Computational Physics

Basic Equations of MHD

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\vec{v}) = 0, \quad \frac{\partial(\rho\vec{v})}{\partial t} + \nabla\cdot\left[\rho\vec{v}\vec{v} - \vec{B}\vec{B} + P^*\right] = 0, \quad \frac{\partial E}{\partial t} + \nabla\cdot\left[\left(E+P^*\right)\vec{v} - \vec{B}(\vec{B}\cdot\vec{v})\right] = 0,$$

$$P^* = P + \frac{\vec{B}\cdot\vec{B}}{2} \qquad E = \frac{P}{\gamma-1} + \frac{\rho(\vec{v}\cdot\vec{v})}{2} + \frac{\vec{B}\cdot\vec{B}}{2}$$

What can a computer do? $+, -, \div, \times$

need to convert $\int, \frac{d}{dq}, \frac{\partial}{\partial q}, \vec{\nabla}, \vec{\nabla}\cdot, \vec{\nabla}\times \rightarrow +, -, \div, \times$

Basics → Bit yes/no, True/False, 0/1

Byte → 8 bits 8 yes or no

Single → 32 bits, 4 bytes → 7 digits $3.4\cdot10^{38}$

double → 64 bits 8 bytes → 15 digits $1.8\cdot10^{308}$

Example above $\rho, \vec{v}, \vec{B}, E, P$ → 9 Variables 36 and 72 bytes to store

1 grid point

Problems are solved on grids

1D 512 array 36,864 bytes 1 Time Step, 36,864,000 bytes 1000 Steps

2D ~ 18.9 gigabytes

3D ~ 9.7 Terabytes

gridding, data storage important AMR

$0 \sim 0$ $\quad 1 - 1$ $\quad 2 - 10$ $\quad 3 - 11$ $\quad 8 \sim 1000$

$\quad\quad\quad\quad 2^0 \quad\quad 2^1+0 \quad\quad 2^1+2^0 \quad\quad 2^3+0+0+0$

$125_{10} \to 1\cdot 10^2 + 2\cdot 10^1 + 5\cdot 10^0$

$125_2 \to 1111101 \to 2^6+2^5+2^4+2^3+2^2+0+2^0 = 64+32+16+8+4+0+1 = 125$

Fractions? $\frac{1}{3} \approx .01010101$

$0+\frac{1}{2^2}+0+\frac{1}{2^4}+0+\frac{1}{2^6}+0+\frac{1}{2^8} = \frac{1}{4}+\frac{1}{16}+\frac{1}{64}+\frac{1}{256} = .332031$ in Single

$\neq \frac{1}{3}$ rounding error. Only numbers of the form $\sum \frac{1}{2^n}$ are exact

<u>Error</u>

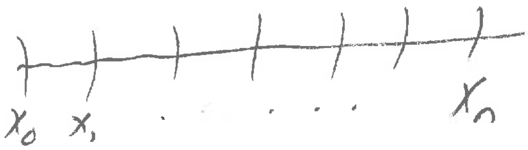
non integers are generally NOT exact.

Lets Start how to go from $\frac{dF}{dx}$ to $+, -, \div, \times$

$$\frac{dF}{dx} = \lim_{h\to 0} \frac{F(x+h)-F(x)}{h} \quad \text{also} \quad \frac{F(x)-F(x-h)}{h}$$

just Slope of Tangent line

define a 1D grid



define $F(x_i)$ on grid $\quad \frac{dF}{dx} \sim \frac{F(x+h)-F(x)}{h}$

where $h \neq 0$ $\quad$ Clearly x_0 or x_n is lost

Pseudo code $\dfrac{F(x) - np.Roll(F(x),-1)}{h} \simeq \dfrac{dF}{dx}$

board example x^2 10 grid points

Code example $h\downarrow$ Still ugly at 0, have to be careful here. Problem $\dfrac{dF}{dx}$ not equal $\dfrac{F(x+h)-F(x)}{h}$ if $h=0$

in computer, $h=0$ = problem

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how to construct approximations and Truncation error.

Start here Taylor Expansions

$$F(x+h) = F(x) + \frac{\partial F}{\partial x} h + \frac{\partial^2 F}{\partial x^2}\frac{h^2}{2!} + \cdots \frac{\partial F}{\partial x^n}\frac{h^n}{n!}$$

$h \longleftrightarrow \Delta x$

$$\underbrace{\frac{F(x+h) - F(x)}{h} = \frac{\partial F}{\partial x}}_{\text{approximation}} + \underbrace{F''\frac{h}{2!} + \cdots F^n\frac{h^{n-1}}{n!}}_{\text{Truncation error}}$$

Forward difference

$$F(x-h) = F(x) - F'(x)h + \frac{F''(x)h^2}{2!} - \frac{F'''(x)h^3}{3!} + \cdots \frac{F^n(x)}{n!}(-h)^n$$

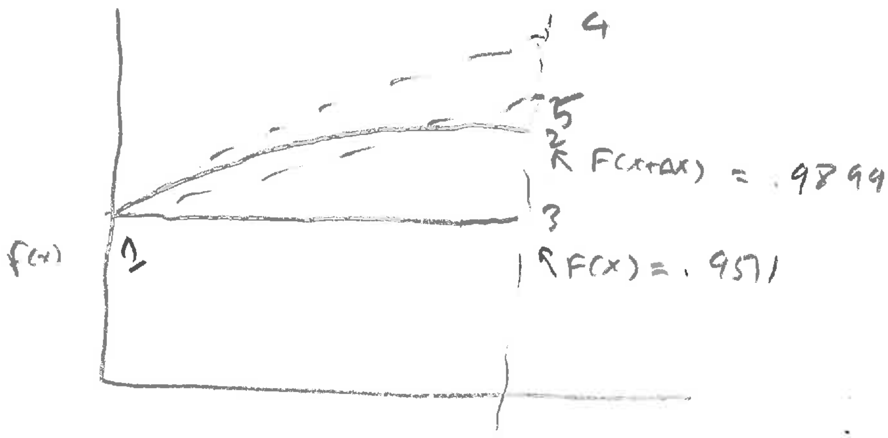
$$\frac{F(x) - F(x-h)}{h} = F'(x) - \frac{F''(x)h^2}{2!} + \frac{F'''(x)h^3}{3!} - \cdots \frac{F^n(x)}{n!}(-h)^n$$

backward difference

Example $F(x) = \sin(2\pi x)$

$X = .2 \quad F(.2) = .9511$

$F(.22), \ \Delta x = .02 = .9899$



2 = $F(x+h)$ 3. $F(x)$ 4. $F(x) + F'(x)\Delta x$ .9899 .775% error

5 = $F(x) + F'(x)\Delta x + F''(x)\frac{\Delta x^2}{2}$ = .9824 = .01% error

Truncation error

$$\frac{dF}{dx} = \underbrace{\frac{F(x+h) - F(x)}{h}}_{\text{approximation}} \underbrace{- \frac{F''h}{2} - \frac{F'''}{6}\frac{h^2}{6} + \cdots}_{\text{Truncation error}}$$

There is ALWAYS error

Can we do better?

A $\quad F(x+\Delta x) = F(x) + F'\Delta x + \frac{F''\Delta x^2}{2} + F'''\frac{\Delta x^3}{3!} + \cdots F^n(x)\frac{\Delta x^n}{n!}$

B $\quad F(x-\Delta x) = F(x) - F'(x)\Delta x + F''\frac{(x)\Delta x^2}{2} - F'''\frac{(x)\Delta x^3}{3!} + \cdots F^n(x)\frac{(-\Delta x)^n}{n!}$

$A-B = 2F'\Delta x + O(\Delta x)^2$

error $\sim \Delta x^2$ not Δx

or $\quad \frac{F(x+\Delta x) - F(x-\Delta x)}{2\Delta x} = \frac{dF}{dx} + O(\Delta x^2)$ Truncation error

Central difference

Vs $\quad \frac{F(x+\Delta x) - F(x)}{\Delta x} = \frac{dF}{dx} + O(\Delta x)$ Truncation error

$\Delta x = .1$ FD BD .1 error CD $\sim (.1)^2$ error

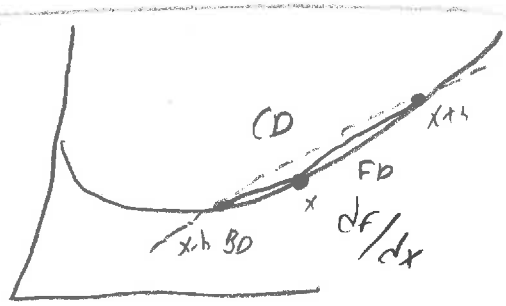
4th order $\quad F'(x) = \frac{-F(x+2h) + F(x+h) - 8F(x-h) + F(x-2h)}{12h} + O(h)^4$ Truncation error

how to derive? Change $\Delta x \rightarrow 2\Delta x, 3\Delta x$ in A and B

add subtract

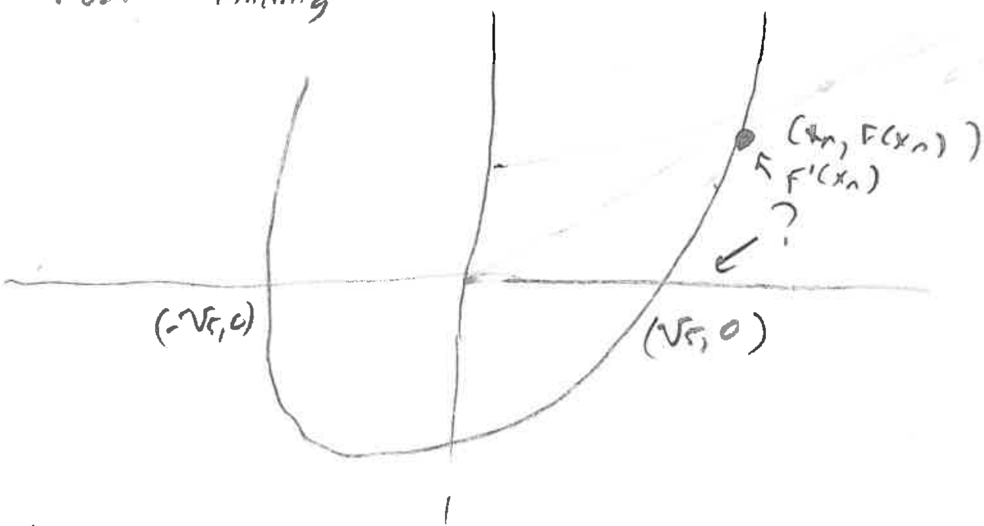
Segue Newton's Method

$\downarrow$



$x^2 = 5$? how about $x^2 - 5 = 0$

root Finding



Point Slope Formula $y - y_1 = m(x - x_1)$ $m =$

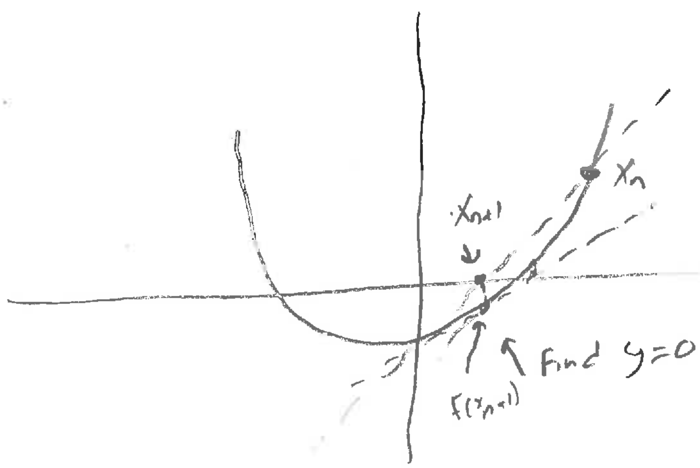
$$y - F(x_n) = F'(x_n)(x - x_n)$$

$$y = F'(x_n)(x - x_n) + F(x_n)$$

$$F'(x_n)(\underset{\uparrow \, x_{n+1}}{x} - x_n) + F(x_n) = 0$$

Solve $x_{n+1} = x_n - \dfrac{F(x_n)}{F'(x_n)}$

Iterate



guess root, The better the guess the Faster the convergence.

$x^2=5 \to F(x)=x^2-5$ Answer = 2.23607

$x=\pm\sqrt{5}$ $\sqrt{4}<\sqrt{5}<\sqrt{9}$ Try 2.5 For x_n

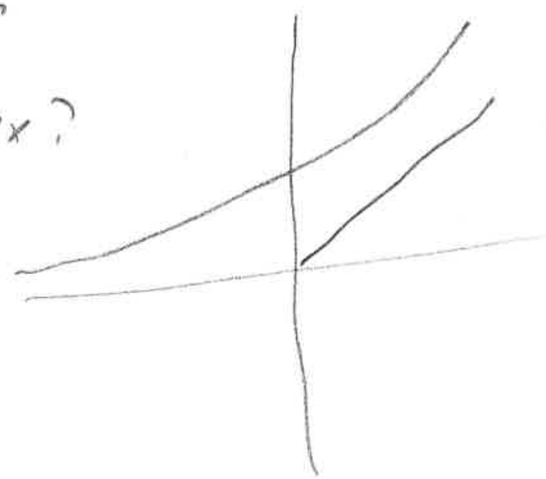
$$x_{n+1} = x_n - \frac{F(x_n)}{F'(x_n)} = x_n - \frac{(x_n^2-5)}{(2x_n)} = 2.5 - .25 = 2.25$$

$\frac{x_{n+1}}{real} = 1.00623$

$2.25 - .013889 = 2.23611 = x_{n+2}$ $\frac{x_{n+2}}{real} = 1.00002$

good enough

Pathological → $e^x = 2x$?



no intersection

Next 2nd order derivatives, Partial derivatives,

Vector Operations.

2nd order: 2 ways (infinite actually)

1: Treat $\frac{dF}{dx}$ as $g(x)$ and repeat or

Taylor Expansion again

$$F(x+\Delta x) \approx F(x) + F'(x)\Delta x + \frac{F''(x)}{2}(\Delta x)^2 + \frac{F'''(x)}{6}(\Delta x)^3 + \dots$$

$$F(x-\Delta x) = F(x) - F'(x) + \frac{F''(x)(\Delta x)^2}{2} - \frac{F'''(x)(\Delta x)^2}{6} + \dots$$

$$F(x+\Delta x) + F(x-\Delta x) \approx 2F(x) + F''(x)(\Delta x)^2 + \dots$$

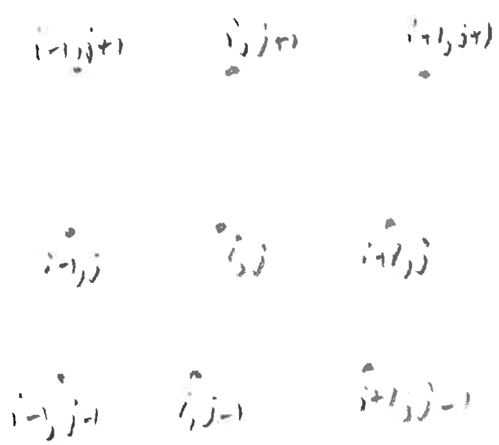
$$\boxed{\frac{F(x+\Delta x) + F(x-\Delta x) - 2F(x)}{\Delta x^2} \approx F''(x)}$$

Mixed Partial derivatives $\frac{\partial^2 F}{\partial x \partial y}$

Need a 2 D Grid!

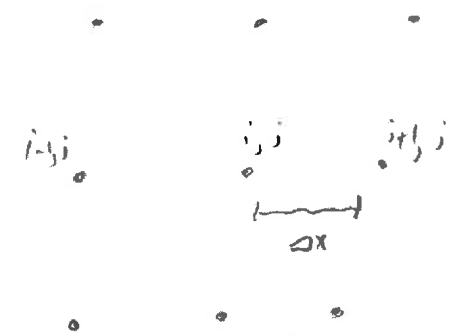
Now $F = F(x,y)$

going to Switch Notation now For convenience
also, assume $\Delta x = \Delta y$ harder otherwise.



$F(x,y) = U(x,y)$

representations



$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u}{\Delta x} \quad \text{Forward}$$

$$= \frac{u_{i,j} - u_{i-1,j}}{\Delta x} \quad \text{backward}$$

$$\boxed{\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2}}$$

$$= \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}$$

A $\quad U_{i+1,j} = U_{i,j} + (u')_{i,j}\,\Delta x + \frac{(u'')_{i,j}\,\Delta x^2}{2} + \cdots \frac{(u^n)_{i,j}(\Delta x^n)}{n!}$

Note ' wrt x

B $\quad U_{i-1,j} = V_{i,j} - (u')_{i,j}\,\Delta x + (u'')_{i,j}\frac{(-\Delta x)^2}{2} + \cdots \frac{(u^n)_{i,j}(-\Delta x)^n}{n!}$

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} = \left(\frac{\partial u}{\partial y}\right)_{i,j} + \left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j}\Delta x + \left(\frac{\partial^3 u}{\partial x^2 \partial y}\right)_{i,j}\frac{(\Delta x)^2}{2} + \cdots$$

$$\left(\frac{\partial u}{\partial y}\right)_{i-1,j} = \left(\frac{\partial u}{\partial y}\right)_{i,j} - \left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j}\Delta x + \left(\frac{\partial^3 u}{\partial x^2 \partial y}\right)_{i,j}\frac{(\Delta x)^2}{2} + \cdots$$

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} - \left(\frac{\partial u}{\partial y}\right)_{i-1,j} = 2\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j}\Delta x$$

$$\frac{\overset{1}{\left(\frac{\partial u}{\partial y}\right)_{i+1,j}} - \overset{2}{\left(\frac{\partial u}{\partial y}\right)_{i-1,j}}}{2\,\Delta x} = \left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j} + O(\Delta x^2)$$

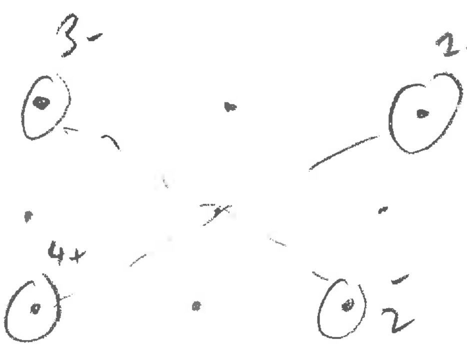
1 $\frac{\partial u}{\partial y}$ at i+1

use centered

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} = \frac{u_{i+1,j+1} - u_{i+1,j-1}}{2\Delta y}$$

$\frac{\partial u}{\partial y}$ at i-1 $= \left(\frac{\partial u}{\partial y}\right)_{i-1,j} = \dfrac{u_{i-1,j+1} - u_{i-1,j-1}}{2\Delta y}$

$$\boxed{\text{So } \left(\frac{\partial^2 u}{\partial x, \partial y}\right)_{i,j} = \frac{\overset{1}{u_{i+1,j+1}} - u_{i+1,j-1} - u_{i-1,j+1} + \overset{4}{u_{i-1,j-1}}}{4\,\Delta x \Delta y} + O\left[(\Delta x)^2, (\Delta y)^2\right]}$$



$$\frac{(1+4) - (2+3)}{4\,\Delta x \Delta y}$$

We will return to the topic of mixed and 2nd order derivatives later. For now, you should be starting to see how we numerically compute

$\vec{\nabla} F$, $\nabla^2 F$, $\nabla \cdot \vec{A}$, $\vec{\nabla} \times \vec{A}$

Ex $\rightarrow$ $\vec{\nabla} \times \vec{A} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \partial_x & \partial_y & \partial_z \\ A_x & A_y & A_z \end{vmatrix}$ Ex $\vec{A} = A_x \hat{i} + A_y \hat{j}$

$\vec{\nabla} \times \vec{A} = \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \hat{k}$

= np.gradient(Ay, dx)

− np.gradient(Ax, dy)

We've come farther than you think!

$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$ 1 D heat conduction

Time marching

FD good

BD/CD No good

$\frac{\partial T}{\partial t} \sim \frac{T_i^{n+1} - T_i^n}{\Delta t}$ $\left(\frac{\partial^2 T}{\partial x^2} \right)_i^n \sim \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta x)^2}$

$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = 0 = \left[\frac{T_i^{n+1} - T_i^n}{\Delta t} - \alpha \frac{(T_{i+1}^n - 2T_i^n + T_{i-1}^n)}{(\Delta x)^2} \right]$$

Solve

Truncation error $\xrightarrow{+}$ $\left[-\left(\frac{\partial^2 T}{\partial t^2} \right)_i^n \frac{\Delta t}{2} + \alpha \left(\frac{\partial^4 T}{\partial x^4} \right)_i^n \frac{(\Delta x)^2}{12} + \dots \right]$ (11)

1st order in time 2nd order in space.

All you need is appending and a for loop.

LATER !!!

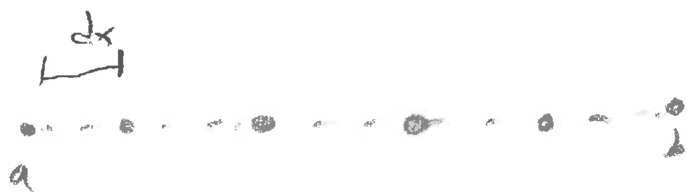
Integrals $\int F(x)\,dx$? No

$$\int_a^b F(x)\,dx, \quad \int_0^x F(x)\,dx = G(x), \quad \int_{-\infty}^{\infty} F(x)\,dx, \quad \int_c^d \int_{a(x)}^{b(x)} F(x,y)\,dx\,dy$$

Yes

Fundamentally

$$\lim_{dx \to 0} \sum F(x)\,dx = \int F(x)\,dx$$



define $F(x) = x^2$

$$\int_0^1 x^2\,dx = \frac{x^3}{3}\Big|_0^1 = \frac{1}{3}$$

Let's do this by hand

With n= 10 1.9% accuracy. We can do better but later.

How about $G(x) = \int_0^x F(x)\,dx$?

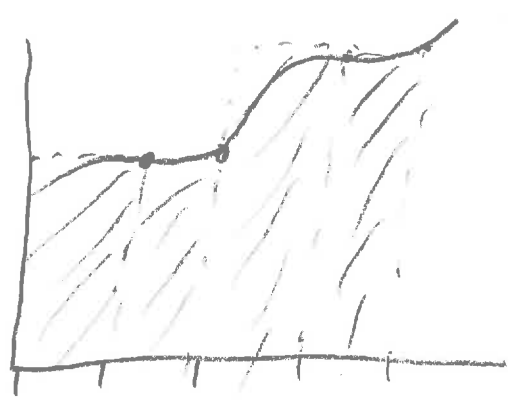

```
G(x) =    out = np.zeros(len(x))
          for i in range (0,num)
               out[i] = sum (F[0:i] . dx)
          return out
```

iterate

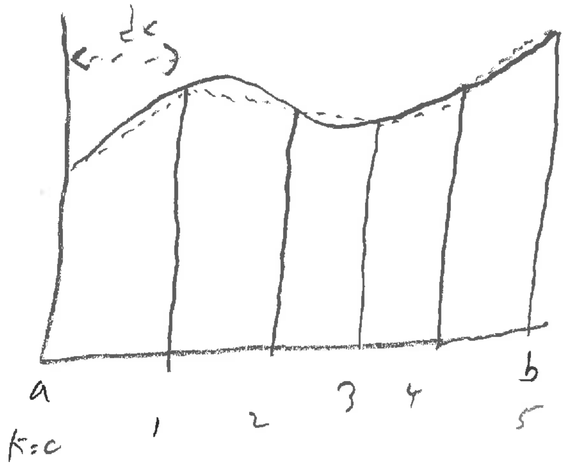
Can We do better?

$\int \sim \sum F(x)\,dx$

Squares



Trapezoidal Rule



book example

$$A_k = \frac{1}{2} dx \left[F(a+(k-1)dx) + F(a+k\,dx) \right]$$

$N = 10 \quad k \in 1, 10$

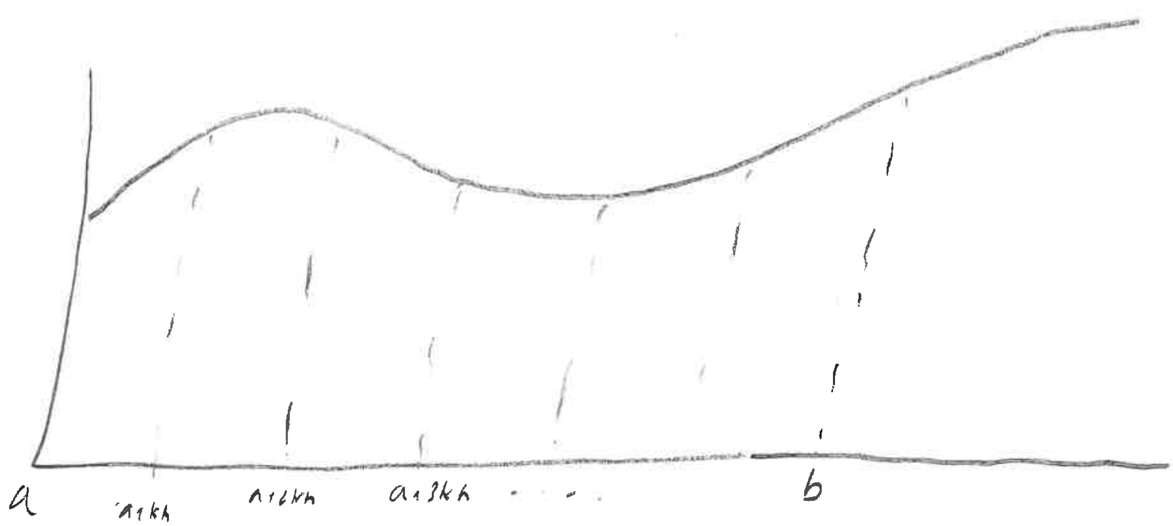
$$I(a,b) \simeq \sum_{k=1}^{N} \frac{1}{2} dx \sum_{k=1}^{N} F(a+(k-1)dx) + F(a+k\,dx)$$

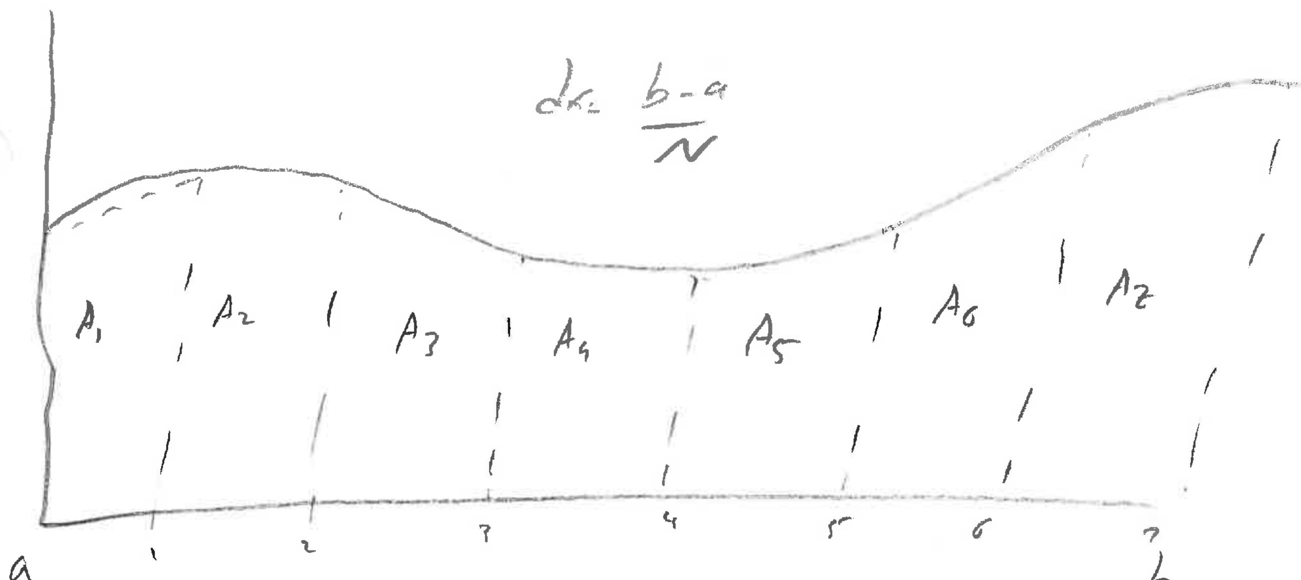
$$= \frac{1}{2} dx \left[F(a) + 2F(a+h) + 2F(a+2h) + \cdots \right]$$

$$\boxed{= dx \left[\frac{1}{2} F(a) + \frac{1}{2} F(b) + \sum_{k=1}^{N-1} F(a+kh) \right]}$$

How about $I(a,x)$?

Trickier, Let's be careful





$$A_1 = \frac{1}{2} dx \left(F(a) + F(a+dx) \right)$$

$$A_2 = \frac{1}{2} dx \left(F(a+dx) + F(a+2dx) \right)$$

$$A_3 = \frac{1}{2} dx \left(F(a+2dx) + F(a+3dx) \right)$$

$$A_7 = \frac{1}{2} dx \left(F(a+6dx) + F(b) \right)$$

$$I(a,x) = dx \left[\frac{1}{2} F(a) + \frac{1}{2} F(x) + \sum_{k=1}^{N-1} F(a+k\,dx) \right]$$

$$I(0) = \frac{1}{2} F(a)$$

$$I(1) = \frac{1}{2} \left(F(a) + F(a+dx) \right)$$

---

can be made with non constant dx

need IF statements

Next Simpsons, Romberg integration, improper integrals, infinite limits

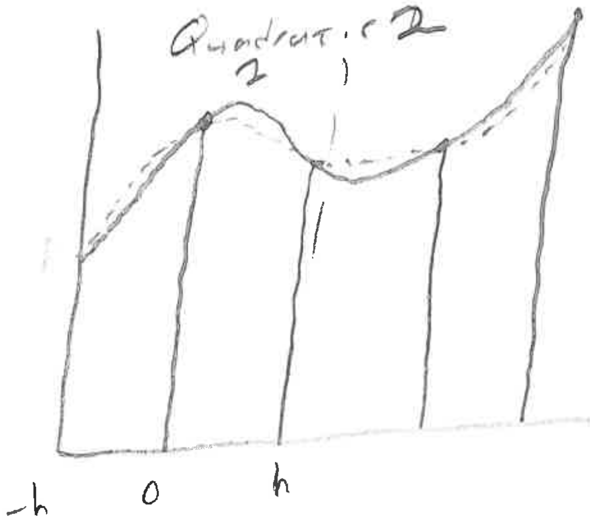
OK

1 pt

$\sum F(x)\,dx$  Trapezoid

2 pts 3 ?

SIMPSON'S RULE



$Ax^2+Bx+C = F(x)$

$F(h) = Ah^2+Bh+C$

$F(0) = C$

$F(-h) = Ah^2-Bh+C$

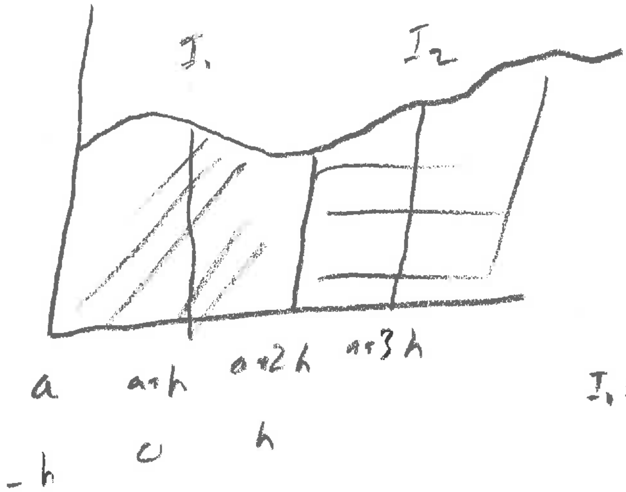
$$A = \frac{1}{h^2}\left[\frac{1}{2}F(-h) - F(0) + \frac{1}{2}F(h)\right],$$

$$B = \frac{1}{2h}\left[F(h) - F(-h)\right], \quad C = F(0)$$

$$\int_{-h}^{h}(Ax^2+Bx+C)\,dx = \frac{2}{3}Ah^3 + 2Ch = \frac{1}{3}h\left[F(-h) + 4F(0) + F(h)\right]$$

$I(a,x)$ Start at $x = a$

↓



$$\frac{1}{3}h\left[F(-h) + 4F(0) + F(h)\right]$$

$$\downarrow$$

$$I_1 = \frac{1}{3}h\left[F(a) + 4F(a+h) + F(a+2h)\right]$$

$$I_2 = \frac{1}{3}h\left[F(a+2h) + 4F(a+3h) + F(a+4h)\right]$$

$$+$$

$$I(a,x) = \frac{1}{3}h\left[F(a) + F(x) + 4\sum_{k=1}^{N/2} F(a+(2k-1)h) + 2\sum_{k=1}^{N/2-1} F(a+2kh)\right]$$

$$\text{or} = \frac{1}{3}h\left[F(a) + F(x) + 4\sum_{\substack{k\text{ odd}\\1\ldots N-1}} F(a+kh) + 2\sum_{\substack{k\text{ even}\\2\ldots N-2}} F(a+kh)\right]$$

Code I(a,x)

Note even = a[2:num-1:2] Then 4*sum(odd)
odd = a[1:num:2] 2*sum(even)

MUCH Faster.

For loops suck