G(x,s)f(s)\,ds$

$\Rightarrow$ Approximations using Particles:

$u(x) \approx \sum G(x, x_p) f(x_p) h$ where h is mesh size from before.

<u>Summarize</u>

Integrals

evaluate fncs through delta fncs
$f(x) = \int f(y)\delta(x-y)\,dy$

soln to ODE/PDE through Green's fncs
$*\left(u(x) = \int_{-\infty}^{\infty} G(x,s) f(s)\,ds\right)$

~~Then~~ In both cases
<u>PARTICLES</u>
can be used as quadrature pts to approximate these integrals

Smooth Approximations to the δ-function

So we have shown

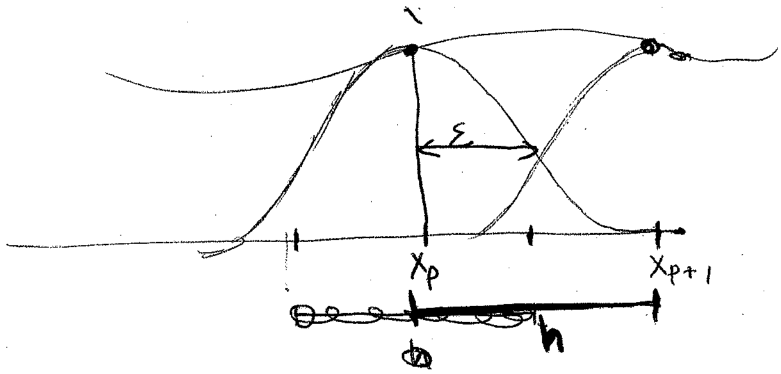
$$f(x) \approx \sum_p f(x_p)\, h\, \delta(x-x_p) \qquad (\text{in 1D})$$

Now let $w_p = f(x_p)h$ $\Rightarrow$ $f(x) \approx \sum_{p=1}^{N} w_p\, \delta(x-x_p) \equiv f^h(x)$ (in 1D)

weights

$\Rightarrow$ we can approximate the $\delta(x-x_p)$ w/ some smooth fnc ξ_ε

$$f(x) \approx f^h(x) \approx f^{\varepsilon}_{h}(x) \equiv \sum_{p=1}^{N} w_p\, \xi_\varepsilon(x-x_p)$$



Ex $\xi_\varepsilon = \xi\left(\frac{\|x\|}{\varepsilon^d}\right)\frac{1}{\varepsilon^d} = \xi\left(\frac{\|x\|}{\varepsilon}\right)\frac{1}{\varepsilon}$ $d \to$ dim

when $d=1$

and let $\xi(x) = \dfrac{e^{-x^2}}{(\pi/2)}$

$\varepsilon \to$ smoothing length so as $\varepsilon \to 0$ $\xi_\varepsilon \to \delta \Rightarrow$ point particles

(if $d>1 \Rightarrow f(x) \approx \sum_p \underbrace{f(x_p)h^d}_{w_p}\, \xi_\varepsilon(x-x_p)$)

often h will be called the volume of the particle!

$\Rightarrow$ For smooth particle methods we have 2 length scales:

1. Volume/distance btn particles
2. Smoothing Length

Error

$$|f(x) - f_\varepsilon^h(x)| = |f(x) - f_\varepsilon(x) + f_\varepsilon(x) - f_\varepsilon^h(x)|$$

$$\leq \underbrace{|f(x) - f_\varepsilon(x)|}_{\text{1 (SMOOTHING ERROR) MOLLIFICATION ERROR}} + \underbrace{|f_\varepsilon(x) - f_\varepsilon^h(x)|}_{\text{2 DISCRETIZATION ERROR}}$$

1. Mollification error - related to δ being approximated by ζ_ε

$$\left| \int_{-\infty}^{\infty} f(y)\,\delta(x-y)\,dy - \int_{-\infty}^{\infty} f(y)\,\zeta_\varepsilon(x-y)\,dy \right|$$

2. Discretization error - error made by quadrature

$$\left| \int_{-\infty}^{\infty} f(y)\,\zeta_\varepsilon(x-y)\,dy - \sum_{p=1}^{N} w_p\,\zeta_\varepsilon(x-x_p) \right|$$