Numerical Methods: If your (difficult) problem can not be solved by the regular math you've learned so far, solve it approximately by simple operations.

Numerical methods:

- do not represent the physics of the problem
- need a mathematical model
- need a numerical scheme
- are not always reliable
- can be computationally demanding
- can be very fast flexible economical
- approximate answer

input → Algorithm → output

(a series of strictly defined operations)

Estimating Error:

Error: ε

absolute true error → $\varepsilon_{at} = \left| \text{true answer} - \text{calculated result} \right|$

relative true error → $\varepsilon_{rt} = \dfrac{\varepsilon_{at}}{|\text{true}|}$ can be percentile

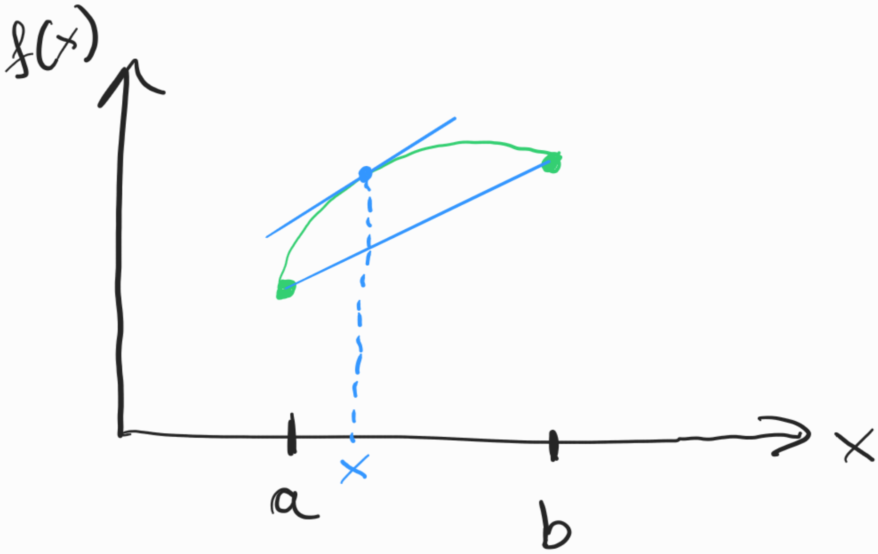
true answer is unknown → approximate error

absolute approximate error $\varepsilon_{aa} = |\text{result}_i - \text{result}_{i-1}|$

relative approximate error $\varepsilon_{ra} = \dfrac{\varepsilon_{aa}}{|\text{result}_i|}$

Tolerance: How much error can we accept?

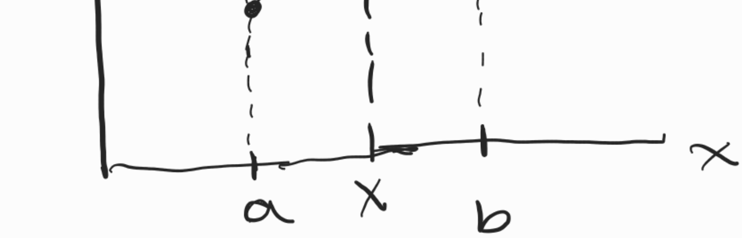
Mean Value Theorem for the Derivative



$$\exists x \in (a,b)$$

$$f'(x) = \frac{f(b)-f(a)}{b-a}$$

First Law of the Mean



$$\exists x \in (a,b)$$

$$\int_a^b f(x)\,dx = (b-a)\cdot f(x)$$

if $f(x) \leq M$ between $(a,b) \Rightarrow \int_a^b f(x)\,dx \leq (b-a)\cdot M$

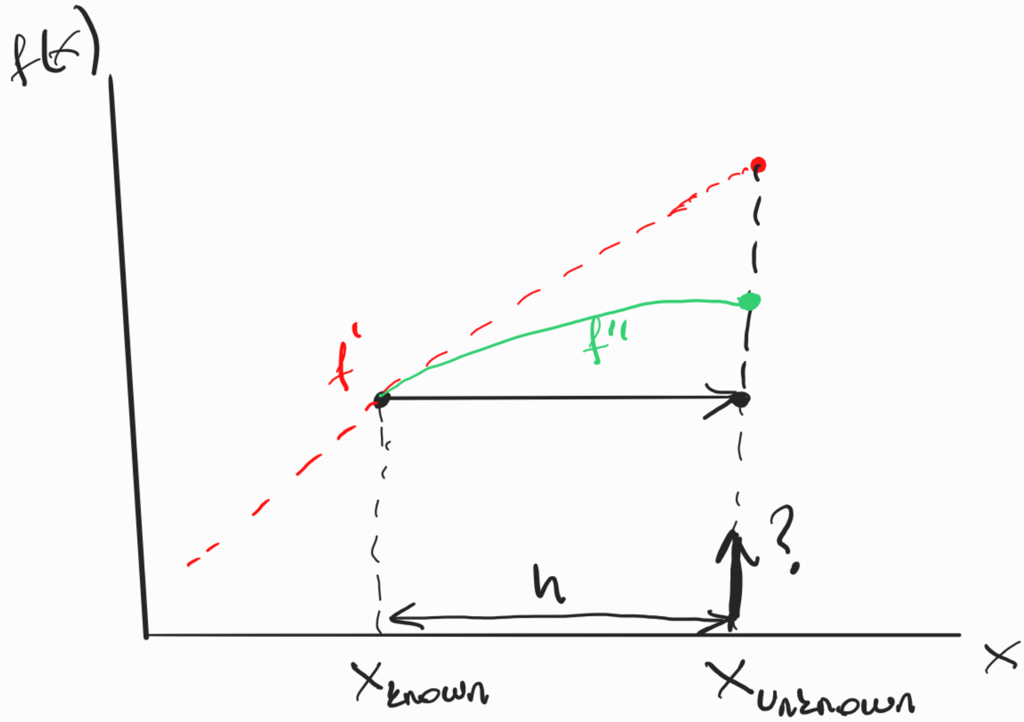
Rolle's Theorem

if $f(a) = f(b)$

$\exists\, x \in (a,b)$

$f'(x) = 0$

Taylor's Expansion



$f'(x_k)$ is known

$f''(x_k)$

f'''

h is small

$$\underbrace{\underbrace{f(x_u) \cong f(x_k)}_{\text{0th order}} + h \cdot f'(x_k) + \frac{h^2}{2!} f''(x_k)}_{\text{2nd order}} + \frac{h^3}{3!} \cdot f'''(x_k)$$

f is same everywhere

f' is constant

f'' ~~is constant~~

nth order

$$f(x_u) = \sum_{i=0}^{n} \frac{(x_u - x_k)^i}{i!} \cdot \left.\frac{d^i f}{dx^i}\right|_{x=x_k} + \frac{(x_u - x_k)^{n+1}}{(n+1)!} \left.\frac{d^{n+1} f}{dx^{n+1}}\right|_{x=x}$$

Order of error = n+1

Order of approximation ↑ truncation error ↓

$\rightarrow f' = 0$ olursa oluyor galiba

truncation error: error due to the absence of remaining iterations or terms

$$f(x_i) = f(x_{i-1}) + f'(x_{i-1})(x_i - x_{i-1}) + f''(x_{i-1})\frac{(x_i - x_{i-1})^2}{2} + \ldots$$

Taylor series where $x_\ell = 0$ is also called Maclaurin series

Reminder;

$$f(x_u) = f(x_\ell) + f'(x_\ell)(x_u - x_\ell) + \frac{f''(x)}{2!}(x_u - x_\ell)^2 \ldots$$

$$\sin x = \sin 0 + \cos 0 \cdot x + -\sin 0\left(\frac{x^2}{2!}\right) + -\cos 0 \cdot \frac{x^3}{3!} \ldots$$

around $x_\ell = 0$

$$= x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \frac{x^9}{9!} - \frac{x^{11}}{11!} + \ldots$$

e^{2x} at $x_u = 0.5$

$x_\ell = 0$

Taylor

$$f(x_u) = f(x_\ell) + f'(x_\ell)\cdot(x_u - x_\ell) + \frac{f''(x_\ell)}{2!}(x_u - x_\ell)^2 \ldots = \sum_{i=0}^{n} \frac{(x_u - x_\ell)^i}{i!} \left.\frac{d^i f}{dx_i}\right|_{x = x_\ell}$$

$$e^{2x} = 1 + 2x + 4\frac{x^2}{2!} + 8\frac{x^3}{3!} + \ldots + 2^i\frac{x^i}{i!} \ldots$$

n	i^{th} term	$f(x_u)=\sum_{i=0}^{n}$ terms	ε_{at}
0	1	1	1.71828
1	1	2	0.71828
2	0.5	2.5	0.21828
3	0.16667	2.6667	0.05162
4	0.04167	2.70833	0.00995
5	0.00833	2.71667	0.00162
6	0.00139	2.71806	0.00023

error is decreasing as you add calculation steps

$\Downarrow$

convergence

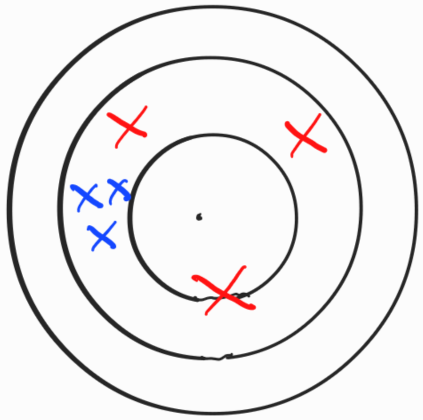
$\pi \approx 3.14 \rightarrow$ more accurate

$\approx 3.1782 \mp 0.00005 \rightarrow$ more precise

accuracy: How close to the true answer

precision: How detailed is your answer

they don't guarantee each other but precision helps accuracy



Precise

accurate

Significant Figures

0.19 2 s.f.

3.14 4 s.f. between 3.135 and 3.145

3.140 4 s.f. between 3.1395 and 3.1405

3.14
0.01 precision = correct to 2 decimal digits

$$t$$

$$\text{error} = \mp \frac{10^{-t}}{2}$$

rounding

3.134 → 3.13

→3.135 → 3.14 (çift tarafa yuvarlanır 5 ile bitiyorsa)

3.136

3.144

→3.145

3.14501 → 3.15

3.14 3 s.f. between 3.135 and 3.145

3.140 4 s.f. between 3.1395 and 3.1405 ∓ 0.0005

(0.001 precision)

0.02 1 s.f. between 0.015 and 0.025

∓ 0.005 abs. error

25% relative error

Errors in each number accumulate over calculations

$$\begin{array}{rl} & 3.14 \mp 0.005 \\ + & 2.72 \mp 0.005 \\ \hline & 5.86 \mp 0.01 \\ & 0.005 \end{array}$$

$$f(x \mp \Delta x, y \mp \Delta y, z \mp \Delta z) = f(x, y, z) \mp (f_x \Delta x + f_y \Delta y + f_z \Delta z)$$

single precision: 7 sig. fig.

double precision: 15 sig. fig.

Non-linear equations with single variable

Bracketing Methods

Bound the root in an interval and shrink the interval at every calculation step

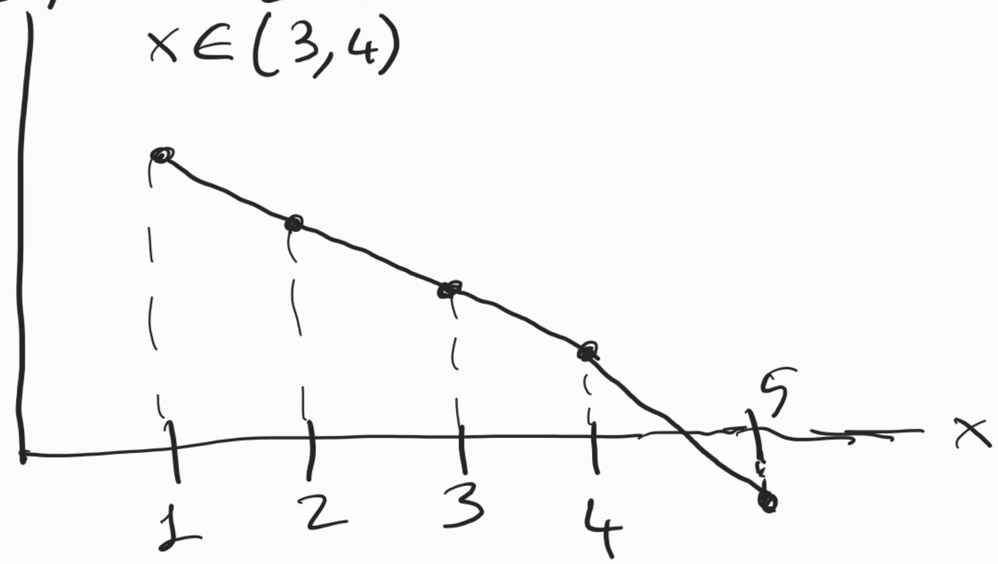
Open Methods

Taylor series like extrapolation from known points

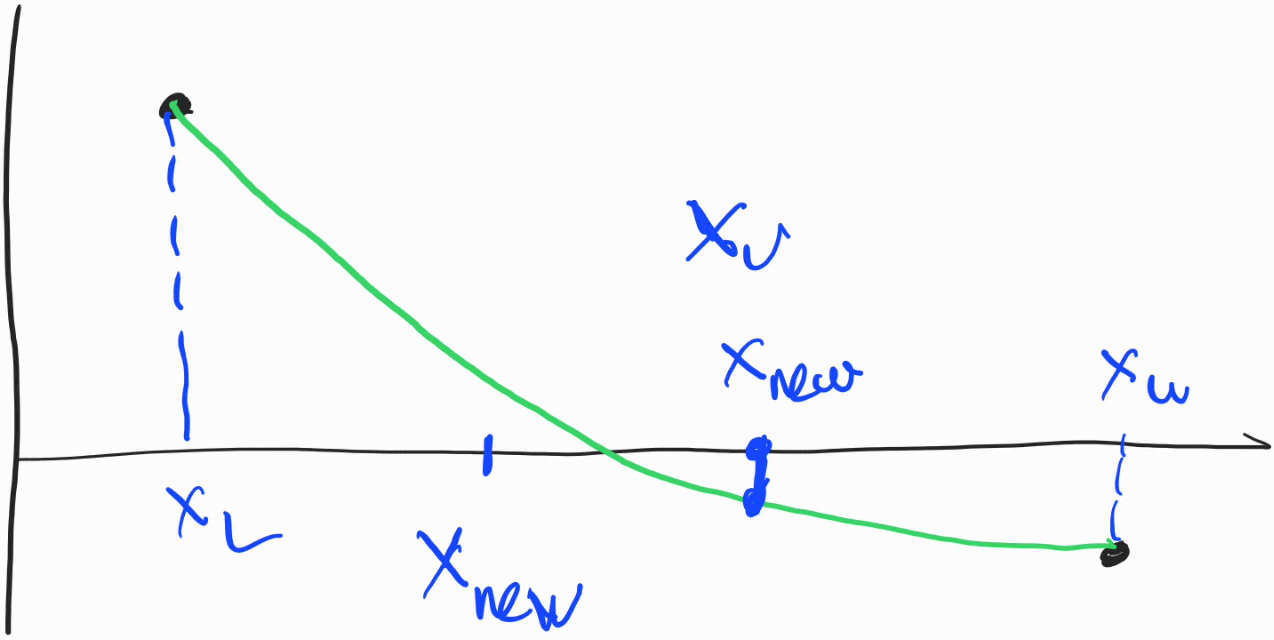
1. Graphical Method

$f(x)$ $x \in [1,5]$

$x \in (3,4)$



2. Bisection Method



check $\quad f(x_L)\cdot f(x_u) < 0$

tolerance = 0.001

x_L = ...

x_u = ...

for i=1 to 1000

new(i) = $(x_L + x_u)/2$

if (f(x_L)) f(new) < 0

x_u = new(i)

else x_L = new(i)

end

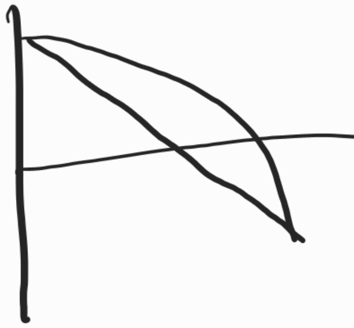
error(i) = $|x_u - x_L|$

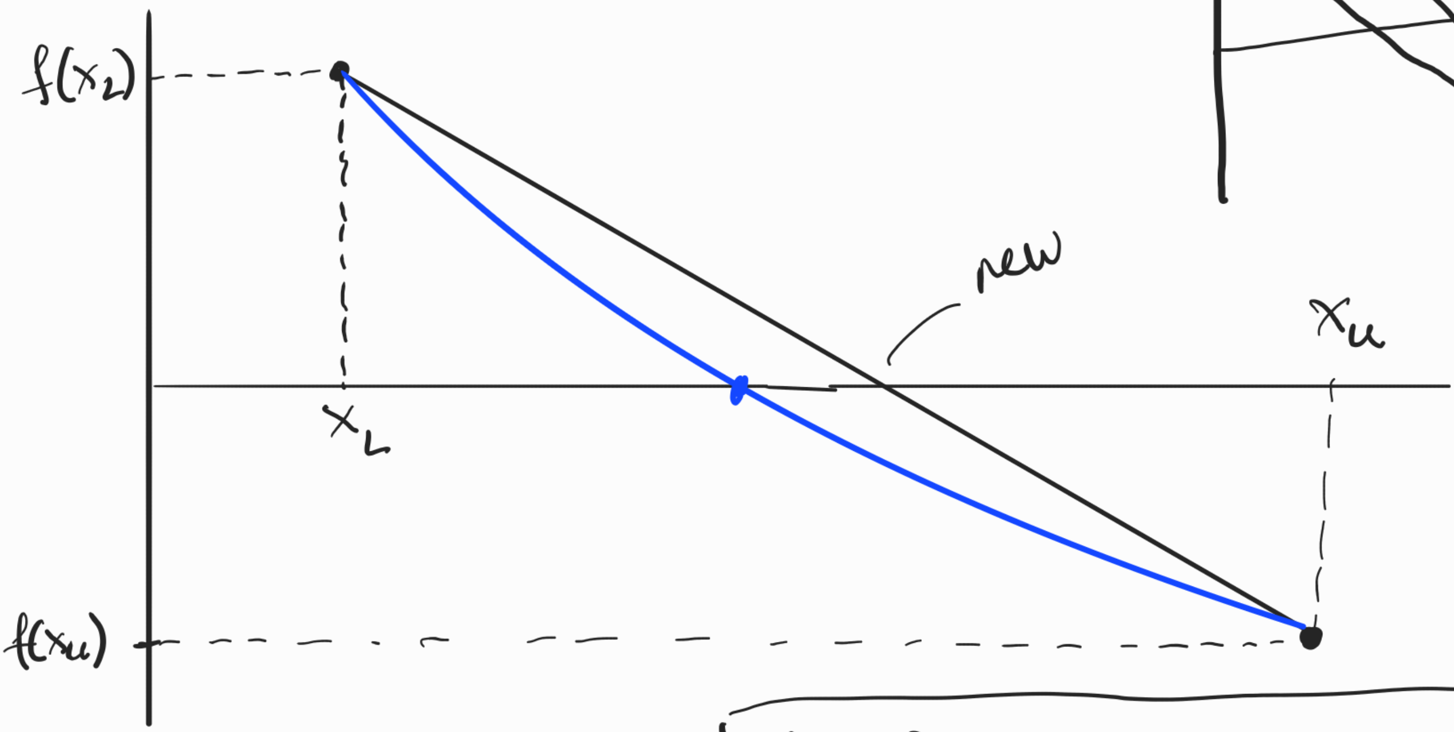
if error(i) < tolerance then stop

3. False Position

(Regula Falsi)

Same as bisection but instead of guessing at the mid-point, use linear interpolation.





$$new = x_L - \frac{f(x_L)}{slope}$$

$$new = x_u - \frac{f(x_u)}{slope}$$

$$\frac{f(x_u) - 0}{x_u - new} = slope$$

$$\frac{f(x_L) - 0}{x_L - new} = slope$$

$$f(x_L) = (x_L - new)\, slope$$

$$\frac{f(x_L)}{slope} = x_L - new$$

$$x_L - \frac{f(x_L)}{slope} = new$$

$$(x_u - new)\, slope = f(x_u)$$

$$\frac{f(x_u)}{slope} = x_u - new \Rightarrow new = x_u - \frac{f(x_u)}{slope}$$

I am trying to find the root of $f(x) = x\sin x - 1$

$x \cdot \sin x = 1 \longrightarrow f(x) = 0$ $\quad x \in [0.5, 1.5]$

$x = ?$

relative error tolerance 5×10^{-5}

Bisection Method

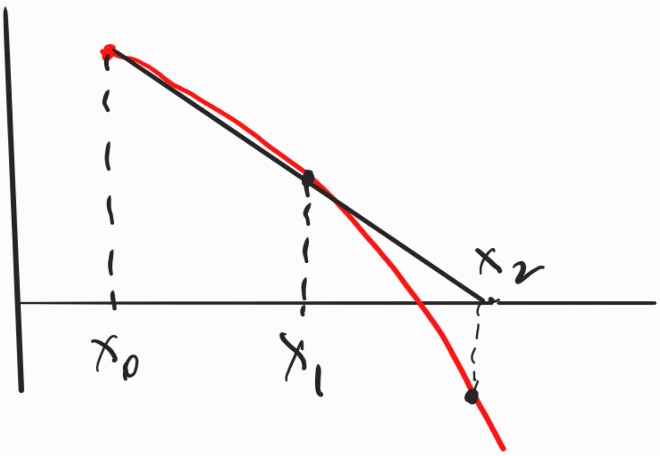
x_L	$f(x_L)$	x_u	$f(x_u)$	x_{new}	$f(x_{new})$	$\varepsilon_{ra} = \left\lvert \frac{x_i - x_{i-1}}{x_i} \right\rvert$
0.5	−0.76	1.5	0.5	$\frac{0.5+1.5}{2} = 1$	−0.16	−
1	−0.16	1.5	+0.5	$\frac{1+1.5}{2} = 1.25$	+0.19	$\left\lvert \frac{1.25-1}{1.25} \right\rvert = 0.2$
1	−0.16	1.25	0.19	$\frac{1+1.25}{2} = 1.125$	+0.015	$\left\lvert \frac{1.125-1.25}{1.125} \right\rvert = 0.111$
1	−0.16	1.125	0.015			
⋮	⋮	⋮	⋮	⋮	⋮	⋮

False-Position (Regula Falsi) Method

x_L	$f(x_L)$	x_u	$f(x_u)$	$x_{new} = x_L - \frac{f(x_L)(x_u - x_L)}{f(x_u) - f(x_L)}$	$f(x_{new})$
0.5	−0.760	1.5	0.496	$0.5 - \frac{-0.760 \times (1.5-1)}{0.496 - 0.76} = 1.105$	−0.0126
1.105	−0.0126	1.5	0.496	$1.105 - \frac{-0.0126 \times (1.5 - 1.105)}{0.496 - 0.0126} = 1.11487$	+0.00099
1.10507	−0.0126	1.11487	0.00099	$1.10507 - \frac{-0.0126 \times (1.11487 - 1.10507)}{0.00099 - (-0.0126)} = 1.11416$	

Open Methods:

Secant Method → Same as false position, without having to bracket, so you can interpolate or extrapolate



False Position → Interpolates
Secant → Inter or Extrapolates

$$x_i = x_{i-1} - \frac{f(x_{i-1})}{\text{slope}}$$

$$\text{slope} = \frac{f(x_{i-1}) - f(x_{i-2})}{x_{i-1} - x_{i-2}}$$

Secant Method

Example: $x \cdot \sin x = 1 \qquad x \in [0.5, 1.5]$

$x_0 = 0.5$; $f_0 = x_0 \sin x_0 - 1$

$x_1 = 1.5$; $f_1 = x_1 \sin x_1 - 1$

for $i = 2$ to 1000

$x_i = x_{i-1} - f_{i-1} \cdot (x_{i-1} - x_{i-2}) / (f_{i-1} - f_{i-2})$

$x_i = x_{i-1} - f_{i-1} \cdot (x_{i-1} - x_{i-2}) / (f_{i-1} - f_{i-2})$

$f_i = x_i \cdot \sin(x_i) - 1$

approx. relative $error_i = |(x_i - x_{i-1})/x_i|$

if $error_i < 0.00005$ then stop

end

Newton-Raphson Method

$$x_i = x_{i-1} - \frac{f(x_{i-1})}{f'(x_{i-1})}$$

$x_0 = 0.5$; $f_0 = x_0 \sin(x_0) - 1$

$slope_0 = x_0 \cos(x_0) + \sin(x_0)$

for $i = 1$ to 1000

$x_i = x_{i-1} - f_{i-1}/slope_{i-1}$

$f_i = x_i \cdot \sin(x_i) - 1$

$slope_i = x_i \cos(x_i) + \sin(x_i)$

if $\underbrace{|f_i/slope_i/x_i|}_{\text{relative error}} < 0.00005$ then stop

end

$x_0 = 0.5$

for $i = 1:1000$

$f_{i-1} = x_{i-1} \cdot \sin x_{i-1}$

$Slope_{i-1} = x_{i-1} \cdot \cos x_{i-1} + \sin x_{i+1}$

if _ _ _ _

end

Fixed Point Iteration

$f(x) = 0 \Longrightarrow x = ?$

$\downarrow$

$x = g(x)$

$x_i = g(x_{i-1})$

$f(x) = x \cdot \sin x - 1 = 0$

$x = \dfrac{1}{\sin x}$

$x = \arcsin\left(\dfrac{1}{x}\right)$

$x_6 = g(g(g(g(g(g(x_0))))))$

bunlar radyan

x	$1/\sin x$
0.5	2.0858
2.0858	1.14906
1.14906	1.09603

$x_0 = 0.5$

for $i = 1:1000$

$x_i = 1/\sin x_{i-1}$

if error_ _ _

end

converges if $|g'(x)| < 1$

$error_i = g'(x) \cdot error_{i-1}$

$$\frac{\sqrt[3]{x} - 2^x + 1.5}{10^x} = 0$$

$x = (2^x - 1.5)^3$ → Start from $x < -1$ converges to $x = -1.63$

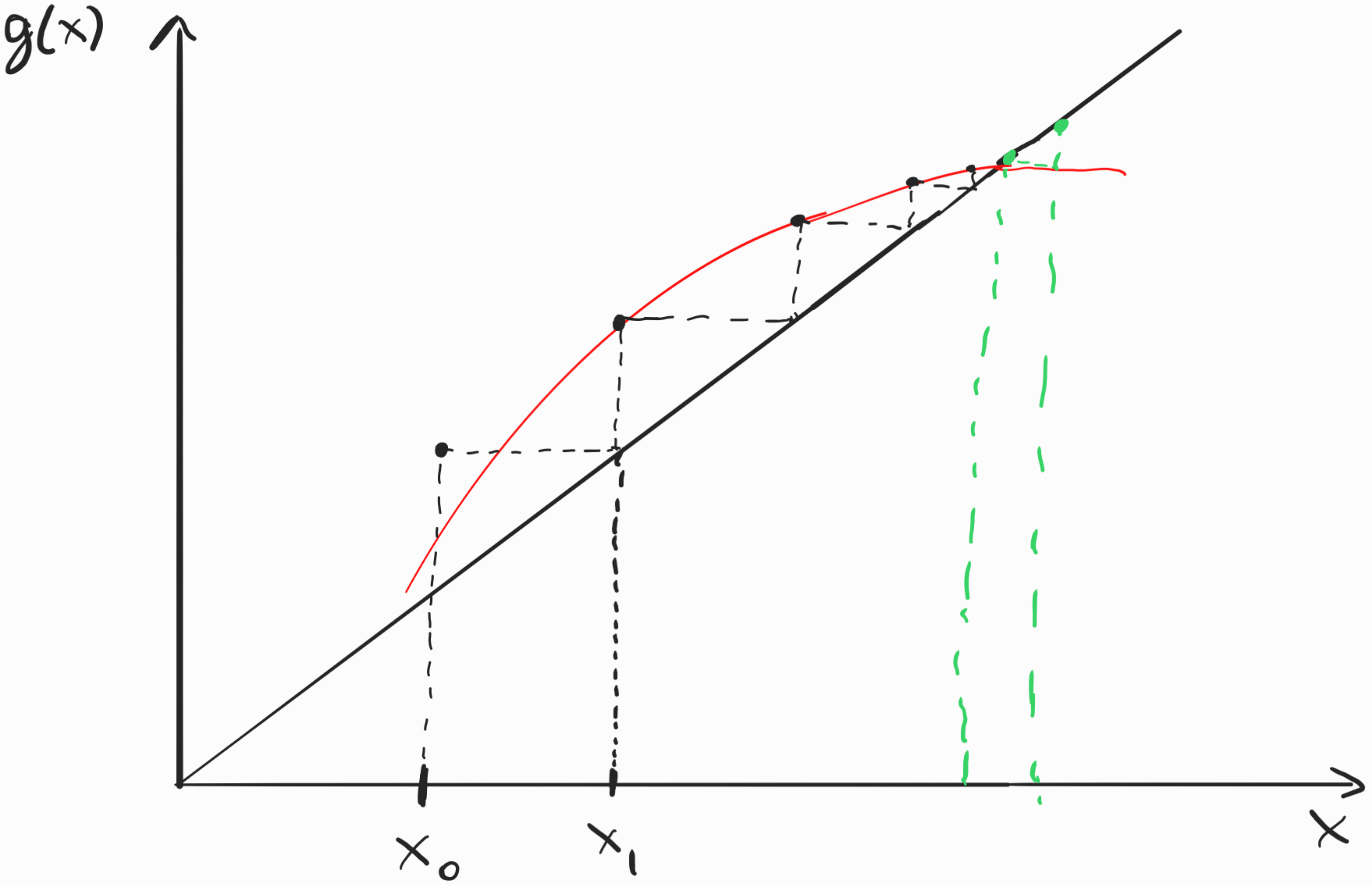
→ Start from $-1 < x < 1$ converges $x = -0.48$

$x = \log_2(\sqrt[3]{x} + 1.5)$

$x = \log_2(\sqrt[3]{x} + 1.5)$ → Start $-1.6 < x < -0.5$ Converges to x

→ Start $x > -0.5$ converges to $x = 1.37$

$g' = \ln 2 \cdot 2^x \cdot 3(2^x - 1.5)^2$



$x = \cancel{g(x)}$

$x = y$

$|g'(x)| < 1$

Monotonic convergence

Linear Algebra

$$A\vec{x} = \vec{b}$$

$\text{rank}[A] = \text{rank}[A:b]$

consistent system

$\text{rank}[A] = \#\text{unknowns}$

there is a solution

$x - y + z = 0$
$-x + 11y + 24z = 0$
$10y + 25z = 0$
$20x + 10y + 80z = 80$

consistent because
Rank $[A]$ = Rank $[A:b] = 3$

homogenous system
$\vec{b} = 0$

Norm of a Vector

L_1 norm of $\vec{x} = \sum_{i=1}^{n} |x_i|$

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

L_2 norm of $\vec{x} = \sqrt{\sum_{i=1}^{n} x_i^2}$
(Euclidian norm)

$||\vec{x}||_p = L_p = \left(\sum_{i=1}^{n} |x_i|^p\right)^{1/p}$

$$\begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$$

$||\vec{x}||_\infty = L_\infty = \sqrt[\infty]{\sum_{i=1}^{n} |x_i|^\infty}$

Maximum norm $L_\infty = \sqrt[\infty]{\sum_{i=1}^{n} |x_i|^\infty}$

gives $\max |x_i|$

$L_\infty = \sqrt[\infty]{1^\infty + 2^\infty + 3^\infty + 4^\infty}$
$= 4$

Matrix Norm

$$\|A\|_2 = \sqrt{\sum_i \sum_j a_{ij}^2}$$

$\|A\|_\infty$

$$\begin{array}{cccc} 12 & 15 & 18 & \\ \left[\begin{array}{ccc} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{array}\right] & & & \begin{array}{c} 6 \\ 15 \\ 24 \end{array} \end{array}$$

$\|A\|_\infty$

uniform column area or column sum norm $\max\limits_{1 \leq j \leq n} \sum_{i=1}^{m} |a_{ij}| = 18$

Uniform row no $\max\limits_{1 \leq i \leq m} \sum_{j=1}^{n} |a_{ij}| = 24$

! Reminder !

Matrix Inversion

$A \cdot A^{-1} = I$ (Identity matrix)

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} = \begin{bmatrix} 15+2\times7 & 1\times6+2\times8 \\ 3\times5+4\times7 & 3\times6+4\times8 \end{bmatrix}$$

$[A : I]$ do row op. to obtain

$[I : A^{-1}]$

Condition Number

$$\text{cond}(A) = \|A\|_\infty \cdot \|A^{-1}\|_\infty$$

If it is big, your equation is ill-conditioned; the solution ($\vec{x}$) is sensitive to little errors in the coefficients (A)

(large condition number)

ill-conditioned system: Results are sensitive to tiny changes

$$\begin{bmatrix} 5 & 4\times10^5 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 10^6 \\ 3 \end{bmatrix}$$

$$\xrightarrow{R_2 - \frac{R_1}{5}} \begin{bmatrix} 5 & 4\times10^5 \\ 0 & -8\times10^5 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 10^6 \\ -2\times10^5 \end{bmatrix}$$

$$y = \frac{-2\times10^5}{-8\times10^4} = 2.5$$

$$5x + 4\times10^5 y = 10^6 \Rightarrow x = 0$$

$$\left[\begin{array}{cc|c} 5 & 400000 & 1000000 \\ 1 & 1 & 3 \end{array}\right]$$

$$\left[\begin{array}{cc|c} 5 & 400000 & 1000000 \\ 0 & -79999 & -199997 \end{array}\right]$$

$$y = \frac{-199997}{-79999} = 2.499994$$

$$5x + 400000 = 1000000$$
$$\Rightarrow x = 0.500006$$

Scaling: Proportionate each row such that its largest coefficient

$$\left[\begin{array}{cc|c} 5 & 4\times10^5 & 10^6 \\ 1 & 1 & 3 \end{array}\right]$$

Pivoting: Shift rows such that largest coefficient in each column or row is on the main diagonal as much as possible

$$R_2 - 5R_1 \quad \left[\begin{array}{cc|c} 1 & 1 & 3 \\ 5 & 4e^5 & 10^6 \end{array}\right]$$

$$\left[\begin{array}{cc|c} 1 & 1 & 3 \\ 0 & 4\times10^5 & 10^6 \end{array}\right] \qquad \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0.5 \\ 2.5 \end{bmatrix}$$

Partial pivoting: Bring largest element on the main diagonal

Scaled pivoting: largest relative to the rest of the row on main diagonal

$$\begin{bmatrix} 5 & 4\times10^5 \\ 1 & 2 \end{bmatrix}$$

Direct Methods:

not applicable for large systems

- **Graphical** (2-3 unknowns)

  plot the equations and solution is at the intersection

- **Cramer's Rule**

  not applicable for large systems

$$x_1 = \frac{\begin{vmatrix} b_1 & a_{12} & a_{13} \\ b_2 & a_{22} & a_{23} \\ b_3 & a_{32} & a_{33} \end{vmatrix}}{|A|}$$

- **Elimination of unknowns**

  too long

$$x = f(y, z)$$

  ↳ plug it into other equations

- Matrix Inversion too long

$$A\vec{x}=\vec{b} \Rightarrow \vec{x}=\vec{A}^{-1}\cdot\vec{b}$$

- Gauss Elimination: row operations on $[A:b]$ to get upper triangular coefficient matrix. Then pull out the bottom unknown, substitute in preceding equation

- Gauss-Jordan Equation: Row operations on $[A:b]$ to get Identity matrix as coefficients, then the right side is the solution

$$\left[\begin{array}{ccc|c} 1 & 0 & 0 & - \\ 0 & 1 & 0 & - \\ 0 & 0 & 1 & - \end{array}\right] \quad [A:b] \rightarrow [I:x]$$

if diagonal is zero at some point, switch rows)

Triangular Decomposition (L-U)

① $A\vec{x}=\vec{b}$

$\hookrightarrow A = L\cdot U$

Lower triangular — Upper triangular

$$L\underbrace{U\vec{x}}_{\vec{y}}=\vec{b}$$

② $L\vec{y}=\vec{b}$

③ $U\vec{x}=\vec{y}$

$$\begin{bmatrix} - & - & - & - \\ - & - & - & - \\ - & - & - & - \\ - & - & - & - \end{bmatrix} = \begin{bmatrix} - & 0 & 0 & 0 \\ - & - & 0 & 0 \\ - & - & - & 0 \\ - & - & - & 1 \end{bmatrix} \begin{bmatrix} - & - & - & - \\ 0 & - & - & - \\ 0 & 0 & - & - \\ 0 & 0 & 0 & - \end{bmatrix}$$

L-U starting assumptions

- Do little diagonal of L is 1
- crout diagonal of U is 1
- Choleski $U_{ii} = L_{ii}$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ L_{21} & 1 & 0 & 0 \\ L_{31} & L_{32} & 1 & 0 \\ L_{41} & L_{42} & L_{43} & 1 \end{bmatrix} \cdot \begin{bmatrix} U_{11} & U_{12} & U_{13} & U_{14} \\ 0 & U_{22} & U_{23} & U_{24} \\ 0 & 0 & U_{33} & U_{34} \\ 0 & 0 & 0 & U_{44} \end{bmatrix}$$

$a_{11} = 1 \cdot U_{11}$

$a_{12} = 1 \cdot U_{12}$

$a_{13} = 1 \cdot U_{13}$

$a_{14} = 1 \cdot U_{14}$

$a_{21} = L_{21} \cdot U_{11} + 1 \times 0$

$a_{31} = L_{31} \cdot U_{11}$

$a_{41} = L_{41} \cdot U_{11}$

$a_{22} = L_{21} \cdot U_{12} + 1 \cdot U_{22}$

$a_{23} = L_{21} \cdot U_{13} + 1 \cdot U_{23}$

$a_{24} = L_{21} U_{14} + 1 U_{24}$

$a_{33} = L_{31} U_{13} + L_{32} \cdot U_{23} + 1 U_{33}$

$a_{34} = L_{31} U_{14} + L_{32} U_{24} + 1 U_{34}$

$a_{43} = L_{41} U_{13} + L_{42} U_{23} + L_{43} \cdot U_{33}$

$a_{44} = L_{41} U_{14} + L_{42} \cdot U_{24} + L_{43} \cdot U_{34} + 1 \cdot U_{44}$

$$\begin{bmatrix} 2 & 6 & 9 \\ 1 & -4 & 5 \\ 3 & 4 & -1 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 27 \\ 57 \end{bmatrix}$$

1. $A = L \cdot U$
2. $L\vec{y} = \vec{b}$
3. $U\vec{x} = \vec{y}$

$$\begin{bmatrix} 1 & 0 & 0 \\ L_{21} & 1 & 0 \\ L_{31} & L_{32} & 1 \end{bmatrix} \cdot \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix}$$

$U_{11} = 2$

$U_{12} = 6$

$U_{13} = 9$

$1 = L_{21} \cdot U_{11} \Rightarrow L_{21} = \frac{1}{2}$

$3 = L_{31} \cdot U_{11} \Rightarrow L_{31} = \frac{3}{2}$

$$4 = \underbrace{L_{31}}_{3/2} \cdot \underbrace{U_{12}}_{6} + L_{32} \cdot \underbrace{U_{32}}_{-7} \Rightarrow L_{32} = \frac{5}{7}$$

$-4 = L_{21} \cdot U_{12} + 1 \cdot U_{22} \Rightarrow U_{22} = -7$

$$5 = \underbrace{L_{21}}_{1/2} \cdot \underbrace{U_{13}}_{9} + 1 \cdot U_{23} \Rightarrow U_{23} = \frac{1}{2}$$

$$-1 = \underbrace{L_{21}}_{3/2} \cdot \underbrace{U_{13}}_{9} + \underbrace{L_{32}}_{5/7} \cdot \underbrace{U_{23}}_{1/2} + 1 \cdot U_{33} \Rightarrow U_{33} = -\frac{104}{7}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 3/2 & 5/7 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 27 \\ 57 \end{bmatrix}$$

$$1 \cdot y_1 = 3$$

$$\frac{1}{2} y_1 + 1 \cdot y_2 = 27$$

$$y_2 = 25.5$$

$$\frac{3}{2} y_1 + \frac{5}{7} y_2 + y_3 = 57$$

$$9/2 + \frac{255}{14} + y_3 = 57$$

$$y_3 = 34.285714$$

$$\begin{bmatrix} 2 & 6 & 9 \\ 0 & -7 & 1/2 \\ 0 & 0 & -\frac{104}{7} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 25\frac{1}{2} \\ 34\frac{2}{7} \end{bmatrix}$$

$$-\frac{104}{7} x_3 = \frac{240}{7} \Rightarrow x_3 = -\frac{30}{13}$$

$$-7x_2 + \frac{1}{2} x_3 = 5 1/2$$

$$-7x_2 = \frac{51}{2} + \frac{15}{13} \Rightarrow x_2 = -3.808$$

$$2x_1 + 6x_2 + 9x_3 = 3$$

$$\hookrightarrow x_1 = \frac{3 - 6x_2 - 9 \cdot \frac{-30}{13}}{2}$$

Gauss Jacobi

(fixed point iteration for a system) (FPI)

$$f(x) = 0 \implies x = g(x) \quad \text{where } |g'(x)| < 1$$

$$x_k = g(x_{k-1})$$

$$Ax = b$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

1st eq.

$$a_{11}x + a_{12}y + a_{13}z = b_1$$

$$x_k = \frac{b_1 - a_{12}y_{k-1} - a_{13}z_{k-1}}{a_{11}}$$

2nd eq.

$$y_k = \frac{b_2 - a_{21}x_{k-1} - a_{23}z_{k-1}}{a_{22}}$$

3^{rd} eqn.

$$z_k = \frac{b_3 - a_{32}x - a_{32}y_{k-1}}{a_{33}}$$

$$x_{i,k} = g_i(x_{i,k-1}) \qquad \sum_j \left| \frac{\partial g_i}{\partial x_j} \right| < 1$$

$$\frac{a_{12}}{a_{11}} + \frac{a_{13}}{a_{11}}$$

Ex:

$$\begin{bmatrix} 2 & 6 & 9 \\ 1 & -4 & 5 \\ 3 & 4 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 27 \\ 57 \end{bmatrix} \xrightarrow{R_1 \leftrightarrow R_3}$$

$$\left[\begin{array}{ccc|c} 3 & 4 & -1 & 57 \\ 1 & -4 & 5 & 27 \\ 2 & 6 & 9 & 3 \end{array}\right] \xrightarrow{R_1 + R_2 = R_1} \left[\begin{array}{ccc|c} 4 & 0 & 4 & 84 \\ 1 & -4 & 5 & 27 \\ 2 & 6 & 9 & 3 \end{array}\right] \xrightarrow{R_2 = R_1 - R_2}$$

$$\left[\begin{array}{ccc|c} 4 & 0 & 4 & 84 \\ 3 & 4 & -1 & 57 \\ 2 & 6 & 9 & 3 \end{array}\right] \rightarrow$$

$$x_1 = \frac{84 - 4x_3}{4} = 21 - x_3$$

$$x_2 = \frac{57 - 3x_1 + x_3}{4}$$

$$x_3 = \frac{3 - 2x_1 - 6x_2}{9}$$

$$x_{i,t+1} = \frac{b_i - \sum_{j=1}^{n} a_{ij} x_{j,t}}{a_{ii}}$$

t	x_1	x_2	x_3
0	0	0	0
1	21	$57/4$	$1/3$
2	$20\frac{2}{3}$	$\frac{57-3\cdot 21+\frac{1}{3}}{4}$	$\frac{3-2\cdot 21-6\cdot\frac{57}{4}}{9} =$

Gauss - Jacobi

$$f_1(x_1, x_2, x_3 \ldots x_n) = 0 \rightarrow x_1^{t+1} = g_1(x_2^t \ldots x_n^t)$$

$$f_2(x_1, x_2, \ldots x_n) = 0 \rightarrow x_2^{t+1} = g_2(x_1^t, x_2^t, x_3^t \ldots x_n^t)$$

$$\vdots$$

$$f_n(x_1, x_2, \ldots x_n) = 0 \longrightarrow x_n^{t+1} = g_n(x_1^t, x_2^t \ldots x_{n-1}^t)$$

Gauss Seidel

$$f_1(x_1, x_2, x_3 \ldots x_n) = 0 \rightarrow x_1^{t+1} = g_1(x_2^t \ldots x_n^t)$$

$$f_2(x_1, x_2, \ldots x_n) = 0 \rightarrow x_2^{t+1} = g_2(x_1^{t+1}, x_2^t, x_3^t \ldots x_n^t)$$

$$\vdots$$

$$f_n(x_1, x_2, \ldots x_n) = 0 \longrightarrow x_n^{t+1} = g_n(x_1^{t+1}, x_2^{t+1} \ldots x_{n-1}^{t+1})$$

Example

$$\begin{bmatrix} 6 & 2 & -1 \\ -1 & 4 & 1 \\ 1 & -2 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 5 \\ 3 \\ 10 \end{bmatrix}$$

diagonally dominant

Yes

No → row op.s to make it so

$x_i = g_i(x \ldots)$

k	$x_1^{k+1} = \dfrac{5-2x_2^k+x_3^k}{6}$	$x_2^{k+1} = \dfrac{3+x_1^k-x_3^k}{4}$	$x_3^{k+1} = \dfrac{10-x_1^k+2x_2^k}{5}$	approximate error ε_{aa}
0	0	0	0	$\begin{bmatrix} x_1^{k+1}-x_1^k \\ x_2^{k+1}-x_2^k \\ \vdots \end{bmatrix}$
1	$5/6 = 0.8\bar{3}$	$3/4 = 0.75$	2	
2	$\dfrac{5-2\cdot\frac{3}{4}+2}{6} = 0.91\bar{6}$	$\dfrac{3+\frac{5}{6}-2}{4} = 0.458\bar{3}$	$\dfrac{10-\frac{5}{6}+2\cdot\frac{3}{4}}{5} = 2.1\bar{3}$	$\begin{bmatrix} 0.08\bar{3} \\ 0.291\bar{6} \\ 0.1\bar{3} \end{bmatrix}$

check $\|\varepsilon\|_{1,2,\infty} < \text{tolerance}$

Gauss Seidel

k	$x_1^k = \dfrac{5-2x_2^{k-1}+x_3^{k-1}}{6}$	$x_2^k = \dfrac{3+x_1-x_3}{4}$	$x_3 = \dfrac{10-x_1+2x_2}{5}$
0	0	0	0
1	$\dfrac{5-0-0}{6} = \dfrac{5}{6}$ →	$\dfrac{3+\frac{5}{6}-0}{4} = 0.958\bar{3}$ →	$\dfrac{10-\frac{5}{6}+2\times 0.958\bar{3}}{5} = 2.21\bar{6}$
2	$\dfrac{5-2\times 0.958\bar{3}+2.21\bar{6}}{6} = 0.88\bar{3}$ →	$\dfrac{3+0.88\bar{3}-2.21\bar{6}}{4} = 0.41\bar{6}$ →	$\dfrac{10-0.88\bar{3}+2\times 0.41\bar{6}}{5} = 1.99$

Example:

$$4x - y + z = 7$$
$$4x - 8y + z = -21$$
$$-2x + y + 5 = 15$$

$$A = \begin{bmatrix} 4 & -1 & 1 \\ 4 & -8 & 1 \\ -2 & 1 & 5 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ L_{21} & 1 & 0 \\ L_{31} & L_{32} & 1 \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix}$$

$U_{11} = 4$
$U_{12} = -1$
$U_{13} = 1$

$L_{21} \cdot U_{11} + 1 \cdot 0 = 4 \Rightarrow L_{21} = 1$
$L_{31} \cdot U_{11} = -2 \Rightarrow L_{31} = -0.5$

$-8 = \underset{1}{L_{21}} \cdot \underset{-1}{U_{12}} + 1 \cdot U_{22} \Rightarrow U_{22} = -7$

$1 = \underset{1}{L_{21}} \cdot \underset{1}{U_{13}} + 1 \cdot U_{23} = U_{23} = 0$

$5 = \overset{-0.5}{L_{31}} \cdot \overset{1}{U_{13}} + L_{32} \cdot \overset{0}{U_{23}} + 1\, U_{33} \rightarrow U_{33} = 5.5$

$1 = \underset{-0.5}{L_{31}} \cdot \underset{-1}{U_{12}} + L_{32} \cdot U_{22}$

$L_{32} = -0.0714825$

$Ax = b$
$\underbrace{L \cdot U \cdot X}_{Y} = b$

$A = L \cdot U$ (1)
$Ux = Y$ (3)
$LY = b$ (2)

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ -0.5 & -1/14 & 1 \end{bmatrix} \begin{bmatrix} 4 & -1 & 1 \\ 0 & -7 & 0 \\ 0 & 0 & 5.5 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ -1/2 & -1/14 & 1 \end{bmatrix} \begin{bmatrix} 7 \\ -28 \\ 16.5 \end{bmatrix} = \begin{bmatrix} 7 \\ -21 \\ 15 \end{bmatrix}$$

$$\underset{U}{\begin{bmatrix} 4 & -1 & 1 \\ 0 & -7 & 0 \\ 0 & 0 & 5.5 \end{bmatrix}} \underset{\vec{x}}{\begin{bmatrix} x \\ y \\ z \end{bmatrix}} = \underset{\vec{y}}{\begin{bmatrix} 7 \\ -28 \\ 16.5 \end{bmatrix}}$$

$5.5z = 16.5 \Rightarrow z = 3$
$-7y = -28 \Rightarrow y = 4$
$4x - y + z = 7 \Rightarrow x = 2$

Gauss Seidel method example

$$4x - y - z = 7$$
$$4x - 8y + z = -21$$
$$-2x + y + 5z = 15$$

1^{st} step make it diagonally dominant

$$x = \frac{7+y+z}{4}$$

$$y = \frac{21+4x+z}{8}$$

$$z = \frac{15+2x-y}{5}$$

Initial guess	iteration 1	iteration 2	iteration 3
0	$7/4 = 1.75$	$\frac{7+3.5+3}{4} = 3.375$	3.775
0	$\frac{21+4\frac{7}{4}+0}{8} = 3.5$	$\frac{21+4\frac{13.5}{4}+3}{8} = 4.6875$	4.939
0	$\frac{15+2\cdot\frac{7}{4}-3.5}{5} = 3$	$\frac{15+2\times3.3375-4.6875}{5}$	3.522

$\varepsilon_{aa} = \max(1.75, 3.5, 3) = 3.5$ $\quad \max(1.625, 1.1875, 0.4125)$ $\quad \|0.4, 0.2515, 0.1105\|$

$0.4 > 0.05$ (tolerance) $\to$ continue

$$\varepsilon_{aa} = \|\vec{x}_k - \vec{x}_{k-1}\|_\infty$$

```
A = [4 -1 -1 ; 4 -8 1 ; -2 1 5]
x(1)=0 ; y(1)=0 ; z(1)=0
for k=1:100
   x(k+1) = (7 + y(k) + z(k))/4 ;
   y(k+1) = (21 + 4.x(k+1) + z(k))/8 ;
   z(k+1) = (15 + 2.x(k+1) - y(k+1))/5 ;
   error(k+1) = max([abs(x(k+1) - x(k));
                     abs(y(k+1) - y(k));
                     abs(z(k+1) - z(k))]);
   if error(k+1) < 0.05 ; break; end
end
x
y
z
```

MT 1

Gauss Seidel'a kadar (Gauss Seidel dahil)

Non-linear Equation

System of linear equations

System of Non-linear equations

$$4x^2 - y^2 = 0$$

$$4xy^2 - x = 1$$

A pull out

Fatoyu gelir

Fixed Point iteration

$x^2 = \sin y$ $\qquad$ $x^2 - \sin y = 0$

$\ln\left(\frac{1}{x}\right) = e^y$ $\qquad$ $\ln\frac{1}{x} - e^y = 0$ $\Rightarrow J = \begin{bmatrix} 2x & -\cos y \\ -\frac{1}{x} & -e^y \end{bmatrix}$

$X = \begin{bmatrix} x_1 & x_2 & x_3 & \cdots \\ y_1 & y_2 & y_3 & \cdots \end{bmatrix}$

k

```
x(1:2,1) = [0.5;0.5]
for k = 1:100
F = [x(1,k)^2-sin(2,k); ln(1/x(1,k)) - exp(x(2,k))]
J = [2.*x(1,k)  -cos(x(2,k)); -1/x(1,k)  -exp(x(2,k))]
error = J^-1.F;
x(1:2,k+1) = x(1:2,k) -error;
if max(abs(error)) < 0.005; break; end
end
```

Review for MT1

Taylor $f(x) = \sum_{n=0}^{\infty} \left.\frac{d^n f}{dx^n}\right|_a \cdot \frac{(x-a)^n}{n!}$ where $f(a)$, is known

true vs approx ⎤
relative vs absolute ⎦ error

decimal digits vs significant figures and rounding errors

Single Non-Linear Equation

Bracketing Methods

- graph
- bisection
- false position

Open Methods

- Secant
- Newton Raphson
- FPI

Norm $(1, 2, \infty)$, condition number, diagonally dominant,
Gauss Jordan, scaling, Pivoting

LU: $Ax = b \longrightarrow A = LU$

$Ly = b$

$Ux = y$

$\downarrow$

$L\underbrace{Ux}_{y} = b$

FPI: Gauss Jacobi use X_k

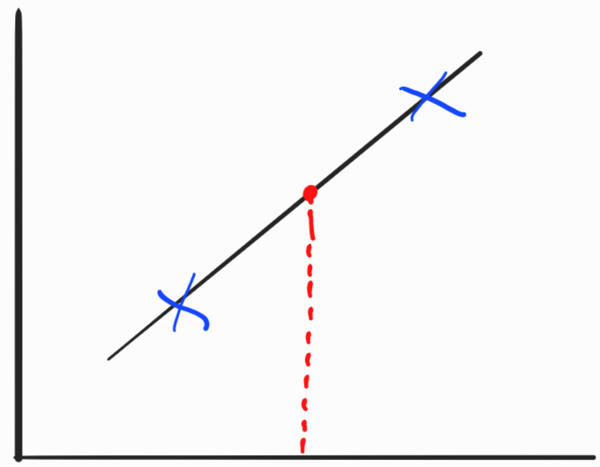
Gauss Seidel use X_k or X_{k+1} if it is available

Newton Jacobi: Newton Raphson for system

Up to now: known functions, unknown points (derivatives)

From now on: known points, unknown functions (derivatives) (integrals)

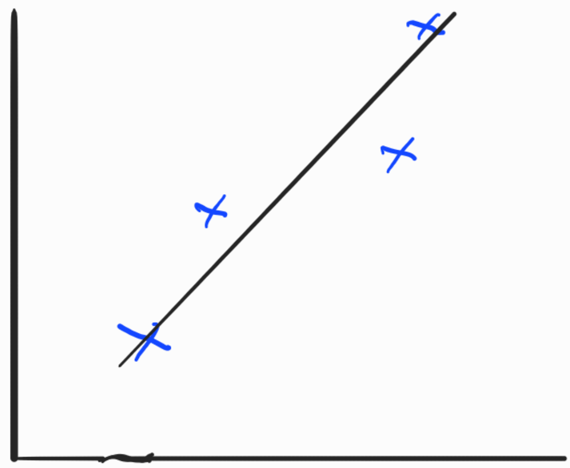
Approximation of Functions



Interpolation

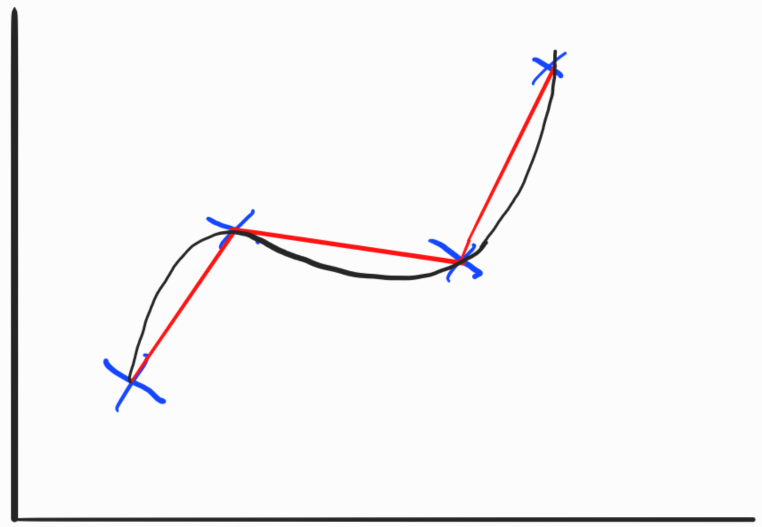
(passes through every point)

"Collocation"



fit

least distant to all points, doesn't have to pass through any



each pair can have a line

OR

you can fit n^{th} degree polynomial on $n+1$ points

$$ax^3+bx^2+cx+d=y$$

collocation $\rightarrow$ x_i, y_i satisfies it

4 eqs. 4 unknowns

OR

Lagrange Polynomial

$$f(x)=\sum_{i=0}^{n}\left[\prod_{\substack{j=0\\ j\neq i}}^{n}\left(\frac{x-x_i}{x_i-x_j}\right)\cdot f(x_i)\right]$$

$x \quad f(x)$

$\downarrow \quad \downarrow$

$x_0, \; y_0$

$x_1, \; y_1$

$x_2, \; y_2$

fit a parabola

$$\underbrace{\frac{x-x_1}{x_0-x_1}}_{j=1} \cdot \underbrace{\frac{x-x_2}{x_0-x_2}}_{j=2} \cdot y_0 + \underbrace{\frac{x-x_0}{x_1-x_0}}_{j=0} \cdot \underbrace{\frac{x-x_2}{x_1-x_2}}_{j=2} \cdot y_1 + \underbrace{\frac{x-x_0}{x_2-x_0}}_{j=0} \cdot \underbrace{\frac{x-x_1}{x_2-x_1}}_{j=1} \cdot y_2$$

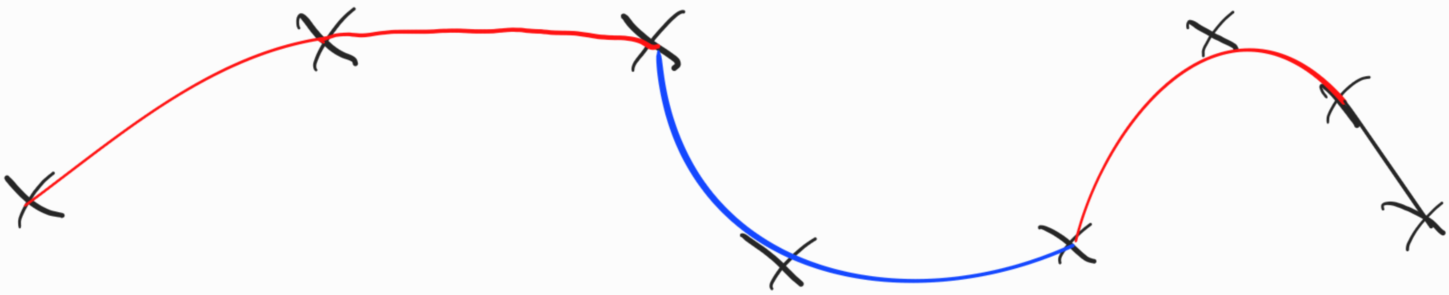
$i=0$ $\qquad i=1$ $\qquad i=2$

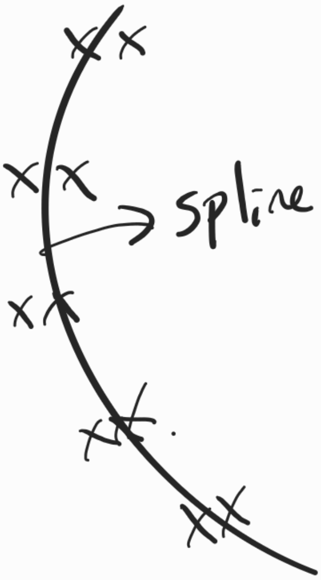
$x = [1 \;\; 2 \;\; 3 \;\; 4]$ evaluate at 2.5

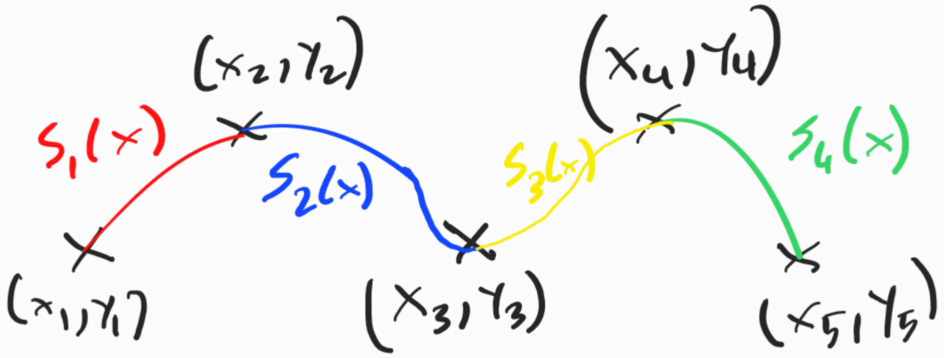
$y = [5 \;\; 8 \;\; 7 \;\; 3]$

```
F=0;
for i=1:size(x)
    P=1;
    for j=1:size(x)
        if j <> i
        P=P*(2.5-x(j))/x(i)-x(j));
        end
    end
  F=F+P*y(i);
end
```

Cubic Spline







- It has to pass exactly through every data point (collocation)

$$S_i(x_i) = y_i \rightarrow S_{i+1}(x_{i+1}) = y_{i+1} \longleftrightarrow S_i(x_{i+1}) = y_{i+1}$$

- it has to be <u>continuous</u>
- It has to be smooth

$$S_i'(x_{i+1}) = S_{i+1}'(x_{i+1})$$

$n-1$ equations

- Second derivative is continuous

$$S_i''(x_{i+1}) = S_{i+1}''(x_{i+1})$$ n-1 equations

$$S_i(x) = a_i x^3 + b_i x^2 + c_i x + d_i$$

4n unknowns

- Natural boundary conditions
(no curvature the ends)

$$S_1''(x_1) = 0 \ , \quad S_n''(x_{n+1}) = 0$$ 2eq.

$$S_i(x) = a_i x^3 + b_i x^2 + c_i x + d_i$$

4n unknowns

Example:

$$S_i(x) = a_i x^3 + b_i x^2 + c_i x + d_i$$

$$S_i'(x) = 3x^2 a_i + 2x b_i + c_i$$

$$S_i''(x) = 6x a_i + 2b_i$$

i	time	u (speed)
1	0	9.85
2	6	8.87
3	12	9.85
4	18	9.17
5	24	4.95

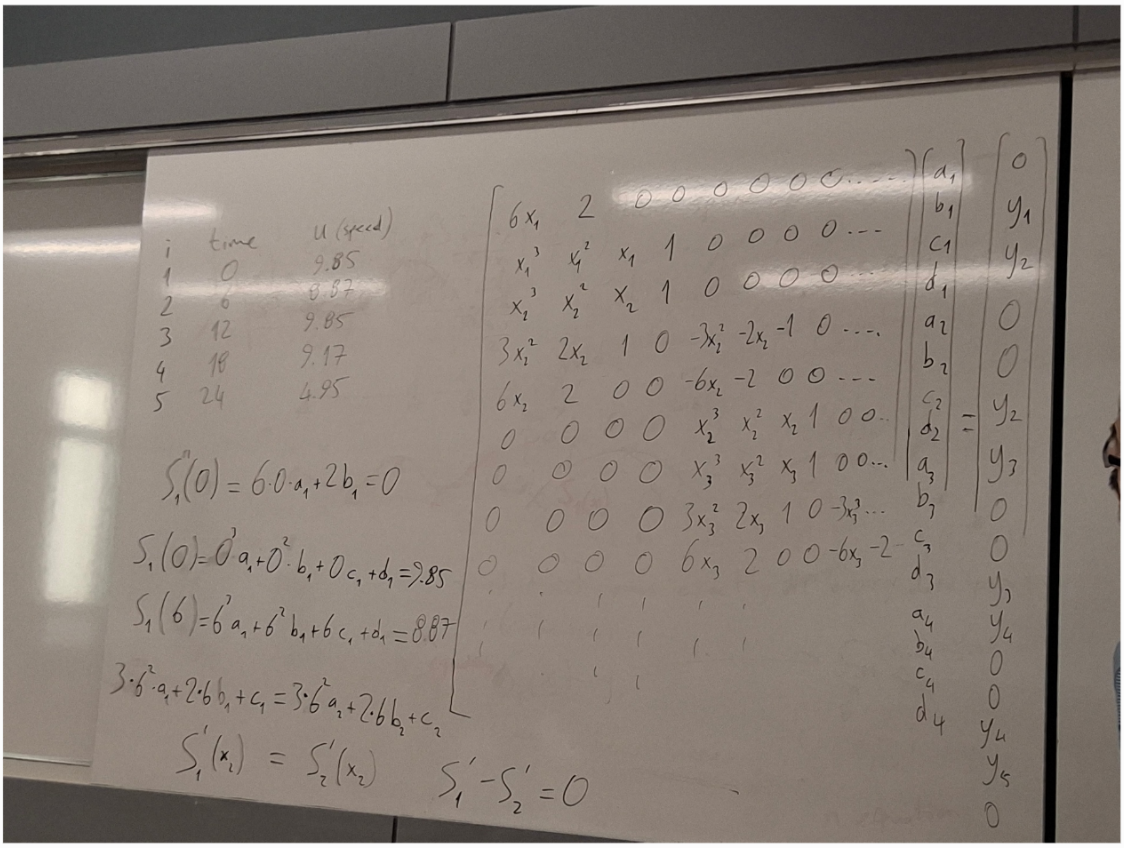
$$S_1''(0) = 6 \cdot 0 \cdot a_1 + 2b_1 = 0$$

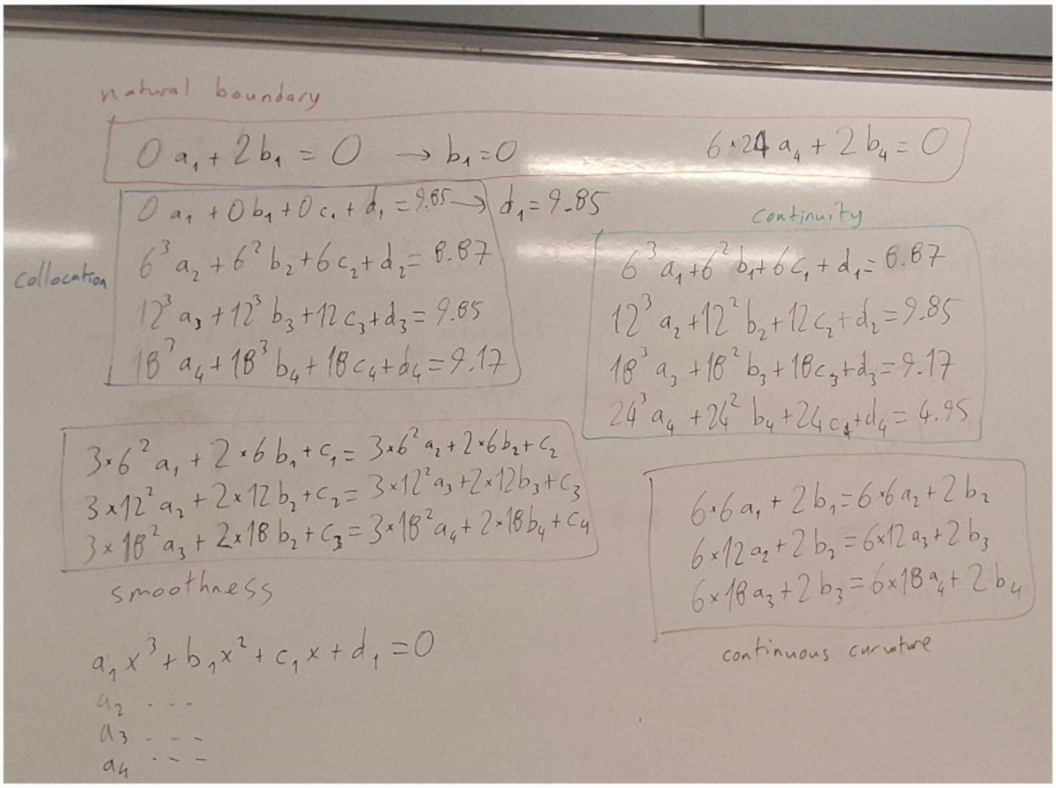
$$S_1(0) = 0^3 \cdot a_1 + 0^2 b_1 + 0c_1 + d_1 = 9.85$$

$$S_1(6) = 6^3 a_1 + 6^2 b_1 + 6c_1 + d_1 = 8.87$$

$$3 \cdot 6^2 \cdot a_1 + 2 \cdot 6 \cdot b_1 + c_1 = 3 \cdot 6^2 a_2 + 2 \cdot 6 b_2 + c_2$$

$$S_1'(x_2) = S_2'(x_2)$$





Curve fitting

We have known data points (x_i, y_i) aim is to approximate $f(x_i) \simeq y_i$ such that error is minimized

Let's define everything in vector form

$$\vec{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \quad \vec{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad \vec{F} = \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_n) \end{bmatrix}$$

$$\vec{E} = \vec{F} - \vec{Y}$$

Max error : $\|E\|_\infty$

average error : $\dfrac{\|E\|_1}{n}$

Root mean Square error (RMS) : $\dfrac{\|\vec{E}\|_2}{n}$

fitting a line:

$f(x) = Ax + B$ find A & B that result in minimum RMSE

minimize inside of square root

$$\sum_{i=1}^{n} (f(x_i) - y_i)^2$$

$$\sum_{i=1}^{n} [Ax_i + B - y_i]^2 = \varepsilon$$ (x_i and y_i are known) (A and B are unknowns)

$$\frac{\partial \varepsilon}{\partial A} = 2\sum_{i=1}^{n} \left[2(Ax_i + B - y_i) \cdot x_i\right]$$ We took derivative and equated to zero

$$= 2\left[A \cdot \sum x_i^2 + B \cdot \sum x_i - \sum x_i \cdot y_i\right] = 0$$

$$A \sum x_i^2 + B \sum x_i = \sum x_i y_i$$

$$\frac{\partial \Sigma}{\partial B} = 0 = \sum_{i=1}^{n} \left[2(Ax_i + B - y_i) \cdot 1\right]$$

$$0 = 2\left(\sum Ax_i + \sum B - \sum y_i\right)$$

$$\Rightarrow A\cdot\sum_{i=1}^{n} x_i + \underbrace{B\sum_{i=1}^{n} 1}_{B\cdot n} = \sum_{i=1}^{n} y_i$$

We get:

2 eqs.
2 unknowns
A, B

$$\begin{cases} A\sum_{i=1}^{n} x_i + \underbrace{B\sum_{i=1}^{n} 1}_{B\cdot n} = \sum_{i=1}^{n} y_i \\ A\sum x_i^2 + B\sum x_i = \sum x_i y_i \end{cases}$$

$$\begin{bmatrix} \sum x_i & \sum 1 \\ \sum x_i^2 & \sum x_i \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \end{bmatrix}$$

Example:

X	Y	X^2	XY
0	3	0	0
1	6	1	6
2	8	4	16
3	13	9	39
4	15	16	60
+5	+18	+25	+90
15	63	55	211

$$\begin{bmatrix} 15 & 6 \text{ (datapoints)} \\ 55 & 15 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 63 \\ 11 \end{bmatrix}$$

$$f = Ax^2 + Bx + C$$

$$RMS^2 = \sum (Ax^2 + Bx + C - y)^2$$

$$\frac{\partial}{\partial A} = \frac{\partial}{\partial B} = \frac{\partial}{C} = 0$$

$$2\sum\left[(Ax^2+Bx+C-y)\cdot x^2\right]=0 \Longleftrightarrow \frac{\partial}{\partial A}=0$$

$$\sum(Ax^4+Bx^3+Cx^2-x^2y)=0$$

$$\sum Ax^4+\sum Bx^3+\sum Cx^2-\sum x^2y$$

$$A\cdot\sum x^4+B\sum x^3+C\cdot\sum x^2=\sum x^2y$$

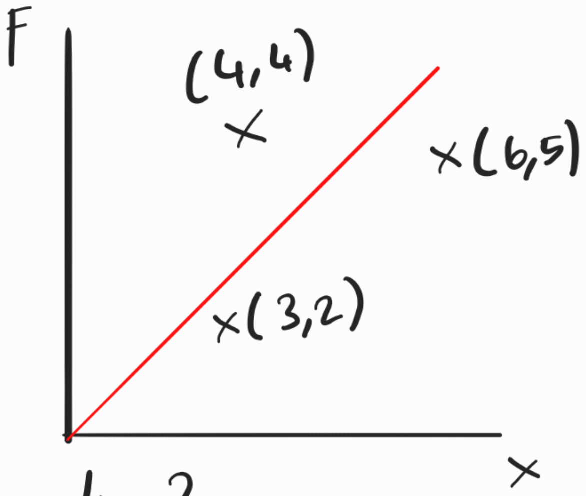
$$\frac{\partial}{\partial B}=0 \Rightarrow A\sum x^3+B\sum x^2+C\sum x=\sum xy$$

$$\frac{\partial}{\partial C}=0 \Rightarrow A\sum x^2+B\sum x+C\sum 1=\sum y$$

$$\begin{bmatrix}\sum x^4 & \sum x^3 & \sum x^2\\ \sum x^3 & \sum x^2 & \sum x\\ \sum x^2 & \sum x & \sum 1\end{bmatrix}\begin{bmatrix}A\\ B\\ C\end{bmatrix}=\begin{bmatrix}\sum x^2y\\ \sum xy\\ \sum y\end{bmatrix}$$

Example:

$$F=k\cdot x$$



$k=?$

$$\frac{\partial}{\partial k}\sum(kx-F)^2=0$$

$$\sum\left[(kx-F)\cdot x\right]=0$$

$$\sum kx^2-\sum Fx=0$$

$$k\cdot\sum x^2=\sum(Fx)$$

$$k(3^2+4^2+6^2)=(3\cdot 2+4\cdot 4+6\cdot 5)$$

$$k=\frac{52}{61}$$

Exponential curve

$$y = C \cdot e^{Ax}$$

$$\frac{\partial}{\partial A} \sum \left(Ce^{Ax} - y \right)^2$$

$$\sum \left[\left(Ce^{Ax} - y \right) C \cdot x e^{Ax} \right] = 0$$

$$\sum C^2 x e^{2Ax} \; - - - -$$

can't get A out of Σ

x	y	f(x)	RMS
⋮	⋮	Ce^{Ax}	$(Ce^{Ax}-y)^2$
			⋮
			$+$
			Σ minimize

Excel has a solver tool that can minimize a target cell by changing one or more input cells

Linearization

$$\ln y = \ln \left(Ce^{Ax} \right)$$

$$\underbrace{\ln y}_{Y} = \underbrace{\ln C}_{B} + Ax$$

$$\begin{bmatrix} \Sigma x^2 & \Sigma x \\ \Sigma x & \Sigma 1 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} \Sigma xY \\ \Sigma Y \end{bmatrix}$$

$$Y = \frac{A}{x} + B$$

$$X = \frac{1}{x}$$

$$Y = AX + B$$

x	y	X
1		1
2		0.5
3		$0.\bar{3}$
4		0.25

Another example for substitution

$$Y = \frac{D}{x+C}$$

$$Yx + Yc = D$$

$$\underbrace{Yx}_{Y} = \underbrace{-C}_{A} \cdot \underbrace{Y}_{x} + \underbrace{D}_{B}$$

xy	x	y	z
0	1	0	2
1	1	1	5
0	2	0	4
2	2	1	7

calculate z	$(\text{error in } z)^2$
	$(z_{calc} - z)^2$

+

$\sum \text{error}^2$

minimize this by changing a, b, c

$$z = ax + by + c$$

$a =$

$b =$

$c =$

$$\sum_{\text{data points}} (ax_i + by_i + c - z_i)^2$$

$$\frac{1}{2}\frac{\partial \Sigma}{\partial a} = 0 = \sum x_i \cdot (ax_i + by_i + c - z_i) = \sum ax_i + \sum bx_iy_i + \sum cx_i - \sum x_iz_i \quad (1)$$

$$= a\sum x_i^2 + b\sum x_iy_i + c\sum x_i - \sum x_iz_i$$

$$\frac{\partial \varepsilon}{\partial b} = 0 = a\sum x_iy_i + b\sum y_i^2 + c\sum y_i - \sum y_iz_i \quad (2)$$

$$\frac{\partial \varepsilon}{\partial c} = 0 = a\sum x_i + b\sum y_i + c\sum 1 - \sum z_i \quad (3)$$

(1): $10a + 3b + 6c = 29$

(2): $3a + 2b + 2c = 12$

(3): $6a + 2b + 4c = 18$

$y = cx^a \Rightarrow \ln y = \ln c + a\ln x$

$y = ax + b$

$\sum (ax + b - y)^2$

$$\underbrace{\begin{bmatrix} \sum x^2 & \sum x \\ \sum x & \sum 1 \end{bmatrix}}_{M} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum xy \\ \sum y \end{bmatrix}$$

$$\begin{bmatrix} \sum (\ln x)^2 & \sum \ln x \\ \sum \ln x & \end{bmatrix}$$

Example

$$y = (ax+b)^2$$

$$\underbrace{\sqrt{y}}_{Y} = ax+b$$

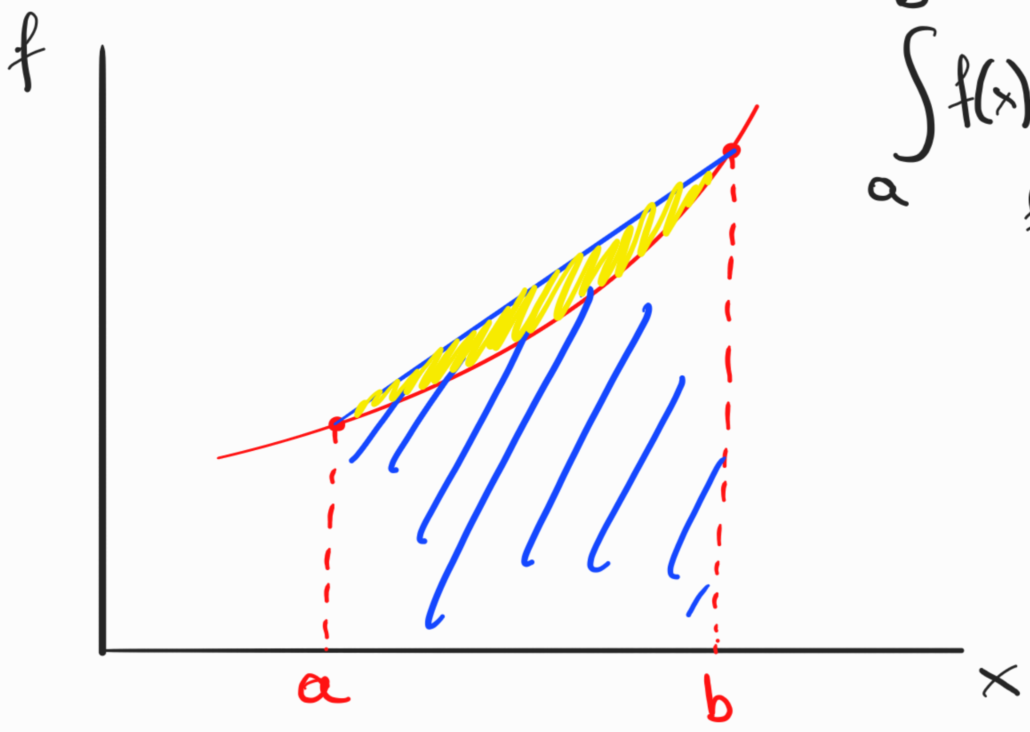
$$\sum \left[(ax+b)^2 - y \right]^2$$

Trapezoidal Rule

area of trapezoid

$$\int_a^b f(x)\,dx = \frac{f(a)+f(b)}{2} \cdot (b-a)$$

first order approximation

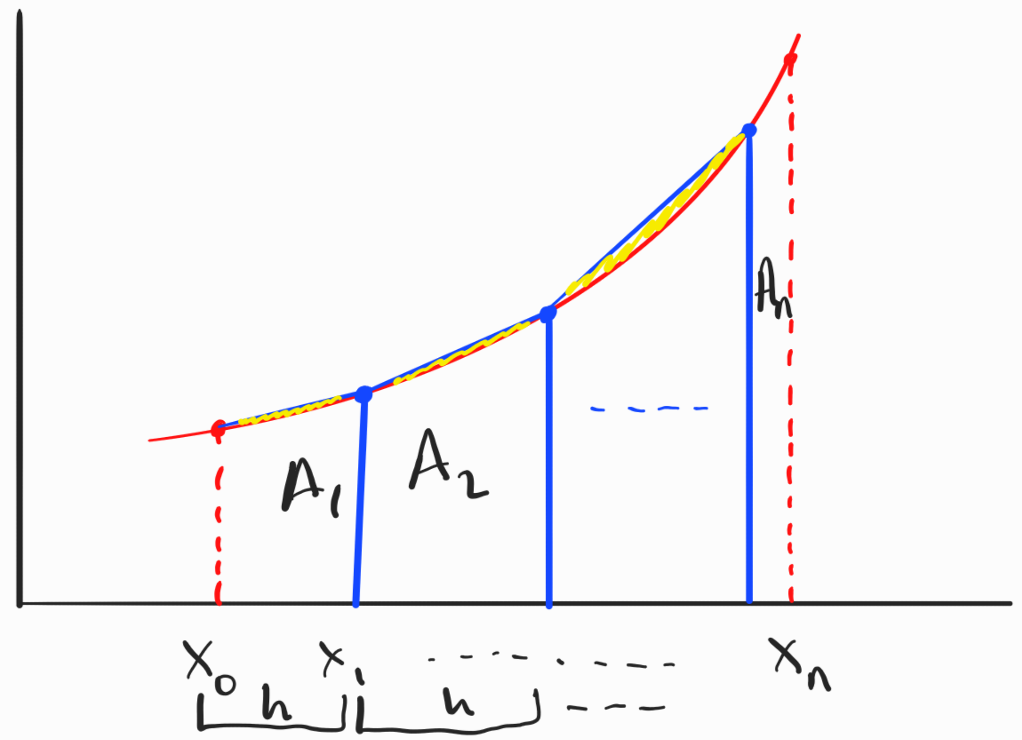


first order approximation

$$E_{at} = -\frac{(b-a)^3}{12} \cdot f''(\xi) \qquad a<\xi<b$$

Not good if $b-a$ is not tiny.

Composite Trapezoid Method



$$A_i = \frac{f(x_{i-1})+f(x_i)}{2}\underbrace{(x_i - x_{i-1})}_{\text{constant}}$$

$$\sum_{i=1}^{n} A_i \qquad \frac{h}{2}\sum_{i=1}^{n} \left[f(x_{i-1})+f(x_i)\right]$$

$f(x_1)$ is summed up twice

once for A_1, once for A_2

$$\frac{b-a}{n}$$

$$h \cdot \left[\frac{f(x_0) + f(x_n)}{2} + \sum_{i=1}^{n-1} f(x_i) \right] + \underbrace{\frac{-h^3}{12} \cdot f'' \cdot n}_{\text{error}}$$

$$-\cancel{n} \cdot \frac{(b-a)^3}{12 n^{\cancel{3}2}} \cdot f''$$

Example:

x	$f(x)$
0	0
1	2
2	4
3	5
4	6
5	4

$$\int_0^5 f(x)\,dx$$

$$h = 1$$

$$1 \left[\frac{0+4}{2} + (2+4+5+6) \right]$$

Composite Trapezoid

$$\frac{h}{2}\left[f(0)+f(n)+2\cdot\sum_{i=1}^{n-1} f(i)\right]$$ equal intervals of x

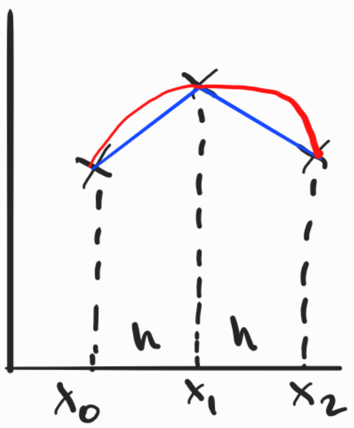
if data intervals are unequal:

x	f
0	1
1	2
2.2	4
3	6
4.5	7

$$\text{Area} = (x_i - x_{i-1})\cdot\frac{f(x_i)+f(x_{i-1})}{2}$$

$$\left.\begin{array}{l}(1-0)\cdot\frac{2+1}{2}\\(2.2-1)\cdot\frac{4+2}{2}\\(3-2.2)\cdot\frac{6+4}{2}\\(4.5-3)\cdot\frac{7+6}{2}\end{array}\right\rbrace \Sigma$$

Simpson's 1/3 Method

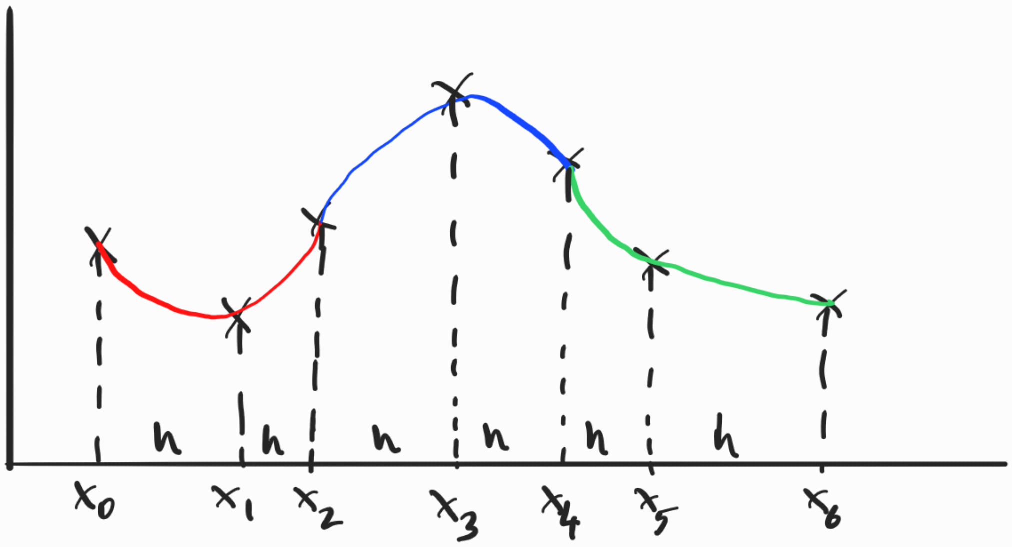


$$A = \frac{h}{3}\left(f(x_0)+4f(x_1)+f(x_2)\right)$$

$$\varepsilon_{AT} = -\frac{h^5}{90} f''''(\xi)$$

4^{th} order error

Composite Simpson



$$\frac{h}{3}\left[f(x_0) + 4\sum f(x_{odd}) + 2\underbrace{\sum f(x_{even})}_{\text{except the two ends}} + f(x_6)\right]$$

$n/2$ parabolas

$$h = \frac{b-a}{n} \qquad \varepsilon = -\frac{(b-a)^5}{90n^5}\cdot\frac{n}{2}\cdot\overline{f''''}$$

It gives exact result for 2^{nd} and 3^{rd} degree polynomials.

Example:

x	$f(x)$
-1	-0.5
0	1
1	1
2	0
3	-1
4	0
5	7

$$\int_{-1}^{5} f(x)\,dx \qquad 2^x - x^2$$

a) Comp. Trapezoid

b) Comp. Simpson

c) Analytical solution

d) $\int_0^4 f(x)dx$ by Simpson

a)

$$\frac{1}{2}\left[-0.5+7+2(1+1+0-1+0)\right]=4.25$$

b)

$$\frac{1}{3}\left[-0.5+4\times(1+0+0)+2\times(1-1)+7\right]$$

$$=3.5$$

c)

$$\int_{-1}^{5}(2^x-x^2)\,dx=\frac{2^x}{\ln 2}-\frac{x^3}{3}\Bigg|_{-1}^{5}$$

$$=\frac{2^5}{\ln 2}-\frac{5^3}{3}-\left(\frac{2^{-1}}{\ln 2}-\frac{-1^3}{3}\right)=3.449$$

d) Simpson is applied over even number of intervals

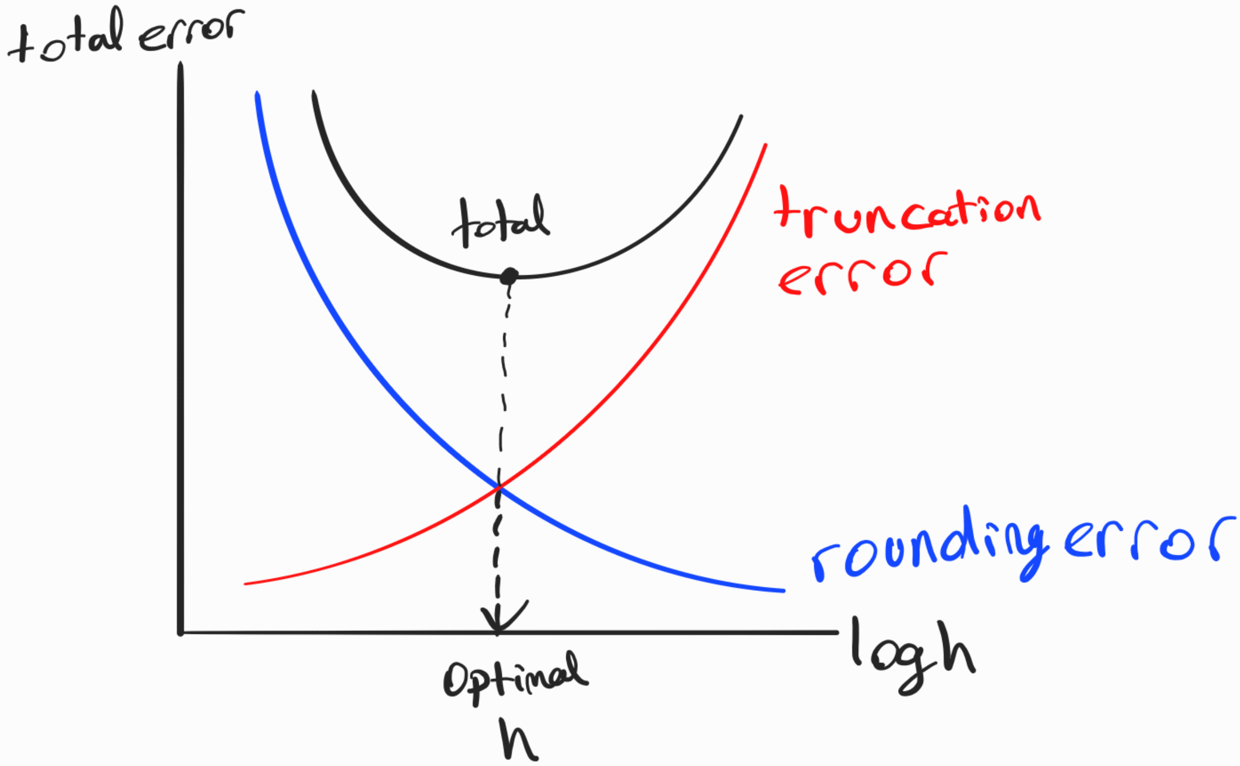
odd number of data points:

$$\int_{-1}^{4}f(x)dx=\underbrace{\int_{-1}^{3}f(x)dx}_{\text{Simpson}}+\underbrace{\int_{3}^{4}f(x)dx}_{\text{trapezoid}}$$

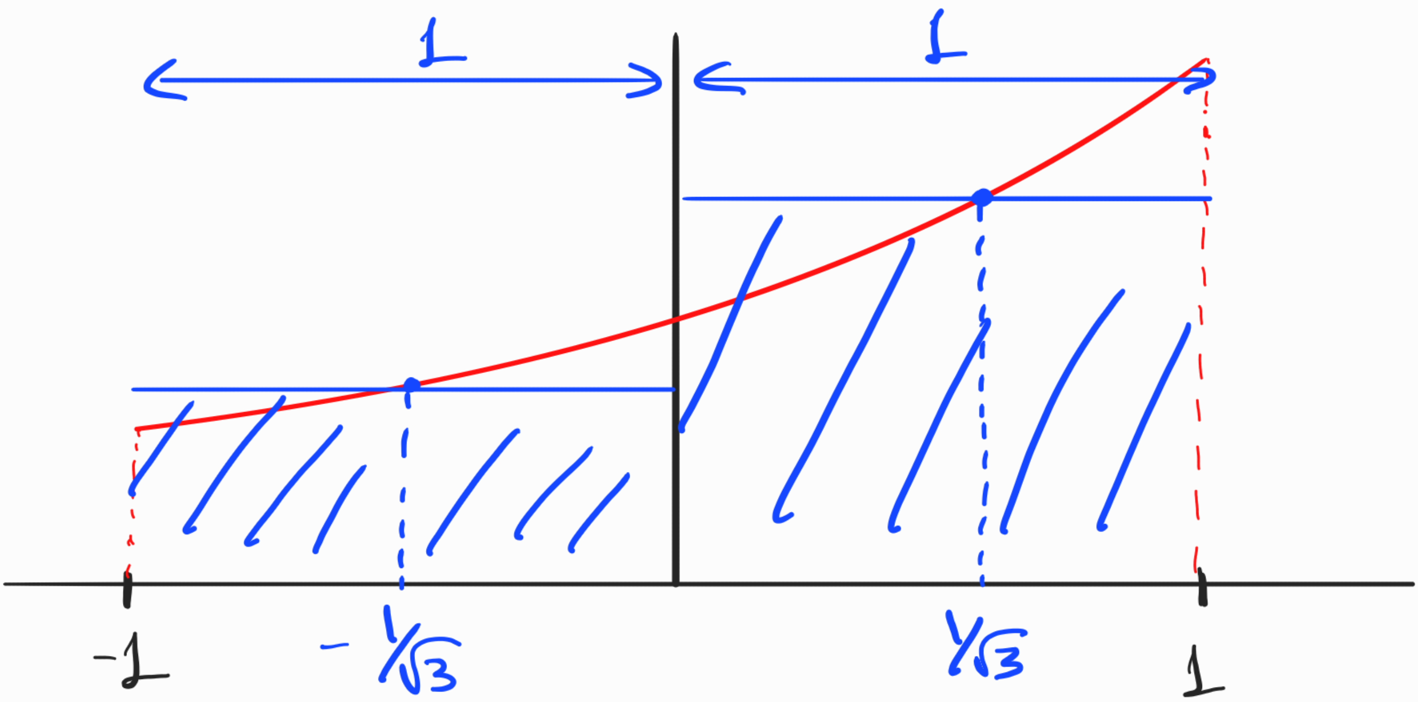
In slice methods with smaller h more intervals
truncation error ↓

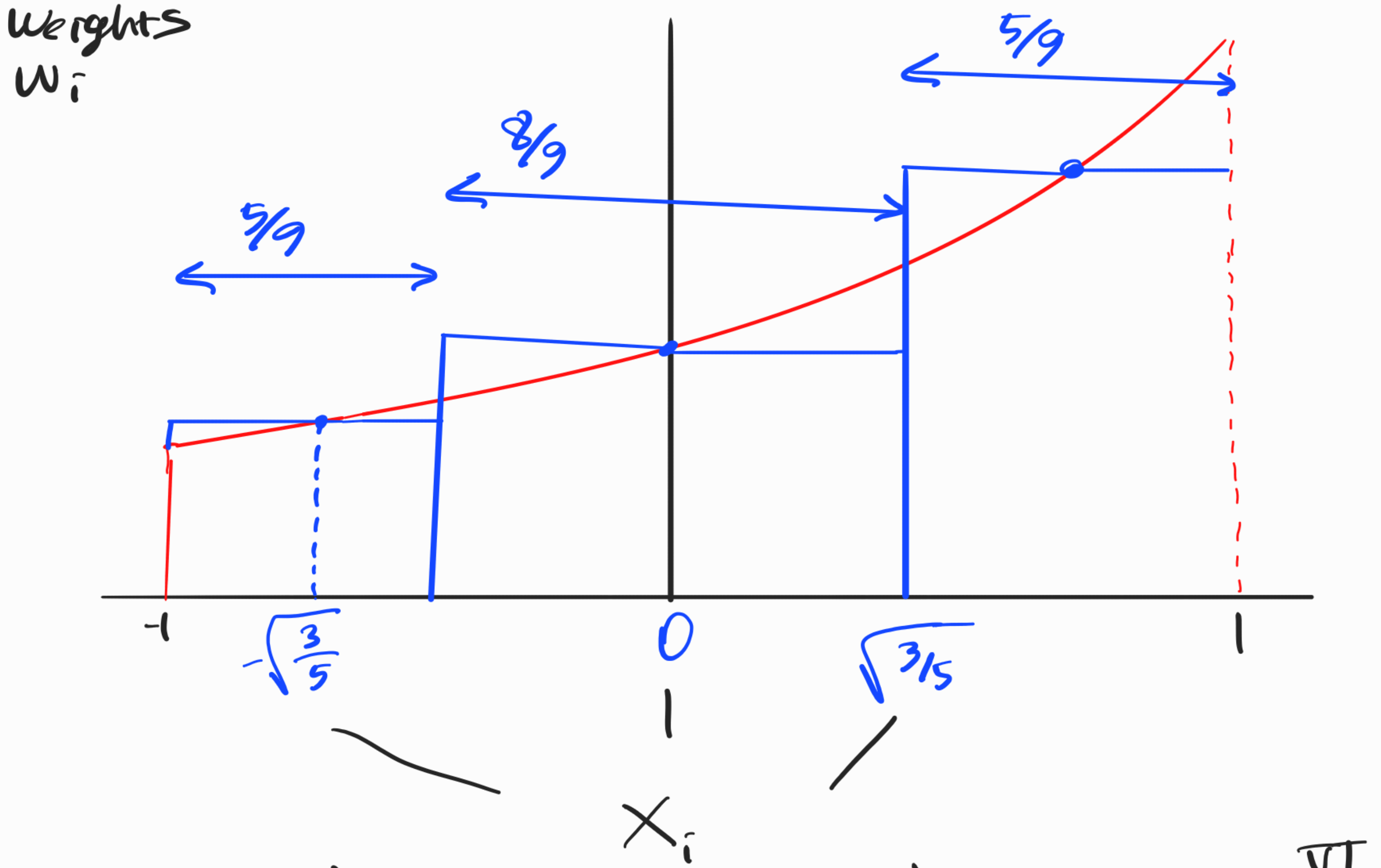
But rounding errors accumulate

Comp. Trapezoid $\varepsilon = -\frac{h^3}{12} n \cdot f''$



Gaussian Quadrature on Legendre Polynomials





$$\frac{5}{9}f\left(-\sqrt{\frac{3}{5}}\right)+\frac{8}{9}f(0)+\frac{5}{9}f\left(\sqrt{\frac{3}{5}}\right) \quad \text{error} \propto f^{VI}$$

error $\propto f''''$ $\quad \sum w_i f(x_i)$

∇ The only issue is to convert $\int_a^b$ into $\int_{-1}^{1}$ or vice verse

Method 1: Convert your problem into $\int_{-1}^{1}$

Method 2: Convert Gaussian solution into $\int_a^b$

Method 1: Transform f such that it fits the quadrature $\int_{t=a}^{t=b} g(t)\,dt$ replace $t=\frac{a+b}{2}+\frac{b-a}{2}x$

$$\underbrace{\int_{-1}^{1} g\left(\frac{a+b}{2} + \frac{b-a}{2}x\right)\frac{b-a}{2}}_{f(x)} dx = \int_{-1}^{1} f(x)dx = \sum w_i f(x_i)$$

x_i $\quad -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}$

w_i $\quad 1, 1 \qquad \sum w_i = 2$

Method 2: rescale quadrature w_i & x_i to fit the problem

- new w_i will be (Gaussian w_i) $\times \frac{b-a}{2}$
- each x_i will transform into

new $x_i = \frac{a+b}{2} + \frac{b-a}{2}$ (Gaussian x_i)

Ex: $\displaystyle\int_{-1}^{5} (2^x - x^2)\,dx$ using 3 point Gauss Q.

$$\int_{-1}^{1} f(x)\,dx \approx \sum_i w_i \cdot f(x_i)$$

w_i	x_i
$5/9$	$-\sqrt{3/5}$
$8/9$	0
$5/9$	$\sqrt{3/5}$

Method 1: Transform the function such that it fits the quadrature

$$t = \frac{a+b}{2} + \frac{b-a}{2}x = \frac{-1+5}{2} + \frac{5--1}{2}x = 2+3x$$

$$dt = \frac{b-a}{2}dx \Rightarrow dt = 3dx$$

$$\int_a^b g(t)\,dt = \int_{-1}^{5} (2^t - t^2)\,dt = \int_{-1}^{1} \left[2^{2+3x} - (2+3x)^2\right] 3\,dx$$

$$= \frac{5}{9}\left[2^{2-3\sqrt{3/5}} - \left(2-3\sqrt{3/5}\right)^2\right]3 +$$

$$= \frac{8}{9}\left[2^{2-3\times 0} - (2-3\times 0)^2\right]3 + \frac{5}{9}\left[2^{2+3\sqrt{3/5}} - \left(2+3\sqrt{3/5}\right)^2\right]\cdot 3$$

$=3.37466$

Method 2: Transform the Quadrature to fit the question

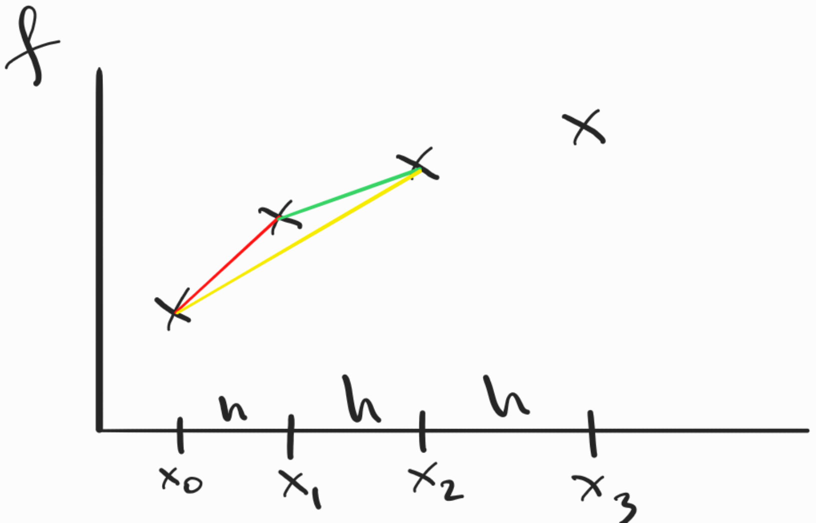
w_i	t_i
$3\times\frac{5}{9}$	$2+3\left(-\sqrt{3/5}\right)=-0.32379$
$3\times\frac{8}{9}$	$2+3\times 0=2$
$3\times\frac{5}{9}$	$2+3\left(\sqrt{3/5}\right)=4.32379$

$$\frac{5}{3}\left[2^{-0.32379}-(-0.32379)^2\right]+\frac{8}{3}\left[2^2-2^2\right]+\frac{5}{3}\left[2^{4.32379}-4.32379^2\right]$$

Romberg Integration

- apply composite trapezoid method with different interval sizes.
- figure out the relation between error vs h.
- extrapolate what the result would be as $h\to 0$

Numerical Differentiation



$$f'(x_1) = \frac{f(x_1) - f(x_0)}{h}$$ backward differentiation

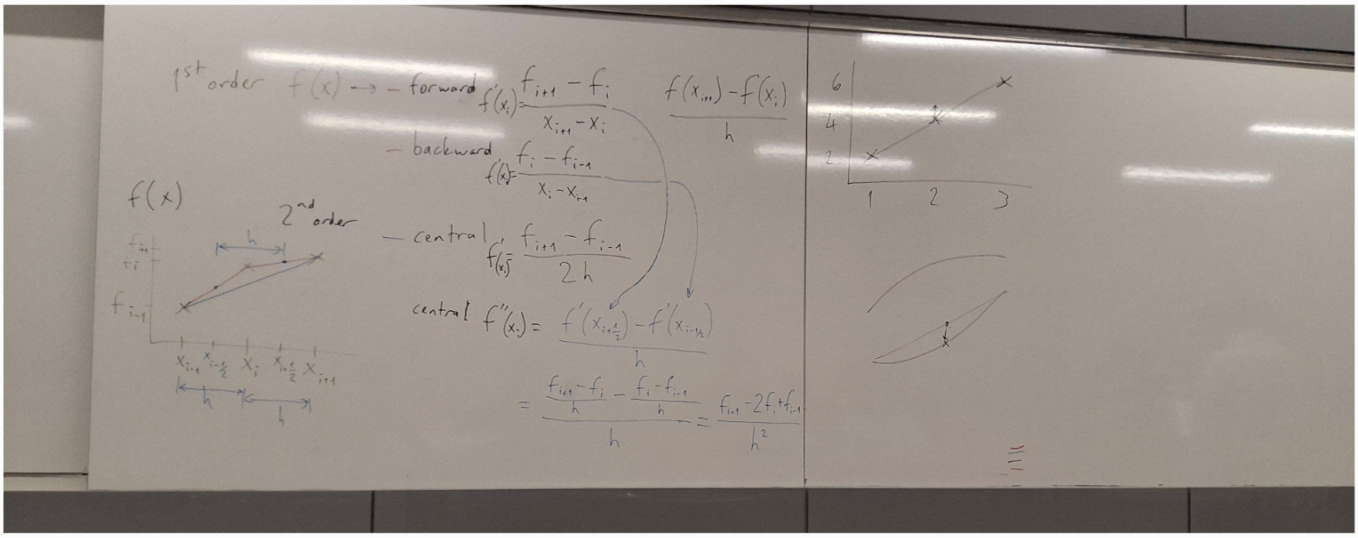
$$f'(x_1) = \frac{f(x_2) - f(x_1)}{h}$$ forward differentiation

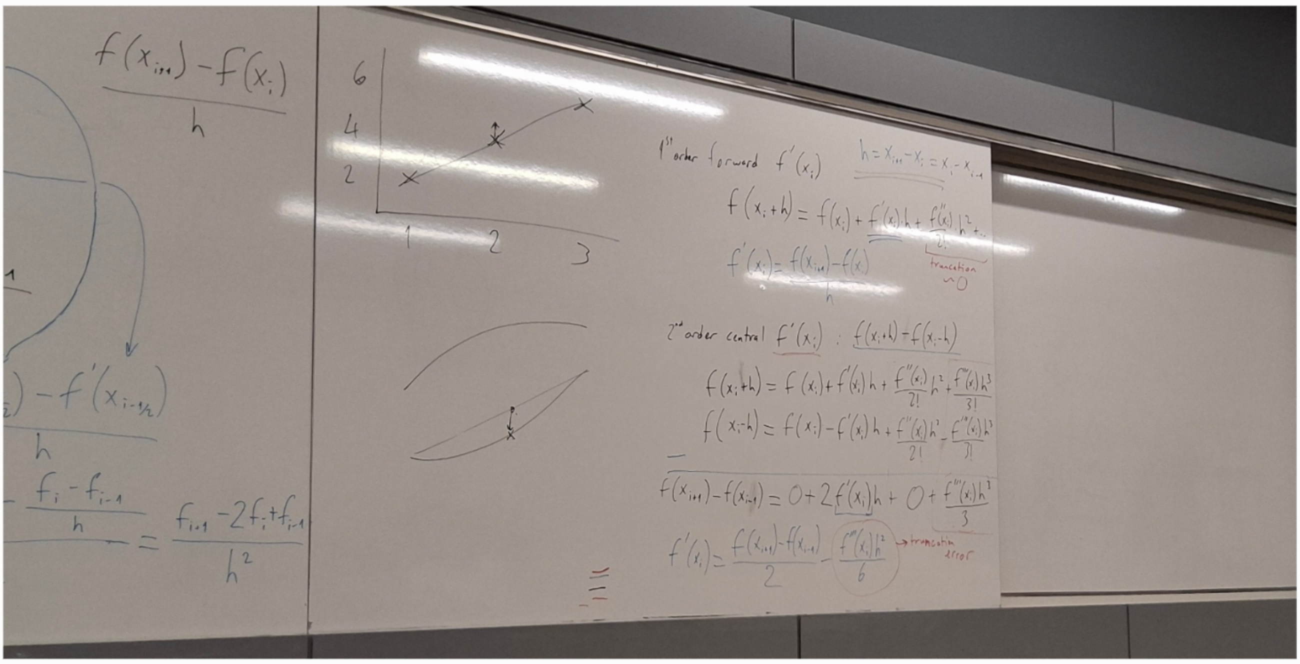
1st order

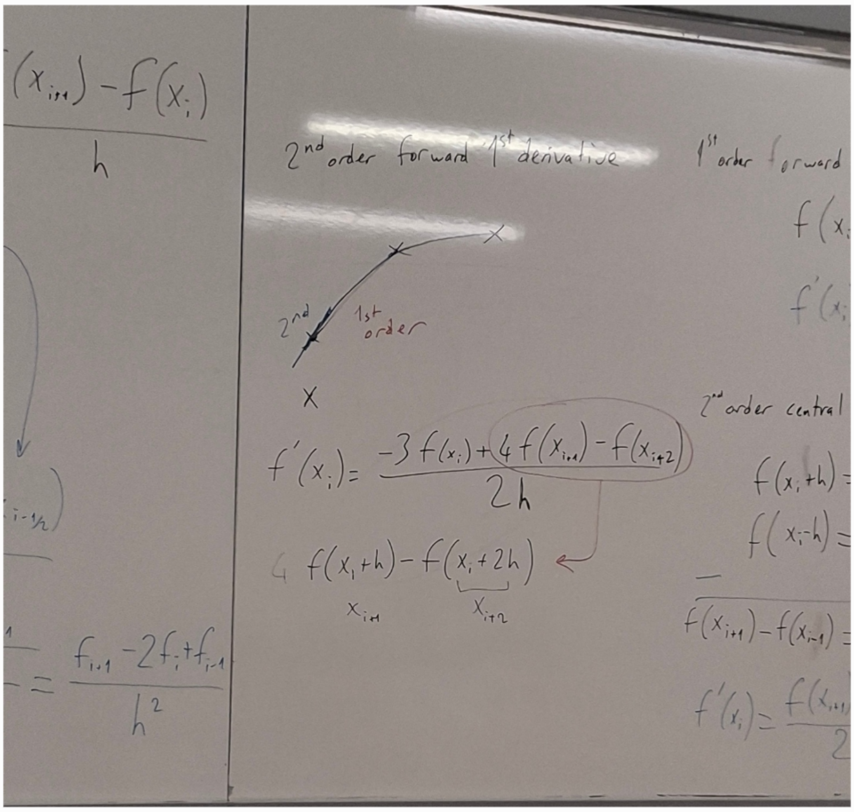
$$\frac{\frac{f(x_1) - f(x_0)}{h} + \frac{f(x_2) - f(x_1)}{h}}{2}$$

$$f'(x_1) = \frac{f(x_2) - f(x_0)}{2h}$$ → central difference formula

2nd order







Ex:

x	Y
0	1
1	3
2	4
3	2

estimate y' at each x, using $O(h^2)$ accuracy

at $x=0$

$$y'(0) = \frac{-3y_i + 4y_{i+1} - y_{i+2}}{2h}$$

$$= \frac{-3\times 1 + 4\times 3 - 4}{2\times 1} = 2.5$$

at $x=1$ central

$$y'(1) = \frac{y_{i+1} - y_{i-1}}{2h} = \frac{4-1}{2} = 1.5$$

at $x=2$ same $\rightarrow y' = \frac{2-3}{2} = -0.5$

at $x=3$ backward

$$y'(3) = \frac{y_{i-2} - 4y_{i-1} + 3y_i}{2h}$$

$$y'(3) = \frac{1 - 4\times 2 + 3\times 2}{2} = -\frac{7}{2} = -3.5$$

Differential Equations

unknown function $y(x)$

$$\frac{d^2y}{dx^2} + \frac{dy}{dx} = y + x$$ Ordinary Differential Equation

$z(x,y)$ $$\frac{\partial z}{\partial x} + \frac{\partial z}{\partial y} = z$$ Partial Differential Equation

$\rightarrow$ known boundary condition(s)

$y'=1$

$y=x$ $\quad y=x+1$

n^{th} order ODE needs n boundary conditions $\rightarrow$ known values of the function or its derivatives

- If all B.C. (boundary conditions) are at the same point

$y(0)=1,\ y'(0)=0$ initial value problem

Otherwise

$y(0)=1, \quad y(5)=8$ boundary value problem

Examples in CE

$$y'' = \frac{M}{EI}$$

$$m\ddot{x} + c\dot{x} + kx = F(t)$$

$$\frac{k}{\gamma_w} \frac{\partial^2 u_e}{\partial z^2} = m_v \frac{\partial u_e}{\partial t}$$

Navier Stokes

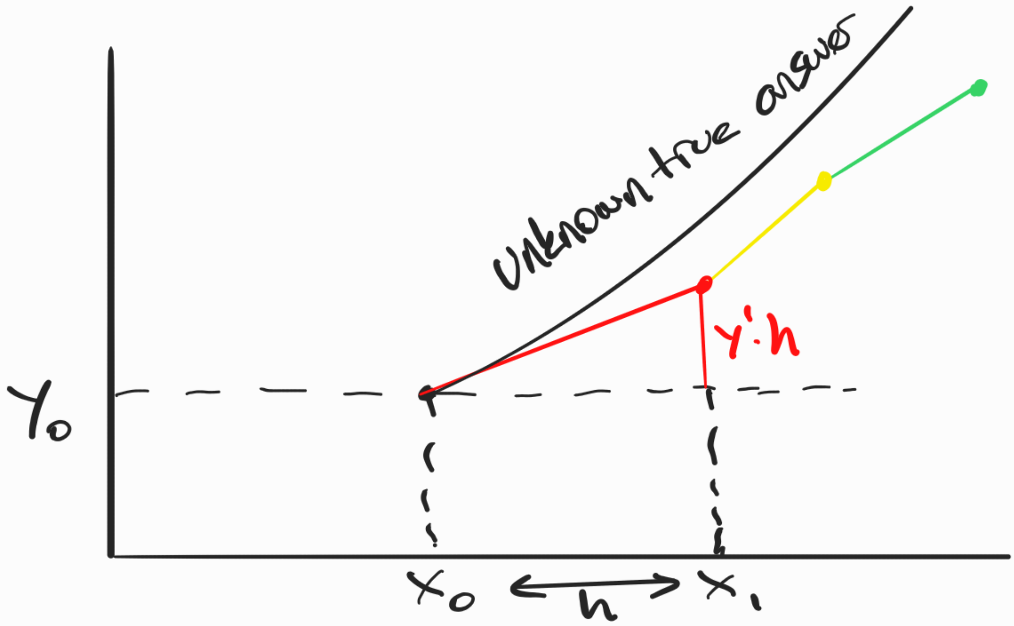
Transport / Flow $\quad \nabla \cdot q = \frac{\text{amount}}{\text{Volume}}$

Euler Method

$$y' = f(x,y), \quad y(x_0) = y_0$$

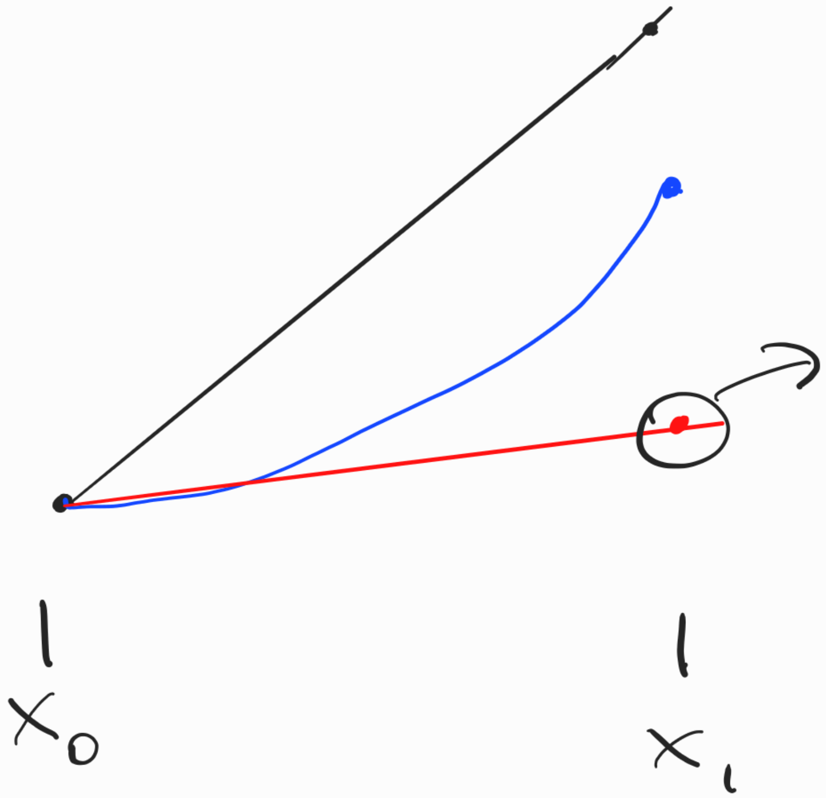
$$y(x+h) = y(x) + y'(x)\cdot h \underbrace{+ y''\frac{h^2}{2}}_{\text{truncation error}}$$

$$y_{i+1} = y_i + h\cdot f(x_i, y_i)$$



Heun's Method
(Improved Euler)
(Predictor - Corrector)

as Euler method but improve each step with a better estimation of slope



calculate y' based on (x_1, y_E)

take average of two slopes

$$\text{slope} = \frac{f(x_0, y_0) + f(x_1, y_E)}{2}$$

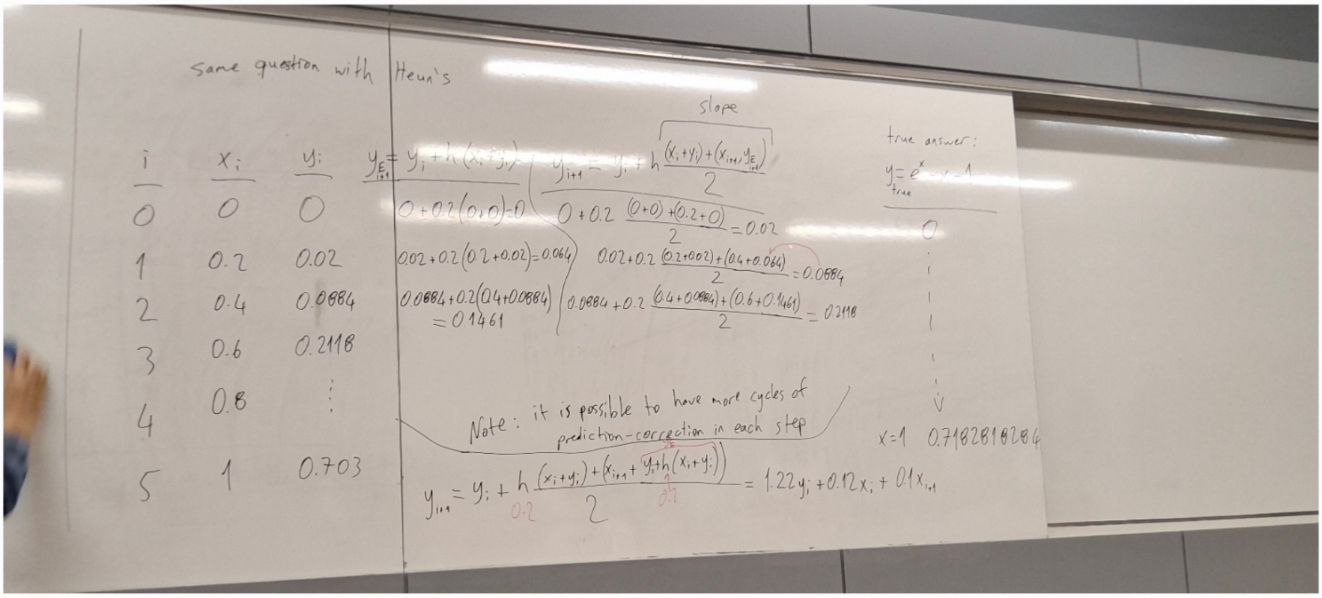
Example:

$y' = y + x$, $y(0) = 0$ use $h = 0.2$ solve for $0 \leq x \leq 1$

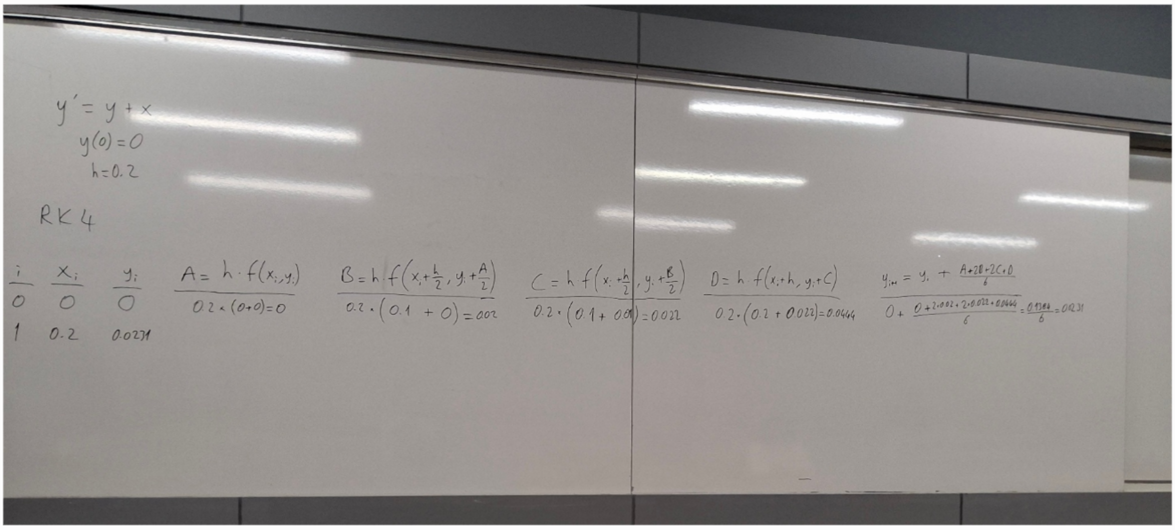
i	x_i	y_i	$y_{i+1} = y_i + h\overbrace{(x_i + y_i)}^{f = \text{slope}}$
0	0	0	$0 + 0.2(0+0) = 0 = y_1$
1	0.2	0	$y_2 = 0 + 0.2(0.2+0) = 0.04$
2	0.4	0.04	$y_3 = 0.04 + 0.2(0.4 + 0.04) = 0.128$
3	0.6	0.128	$0.128 + 0.2(0.6 + 0.128) = 0.274$
4	0.8	0.274	$0.274 + 0.2(0.8 + 0.274) = 0.489$

Same question with Heun's

i	x_i	y_i	$y_{E_i} = y_i + h(x_i + y_i)$	$y_{i+1} = y_i + h\overbrace{\frac{(x_i + y_i) + (x_{i+1}, y_{E_i})}{2}}^{\text{slope}}$
0	0	0	$0 + 0.2(0+0)$	$0 + 0.2 \times (0+0)$



Heun's



RK4

Example!

ODE systems, initial value problems

$$y' = x + z = f(x,y,z)$$

$$z' = x - y + z = g(x,y,z)$$

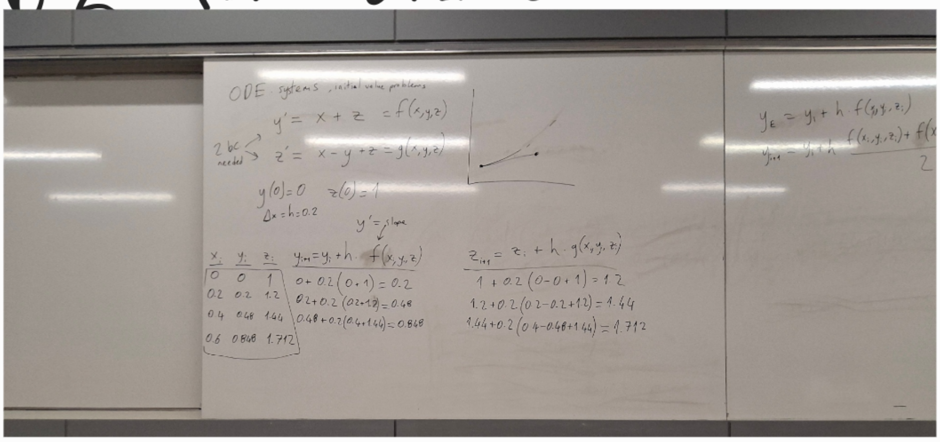
You need 2 boundary conditions

$$y(0) = 0 \qquad z(0) = 1$$

$$\Delta x = h = 0.2$$

y' slope

x_i	y_i	z_i	$y_{i+1} = y_i + h \cdot f(x_i, y_i, z_i)$	$z_{i+1} = z_i + h \cdot g(x_i, y_i, z_i)$
0	0	1	$0 + 0.2(0+1) = 0.2$	
0.2	0.2	1.2	$0.2 + 0.2(0.2$	

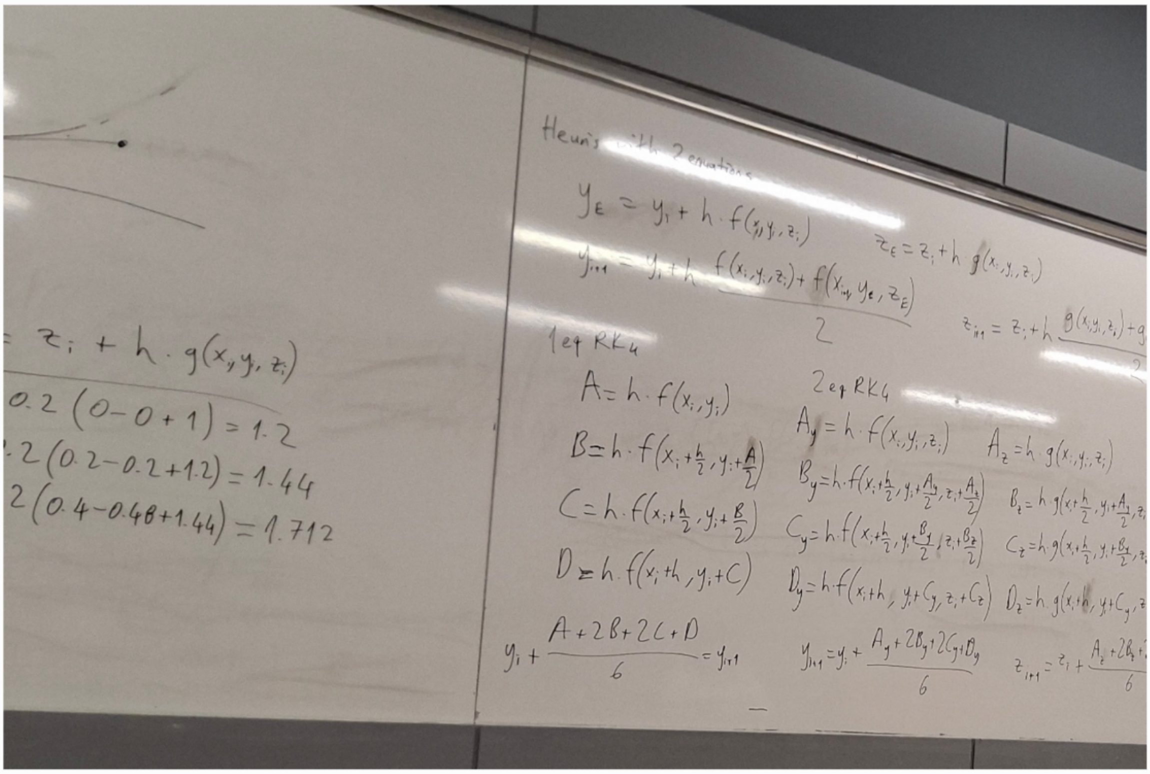


Euler

Heun's with 2 equations

$$y_E = y_i + h \cdot f(x_i, y_i, z_i) \qquad z_E = z_i + h\, g(x_i, y_i, z_i)$$

$$y_{i+1} = y_i + h\,\frac{f(x_i, y_i, z_i) + f(x_{i+1}, y_E, z_E)}{2}, \quad z_{i+1} = z_i + h\,\frac{g(x_i, y_i, z_i) + g(x_{i+1}, y_E, z_E)}{2}$$



Matlab notes:

$Y(3) = 1 \Rightarrow \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$

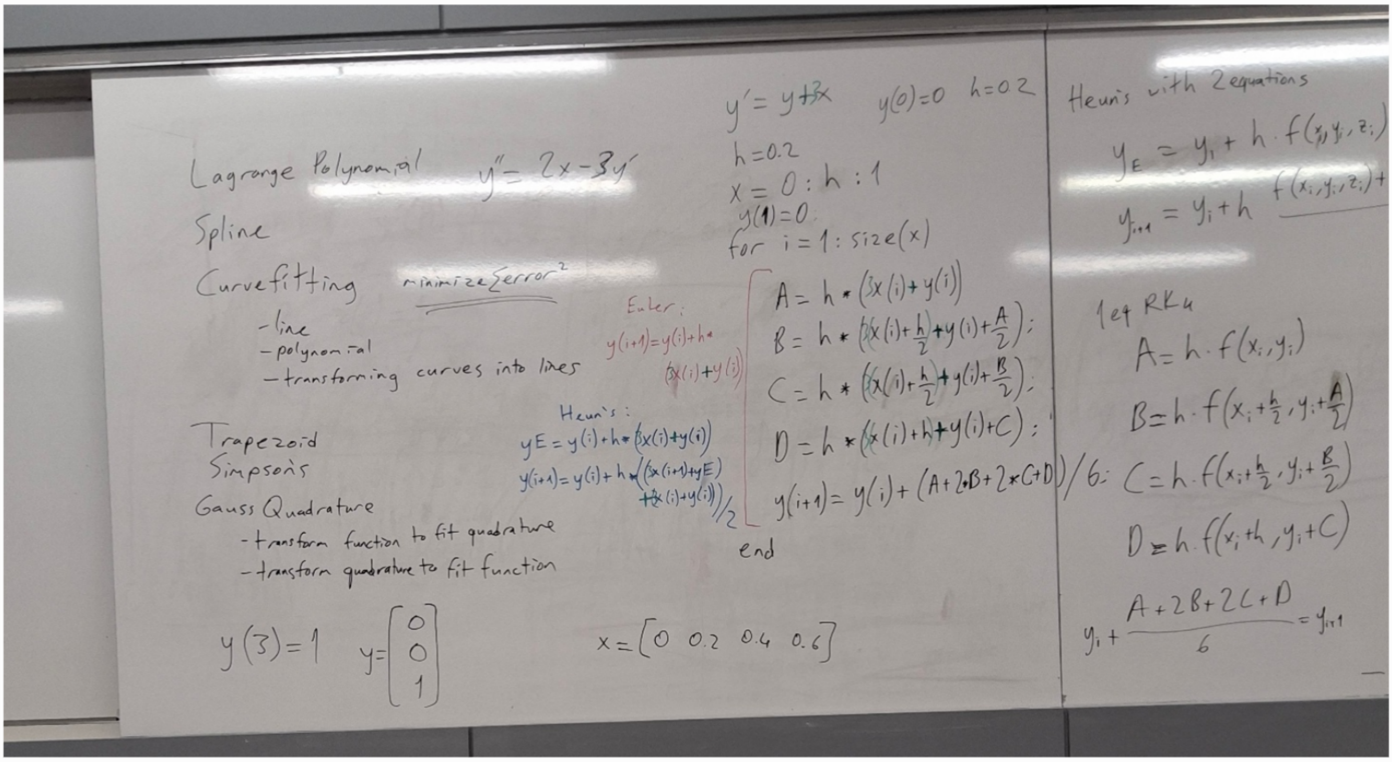
```
h = 0.2
x = 0: h: 1
y(1) = 0
for i = 1 : size(x)
    A = h · (x(i) + y(i))
    B = h · (x(i) + h/2 + y(i) + A/2)
    C = h · (x(i) + h/2 + y(i) + B/2)
    D = h · (x(i) + h + y(i) + C)
    y(i+1) = y(i) + (A + 2B + 2·C + D)/6
end
```

Euler:
$y(i+1) = y(i) + h \cdot (x(i) + y(i))$

Heun's:

$$Y_E = Y(i) + h \cdot (x(i) + y(i))$$

$$Y(i+1) = Y(i) + h \cdot ((x(i+1) + YE) + (x(i) + Y(i)))/2$$



ODE 1st order

- Euler
- Heun's
- RK4

Systems of 1st order ODE (IVP)

$$y' = f(x, y, z)$$

$$z' = g(x, y, z)$$

Higher Order ODE (IVP)

$$y'' + 2y' = x + y$$

substitute

$$z = y'$$

I.V.P.

$$Y(0) = 1$$

$$y'(0) = 2$$

Boundary Condition Problem

$$Y(0) = 1$$

$$Y(2) = 2$$

Finite Difference Method

can solve both initial and boundary value problems

transform the problem into a system of non-differential equations, with each point as an unknown.

Example:

use 2nd order approximation

$$y'' + 2y' + 3y = 4x + 5$$

$y(0) = -1$ $\qquad y(0.5) = ?$

$y(2) = 1$ $\qquad y(1) = ?$

$h = 0.5$ $\qquad y(1.5) = ?$

$$y_i'' = \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2}$$

$$y_i' = \frac{y_{i+1} - y_{i-1}}{2h}$$

central 2nd order

for i^{th} point

$$\underbrace{\frac{y_{i-1} - 2y_i + y_{i+1}}{0.5^2}}_{y''} + 2 \cdot \underbrace{\frac{y_{i+1} - y_{i-1}}{2 \times 0.5}}_{y'} + 3y_i = 4x_i + 5$$

$$i=1: \quad \frac{y_0 - 2y_1 + y_2}{0.25} + \frac{\cancel{2}\, y_2 - y_0}{\cancel{2} \times 0.5} + 3y_1 = 4x_1 + 5$$

$$4(-1 - 2y_1 + y_2) + 2(y_2 - (-1)) + 3y_1 = 4 \times 0.5 + 5$$

$$2(-1) - 5y_1 + 6y_2 = 7$$

$$i=2: \quad 4(y_1 - 2y_2 + y_3) + 2(y_3 - y_1) + 3y_2 = 4 \times 1 + 5$$

$$2y_1 - 5y_2 + 6y_4 = 9$$

$$i=3: \quad 4(y_2 - 2y_3 + y_4) + 2(y_4 - y_2) + 3y_3 = 4 \times 1.5 + 5$$

$$2y_2 - 5y_3 + 6 = 11$$

$$\begin{bmatrix} -5 & 6 & 0 \\ 2 & -5 & 6 \\ 0 & 2 & -5 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 9 \\ 9 \\ 5 \end{bmatrix}$$

Tri-diagonal (banded) Matrix

Example:

use 2^{nd} order approximation

$$y'' + 2y' + 3y = 4x + 5$$

(IVP) $y(0) = -1$
$y'(0) = 0$

$h = 0.5$

$y_1 = y(0.5) = ?$
$y_2 = y(1) = ?$
$y_3 = y(1.5) = ?$
$y_4 = y(2) = ?$

$y'(0) = 0$ this condition

$i = 0$

(forward)

$$y_i' = \frac{-3y_i + 4y_{i+1} - y_{i+2}}{2h} = \frac{-3y_0 + 4y_1 - y_2}{2\times 0.5} = 3 + 4y_1 - y_2 = 0$$

$$\begin{bmatrix} 4 & -1 & 0 & 0 \\ -5 & 6 & 0 & 0 \\ 2 & -5 & 6 & 0 \\ 0 & 2 & -5 & 6 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} -3 \\ 9 \\ 9 \\ 11 \end{bmatrix}$$

HWS $y'' = y \cdot \ln y'$ solve it by Euler's method

$z' = y \cdot \ln z$
$y'' = y \cdot \ln y'$

$\boxed{z = y'}$

FDM can be applied to non-linear differential equations

$$\sqrt{2+y''} = y \cdot \ln y' \longrightarrow$$ non-linear system of n equations n unknowns ($n = \#$ points)

Newton jacobi

Forced-damped vibration eq.

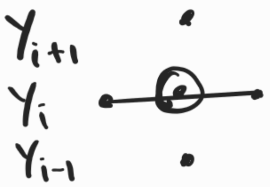
$$m\ddot{u} + c\dot{u} + ku = F(t)$$

$$\ddot{u}_i = \frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta t)^2}$$

u_i, u_{i+1} are displacements at different times

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = k$$

$$f(x_{i-1}, y_i) - 2f(x_i, y_i) + f(x_{i+1}, y_i)$$



$$\frac{f(x_{i-1}, y_i) - 2f(x_i, y_i) + f(x_{i+1}, y_i)}{(\Delta x)^2} + \frac{f(x_i, y_{i-1}) - 2f(x_i, y_i) + f(x_i, y_{i+1})}{(\Delta y)^2}$$

$$k \cdot h^2 = \sum f_{\text{neighbors}} - 4f(x_i, y_i)$$

$$f(x_i, y_i) = f_{\substack{\text{average of} \\ \text{four neighbors}}} + \frac{kh^2}{4}$$