

CSS322 Midterm Summary

► System of Linear Equations (L2)

solve n equations with n unknowns

$$\hookrightarrow Ax = b$$

↳ Unique solution

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ \vdots & \ddots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

$\Rightarrow A$ is nonsingular matrix
 $\det(A) \neq 0$
 \Rightarrow solution $x = A^{-1}b$

① L: Lower-Triangular Matrix

$$\begin{bmatrix} l_{11} & 0 & \dots & 0 \\ l_{21} & l_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ l_{n1} & \dots & \dots & l_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

Solve by "forward substitution"

② U: Upper-Triangular Matrix

$$\begin{bmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ 0 & u_{22} & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \dots & u_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

Solve by "backward substitution"

► LU-factorization / -decomposition

$$A = LU$$

↳ plain GE (Gaussian Elimination)

$$\begin{bmatrix} a_{11} & - & - & \dots & - \\ , & a_{22} & - & \dots & - \\ ; & - & a_{33} & \dots & - \\ ; & - & - & \ddots & \dots & a_{nn} \end{bmatrix}$$

! Pivot may be 0 even if matrix is nonsingular

solve linear equations \rightarrow

$$Ax = b$$

$$\textcircled{1} \quad A = LU$$

$$\textcircled{2} \quad Lw = b \rightarrow \text{solve for } w \rightarrow \text{"forward substitution"}$$

$$\textcircled{3} \quad UX = w \rightarrow \text{solve for } X \rightarrow \text{"backward substitution"}$$

$$\text{ex} \quad \begin{cases} x_1 + 2x_2 + x_3 = -1 \\ -3x_1 + x_2 + x_3 = 0 \\ x_1 + 3x_3 = 1 \end{cases} \quad Ax = b$$

$$\text{sol} \quad \begin{bmatrix} 1 & 2 & 1 \\ -3 & 1 & 1 \\ 1 & 0 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$$

Plain GE :

$$R_2 - (-3)R_1 \rightarrow \begin{bmatrix} 1 & 2 & 1 \\ 0 & 7 & 4 \\ 0 & -2 & 2 \end{bmatrix} \rightarrow R_3 - \left(\frac{-2}{7}\right)R_2 \rightarrow \begin{bmatrix} 1 & 2 & 1 \\ 0 & 7 & 4 \\ 0 & 0 & 22/7 \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ -3 & 1 & 0 \\ 1 & -2/7 & 1 \end{bmatrix}$$

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$$U = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 7 & 4 \\ 0 & 0 & 22/7 \end{bmatrix}$$

②

$$\rightarrow Lw = b \quad \begin{bmatrix} 1 & 0 & 0 \\ -3 & 1 & 0 \\ 1 & -2/7 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$$

$$\rightarrow w_1 = -1$$

$$\rightarrow -3w_1 + w_2 = 0$$

$$\rightarrow w_2 = 3w_1 = 3(-1) = -3$$

$$\rightarrow w_1 - \frac{2}{7}w_2 + w_3 = 1$$

$$w_3 = 8/7$$

$$\Rightarrow w = \begin{bmatrix} -1 \\ -3 \\ 8/7 \end{bmatrix}$$

③

$$\rightarrow Ux = w$$

$$\begin{bmatrix} 1 & 2 & 1 \\ 0 & 7 & 4 \\ 0 & 0 & 22/7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -3 \\ 8/7 \end{bmatrix}$$

$$\rightarrow \frac{22}{7}x_3 = \frac{8}{7} \Rightarrow x_3 = \frac{4}{11}$$

$$7x_2 + 4x_3 = -3$$

$$7x_2 + \frac{16}{11} = -3$$

$$x_2 = \left(-3 - \frac{16}{11} \right) / 7 = -\frac{7}{11}$$

$$x_1 + 2x_2 + x_3 = -1$$

$$x_1 = -1 - 2\left(-\frac{7}{11}\right) - \frac{4}{11} = -\frac{1}{11}$$

$$X = \begin{bmatrix} -1/11 \\ -7/11 \\ 4/11 \end{bmatrix} *$$

How to solve problem of Plain GE?

→ Permutation matrix P
 ↳ only contains 0's and 1's
 ↳ 1's per row / per column (1)

$$\text{ex. } \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

mat. A perm. mat. P.

left PA \Rightarrow exchange rows
right AP \Rightarrow exchange columns

$$P^T = P^{-1}$$

we can exchange rows
 → GEPP

"P^TLU factorization"

Gaussian Elimination with partial pivoting

→ select pivot at maximum absolute value

$$A = P^T LU \rightarrow \text{solve linear equation of } Ax = b$$

- ① $A = P^T LU$
- ② $\hat{b} = Pb \Rightarrow$ exchange row of b
- ③ $Lw = \hat{b}$
- ④ $Ux = w \Rightarrow x$ is ans.

$$\text{ex: } \begin{bmatrix} 1 & 2 & 1 \\ -3 & 1 & 1 \\ 1 & 0 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$$

exchange Row 1 & 2

$$\text{① } \begin{bmatrix} 1 & 2 & 1 \\ -3 & 1 & 1 \\ 1 & 0 & 3 \end{bmatrix} \rightarrow \begin{bmatrix} -3 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 0 & 3 \end{bmatrix} \rightarrow R_2 - \frac{1}{(-3)}R_1 \begin{bmatrix} -3 & 1 & 1 \\ 0 & 7/3 & 4/3 \\ 1 & 0 & 3 \end{bmatrix} \rightarrow R_3 - \frac{1}{7/3}R_2 \begin{bmatrix} -3 & 1 & 1 \\ 0 & 7/3 & 4/3 \\ 0 & 0 & 66/21 \end{bmatrix} = U$$

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

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

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

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

$$L = \begin{bmatrix} 1 & 0 & 0 \\ -1/3 & 1 & 0 \\ -1/3 & 1/7 & 1 \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ -1/3 & 1 & 0 \\ -1/3 & 1/7 & 1 \end{bmatrix}$$

$$\begin{cases} w_1 = 0 \\ -\frac{1}{3}w_1 + w_2 = -1 \Rightarrow w_2 = -1 \\ -\frac{1}{3}w_1 + \frac{1}{7}w_2 + w_3 = 1 \end{cases}$$

$$w_3 = 1 + \frac{1}{7} = \frac{8}{7}$$

$$w = \begin{bmatrix} 0 \\ -1 \\ 8/7 \end{bmatrix}$$

$$\frac{66}{21}x_3 = \frac{8}{7} \Rightarrow x_3 = \frac{8}{7} \cdot \frac{21}{66} = \frac{4}{11}$$

$$\frac{7}{3}x_2 + \frac{9}{3}x_3 = -1$$

$$x_2 = \left[-1 - \frac{4}{3} \left(\frac{4}{11} \right) \right] \times \frac{3}{7} = -7/11$$

$$-3x_1 + x_2 + x_3 = 0$$

$$x_1 = \left[\left(-\frac{4}{11} \right) - \left(-\frac{7}{11} \right) \right] / -3 = \frac{3}{11} > \frac{1}{3} = \frac{-1}{11}$$

$$\therefore x = \begin{bmatrix} -1/11 \\ -7/11 \\ 4/11 \end{bmatrix}$$

finding inverse matrix?

* $A\bar{A}^{-1} = I$ A GEPP is the best way to solve $Ax = v$

$$A[x_1 \ x_2 \ \dots \ x_n] = [e_1 \ e_2 \ \dots \ e_n]$$

$$[Ax_1 \ Ax_2 \ \dots \ Ax_n] = [e_1 \ e_2 \ \dots \ e_n]$$

$$\hookrightarrow Ax_1 = e_1, \ Ax_2 = e_2, \ Ax_3 = e_3$$

* factorization (PTLU) of A only once

then use it to solve $Ax_i = e_i \quad i=1, \dots, n$

$$\bar{A}^{-1} \begin{bmatrix} \vdots & \vdots & \vdots \\ x_1 & x_2 & \dots & x_n \\ \vdots & \vdots & & \vdots \end{bmatrix}$$

4 step method

$$\hat{b}_i = Pb_i \rightarrow Lw_i = \hat{b}_i \rightarrow Ux_i = w_i$$

Norms (13)

* Triangle inequality : $\|x+y\| \leq \|x\| + \|y\|$

Vector norms

① 2-norms / euclidean norms

$$\|v\|_2 = \sqrt{\sum_{i=1}^n v_i^2}$$

② 1-norm

$$\|v\|_1 = \sum_{i=1}^n |v_i|$$

③ ∞ -norm

$$\|v\|_\infty = \max_{i=1}^n \{|v_i|\}$$

(maximum absolute value)

④ p-norm

$$\|v\|_p = \left(|v_1|^p + |v_2|^p + \dots + |v_n|^p \right)^{1/p}$$

$; p \geq 1$

Matrix norms

* Frobenius norm

$$\|B\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n b_{ij}^2}$$

* 1-norm

$\|B\|_1 =$ maximum absolute column sum

$$A = \begin{bmatrix} 1 & -2 \\ -3 & 4 \end{bmatrix} \Rightarrow \|A\|_1 = \max\{|1+|-3|, |-2|+|4|\} = \max\{4, 6\} = 6$$

* ∞ -norm

$\|B\|_\infty =$ maximum absolute row sum

$$\Rightarrow \|A\|_\infty = \max\{|1|+|-2|, |-3|+|4|\} = \max\{3, 7\}$$

• Approximation (L4)

- store decimal number in computer using floating-point format

⇒ can cause inaccurate / round off / inexactness

• error

$$\text{absolute error} = |\text{approx. value} - \text{true value}|$$

$$\text{relative error} = \frac{\text{absolute error}}{\text{true value}}$$

→ \hat{x} → approximate number $\rightarrow \frac{|\hat{x}-x|}{|x|}$

↳ approximate vector $\rightarrow \frac{||\hat{x}-x||}{||x||}$

• CATASTROPHIC CANCELLATION

arithmetic \div

- subtracting 2 numbers having same sign and similar magnitude, result becomes smaller magnitude

can be resulted in very large error!

• floating-point arithmetic

$$X = (\underbrace{d_0, d_1, d_2, \dots, d_{p-1}}_{p \text{ digits}}) \times 2^e$$

↳ precision

float : $p=23$
double : $p=52$

$$\text{ex. } 18 = (10010.)_2 = (1.001)_2 \times 2^4$$

$$0.875 = \frac{7}{8} = \frac{4}{8} + \frac{2}{8} + \frac{1}{8}$$

$$= \frac{1}{2} + \frac{1}{4} + \frac{1}{8} = (0.111)_2 \times 2^0 \\ = (1.11)_2 \times$$

• unit round off

$$\hookrightarrow E_{\text{mach}} = 2^{-p}$$

$$\text{ex. } p=3$$

$$x = 12 \Rightarrow (1.10)_2 \times 2^3$$

$$y = 3 \Rightarrow (1.10)_2 \times 2^1$$

$$z = x-y = 9 \Rightarrow (1.001)_2 \times 2^3$$

$$\Rightarrow (1.001)_2 \times 2^3 = 8$$

$$\text{relative error} = \frac{|8-9|}{|9|}$$

$$= 1/9$$

► Conditioning & Stability (LS)

- well-condition \rightarrow input has a small change \rightarrow output has a reasonable change.
- ill-condition \rightarrow output has a very large change

* even in the same problem \rightarrow it can be both well-/ill-condition at the same time

• Condition number

\hookrightarrow ratio of relative change in solution/output to relative change in input.

$$\text{cond. number} = \frac{\text{relative change in solution}}{\text{relative change in input}} \rightarrow \begin{cases} \text{close to } 1 \rightarrow \text{"well-condition"} \\ \text{otherwise} \rightarrow \text{"ill-condition"} \end{cases}$$

A some is hard to compute due to complexity, thus upper bound or rough estimation is used instead.

$$\begin{array}{lll} \text{cond. number} & \Rightarrow \text{cond}(A) = \kappa(A) = \|A\| \cdot \|A^{-1}\| & \rightarrow \text{the larger cond}(A), \\ \text{of non-singular square matrix} & * A \text{ is singular} \rightarrow \text{cond}(A) = \infty & \text{the more ill-condition} \end{array}$$

② Stability

- an algorithm is **stable** if the result it produce is relatively insensitive to perturbation due to approximation during computation

$$f(x) + \epsilon_f$$

◦ forward stable, produce nearly result for exact problem

$$f(x + \epsilon_b) + \epsilon_f$$

◦ conditionally stable, produce nearly result for nearly problem

◦ backward stable, produce exact result $f(x + \epsilon_b)$ for nearly problem
 \hookrightarrow tend to use more in practical

\Rightarrow Plain GE is unstable
GEPP is backward stable

◦ we can expect accurate solution from well-condition problem using stable algorithm

► Cholesky factorization (L6) → any positive definite symmetric matrix A can be

factored into $A = LL^T$ ($L \Rightarrow$ lower triangular matrix)

► Symmetric matrix $\Rightarrow A = A^T$

$$A = \begin{bmatrix} a_{11} & a_{21} & \dots & a_{n1} \\ a_{21} & a_{22} & & \vdots \\ \vdots & & \ddots & \vdots \\ a_{n1} & \ddots & \dots & a_{nn} \end{bmatrix}$$

A

$$\begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ l_{21} & l_{22} & l_{32} \\ l_{31} & l_{32} & l_{33} \end{bmatrix}$$

$$a_{11} = l_{11}^2$$

$$a_{21} = l_{11} l_{21}$$

$$a_{31} = l_{11} l_{31}$$

$$a_{22} = l_{21}^2 + l_{22}^2$$

$$a_{32} = l_{21} l_{31} + l_{22} l_{32}$$

$$a_{33} = l_{31}^2 + l_{32}^2 + l_{33}^2$$

• The efficient way to calculate $A = LL^T$

$$A = L L^T$$

$$\begin{bmatrix} a_{11} & a_{21} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 \\ l_{21} & l_{22} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} \\ 0 & l_{22} \end{bmatrix}$$

- ① $a_{11} = l_{11}^2 \Rightarrow l_{11} = \pm \sqrt{a_{11}} \rightarrow$ (for the sake of good, we will use only positive/larger value)
- ② $a_{21} = l_{11} l_{21} \Rightarrow l_{21} = a_{21} / l_{11}$
- ③ $a_{22} = l_{21}^2 + l_{22}^2 \Rightarrow l_{22} = \pm \sqrt{a_{22} - l_{21}^2}$

• this concept can be applied to all symmetric matrx.

• This algorithm is WELL-DEFINED → the best way to calculate
 & cheaper than GE/GEPP $\rightarrow Ax=b$ when A is symmetric matrix

→ Solving linear system w/ Cholesky factorization ($Ax=b$)

① $A = LL^T$ (factor by using Cholesky factorization)

② $Lw=b$ (solve for w , using forward substitution)

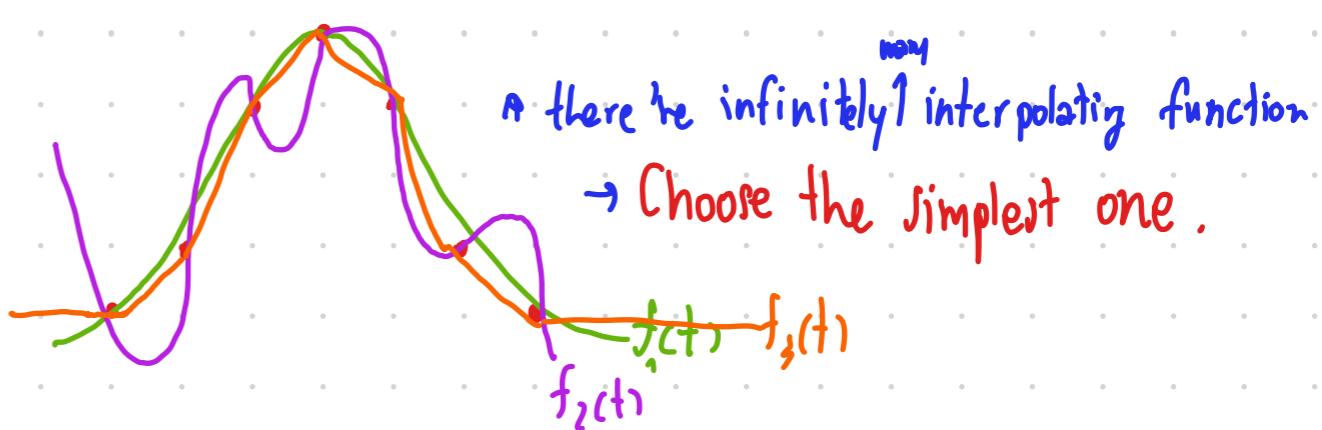
③ $L^T x = w$ (solve for x , using back substitution)

X

► Interpolation (L7)

we have n points (t_i, y_i) for $i = 1, \dots, n$

we want to find function that $f(t_i) = y_i$



► Polynomial Interpolation

simplest / continuous / differentiable / easy to evaluate

ⓐ monomial basis

n points → polynomial of degree $n-1$

$$P_{n-1}(t) = x_1 + x_2 t + x_3 t^2 + \dots + x_n t^{n-1}$$

→ we need to determine $x_i ; i = 1 \dots n$

$$\begin{bmatrix} 1 & t_1 & t_1^2 & \dots & t_1^{n-1} \\ 1 & t_2 & t_2^2 & \dots & t_2^{n-1} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 1 & t_n & t_n^2 & \dots & t_n^{n-1} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

improve efficiency by "Horner's method" → calculate faster

$$P_{n-1}(t) = x_1 + t(x_2 + t(x_3 + t(\dots(x_{n-1} + x_n t)\dots)))$$

ex. $2t^3 + 4t^2 - 3t + 1 = 1 - 3t + 4t^2 + 2t^3$
 $= 1 + t(-3 + 4t + 2t^2)$
 $= 1 + t(-3 + t(4 + 2t))$

⇒ solve for x
 you can use GEPP!
 (8 4 step method)

Vandermonde matrix → if all t_i are distinct
 → non singular matrix

► Lagrange Interpolation

$$l_1(t) = \frac{(t-t_2)(t-t_3) \dots (t-t_n)}{(t_1-t_2)(t_1-t_3) \dots (t_1-t_n)}$$

$$l_j(t) = \frac{\prod_{k=1, k \neq j}^n (t - t_k)}{\prod_{k=1, k \neq j}^n (t_j - t_k)}, \quad j = 1, \dots, n.$$

$$l_2(t) = \frac{(t-t_1)(t-t_3)(t-t_4) \dots (t-t_n)}{(t_2-t_1)(t_2-t_3) \dots (t_2-t_n)}$$

→ we rewrite polynomial as

$$P_{n-1}(t) = \sum_{i=1}^n y_i l_i(t)$$

► Newton Interpolation

→ we write $p_{n-1}(t)$ as $\sum_{i=1}^n x_i \pi_i(t)$
 where $\pi_i(t) = \prod_{j=1}^{i-1} (t - t_j)$
 ↓
 newtonian basis

$$\begin{cases} \pi_1(t) = 1 \\ \pi_2(t) = (t - t_1) \\ \pi_3(t) = (t - t_1)(t - t_2) \\ \vdots \\ \pi_n(t) = (t - t_1)(t - t_2) \dots (t - t_{n-1}) \end{cases}$$

Horner's rules → $p_{n-1}(t) = x_1 + (t - t_1)(x_2 + (t - t_2)(x_3 + \dots x_n(t - t_{n-1}) \dots))$

$$\begin{aligned} & \underline{5(t+1)(t-1)} - 6(t+1)(t-1)(t-2)(t-3) \\ & = (t+1)(t-1)(5 - 6(t-2)(t-3)) \end{aligned}$$

► interpolating complex function to simpler polynomial function

→ sample n points $(t_i, f(t_i))$

error bound.

$$\underbrace{\max_{t \in [t_1, t_n]} |f(t) - p_{n-1}(t)|}_{\text{error from interpolation}} \leq$$



sample how many n points.

maximum gap between t .

$$h = \max\{t_2 - t_1, t_3 - t_2, t_4 - t_3, \dots, t_n - t_{n-1}\}$$

$$|f^{(n)}_{\min}(t)| \leq M$$

derivatives at n order.

first order $f(x)$

second order $f''(x)$

n order $f^{(n)}(x)$

Numerical Integration (L8) $I(f) = \int_a^b f(x) dx$

3 rules

① Mid point Rules \rightarrow 1 point \Rightarrow degree 1

only 1 point \rightarrow center b/w a & b

$$n=1$$

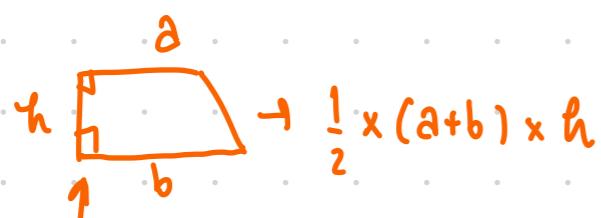
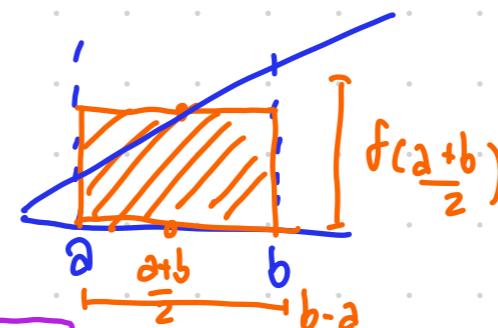
$$\text{at } \left(\frac{a+b}{2}\right) = x_1$$

Polynomial interpolant at $(x_1, f(x_1))$

$$P_0(x) = f\left(\frac{a+b}{2}\right)$$

$$G_1(f) = (b-a) f\left(\frac{a+b}{2}\right) \Rightarrow M(f)$$

mid point rules



Quadrature rule

$$Q_n(f) = w_1 f(x_1) + w_2 f(x_2) + \dots + w_n f(x_n).$$

② Trapezoid Rule \rightarrow 2 points

$$T(f) = \left(\frac{b-a}{2}\right) (f(a) + f(b))$$

A method of undetermined coefficients

$$\begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \\ x_1^{n-1} & x_2^{n-1} & \dots & x_n^{n-1} \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} b-a \\ (b^2 - a^2)/2 \\ \vdots \\ (b^n - a^n)/n \end{bmatrix}$$

→ solve by GEPP

③ Simpson's Rule \rightarrow 3 points \Rightarrow degree 3

$$S(f) = \left(\frac{b-a}{6}\right) \left(f(a) + 4 f\left(\frac{a+b}{2}\right) + f(b) \right)$$

A Midpoint Rule is more accurate than the trapezoid rule \times error

(twice more accurate)

$$E(f) \approx \frac{T(f) - M(f)}{3}$$

A Simpson's rule is much bigger error.

Use to approx. the error of integral

► Gaussian Quadrature

- for each n , there's a unique n -point gaussian quadrature rule gives the degree of $\underline{2n-1}$
- highest possible accuracy of n nodes, but difficult to derive.
find w_i 's and x_i 's so that $\int_a^b dx$, $\int_a^b x dx$, ..., $\int_a^b x^{2n-1} dx$ computed exactly (2n equations)
↳ will result in nonlinear system of equations

- Weights and nodes derived are specific to the particular interval.
- To integrate over other interval, can transform the new interval into the interval for the rule (say, $[-1, 1]$).

► Composite Rules

→ ① Midpoint Composite Rules ($M_k(f)$)

Subdivided into k equals interval

use midpoint rules on subinterval

→ ② Trapezoid Composite Rules ($T_k(f)$)

Subdivided into k equals interval

use trapezoid rules on subinterval

► Numerical Differentiation (L9)

→ function $f(x) : \mathbb{R} \rightarrow \mathbb{R}$

evaluate $f'(x)$ for given input x

* Approximate $f'(x)$ for given input x numerically, without computing formula of $f'(x)$

In general

when $n \gg 1$; it's bounded by largest term

$$\Rightarrow O(n^p) = C_p n^p + C_{p-1} n^{p-1} + \dots + C_0$$

when $0 < n \ll 1$; it's bounded by smallest term

$$\Rightarrow O(h^p) = C_p h^p + C_{p+1} h^{p+1} + \dots$$

for small value

• Forward difference

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

(has the error of $O(h)$)

↑
first order accuracy

• Backward Difference

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

(error is $O(h)$)

• Centered Difference of $f'(x)$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

[second order accuracy] → error of $O(h^2)$

• Centered difference for $f''(x)$:

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

[second order acc.] error of $O(h^2)$

- another way to derive finite difference formula is to interpolate f & find derivative of interpolant.

$t_i, i=1, \dots, n \Rightarrow h = t_{i+1} - t_i \Rightarrow$ equally-spaced points

same as

let $y_i = f(t_i)$; interpolate 2 points (t_i, y_i) & $(t_{i+1}, y_{i+1}) \rightarrow$ forward difference of f'

$(t_{i-1}, y_{i-1}) \& (t_i, y_i) \rightarrow$ backward difference of f'

$(t_{i-1}, y_{i-1}) \& (t_i, y_i) \& (t_{i+1}, y_{i+1}) \rightarrow$ centered difference of f'



To derive higher-order methods or methods for higher derivatives:

- ① Add more data points, e.g., $(t_{i-2}, y_{i-2}), (t_{i+2}, y_{i+2}), (t_{i-3}, y_{i-3}), (t_{i+3}, y_{i+3}), \dots$
- ② Find the interpolant, and
- ③ Take the derivative of the interpolant.

in both integration & differentiation, smaller step size give more accurate result

but step can't be too small b/c computation cost & catastrophic cancellation

• Richardson extrapolation

Suppose $f(h) = a_0 + a_1 h^p + O(h^r)$

as $h \rightarrow 0$ for some $p & r$, w/ $r > p$

thus

$$a_0 = f(h) + \frac{f(h) - f(h/q)}{q^{p-1}}$$

(has the error of $O(h^r)$ which smaller than $f(h)$ & $f(h/q)$)

→ $f(h)$ value obtained from \int method with step h

→ p is the derivative order

→ q is some positive integer

→ a_0 is the extrapolated value