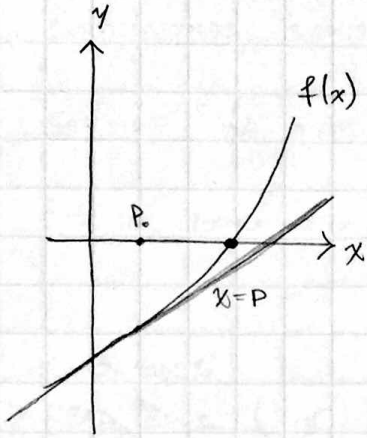


ROOT FINDING:



FIND P SUCH THAT $f(P) = 0$

NEWTON'S METHOD:

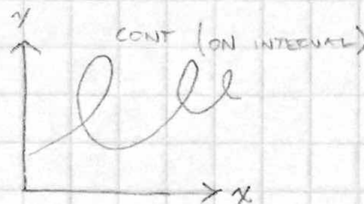
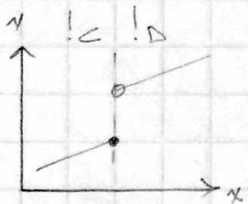
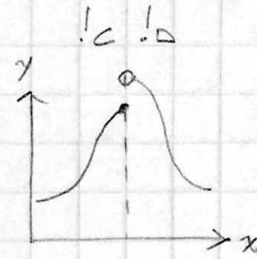
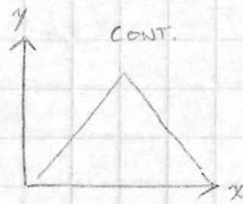
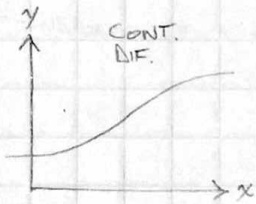
- GUESS P_0
- USE $T \in P_0$ TO FIND P_1
- ITERATE TO FIND $P_j \in$ DETERMINED ACCURACY

50% THEORY : 50% ANALYSIS

EMAIL SOURCE CODE DIRECTLY

NOTES:

MATHEMATICAL PRELIMS



CONTINUITY: $\lim_{x \rightarrow x_0} f(x) = f(x_0)$ EXISTS AND IS SINGLE VALUED (REGARDLESS OF DIR.)

DIFFERENTIABILITY: $\lim_{x \rightarrow x_0} \frac{f(x) - f(x_0)}{x - x_0} = \frac{\partial f(x)}{\partial x} \Big|_{x_0} = f'(x_0)$ EXISTS \therefore IS SINGLE VALUED

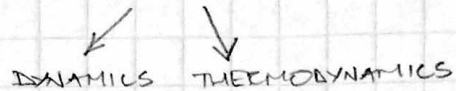
PRESENTATIONS ON FRIDAYS

- SHOULD BE PROFESSIONAL IN NATURE : ON MATERIAL PRESENTED THAT WEEK

CONSTITUTIONAL SUPERCOOLING

SEA-ICE: INDICATOR : PERPETRATOR OF CLIMATE CHANGE

SEA ICE GOVERNED BY "DYNAMIC DUO"



ASSIGNMENTS

* READ BOOK (THE ICE MASTER)

- REPORT ON LEADERSHIP, THE GOOD : BAD. DUE OCTOBER 7
- DID THEY USE TRICAL KNOWLEDGE?

* MAKE A LIST

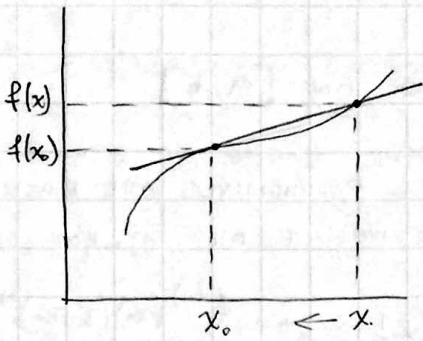
- TOP 10 THINGS TO KNOW ABOUT SEA ICE. SUMMARY OF IMPORT^{ANT} THINGS
- EG. SUMMARY FOR VICE PRESIDENT

- LEADERSHIP STYLE, STRENGTHS, : WEAKNESSES

- HOW DID THEY RESPOND TO ADVERSITY, SUCCESS?

- INDIGENOUS KNOWLEDGE -- DID THEY USE IT?

CONTINUITY / DIFFERENTIABILITY



$$f'(x_0) = \lim_{x \rightarrow x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

MATLAB (ROWS, COLUMNS)

ABSOLUTE ERROR: $|P - P^*|$ (APPROXIMATION)

RELATIVE ERROR: $\frac{|P - P^*|}{|P|}$, SAME AS ABSOLUTE, BUT NORMALIZED BY $|P|$

* LAB 1 PSEUDOCODE

COMPUTE J_2 FROM $J_2(x) \frac{z(z)}{x} = J_{2+1}(x) + J_{2-1}(x)$
 U.K.

n	J_n
0	
1	
2	
3	
4	

NOTES CONT.

- STABLE: SMALL CHANGES IN INPUT \rightarrow SMALL CHANGES IN OUTPUT
 \hookrightarrow COND. STABLE = STABLE BUT ONLY FOR CERTAIN CHOICES OF INITIAL DATA

STABILITY OFTEN ATTRIBUTED TO ERROR

BESELJ $\rightarrow J_n(z)$

- $E_n \approx C N E_0$ (LINEAR)

- $E_n \approx C^n E_0$ (EXPONENTIAL) \rightarrow OFTEN UNSTABLE

$J_0 = \dots$ (FOR $x = 1, 8, 25$)

$J_1 = \dots$ (FOR $x = 1, 8, 25$)

FOR $x = 1, 8, 25$

FOR $n = 1 : 25$

$J_{n+1}(x) = \frac{2n}{x} J_n(x) - J_{n-1}(x)$

\hookrightarrow FORWARD SCHEME

$n=1$
 $J_2(x) = \frac{2^1}{x} J_1(x) - J_0(x)$

$n=2$
 $J_3(x) = \frac{2^2}{x} J_2(x) - J_1(x)$

9/18/2015

* TAYLOR'S THEOREM

IF $f(x)$ HAS $n+1$ DERIVATIVES THAT EXIST ON $[a, b]$
THEN $f(x) = P_n(x) + R_n(x)$

USEFUL BC POLYNOMIALS ARE EASY TO WORK WITH. IE. DIFF, INT, ECT.

• N^{TH} TAYLOR POLYNOMIAL

$$P_n(x) = f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)(x-x_0)^2}{2!} \dots + \frac{f^{(n)}(x_0)(x-x_0)^n}{n!}$$

$$= \sum_{k=0}^n \frac{f^{(k)}(x_0)}{k!} (x-x_0)^k \quad \text{FOR } \begin{matrix} x_0 \in [a, b] \\ x \in [a, b] \end{matrix} \quad \text{IMPORTANT}$$

-NOTE: $P_n(x_0) = f(x_0)$, $k=0, 1, 2, \dots, n$

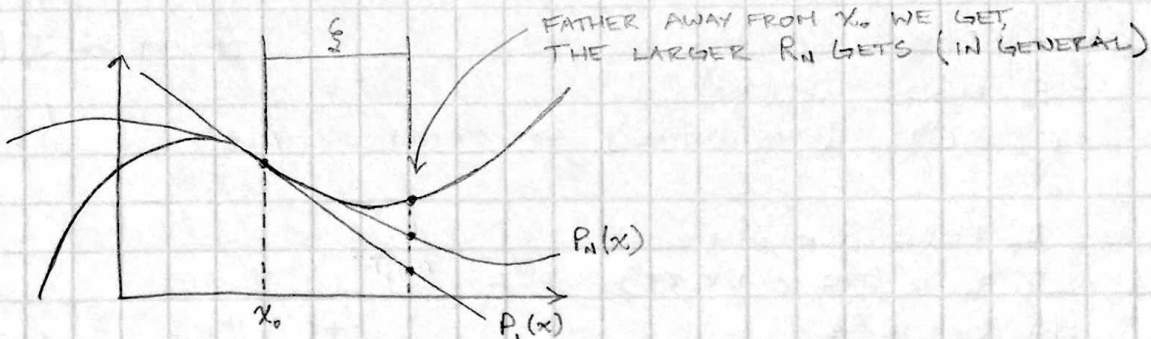
• TAYLOR SERIES:

$$n \rightarrow \infty \rightarrow \begin{matrix} P_n(x) = f(x) \\ \downarrow \\ \infty \end{matrix}$$

• TRUNCATION ERROR (REMAINDER)

$$R_n(x) = \frac{f^{(n+1)}(\xi)(x-x_0)^{n+1}}{(n+1)!}$$

WE DON'T KNOW THIS
 $\xi \in [x, x_0]$



9/18/2015

MATH IN COMPUTERS:

$$\frac{1}{3} = 0.333333... \rightarrow \text{MUST CHOP-OFF / ROUND}$$

- RESULTS IN ROUND OFF ERROR

$$(A+B)+C = A+(B+C)$$

$$(A*B)*C = A*(B*C)$$

$$A*(B+C) = (A*B)+(A*C)$$

} = BECOMES \neq W/ COMPUTERS

IN GENERAL, AS # OF OPERATIONS INCREASES, SO DOES ROUND OFF ERROR

* CLASSES OF ERROR GROWTH:

E_0 = INITIAL ERROR IN SOLUTION

E_N = ERROR AFTER N STEPS

1.) $E_N \propto KNE_0$ (LINEAR GROWTH)

$E_N \propto K^N E_0$ (EXPONENTIAL ERROR GROWTH)

* RECURSIVE RELATIONS

A.) $P_N = \frac{1}{3} P_{N-1}$

B.) $P_N = \frac{10}{3} P_{N-1} - P_{N-2}$

- ASSUME CONSTANTS ARE EXACT

$P_N = \frac{1}{3} P_{N-1}$ EXACT

$\hat{P}_N = \frac{1}{3} \hat{P}_{N-1}$ COMPUTER

\rightarrow

$$P_N - \hat{P}_N = \frac{1}{3} (P_{N-1} - \hat{P}_{N-1})$$

$$E_N = \frac{1}{3} E_{N-1}$$

$$E_1 = \frac{1}{3} E_0$$

$$E_2 = \frac{1}{3} E_1 = \frac{1}{3} (\frac{1}{3} E_0) = (\frac{1}{3})^2 E_0$$

$$E_3 = \frac{1}{3} E_2 = (\frac{1}{3})^3 E_0 \rightarrow E_N = \frac{1}{3} E_{N-1} = (\frac{1}{3})^N E_0$$

$$\lim_{N \rightarrow \infty} E_N = \lim_{N \rightarrow \infty} (\frac{1}{3})^N E_0 = 0$$

\hookrightarrow CANNOT ASSUME CONSTANTS EXACT

9/18/2015

$$\text{LET } \hat{\frac{1}{3}} = \frac{1}{3} - \delta$$

$$P_N = \frac{1}{3} P_{N-1} \rightarrow \hat{P}_N = (\frac{1}{3} - \delta) \hat{P}_{N-1} \rightarrow \epsilon_N = \frac{1}{3} \epsilon_{N-1} + \delta \hat{P}_{N-1}$$

$$\epsilon_1 = \frac{1}{3} \epsilon_0 + \delta \hat{P}_0$$

$$\epsilon_2 = (\frac{1}{3})^2 \epsilon_0 + \frac{1}{3} \delta \hat{P}_0 + \delta \hat{P}_1$$

$$\epsilon_3 = (\frac{1}{3})^3 \epsilon_0 + (\frac{1}{3})^2 \delta \hat{P}_0 + \frac{1}{3} \delta \hat{P}_1 + \delta \hat{P}_2$$

$$\epsilon_N = (\frac{1}{3})^N \epsilon_0 + \underbrace{(\frac{1}{3})^{N-1} \delta \hat{P}_0 + \dots + \delta \hat{P}_{N-1}}_{\substack{N \text{ TERMS, EACH} \\ \text{SMALLER THAN } \delta \hat{P}_0}}$$

$$\epsilon_N \leq (\frac{1}{3})^N \epsilon_0 + n \delta \hat{P}_0 \rightarrow \text{ERRORS ONCE INTRODUCED GROW LINEARLY}$$

B.

$$P_N = \frac{10}{3} P_{N-1} - P_{N-2} \quad (\text{EXACT})$$

$$\hat{P}_N = \frac{10}{3} \hat{P}_{N-1} - \hat{P}_{N-2} \quad (\text{COMPUTE})$$

$$P_N - \hat{P}_N = \frac{10}{3} (P_{N-1} - \hat{P}_{N-1}) - (P_{N-2} - \hat{P}_{N-2})$$

DIFFERENCE EQ. W/ CONSTANT COEFFICIENTS

$$\text{ASSUME } \epsilon_N \propto \lambda^n$$

$$\lambda^n = \frac{10}{3} \lambda^{n-1} - \lambda^{n-2} \rightarrow \lambda^2 - \frac{10}{3} \lambda + 1 = 0 \quad \text{CHARACTERISTIC OR AUXILIARY EQ.}$$

$$\lambda = \frac{-B \pm (B^2 - 4AC)^{1/2}}{2A}$$

$$\epsilon_N = C_1 \underbrace{(\frac{1}{3})^n}_{\rightarrow 0} + C_2 \underbrace{(\frac{1}{3})^n}_{\rightarrow \infty} \rightarrow \lim_{n \rightarrow \infty} = \infty$$

ONE ROOT IN CHARAC. EQ > 1

ONLY THE LARGEST ROOT MATTERS

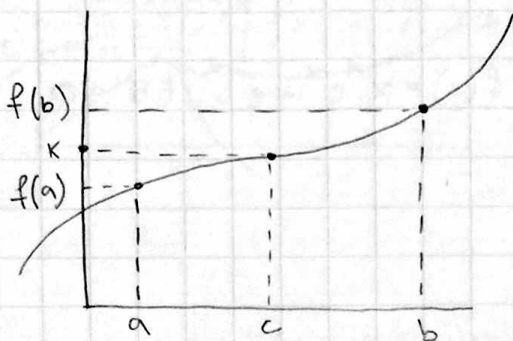
- FOR COMPLEX ROOTS, IT IS THE MAGNITUDE THAT MATTERS

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A FEW IMPORTANT THEOREMS

1. INTERMEDIATE VALUE THEOREM

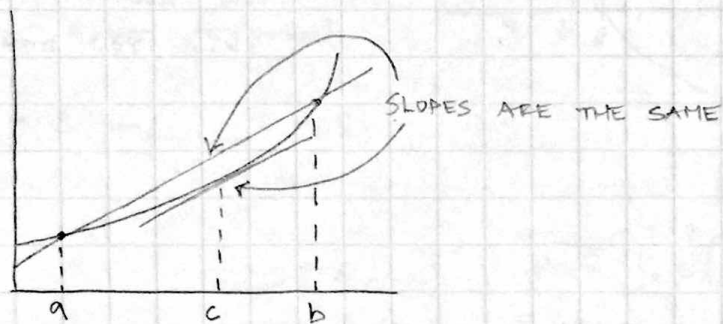
IF $f \in C[a, b]$ AND K IS BETWEEN $f(a)$ AND $f(b)$, THEN THERE EXISTS A NUMBER $c \in (a, b)$ FOR WHICH $f(c) = K$



2. MEAN VALUE THEOREM (MVT)

IF $f \in C[a, b]$ AND DIFFERENTIABLE ON (a, b) , THEN A NUMBER $c \in (a, b)$ EXISTS W/

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



9/21/2015

$$\epsilon_n \propto \lambda^n \rightarrow \epsilon_n = \sum_{j=0}^2 c_j \lambda_j^n, \text{ IF } |\lambda_j| > 1 \rightarrow \underline{\text{EXPONENTIAL}}$$

* SOLUTIONS TO NON-LINEAR EQUATIONS

"ROOT" FINDING PROBLEMS. FINDING p SUCH THAT $f(p) = 0$

EG.

$$x^4 e^x - e^{-2x} = 8 \rightarrow f(x) = x^4 e^x - e^{-2x} - 8 = 0$$

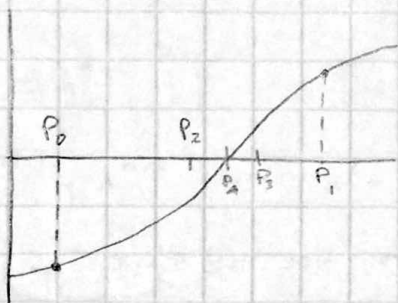
→ ITERATIVE METHODS ←

0.) "SCAN" x UNTIL $f(x) = 0$

- WHAT STEP SIZE? → TERRIBLE METHOD

1.) BISECTION METHOD

IF $f(a)f(b) < 0$, THEN INT GUARENTEE'S A ROOT
 $p \in [a, b]$



PICK TWO POINTS, EVALUATE,
THEN CUT IN HALF, BRACKET
THE ROOT & THROW AWAY
HALF YOU DON'T WANT

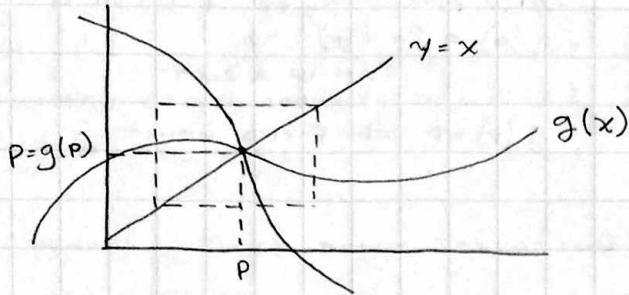
BISECTION METHOD:

- + SIMPLE
- + ALWAYS FINDS A ROOT
- NEED $[a, b]$ SUCH THAT $f(a)f(b) < 0$
- SLOW, $\epsilon_n \leq \frac{b-a}{2^n}$

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* FIXED POINT SCHEME

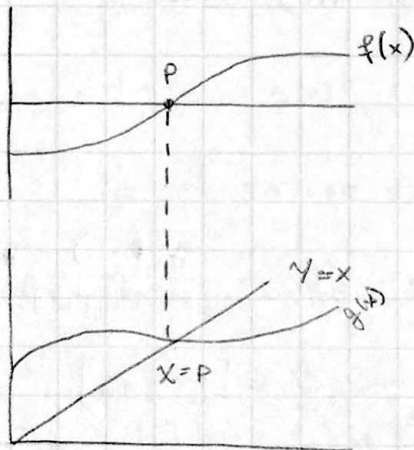
- WILL BE USEFUL FOR ANALYZING CONVERGENCE RATES OF VARIOUS ROOT FINDING TECHNIQUES



PROVABLE COND. FOR FIXED POINT

P IS A FIXED POINT WHEN $g(P) = P$

- i.) $g(x)$ IS CONTINUOUS ON $[a, b]$
- ii.) $g(x)$ IS BOUNDED ON $[a, b]$ BY $[a, b]$
- iii.) $|g'(x)| < 1 \quad x \in [a, b]$

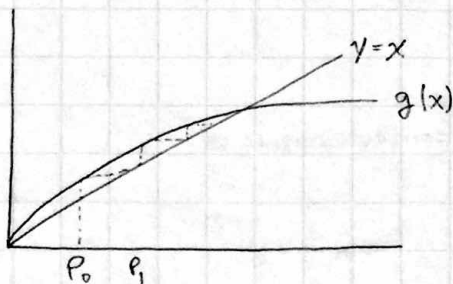


← WHEN $f(x) = 0$, $g(x) = x$
 $g(x) = x - f(x)$
 $g(p) = p - f(p)$
 $g(p) = p$
BY DEF A
FIXED POINT

HOW TO FIND FIXED POINT GIVEN $g(x)$?

→ FIXED POINT ITERATION

$$P_N = g(P_{N-1})$$

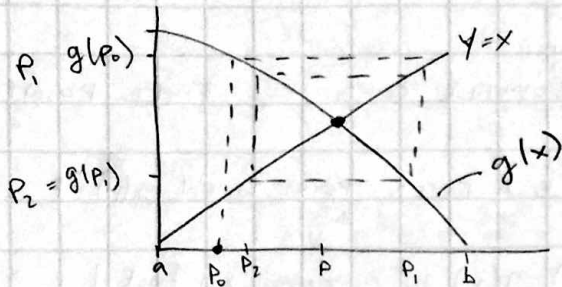


NEED $P_0 \in [a, b]$

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* FIXED POINT ITERATION

$$P_N = g(P_{N-1})$$



$$g(x) = x - f(x)$$

$$g(P) = P - f(P) = 0 \text{ IF A ROOT}$$

$$g(P) = P \Rightarrow \text{FIXED POINT}$$

ESTIMATE ERROR:

- ASSUME FIXED POINT CONTINUOUS i.) ii.) iii.) HOLD

$$P_n = g(P_{n-1}) \quad (\text{COMPUTE})$$

$$P = g(P) \quad (\text{EXACT})$$

$$|P_n - P| = |g(P_{n-1}) - g(P)| \rightarrow \text{MVT: } g'(c) = \frac{g(P_{n-1}) - g(P)}{P_{n-1} - P}$$

$$c \in [P, P_{n-1}]$$

$$E_n = |g'(c)| |P_{n-1} - P|$$

$$E_n = \underbrace{|g'(c)|}_{< 1 \text{ (MANDATED, RULE 3)}} |E_{n-1}|$$

$$E_n = K E_{n-1} = K^n E_0 \quad K < 1$$

$$\lim_{n \rightarrow \infty} E_n = \underbrace{K^n}_{= 0} E_0 = 0$$

GUARANTEED TO CONVERGE

A FEW OBSERVATIONS:

A.) $|g'(x)|$ SMALL \rightarrow QUICK CONVERGENCE

B.) $|g'(x)| > 1 \rightarrow$ DIVERGE

C.) IF $|g'(x)| < 1$ FOR $x \in [a, b]$, CONVERGE FOR ANY $P_0 \in [a, b]$
IF $|g'(P)| < 1$, CONVERGE FOR SOME $P_0 \in [a, b]$

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CONVERGENCE RATES:

- DEFINITION: $\lim_{n \rightarrow \infty} \frac{|E_{n+1}|}{|E_n|^\alpha} = \lambda$ 'ASYMPTOTIC STATEMENT'

α IS THE ORDER OF CONVERGENCE

$$E_{n+1} = \lambda E_n^\alpha \rightarrow \begin{cases} \alpha = 1 & \text{(LINEAR)} \\ \alpha = 2 & \text{(QUADRATIC)} \\ \alpha = 3 & \text{(CUBIC)} \end{cases}$$

DOES NOT HAVE TO BE AN INTEGER

ASYMPTOTIC ERROR CONSTANT, WANT TO BE SMALL

GENERAL FIXED POINT ITERATION

$p_{n+1} = g(p_n)$ COMPUTE

$p = g(p)$ EXACT

$E_{n+1} = |g(p_n) - g(p)|$

↳ TAYLOR EXPAND $g(p_n)$ ABOUT p

$$g(p_n) = |g(p) + g'(p)(p-p_n) + \frac{g''(p)(p-p_n)^2}{2!} + \frac{g^{(3)}(p)(p-p_n)^3}{3!} \dots|$$

$$E_{n+1} = |g'(p)(p-p_n) + \frac{g''(p)(p-p_n)^2}{2!} + \frac{g^{(3)}(p)(p-p_n)^3}{3!} + \dots|$$

$$E_{n+1} = |g'(p)E_n + \frac{g''(p)E_n^2}{2!} + \frac{g^{(3)}(p)E_n^3}{3!} + \dots|$$

$\lim_{n \rightarrow \infty} E_{n+1} = |g'(p)|E_n \rightarrow \alpha = 1$ ← LINEAR CONVERGENCE
 $\lambda = |g'(p)|$

(2) (2)²

9/22/2015

NEWTON'S METHOD

IF $g(x) = x - \phi(x)f(x)$

\swarrow FUNCTION FOR WHICH WE WANT ROOT
 \uparrow SCALING FUNCTION

THEN $g(p) = p - \phi(p)f(p)$
 $g'(p) = 1 - \phi'(p)f(p) - \phi(p)f'(p)$

$g(p) = p$ \rightarrow $g'(p) = 1 - \phi'(p)f(p) - \phi(p)f'(p)$
 $g'(p) = 1 - \phi(p)f'(p) = 0$ \rightarrow FORCE QUADR. CONVERGE

$= 0$, IT'S A ROOT!

$$\phi(p) = \frac{1}{f'(p)}$$

$$\phi(x) = \frac{1}{f'(x)}$$

$g(x) = x - f(x)/f'(x)$ FIXED POINT FUNCTION FOR NEWTON'S METHOD

$$P_{N+1} = P_N - \frac{f(P_N)}{f'(P_N)}$$

NEWTON'S METHOD

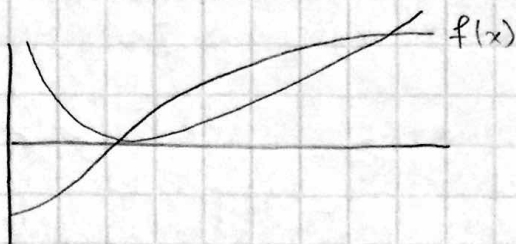
GUARANTEED QUADRATIC CONVERGENCE FOR $P_0 \in [a, b]$
 PROVIDED $f'(p) \neq 0$

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NEWTON'S METHOD

$P_{N+1} = P_N - \frac{f(P_N)}{f'(P_N)}$ FOR $f'(p) \neq 0$

WHAT IF $f'(p) = 0$



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"DERIVED" NEWTON'S METHOD

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

$$g'(x) = \frac{d}{dx} \left[x - \frac{f(x)}{f'(x)} \right] = 1 - \frac{f'(x)}{f'(x)} + \frac{f(x)f''(x)}{(f'(x))^2}$$

$$g'(x) = \frac{f(x)f''(x)}{[f'(x)]^2} \Rightarrow g'(p) = \frac{f(p)f''(p)}{[f'(p)]^2} = \frac{0}{0}$$

→ L'HOPITALS RULE ←

$$\frac{f'(p)f''(p) + f(p)f'''(p)}{2f'(p)f''(p)} = \frac{0}{0} \rightarrow \text{DO AGAIN}$$

$$\frac{[f''(p)]^2 + f'(p)f'''(p) + f'(p)f'''(p) + f(p)f''(p)}{2[f''(p)]^2 + 2f'(p)f'''(p)} = \frac{1}{2} \neq 0$$

- STILL CONVERGES, BUT $\alpha=1$ (LINEARLY) WHEN $f'(p)=0$

↳ SLOPE OF f
@ p

GENERALIZE THE ROOT OF MULTIPLICITY m

$$f(x) = (x-p)^m q(x), \quad \lim_{x \rightarrow p} q(x) = 0$$

$f(x) = (x-p)^m q(x)$ WHERE WHICH ENSURES $q(x)$ CONTAINS NO ROOTS

9/23/2015

* MODIFIED NEWTON'S METHOD (FOR $m \geq 2$)

- FOR $m=2$; $f(p)=0$; $f'(p)=0$; BUT $f''(p) \neq 0$

DEFINE $u(x) = \frac{f(x)}{f'(x)}$

i.) $u(p) = \frac{f(p)}{f'(p)} = 0 \rightarrow \text{L'HOPITALS} \rightarrow \frac{f'(p)}{f''(p)} = 0$

- SO $u(x)$ HAS SAME ROOT AS $f(x)$

ii.) $u'(p) = 1 - \frac{ff''}{[f']^2} \Big|_{x=p} = \frac{1}{2}$ (SIMPLE ROOT) WHICH MEANS QUADRATIC CONVERGENCE,

iii.) APPLY NEWTON'S METHOD TO $u(x)$

$$P_{n+1} = P_n - \frac{u(P_n)}{u'(P_n)} \leftarrow \text{'MODIFIED' NEWTON'S METHOD}$$

$$g(x) = x - \frac{u(x)}{u'(x)}, \quad g'(p) = 0 \rightarrow \alpha = 2$$

$$\lambda = u''(p) = \frac{-f'''(p)}{6f''(p)} \neq 0, \text{ TEXT SHOWS THIS METHOD}$$

FOR $u'(p) = \frac{1}{m}$, FOR LARGE m $u'(p) \rightarrow 0$

* SECANT METHOD

- MAKE APPROX. TO DERIVATIVE OF $f'(x)$ IN NEWTON'S METHOD

- $f'(x)$ CAN BE DIFFICULT TO COMPUTE

- "DISCRETE VERSION OF NEWTON'S METHOD"

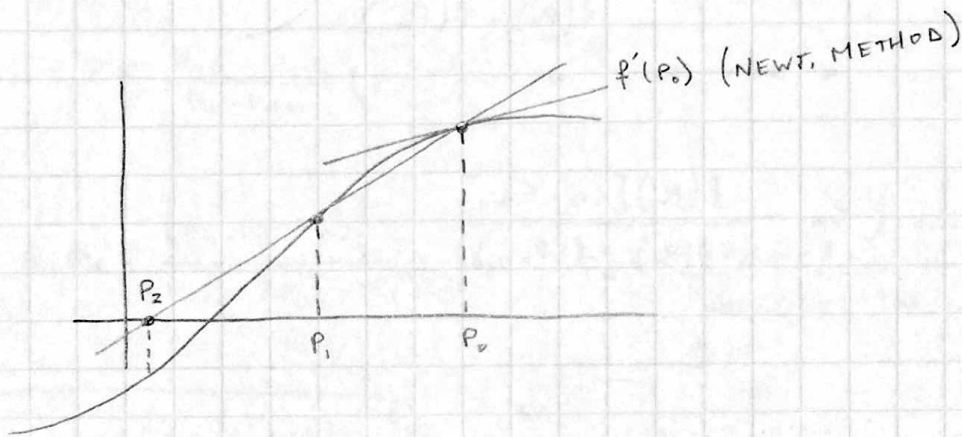
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$$f'(p_n) \equiv \lim_{x \rightarrow p_n} \frac{f(x) - f(p_n)}{x - p_n} \rightarrow \text{USE } x = p_{n-1}$$

$$\rightarrow f'(p_n) \approx \frac{f(p_{n-1}) - f(p_n)}{p_{n-1} - p_n}$$

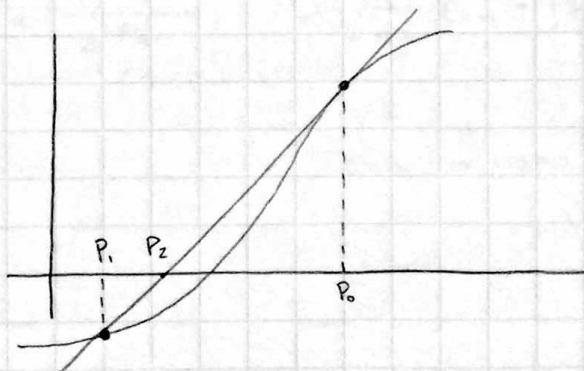
$$p_{n+1} = p_n - \frac{f(p_n)(p_n - p_{n-1})}{f(p_n) - f(p_{n-1})} \rightarrow \text{NEED TWO STARTING VALUES. DO NOT NEED TO BRACKET THE ROOT}$$

- SLOWER CONVERGENCE
- BUT DO NOT HAVE TO EVALUATE $f'(p_n)$



* METHOD OF FALSE POSITION

- SECANT METHOD BUT ALWAYS BRACKET THE ROOT



9/23/2015

$$P_{n+1} = P_n - \frac{f(P_n)(P_n - P_{n+1})}{f(P_n) - f(P_{n+1})} = g(P_n, P_{n+1})$$

WANT $\epsilon_{n+1} = f(\epsilon_n)$

$$\underbrace{|P_{n+1} - P|}_{\epsilon_{n+1}} = |g(P_n, P_{n+1}) - g(P, P)| = P_n - \frac{f(P_n)(P_n - P_{n+1})}{f(P_n) - f(P_{n+1})} - P$$

$$\epsilon_{n+1} = P_n - P - \frac{f(P_n)(P_n - P - P_{n+1} + P)}{f(P_n) - f(P_{n+1})}$$

$$\epsilon_{n+1} = \epsilon_n - \frac{f(P_n)[\epsilon_n - \epsilon_{n+1}]}{f(P_n) - f(P_{n+1})}$$

⋮

$$\lim_{n \rightarrow \infty} \epsilon_{n+1} = \frac{1}{2} \frac{f''(P)}{f'(P)} \epsilon_n \epsilon_{n-1} \dots \epsilon_{n+1} = \lambda \epsilon_n^{\frac{\sqrt{5}+1}{2}}$$

$$\lambda = \frac{\sqrt{5}+1}{2} \rightarrow \text{"SUPER LINEAR"}$$

9/25/2015

* ACCELERATING LINEARLY CONVERGING PROCESSES

MOTIVATION: CONSTRUCT A NEW SET OF ITERATES $\{\tilde{P}_n\}$
 THAT CONVERGE MORE RAPIDLY TO P THEN DOES $\{P_n\}$

$$\lim_{n \rightarrow \infty} \epsilon_{n+1} = g'(P) \epsilon_n, \quad \text{LINEAR } \alpha = 1$$

$$\lambda = g'(P)$$

$$\lim_{n \rightarrow \infty} P_{n+1} - P = g'(P)(P_n - P)$$

$$\lim_{n \rightarrow \infty} P_{n+2} - P = g'(P)(P_{n+1} - P)$$

$$P_{n+1} - P_{n+2} = g'(P)(P_n - P_{n+1}) \rightarrow g'(P) \cong \frac{P_{n+1} - P_{n+2}}{P_n - P_{n+1}} \quad \text{FOR LARGE } n \text{ (ESTIMATE)}$$

$$P_{n+1} - P \cong \frac{P_{n+1} - P_{n+2}}{P_n - P_{n+1}} (P_n - P) \rightarrow \text{SOLVE FOR } P$$

$$P \cong P_n - \frac{(P_{n+1} - P_n)^2}{P_{n+2} - 2P_{n+1} + P_n} \rightarrow P_n \cong \frac{-(P_{n+1} - P_n)^2}{P_{n+2} - 2P_{n+1} + P_n}$$

$$\tilde{P} = P_n - \frac{(P_{n+1} - P_n)^2}{P_{n+2} - 2P_{n+1} + P_n}$$

AITKENS Δ^2 METHOD

$$\Delta P_n \equiv P_{n+1} - P_n$$

$$\Delta^2(P_n) = \Delta(\Delta P_n) = P_{n+2} - 2P_{n+1} + P_n$$

$$\tilde{P}_n = P_n - \frac{(\Delta P_n)^2}{\Delta^2 P_n}$$

$$\lim_{n \rightarrow \infty} \tilde{\epsilon}_{n+1} = |g'(P)|^2 \epsilon_n$$

$$P_0 = g(P_0) = \tilde{P}_0$$

$$P_2 = g(P_1) = \tilde{P}_1$$

$$P_3 = g(P_2) = \tilde{P}_2$$

$$P_4 = g(P_3)$$

LOOK AT VIDEO

9/25/2015

* CHAPTER 10 - MULTIVARIATE NON-LINEAR EQUATIONS

$$f_1(x_1, x_2, x_3, \dots, x_n) = 0$$

$$f_2(x_1, x_2, x_3, \dots, x_n) = 0$$

\vdots

$$f_n(x_1, x_2, x_3, \dots, x_n) = 0$$

BAR INDICATES VECTOR

$$\rightarrow \underline{F}(\underline{x}) = 0$$

$$\underline{x} = (x_1, x_2, x_3, \dots, x_n)$$

\underline{p} IS A FIXED POINT VECTOR (p_1, p_2, \dots, p_n)

$$\text{IF } \underline{g}(\underline{p}) = \underline{p}$$

$$g_i(p_1, p_2, \dots, p_n) = p_i \quad \text{FOR } i = 1, \dots, n$$

THE EXISTENCE OF \underline{p} IS GUARANTEED BY

i. $\underline{g}(\underline{x})$ IS CONT. ON $a_i \leq x_i \leq b_i$

ii. $\underline{g}(\underline{x})$ IS BOUNDED BY $a_i \leq g_i(x_i) \leq b_i$

iii. $\sum_{j=1}^n \left| \frac{\partial g_i}{\partial x_j} \right| < 1$

• LINEAR $\frac{\partial g_i}{\partial x_i}(f) \neq 0$

• QUADRATIC $\frac{\partial g_i}{\partial x_i} = 0$

• $\frac{\partial^2 g_i}{\partial x_j \partial x_i}(f) = 0$

* NEWTON'S METHOD FOR SYSTEMS OF NONLINEAR EQUATIONS

$$\underline{g}(\underline{x}) = \underline{x} - \underline{A}^{-1}(\underline{x}) \cdot \underline{f}(\underline{x})$$

↑ INVERSE OF MATRIX

← COLUMN OF FUNCTION

9/25/2015

$$g_i(\underline{x}) = x_i - \sum_{j=1}^N b_{ij}(\underline{x}) f_j(\underline{x})$$

$$\underline{A} = \begin{bmatrix} b_{11} & b_{12} & \dots & b_{1n} \\ b_{21} & b_{22} & & b_{2n} \\ \vdots & & \ddots & \vdots \\ b_{n1} & b_{n2} & \dots & b_{nn} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix}$$

\underline{A}^{-1}

FOR NEWTON'S METHOD $\frac{\partial g_i(f)}{\partial x_i} = 0$ FOR EACH i, k

• IF $i = k$

$$\frac{\partial g_i}{\partial x_k} = - \left[\sum_{j=1}^N b_{ij} \frac{\partial f_j}{\partial x_k} + \sum_{j=1}^N \frac{\partial b_{ij}}{\partial x_k} f_j \right] \Big|_{\underline{x}=\underline{x}^k} = 0$$

• IF $i \neq k$

$$\frac{\partial g_i}{\partial x_k} = 0 - \left[\text{SAME } \uparrow \right] = 0$$

$$\sum_{j=1}^N b_{ij} \frac{\partial f_j}{\partial x_k} = \begin{cases} 1 & i = k \\ 0 & i \neq k \end{cases}$$

$$\sum_{j=1}^N b_{ij} f'_{jk} = \begin{cases} 1 & i = k \\ 0 & i \neq k \end{cases}$$

$$\underline{A}^{-1} \cdot \underline{A} = \underline{I}$$

→

$$\underline{A} = \begin{bmatrix} x_1 & \dots & x_n \\ \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_n} \\ \dots & \dots & \dots & \dots \\ \frac{\partial f_n}{\partial x_1} & \dots & \dots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}$$

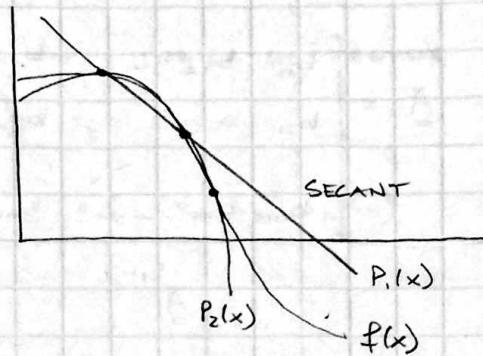
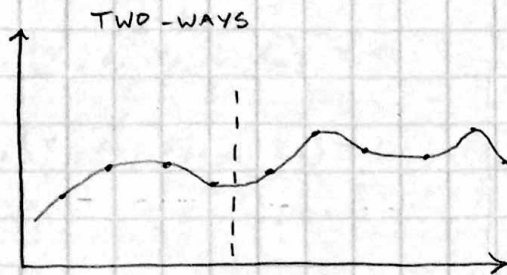
$$\underline{x}_{n+1} = \underline{x}_n - \underline{J}^{-1}(\underline{x}_n) \underline{f}(\underline{x}_n)$$

NEWTON'S METHOD FOR N-L SYS. OF EQUATIONS

L2 NORM FOR STOPPING CRITERIA

9/28/2015

* POLYNOMIAL INTERPOLATION



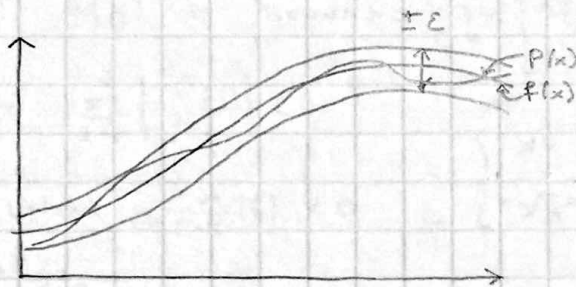
- APPEAL OF POLYNOMIALS:

- EASY TO EVALUATE
- INTEGRATE
- DIFFERENTIATE
- STORE

W/ MORE POINTS \Rightarrow HIGHER ORDER FIT POSSIBLE

- APPROXIMATIONS BASED ON WEIERSTRAUSS APPROXIMATION THEOREM

IF $f(x)$ IS C^0 ON $[a, b]$ AND $\epsilon > 0$, THEN A POLYNOMIAL $P(x)$ EXISTS ON $[a, b]$ SUCH THAT $|f(x) - P(x)| < \epsilon$



DOESN'T SAY ANYTHING ABOUT HOW TO GET $P(x)$

ONE TYPE OF POLYNOMIAL IS A TAYLOR POLYNOMIAL

i. GREAT B/C TRUNCATION ERROR IS EXPLICIT

$$\frac{f^{(n+1)}(\xi)(x-x_0)^{n+1}}{(n+1)!} \quad \{ \xi \in [x, x_0] \}$$

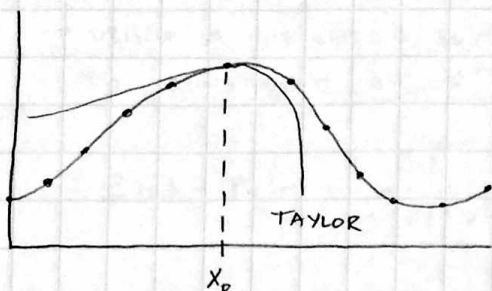
ii. ALL INFORMATION ABOUT $f(x)$ IS AT x_0

$$f^{(k)}(x_0), \quad k = 0, 1, \dots, n$$

iii. "LOCALLY" GOOD BUT GETS WORSE AS $|x-x_0|$ GROWS

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- A BETTER POLYNOMIAL FOR INTERPOLATION $P_N(x)$ MATCHES $f(x)$ AT A FINITE # OF VALUES



- N^{TH} ORDER HAS $N+1$ COEFFICIENTS

$$P_N(x) = a_N x^N + a_{N-1} x^{N-1} + \dots + a_1 x + a_0$$

IF $f(x_i) = P_N(x_i)$ THEN WE NEED $N+1$ x_i 'S TO FIND A UNIQUE SET OF COEFF'S $\{a_i\}$

EG.

$$x_1, x_2, x_3 \quad ; \quad f(x_1), f(x_2), f(x_3)$$

$$P_2(x) = ax^2 + bx + c \quad \rightarrow \quad \text{WANT } P_2(x_i) = f(x_i)$$

$$\begin{aligned} ax_1^2 + bx_1 + c &= f(x_1) \\ ax_2^2 + bx_2 + c &= f(x_2) \\ ax_3^2 + bx_3 + c &= f(x_3) \end{aligned} \quad \rightarrow \quad \begin{bmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ x_3^2 & x_3 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \end{bmatrix}$$

$$A \quad X = B$$

$$\underline{X} \underline{A} = \underline{F} \quad \rightarrow \quad A = \underline{X}^{-1} \underline{F}$$

$$X = A^{-1}B$$

* KEY TO POLYNOMIAL INTERPOLATION

- GIVEN $N+1$ DISTINCT SAMPLES OF $f(x)$, CAN ALWAYS FIND A UNIQUE POLYNOMIAL $P_N(x)$ OF ORDER N SUCH THAT $P_N(x_i) = f(x_i)$, $i=0,1,\dots,N$

- COMPLICATED HOWEVER, INSTEAD USE A 'BASIS' POLYNOMIAL

$$P_N(x) = \sum_{j=0}^N \alpha_j b_j(x) \quad \text{WHERE } b_j(x) \equiv \text{BASIS POLYNOMIAL (KNOWN FUNCTION OF } x)$$

NOTE: IF $b_j(x) = x^j$ THEN $\{\alpha_j\} = \{a_j\}$, $P_N(x) = a_0 x^N + a_{N-1} x^{N-1} + \dots + a_1 x + a_0$

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BY CLEVERLY CHOOSING $\{b_j(x)\}$ WE CAN EASILY IDENTIFY $\{\alpha_j\}$

IF $b_j(x_i) = \delta_{ij} = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$ THEN $P_N(x_i) = \sum_{j=0}^N \alpha_j \delta_{ij} = \alpha_i = f(x_i)$

$$P_N(x) = \sum_{j=0}^N f(x_j) b_j(x)$$

LAGRANGE POLYNOMIAL

$$L_{N,j}(x) = \prod_{\substack{k=0 \\ k \neq j}}^N \frac{x - x_k}{x_j - x_k} = \underbrace{\frac{x - x_0}{x_j - x_0} \cdot \frac{x - x_1}{x_j - x_1} \cdot \frac{x - x_2}{x_j - x_2} \cdots \frac{x - x_N}{x_j - x_N}}_{N \text{ TERMS}}$$

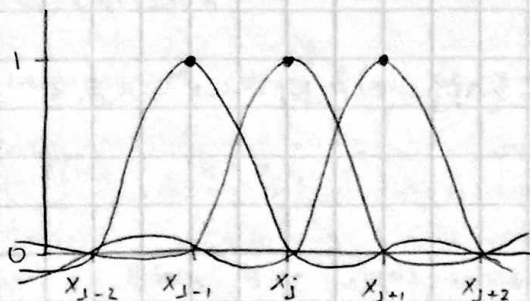
$$L_{N,j}(x_i) = \frac{x_i - x_0}{x_j - x_0} \cdot \frac{x_i - x_1}{x_j - x_1} \cdots \frac{x_i - x_N}{x_j - x_N} \quad \begin{array}{l} \text{IF } i=j = 1 \\ \text{IF } i \neq j = 0 \end{array}$$

EX.

$$P_3(x) = \sum_{j=0}^3 f(x_j) L_{3,j}(x) \\ = f(x_0) L_{3,0}(x) + f(x_1) L_{3,1}(x) + f(x_2) L_{3,2}(x) + f(x_3) L_{3,3}(x)$$

AND

$$L_{3,0}(x) = \frac{x - x_1}{x_0 - x_1} \cdot \frac{x - x_2}{x_0 - x_2} \cdot \frac{x - x_3}{x_0 - x_3} \rightarrow \begin{array}{l} L_{3,0}(x_0) = 1 \\ L_{3,0}(x_1) = 0 \\ L_{3,0}(x_2) = 0 \\ L_{3,0}(x_3) = 0 \end{array}$$



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EASY TO WRITE DOWN, BUT SOMEWHAT INEFFICIENT TO USE

$$P_N(x) = \sum_{j=0}^N f(x_j) L_{N,j}(x)$$

- USING A WEIGHTED SUM OF $N+1$ N^{TH} ORDER POLYNOMIALS TO CONSTRUCT AN N^{TH} ORDER POLYNOMIAL $P_N(x)$

$$f(x) - P_N(x) = \frac{f^{(N+1)}(\xi)}{(N+1)!} \prod_{i=0}^N (x - x_i)$$

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CHEBYSHEV POLYNOMIALS, OPTIMAL POINTS (SECT. 8.3)

- TAYLOR: ALL INFORMATION @ x_0
- LAGRANGE: PASS THROUGH x_0, \dots, x_N (SPREAD OUT ERROR)

DOES THERE EXIST A SET OF POINTS $\{x_i\}$ FOR WHICH THE 'OPTIMAL' INTERPOLATION IS ACHIEVED?

"OPTIMAL" DEFINED AS MINIMIZING THE MAXIMUM ERROR ON $[a, b]$

$$f(x) - P_N(x) = \underbrace{\frac{f^{(N+1)}(\xi)}{(N+1)!}}_{\text{FIXED}} \underbrace{\prod_{i=0}^N (x - x_i)}_{\text{MINIMIZE THE MAX OF THIS}}, \quad \xi \in [x_0, x_N]$$

- CAN PROVE THAT A MINIMAL MAXIMUM EXISTS ON THE INTERVAL $[-1, 1]$ IF WE USE ROOTS OF CHEBYSHEV POLYNOMIALS FOR $\{x_i\}$

$$x_i = \cos \left[\frac{(2i+1)\pi}{2(N+1)} \right] \quad i = 0, 1, 2, \dots, N$$

FOR A GENERAL INTERVAL $[a, b]$

$$x_i = \frac{a+b}{2} + \frac{b-a}{2} \bar{x}_i$$

← CAN BE USED TO DESIGN EXPERIMENTS (INTERVAL SPACING)

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* ITERATIVE INTERPOLATION (SEC. 3.1)

- PRODUCE HIGHER ORDER POLYNOMIALS FROM COMBINATIONS OF LOWER ORDER POLYNOMIALS

$$P_N(x) = \sum_{j=0}^N f(x_j) b_j(x) \quad (\text{GENERAL})$$

$$b_j(x) = L_{N,j}(x) = \prod_{\substack{k=0 \\ k \neq j}}^N \frac{x - x_k}{x_j - x_k} \quad (\text{LAGRANGE})$$

- SOME TERMS:

$$P_{(0)}(x) = f(x_0) b_0(x) = f(x_0)$$

↑ NOT THE ORDER, BUT THE POINT IT PASSES THROUGH

$$P_{(1)}(x) = f(x_1) b_1(x) = f(x_1) \quad (1 \text{ TERM})$$

$$P_{(0,1)}(x) = \overset{P_{(0)}}{f(x_0)} \frac{x - x_1}{x_0 - x_1} + \overset{P_{(1)}}{f(x_1)} \frac{x - x_0}{x_1 - x_0} \quad (2 \text{ TERMS})$$

$$P_{(0,1)}(x) = \frac{P_{(0)}(x)(x - x_1) - P_{(1)}(x)(x - x_0)}{x_1 - x_0}$$

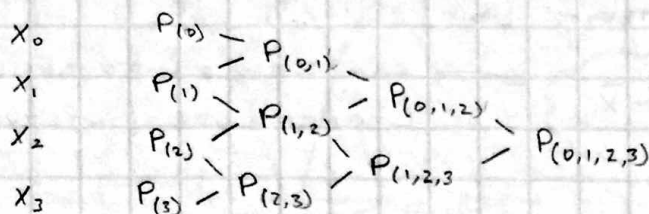
$N=2$

$$P_{(0,1,2)}(x) = f(x_0) b_0(x) + f(x_1) b_1(x) + f(x_2) b_2(x)$$

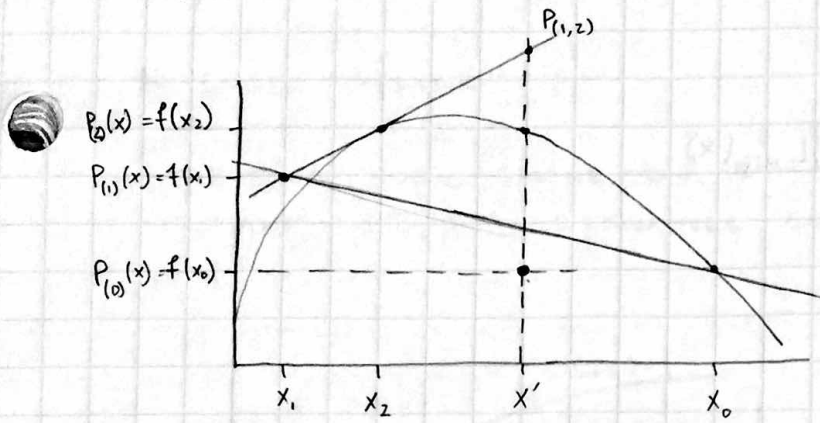
$$= \frac{f(x_0)(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} + \frac{f(x_1)(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} + \frac{f(x_2)(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$

$$= \frac{P_{(1,2)}(x)(x - x_0) - P_{(0,1)}(x)(x - x_2)}{x_2 - x_0} \quad \text{"NEVILLE'S METHOD"}$$

- NEVILLE'S TABLE



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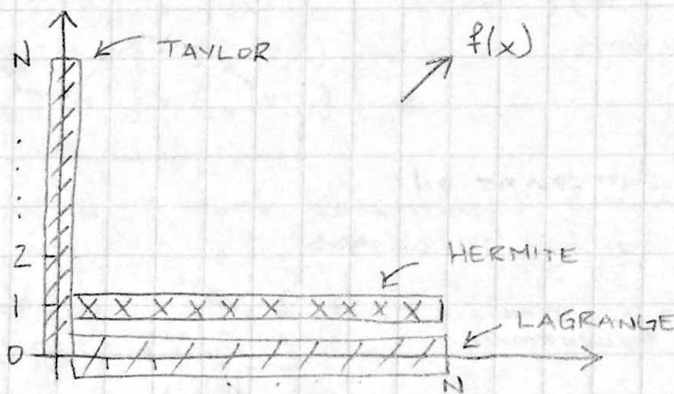


$x_0 \quad P_{(0)}(x')$
 $x_1 \quad P_{(1)}(x') = P_{(0,1)}(x')$
 $x_2 \quad P_{(2)}(x') = P_{(1,2)}(x')$

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* HERMITE POLYNOMIAL

- MATCHES f AND f' AT $N+1$ POINTS $\{x_i\}$



- $2N+2$ CONDITIONS:

$$P(x_j) = f(x_j) \text{ AND } P'(x_j) = f'(x_j) \text{ FOR } j = 0, 1, \dots, N$$

- UNIQUE POLYNOMIAL OF ORDER $2n+1$: $P_{2n+1}(x)$

INTERIMS OF BASIS FUNCTIONS

$$P_{2n+1}(x) = \sum_{j=0}^N f(x_j) H_{2n+1}(x) + \sum_{j=0}^N f'(x_j) \hat{H}_{2n+1}(x)$$

W/ PROPERTIES:

$$H_{2n+1}(x_i) = \delta_{ij}$$

$$\hat{H}_{2n+1}(x_i) = 0$$

$$P_{2n+1}(x_i) = f(x_i)$$

$$\hat{H}_{2n+1}(x_i) = 0$$

$$\hat{H}'_{2n+1}(x_i) = f'(x_i)$$

$$P'_{2n+1}(x_i) = f'(x_i)$$

9/30/2015

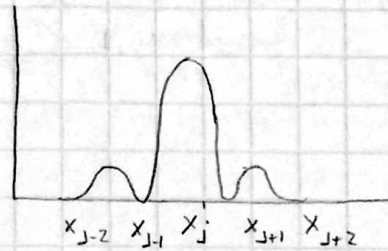
→ FROM TEXT ←

$$H_{2n+1}(x) = [1 - 2(x-x_j)L'_{N_{ij}}(x_j)]L_{N_{ij}}^2(x)$$

$$\hat{H}_{2n+1}(x) = (x-x_j)L_{N_{ij}}^2(x)$$

ERROR TERM:

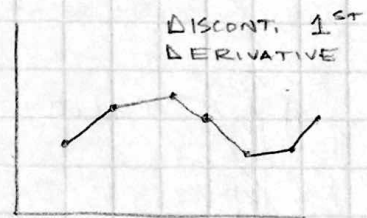
$$\frac{f^{(2n+2)}(\xi)}{(2n+2)!} \prod_{j=0}^N (x-x_j)^2$$



— UP TO THIS POINT, GLOBAL POLYNOMIAL INTERPOLATION

(+) SINGLE FUNCTION (POLYNOMIAL)

(-) 'RINGING' CAN BE SERIOUS



↳ PIECEWISE POLYNOMIAL INTERPOLATION

- LOWER ORDER OVER SMALLER INTERVALS

EG. LINEAR PIECEWISE POLYNOMIAL

$$|P_1(x) - f(x)| \sim O(h^2) \text{ WHERE } h = x_{j+1} - x_j, \frac{f^{(2)}(\xi)}{2!} \frac{(x-x_0)(x-x_1)}{h \cdot h}$$

* HERMITE CUBIC FOR LOCAL INTERPOLATION

$$x_j \quad x_{j+1} \quad f(x_j) \quad f(x_{j+1}) \quad f'(x_j) \quad f'(x_{j+1})$$

+ CONT. FIRST DERIVATIVE

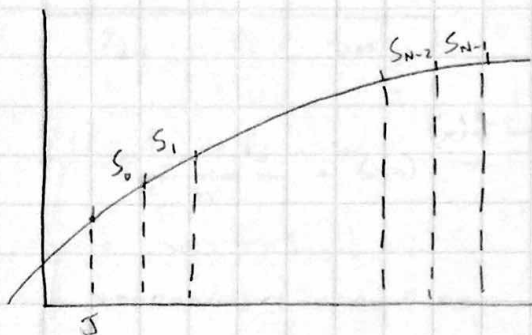
- NEED TO KNOW $f'(x_j)$

- INSTEAD, USE A SPLINE, ONLY REQUIRES DERIVATIVE TO BE CONTINUOUS.

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* CUBIC SPLINE

- USE A CUBIC SPLINE ON EACH INTERVAL
- MAKE 1ST, 2ND DERIVATIVES CONTINUOUS ACROSS INTERVAL



$N+1$ POINTS

N SEGMENTS

$$S_j = a_j + b_j(x-x_j) + c_j(x-x_j)^2 + \dots$$

$4N$ CONDITIONS NEEDED FOR UNIQUE SOLUTION

CONSTRAINTS:

- i.) $S_j(x_j) = f(x_j)$: RIGHT
 - ii.) $S_j(x_{j+1}) = f(x_{j+1})$: LEFT
 - iii.) $S_j'(x_{j+1}) = S_{j+1}'(x_{j+1})$ } ?
 - iv.) $S_j''(x_{j+1}) = S_{j+1}''(x_{j+1})$ }
- CONTINUITY

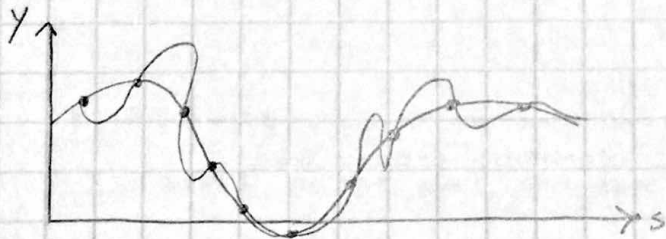
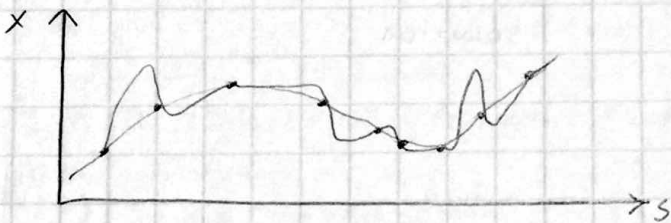
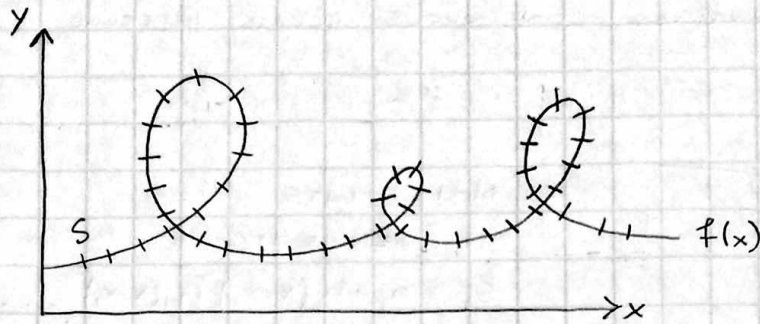
→ NEED 2 MORE CONDITIONS: COMMON STRATEGIES

$$\left. \begin{aligned} S_0'(x_0) &= f'(x_0) \\ S_{N-1}(x_N) &= f'(x_N) \end{aligned} \right\} \text{MOST ACCURATE, BUT REQUIRES KNOWING DERIVATIVES}$$

$$S_0''(x_0) = S_{N-1}''(x_N) = 0 : \text{'NATURAL' SPLINE}$$

10/2/2015

* PARAMETRIC INTERPOLATION



* CHAPTER 4.1: NUMERICAL DIFFERENTIATION

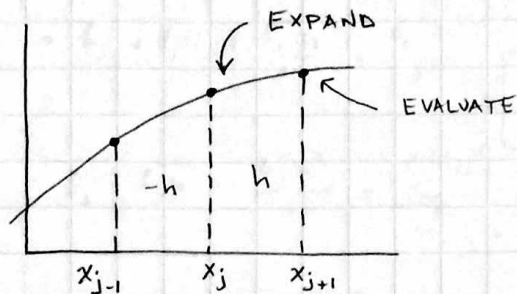
- LOOKING FOR WAYS TO APPROX. FUNCTION DERIVATIVES W/
COMBINATIONS OF FUNCTION EVALUATIONS @ DISCRETE POINTS.

- TEXT: CONSTRUCT A POLYNOMIAL APPROXIMATION TO $f(x)$ THROUGH
EVENLY SPACED SAMPLES OF $f(x_i)$, THEN DIFFERENTIATE

EXPAND $f(x)$ ABOUT x_j - THE POINT WHERE WE WANT THE DERIVATIVE

$$f(x) = f(x_j) + f'(x_j)(x-x_j) + \frac{f''(x_j)}{2!}(x-x_j)^2 \dots$$

10/2/2015



$$f_{j+1} = f_j + hf_j' + \frac{h^2}{2!} f_j'' + \dots$$

$$f_j' = \frac{f_{j+1} - f_j}{h} - \frac{h}{2!} f_j'' + \dots$$

$$f_j' = \frac{f_{j+1} - f_j}{h} + O(h) \rightarrow \text{ERROR} \sim \frac{f_j'' h}{2}$$

APPROXIMATE TO FIRST DERIVATIVE TO ORDER h ACCURACY.

$$f_j' = \frac{\Delta f_j}{h}$$

FIRST FORWARD DIFFERENCE APPROX. TO $O(h)$

$$f_j' = \frac{\nabla f_j}{h}$$

WHERE $\nabla f_j = f_j - f_{j-1}$

CALCULATE f_j''

$$f_{j+2} = f_j + 2hf_j' + \frac{(2h)^2}{2} f_j'' + \frac{(2h)^3}{3!} f_j''' + \dots$$

$$-2[f_{j+1} = f_j + hf_j' + \frac{h^2}{2!} f_j'' + \frac{h^3}{3!} f_j''']$$

$$= f_{j+2} - 2f_{j+1} + f_j = h^2 f_j'' + h^3 f_j''' + \dots \text{ SOLVE FOR,}$$

$$\therefore f_j'' = \frac{f_{j+2} - 2f_{j+1} + f_j}{h^2} + O(h)$$

NOTE: $\Delta^2 f_j = \Delta(\Delta f_j) = \Delta(f_{j+1} - f_j) = \Delta f_{j+1} - \Delta f_j = f_{j+2} - 2f_{j+1} + f_j$

$$f_j'' = \frac{\Delta^2 f_j}{h^2} + O(h) \quad (\text{FORWARD})$$

$$f_j'' = \frac{\nabla^2 f_j}{h^2} + O(h) \quad (\text{BACKWARD})$$

10/2/2015

WANT f'_j TO $O(h^2)$

$$-4 \left[f_{j+1} = f_j + hf_j + \frac{h^2}{2!} f_j'' + \frac{h^3}{3!} f_j''' \right]$$

$$f_{j+2} = f_j + 2hf_j + \frac{4h^2}{2!} f_j'' + \frac{8h^3}{3!} f_j''' + \dots$$

$$f_{j+2} - 4f_{j+1} + 3f_j = -2hf_j' + \frac{4h^3}{6} f_j''' + \dots$$

$$f'_j = \frac{-f_{j+2} + 4f_{j+1} - 3f_j}{2h} + O(h^2)$$

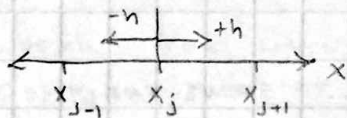
10/5/2015

* NUMERICAL DIFFERENTIATION

N^{th} ORDER DERIVATIVE TO ACCURACY $O(h^m)$ REQUIRES $n+m$ POINTS INVOLVING $n+m-1$ TAYLOR SERIES

CENTRAL DIFFERENCE APPROXIMATIONS

- COMBINE FWD / BWD APPROXIMATIONS TO ELIMINATE HIGHER ORDER TERMS, RESULTING IN A SYMMETRIC SAMPLING AROUND x_j



$$f_{j+1} = f_j + f_j' h + \frac{f_j''}{2!} h^2 + \frac{f_j'''}{3!} h^3 \dots \text{(FORWARD)}$$

$$+ f_{j-1} = f_j - f_j' h + \frac{f_j''}{2!} h^2 - \frac{f_j'''}{3!} h^3$$

$$f_{j+1} - f_{j-1} = 2f_j' h + f_j'' h^2 + O(h^4)$$

$$\rightarrow f_j'' = \frac{f_{j+1} - 2f_j + f_{j-1}}{h^2} + O(h^2)$$

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$$f_{j+h} = f_j + f'_j h + \frac{f''_j h^2}{2!} + \frac{f'''_j h^3}{3!} + \frac{f^{(4)}_j h^4}{4!} + \dots$$

$$f_{j-1} = f_j - f'_j h + \frac{f''_j h^2}{2!} - \frac{f'''_j h^3}{3!} + \frac{f^{(4)}_j h^4}{4!} + \dots$$

$$f_{j+h} - f_{j-1} = 2f'_j h + \frac{f'''_j h^3}{3} + O(h^5)$$

$$f'_j = \frac{f_{j+h} - f_{j-1}}{2h} + O(h^2)$$

EXTRA POINT GIVES $O(h^2)$ ACCURACY INSTEAD OF $O(h)$ W/ TWO POINTS

INTERPRETATION OF $O(h^m)$

IF E_h IS THE ERROR FOR $O(h^m)$, THEN IF $h \rightarrow h/2$

$$E_{h/2} = O\left(\frac{h}{2}\right)^m = E_h \left(\frac{1}{2}\right)^m$$

- NOTICE h IS IN DENOMINATOR FOR ALL DERIVATIVES, HOWEVER IT CAN DESTROY SOLUTION VIA ROUND OFF ERROR. HOWEVER IT'S BETTER FOR TRUNCATION ERROR

* COMPUTER ERRORS WHEN NUMERICALLY DIFFERENTIATING

$$f'_j = \frac{f_{j+h} - f_{j-1}}{2h} - \frac{f'''(\xi)h^2}{6} \Rightarrow \text{EXACT}$$

COMPUTE $\hat{f}_j = f_j + \epsilon_j$ EXACT f_j ROUND OFF

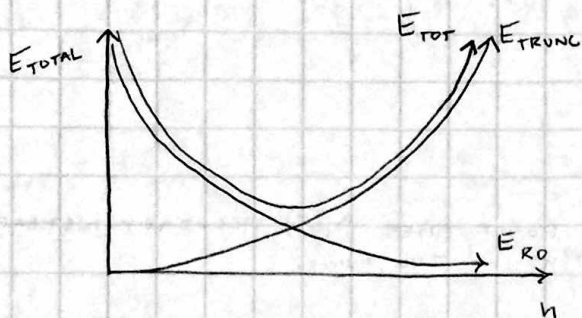
$$\hat{f}'_j = \frac{\hat{f}_{j+h} - \hat{f}_{j-1}}{2h} = \frac{f_{j+h} - f_{j-1}}{2h} + \frac{\epsilon_{j+h} - \epsilon_{j-1}}{2h}$$

$$|\hat{f}'_j - f'_j| = |E_{\text{TRUNC}} - E_{\text{ROUND-OFF}}| \leq |E_{\text{TRUNC}}| + |E_{\text{ROUND-OFF}}|$$

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ASSUME $f'''(\xi)$ IS BOUNDED BY SAME NUMBER, M

$$E_{TOT}(h) = \frac{mh^2}{6} + \frac{\epsilon}{h} \rightarrow \text{RESULTS IN AN ERROR TRADE OFF}$$

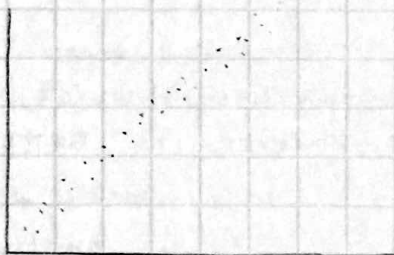


$$\frac{\partial E_{TOT}}{\partial h} = 0$$

$$\frac{mh}{3} = \frac{\epsilon}{h^2}$$

* CURVE FITTING:

- SO FAR ALL INTERPOLANTS PASS EXACTLY THROUGH DATA POINTS $\{x_i\}, \{y_i\}$



WANT A 'BEST FIT' SOLUTION, NOT NECESSARILY AN INTERPOLATION THROUGH POINTS

EVALUATE ERROR - BY MINIMIZING THE SUM OF THE SQUARED ERRORS

TOTAL ERROR $\Rightarrow \epsilon = \sum_{j=0}^N [f(x_j) - \tilde{P}(x_j)]^2$, GOAL IS TO FIND $\tilde{P}(x_j)$ WHICH MINIMIZES ϵ

EG. STRAIGHT LINE THROUGH DATA "LINEAR LEAST SQUARES" FIT

$$\tilde{P}(x) = P_1(x) = a_0 + a_1x, \quad \epsilon = \sum_{j=0}^N [f(x_j) - (a_0 + a_1x_j)]^2$$

$$\frac{\partial \epsilon}{\partial a_0} = \frac{\partial \epsilon}{\partial a_1} = 0 \quad \rightarrow \quad \frac{\partial \epsilon}{\partial a_0} = 0 = -2 \sum_{j=0}^N [f(x_j) - (a_0 + a_1x_j)]$$

$$\frac{\partial \epsilon}{\partial a_1} = 0 = -2 \sum_{j=0}^N [f(x_j) - (a_0 + a_1x_j)] (-x_j) \leftarrow \text{WHY?}$$

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FOR POLYNOMIALS $0, \dots, N$ $\sum_{j=0}^N \rightarrow N+1$

FOR CURVE FITTING $1, \dots, m$ $\sum_{j=1}^m \rightarrow m$ # OF DATA POINTS

NORMAL EQUATIONS

$$a_0 m + a_1 \sum_{j=1}^m x_j = \sum_{j=1}^m y_j$$

$$a_0 \sum_{j=1}^m x_j + a_1 \sum_{j=1}^m x_j^2 = \sum_{j=1}^m x_j y_j$$

$$\begin{bmatrix} m & \sum x_j \\ \sum y_j & \sum x_j^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} \sum y_j \\ \sum x_j y_j \end{bmatrix}$$

$$a_0 = \frac{\sum x_j^2 \sum y_j - \sum x_j y_j \sum x_j}{m \sum x_j^2 - (\sum x_j)^2}$$

$$a_1 = \frac{m \sum x_j y_j - \sum x_j \sum y_j}{m \sum x_j^2 - (\sum x_j)^2}$$

ALL KNOWN INFORMATION

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LEAST SQUARES CURVE FITTING:

$$\text{IF } \tilde{P}(x) = P_0(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0$$

THEN MINIMIZE

$$E = \sum_{i=1}^N [f(x_i) - P_n(x_i)]^2 = \sum_{i=1}^m \left[f(x_i) - \sum_{k=0}^N a_k x_i^k \right]^2$$

$$\frac{\partial E}{\partial a_j} = 0 \quad \text{FOR } j = 0, 1, \dots, N$$

$$\begin{aligned} \frac{\partial E}{\partial a_j} &= 2 \sum_{i=1}^m \left[f(x_i) - \sum_{k=0}^N a_k x_i^k \right] (-x_i^j) = 0 \\ &= -2 \sum_{i=1}^m y_i x_i^j + 2 \sum_{k=0}^N a_k \sum_{i=1}^m x_i^{j+k} = 0 \end{aligned}$$

* $N+1$ NORMAL EQUATIONS:

$$\sum_{k=0}^N a_k \sum_{i=1}^m x_i^{j+k} = \sum_{i=1}^m y_i x_i^j, \quad j = 0, 1, \dots, N$$

EXPAND

$$j=0: a_0 \sum_{i=1}^m x_i^0 + a_1 \sum_{i=1}^m x_i^1 + \dots + a_n \sum_{i=1}^m x_i^N = \sum_{i=1}^m y_i x_i^0$$

$$j=1: a_0 \sum_{i=1}^m x_i^1 + a_1 \sum_{i=1}^m x_i^2 + \dots + a_n \sum_{i=1}^m x_i^{N+1} = \sum_{i=1}^m y_i x_i^1$$

$$j=N: a_0 \sum_{i=1}^m x_i^N + a_1 \sum_{i=1}^m x_i^{N+1} + \dots + a_n \sum_{i=1}^m x_i^{2N} = \sum_{i=1}^m y_i x_i^N$$

$$\underline{X} \underline{A} = \underline{b}$$

$$\underline{A} = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$$

$$\underline{b} =$$

X IS INVERTIBLE AS LONG AS x_i 'S ARE UNIQUE

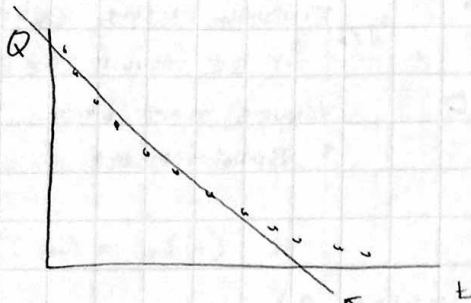
$$\underline{X} = \begin{bmatrix} m \\ \sum x_i^2 \\ \sum x_i^3 \\ \vdots \\ \sum x_i^N \end{bmatrix}$$

LOOK AT VIDEO
↓

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WHAT IF $\tilde{P}(x)$ IS NOT A POLYNOMIAL?

- EG. DATA DOES NOT FIT A POLYNOMIAL



GOES NEGATIVE, NOT A GOOD APPROXIMATION

$$\tilde{P}(x) = b e^{ax}$$

$$E = \sum_{i=1}^m [f(x_i) - b e^{ax_i}]^2$$

$$\frac{\partial E}{\partial b} = 0 = 2 \sum_{i=1}^m [y_i - b e^{ax_i}] [-e^{ax_i}]$$

$$\frac{\partial E}{\partial a} = 0 = 2 \sum_{i=1}^m [y_i - b e^{ax_i}] (-b x_i e^{ax_i})$$

$$\rightarrow b \sum_{i=1}^m e^{2ax_i} = \sum_{i=1}^m y_i e^{ax_i} \quad ; \quad b \sum_{i=1}^m x_i e^{2ax_i} = \sum_{i=1}^m x_i y_i e^{ax_i}$$

↳ PROBLEM: CANNOT WRITE AS $\underline{X} \begin{bmatrix} a \\ b \end{bmatrix} = \underline{b}$, THERE IS NO EXACT SOLUTION

TWO SOLUTIONS:

1.) LINEARIZE

$$\ln \{ \tilde{P}(x) = y = b e^{ax} \} \rightarrow \ln y = \ln b + ax \rightarrow \ln y = ax + \ln b$$

$$Y = B + aX \quad (\text{LINEAR IN THESE VARIABLES})$$

→ APPLY LEAST SQUARES TO THIS EQ. & FIND $a + B$ WHICH MINIMIZE E IN TERMS OF $\{X_i\} + \{Y_i\}$

ROOT \swarrow N.L. \searrow LINEARIZE

$\{P\} = mX + b$
 \sim known \swarrow a_1 \searrow a_0

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ii.) WRITE AS A SYX. OF N-L EQUATIONS AND USE A ROOT FINDING TECHNIQUE

$$f_1(a,b) = b \sum_{i=1}^m e^{2ax_i} - \sum_{i=1}^m y_i e^{ax_i} = 0$$

$$f_2(a,b) = b \sum_{i=1}^m x_i e^{2ax_i} - \sum_{i=1}^m x_i y_i e^{ax_i} = 0$$

FINDING INITIAL GUESS

CAN BE TOUGH. TRY PLOTTING

VALUES THAT LOOK "GOOD".

§ USING THOSE.

* NUMERICAL INTEGRATION, "QUADRATURE" (CHAPTER 8)

-NO 'H'S' IN DENOMINATOR, SO INTEGRATION IS MORE STABLE THAN DIFFERENTIATION.

APPROXIMATE $f(x) \approx \sum_{i=0}^N f_i L_{N,i}(x)$

$$\int_a^b f(x) dx \approx \sum_{i=0}^N f_i \underbrace{\int_a^b L_{N,i}(x) dx}_{a_i} = \sum_{i=0}^N a_i f_i$$

WEIGHTED SUM OF FUNCTION EVALUATIONS
 $a_i \rightarrow$ THIS IS A NUMBER

$$\int_a^b f(x) dx = \underbrace{\sum_{i=0}^N a_i f_i}_{\text{QUADRATURE (NUMERICAL METHOD)}} + \text{ERROR TERM}$$

← QUANTIFY (NUMERICAL ANALYSIS)

TEXT:

$$\int_a^b f(x) dx = \sum_{i=0}^N a_i f_i + \int_a^b \frac{(-1)^N}{(N+1)!} \frac{(x-x_i)}{(N+1)!} f^{(N+1)}(x) dx$$

HORNBECK: TAYLOR SERIES

$$I(x) = \int_a^x f(\tilde{x}) d\tilde{x} \rightarrow \text{EXPAND } I(x) \text{ AROUND } x=a$$

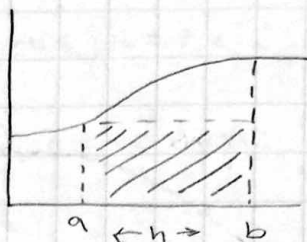
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$$\begin{aligned} I(x) &= I(a) + I'(a)(x-a) \\ &= 0 + f'(a)(x-a) \\ &= f(a) + \frac{f'(a)}{2}(x-a)^2 + \frac{f''(a)}{3!}(x-a)^3 \end{aligned}$$

$$I(b) = f(a)h + \frac{f'(a)h^2}{2} + \frac{f''(a)h^3}{3!} + \dots$$

SIMPLEST SOLUTION,

$$I(b) = hf(a)$$



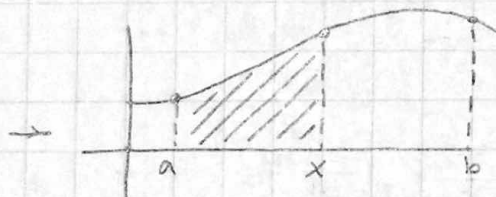
GOOD WHEN h IS SMALL

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NUMERICAL QUADRATURE

$$\int_a^b f(x) dx = \sum_{i=0}^N a_i f_i + \text{ERROR TERM}$$

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



$$I(x) = I(a) + I'(a)(x-a) + \frac{I''(a)}{2!}(x-a)^2 + \dots$$

$$= f(a)(x-a) + \frac{f'(a)}{2!}(x-a)^2 + \dots$$

$$I(b) = f(a)h + \frac{f'(a)h^2}{2!} + \frac{f''(a)h^3}{3!} + \dots \rightarrow \text{KEEP ANOTHER TERM}$$

$$ii.) I(b) = hf_a + \frac{h^2}{2} f'_a + \frac{h^3}{3!} f''_a + \dots$$

\hookrightarrow USE FORWARD DIFFERENCE, $f'_a = \frac{f_b - f_a}{h} - \frac{h}{2} f''(s_0)$

$$I(b) = hf_a + \frac{h^2}{2} \left(\frac{f_b - f_a}{h} \right) - \frac{h^3}{4} f''(s) + \frac{h^3}{6}$$

$$I(b) = hf_a + \frac{h}{2} (f_b - f_a) - \frac{h^3}{12} f''(s)$$

CAN'T CALCULATE THIS

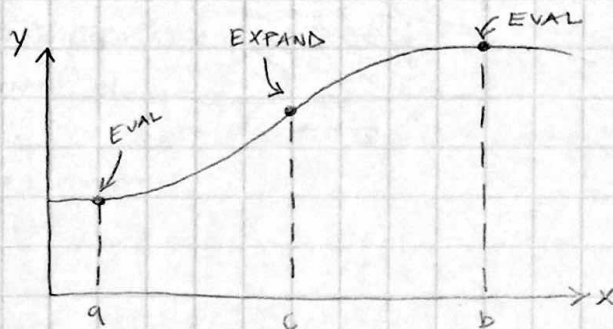
TRAPAZOIDAL RULE

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FOR NUMERICAL INTEGRATION, LOOK @ ORDER OF POLYNOMIAL THAT CAN BE INTEGRATED EXACTLY TO DETERMINE ORDER OF ERROR.

$$\text{I.E. } P_N^{(N+1)}(x) = 0$$

INSTEAD OF USING A FWD DIFFERENCE, USE A CENTER DIFFERENCE



BEFORE: $b-a=h$

NOW: $b-a=2h$

$$I(b) = I(c) + hf_c + \frac{h^2}{2!} f_c' + \frac{h^3}{3!} f_c'' + \dots$$

$$I(a) = I(c) - hf_c + \frac{h^2}{2!} f_c' - \frac{h^3}{3!} f_c'' + \dots$$

$$I(b) = 2hf_c + \frac{2h^3}{3!} f_c'' + \frac{2h^3}{3!} f_c^{(4)} + \dots$$

$$\rightarrow \text{USE C.D. APPROX: } f_c'' = \frac{f_a - 2f_c + f_b}{h^2} - \frac{h^2}{12} f^{(4)}(f)$$

$$I(b) = \frac{h}{3} [f_a + 4f_c + f_b] - \frac{h^5}{90} f^{(4)}(f)$$

← CAN DO A CUBIC EXACTLY, 4TH DERIVATIVE OF A CUBIC = 0, SO ERROR $\rightarrow 0$

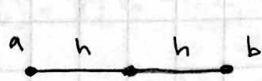
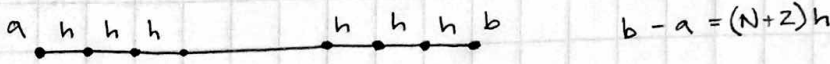
* NEWTON NOTES FORMULAS

- CLOSED FORMULAS INCLUDE END POINTS
- OPENS DO NOT

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* NEWTON-COTES OPEN FORMULAS

- DO NOT INCLUDE LIMITS OF INTEGRATION

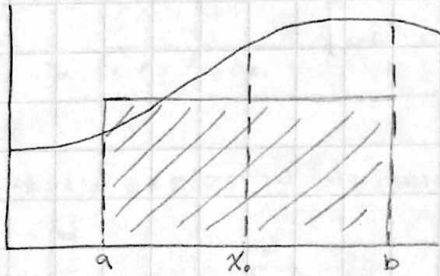


$$I(b) = I(x_0) + hf_0 + \frac{h^2 f_0'}{2!} + \frac{h^3 f_0''}{3!} + \dots$$

$$I(a) = I(x_0) - hf_0 + \frac{h^2 f_0'}{2!} - \frac{h^3 f_0''}{3!} + \dots$$

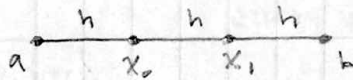
$I(b) = 2hf_0 + \frac{h^3 f''(\xi)}{3}$

MID POINT RULE



FOR LINEAR FUNCTION, ERROR CANCELS OUT

EG. N=1



EXPAND ABOUT x_0

$$I(b) = I(x_0) + 2hf_0 + \frac{(2h)^2}{2!} f_0' + \frac{(2h)^3}{3!} f_0'' + \dots$$

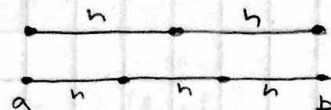
$$I(a) = I(x_0) - hf_0 + \frac{h^3}{2!} f_0' - \frac{h^3}{3!} f_0'' + \dots$$

$$I(b) = 3hf_0 + \frac{3}{2}h^2 f_0' + \frac{ah^3}{6} f''(\xi)$$

↑ FORWARD DIFF.

→ CAN STILL ONLY DO A LINEAR FUNCTION EXACTLY

- SOME ADVANTAGE BC. h IS SMALLER THAN CLOSED CASE:



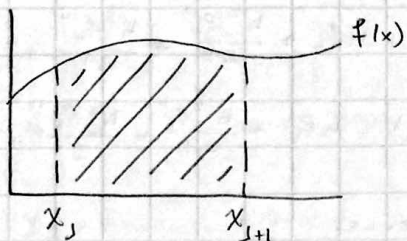
N EVEN: P_{NH} CAN BE INTEGRATED EXACTLY

N ODD: P_N CAN BE INTEGRATED EXACTLY.

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* COMPOSITE INTEGRATION

- USE LOW ORDER N-C FORMULAS ON SUB INTERVALS



$$S_{j+1} = \int_{x_j}^{x_{j+1}} f(x) dx$$

- TRAPEZOIDAL RULE:

$$S_j = \frac{h}{2} [f_{j+1} + f_j] - \frac{h^3}{12} f''(\xi_j) \quad \xi_j \in [x_j, x_{j+1}]$$

- COMPOSITE TRAPEZOIDAL RULE

$$I(b) = \sum_{i=1}^N \frac{h}{2} [f_i + f_{i+1}] - \sum_{i=1}^N \frac{h^3}{12} f''(\xi_i)$$

$$I(b) = \frac{h}{2} \left[2 \sum_{i=1}^{N-1} f_i + f_0 + f_N \right] \quad \leftarrow \text{COMPOSITE TRAPEZOIDAL RULE}$$

INSIDE POINTS OUTSIDE POINTS

- ERROR = $\sum_{j=1}^N \frac{h^3}{12} f''(\xi_j) = \frac{h^3}{12} N \bar{f}''(\xi)$ WHERE \bar{f}'' IS THE AVERAGE VALUE OF $f''(\xi_j)$

$$b-a = Nh \Rightarrow N = \frac{b-a}{h}$$

$$\text{ERROR} = \frac{b-a}{12} h^2 f''(\xi) \quad \text{WHICH IS } O(h^2)$$

APPLICATION OF METHOD N TIMES REDUCES ORDER OF ERROR BY A FACTOR OF h

HIGHER ORDER
N \equiv BETTER/MORE
ACCURATE THE
SOLUTION

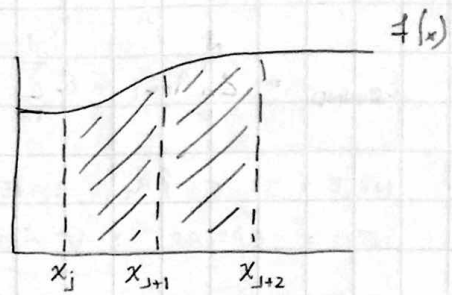
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EG. SIMPSON'S RULE

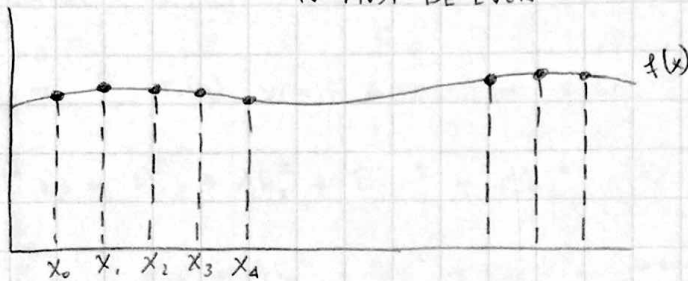
$$I(b) = \frac{h}{3} [f_a + 4f_c + f_b]$$

$$I(b) = \frac{h}{3} \left[f_0 + 2 \sum_{j=1}^{N/2-1} f_{2j} + 4 \sum_{j=1}^{N/2} f_{2j-1} + f_n \right]$$

$$- \frac{(b-a)h^4}{18} f''(\xi)$$



N MUST BE EVEN



ROUNDING ERRORS IN NUMERICAL INTEGRATION

$$\int_a^b f(x) dx = \underbrace{\sum_{i=0}^N a_i f_i}_{\text{QUADRATURE}} + E_{\text{TRUNCATION}}$$

TRUNCATION HAS h IN NUMERATOR
SO $E_{\text{TRUNCATION}} \rightarrow 0$ AS $h \rightarrow 0$

ON COMPUTER:

$$\hat{f}_i = f_i + \epsilon_i \rightarrow \underbrace{\sum_{i=0}^N a_i \hat{f}_i}_{\text{COMPUTED QUADRATURE}} = \underbrace{\sum_{i=0}^N a_i f_i}_{\text{EXACT QUADRATURE}} + \underbrace{\sum_{i=0}^N a_i \epsilon_i}_{\text{ROUND-OFF}}$$

$$E_{\text{TOTAL}} = \left| \int_a^b f(x) dx - \sum_{i=0}^N a_i \hat{f}_i \right| = \left| \sum_{i=0}^N a_i f_i + E_{\text{TRUNC}} - \sum_{i=0}^N a_i f_i - E_{\text{ROUND}} \right|$$

$$= \left| E_{\text{TRUNC}} - E_{\text{ROUND}} \right| \leq \left| E_{\text{TRUNC}} \right| + \left| E_{\text{ROUND}} \right|$$

$$E_{\text{ROUND OFF}} = \sum_{i=0}^N a_i \epsilon_i, \quad \text{TRAPEZOIDAL RULE } \sum_{i=0}^N a_i f_i = \frac{h}{2} [f_0 + f_1]$$

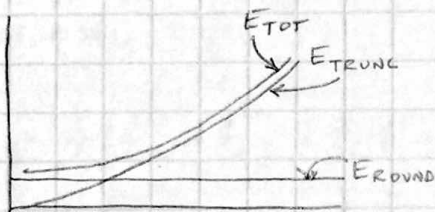
$$a_0 = a_1 = \frac{h}{2}$$

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$$E_{\text{ROUND}} = \sum_{i=0}^N a_i \varepsilon_i \leq \varepsilon \sum_{i=0}^N |a_i| \quad \text{WHERE } \varepsilon \equiv \max |\varepsilon_i|$$

NOTE THAT $\{a_i\}$ HAVE A FACTOR OF h IN NUMERATOR, SO IT WOULD APPEAR THAT $E_{\text{ROUND}} \rightarrow 0$ AS $h \rightarrow 0$

$$\int_a^b dx = b - a = \sum_{i=0}^N a_i(h), \quad E_{\text{ROUND}} \leq \varepsilon(b-a) \quad \text{IE. INDEPENDENT OF } h \text{ AND DOES NOT } \rightarrow 0 \text{ FOR } h \rightarrow 0$$



* ROMBERG INTEGRATION

- CAN BE USED ON ANY N-C FORMULA

IDEA: COMPUTE QUADRATURE RULE W/ TWO DIFFERENT h INTERVALS
? COMBINE TO CANCEL THE LEADING ERROR TERM, GIVING
A BETTER APPROXIMATION

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* ROMBERG INTEGRATION

→ START W/ COMPOSITE TRAPEZOIDAL RULE

$$I(b) = \frac{h}{2} \left[f_0 + 2 \sum_{i=1}^{N-1} f_i + f_N \right] + \underbrace{Ah^2 + Bh^4 + Ch^6 \dots}_{A = \frac{f''(s)}{12}}$$

→ DEFINE

$$R_{N,0} = \frac{h}{2} \left[f_0 + 2 \sum_{i=1}^{N-1} f_i + f_N \right] \quad \text{COMPOSITE TRAPEZOIDAL RULE ON } N \text{ PANELS, SIZE } h$$

LOOK @ $I(b)$ USING DIFFERENT PANEL SIZES, h_1 , AND $h_2 = \frac{h_1}{2}$

$$h \quad I(b) = R_{2N} + Ah_2^2 + Bh_2^4 + Ch_2^6 + \dots$$

$$h_2 \quad I(b) = R_N + Ah_1^2 + Bh_1^4 + Ch_1^6 + \dots$$

$$\hookrightarrow = R_N + A(2h_2)^2 + B(2h_2)^4 + C(2h_2)^6 = R_N + 4Ah_2^2 + 16Bh_2^4 + 64Ch_2^6$$

$$3I(b) = 4R_{2N} - R_N - 12Bh_2^4 - 60Ch_2^6$$

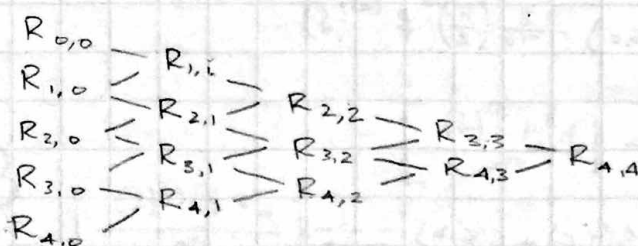
$$I(b) = \frac{4R_{2N} - R_N}{3} - 4Bh_2^4 - 20Ch_2^6$$

$$\begin{aligned} R_N &\rightarrow O(h_1^2) \\ R_{2N} &\rightarrow O(h_2^2) = O\left(\frac{h_1^2}{4}\right) \end{aligned} \quad \left. \vphantom{\begin{aligned} R_N \\ R_{2N} \end{aligned}} \right\} O\left(\frac{h_1^4}{16}\right)$$

EACH APPLICATION INCREASES ORDER OF ERROR TERM BY h_1^2 WHEREAS HALVING REDUCES ONLY BY A FACTOR OF $1/4$. THIS HAS RESULTED IN SIMPSONS RULE

GENERALIZE: $M = \#$ OF PANEL DOUBLINGS
 $J = \#$ OF ERROR REMOVALS

$$R_{m,j} = \frac{A^j R_{m,j-1} - R_{m-1,j-1}}{A^j - 1}$$



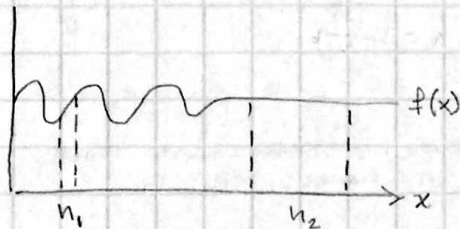
$$O\left(\frac{h}{2^4}\right)^{10} \quad O\left(\frac{h^{10}}{16^{10}}\right)$$

$$O\left(\frac{h}{2^m}\right)^{2m+2}$$

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USE $R_{m,m}$; CONVERGES FASTER

* ADAPTIVE QUADRATURE



$$\text{ERROR} \sim h^m f^{(m)}$$

IF WANT CONSTANT ERROR OVER INTERVAL, $h_1 \ll h_2$

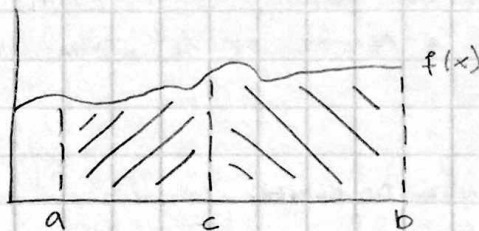
WANT TO UNIFORMLY DISTRIBUTE ERROR

SIMPSON'S RULE:

$$\int_a^b f(x) dx = \frac{h}{3} [f_a + 4f_c + f_b] - \frac{h^5 f^{(4)}(\xi)}{90}$$

DEFINE: $S(a,b) \equiv \text{SIMPSON'S ON } [a,b]$

$$\int_a^b f(x) dx = S(a,b) - \frac{h^5 f^{(4)}(\xi)}{90}$$



$$\int_a^b f(x) dx = S(a,c) - \frac{h^5 f^{(4)}(\xi_1)}{90} + S(c,b) - \frac{h^5 f^{(4)}(\xi_2)}{90}$$

LET $f^{(4)}(\xi) \equiv \frac{f^{(4)}(\xi_1) + f^{(4)}(\xi_2)}{2}$ THEN,

$$\int_a^b f(x) dx = S(a,c) + S(c,b) - \frac{2}{90} \left(\frac{h}{2}\right)^3 f^{(4)}(\xi)$$

$$= S(a,c) + S(c,b) - \frac{1}{16} \left[\frac{h^3 f^{(4)}(\xi)}{90} \right]$$

$$S(a,b) = - \frac{h^5 f^{(4)}(\xi)}{90} = S(a,c) + S(c,b) - \frac{1}{16} \left[\frac{h^5 f^{(4)}(\xi)}{90} \right]$$

ASSUMPTION
 $f^{(4)}(\xi) = \frac{f^{(4)}(\xi_1) + f^{(4)}(\xi_2)}{2}$

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$$\frac{15}{16} \left[\frac{h^5 f^{(4)}(\xi)}{70} \right] \approx S(a,b) - S(a,c) - S(c,b)$$

$$\left| \int_c^b f(x) dx - S(a,c) - S(c,b) \right| \approx \frac{1}{15} \left| S(a,b) - S(a,c) - S(c,b) \right|$$

INTERPRETATION: $S(a,c) + S(c,b)$ APPROXIMATES $\int_a^b f(x) dx$ 15 TIMES

BETTER THAN $S(a,b)$

MIDTERM STUDY GUIDE:

* TAYLORS THEOREM

IF $f(x)$ HAS $N+1$ DERIVATIVES ON $[a,b]$, THEN

$$f(x) = P_N(x) + R_N(x)$$

WHERE $P_N(x) = \sum_{k=0}^N \frac{f^{(k)}(x_0)}{k!} (x-x_0)^k$ BY DEFINITION, $P_N(x_0) = f(x_0)$

$$R_N(x) = \frac{f^{(N+1)}(\xi)}{(N+1)!} (x-x_0)^{N+1} \quad \text{WHERE } \xi \in [x, x_0]$$

* ERROR

LINEAR: $\epsilon = K\epsilon_0$

EXPONENTIAL: $\epsilon = K^n \epsilon_0$

$$P_N = \frac{1}{3} P_{N-1} \quad \rightarrow \quad P_N - \hat{P}_N = \frac{1}{3} (P_{N-1} - \hat{P}_{N-1}) = \epsilon_N = \frac{1}{3} \epsilon_{N-1}$$

$n=1$: $\epsilon_1 = \frac{1}{3} \epsilon_0$

$n=2$: $\epsilon_2 = \frac{1}{3} \epsilon_1 \rightarrow \epsilon_2 = (\frac{1}{3})^2 \epsilon_0$

$n=3$: $\epsilon_3 = \frac{1}{3} \epsilon_2 \rightarrow \epsilon_3 = (\frac{1}{3})^3 \epsilon_0$

$\epsilon_N = (\frac{1}{3})^N \epsilon_0$

$$\lim_{n \rightarrow \infty} \epsilon_N = \lim_{n \rightarrow \infty} (\frac{1}{3})^N \epsilon_0 = \underline{\underline{0}} \quad (\text{CANNOT ASSUME EXACT CONSTANTS})$$

\rightarrow LET $\frac{1}{3} = \frac{1}{3} + \delta \rightarrow \frac{1}{3} = \frac{1}{3} - \delta$

$$\hat{P}_N = (\frac{1}{3} - \delta) \hat{P}_{N-1}, \quad P_N = \frac{1}{3} P_{N-1}$$

$$\epsilon_N = \frac{1}{3} P_{N-1} - (\frac{1}{3} - \delta) \hat{P}_{N-1} \rightarrow \epsilon_N = \frac{1}{3} P_{N-1} - \frac{1}{3} \hat{P}_{N-1} + \delta \hat{P}_{N-1}$$

$$\epsilon_N = \frac{1}{3} \epsilon_{N-1} + \delta \hat{P}_{N-1}$$

$n=1$ $\epsilon_1 = \frac{1}{3} \epsilon_0 + \delta \hat{P}_0$

$n=2$ $\epsilon_2 = \frac{1}{3} \epsilon_1 + \delta \hat{P}_1 = \frac{1}{3} (\frac{1}{3} \epsilon_0 + \delta \hat{P}_0) + \delta \hat{P}_1 = (\frac{1}{3})^2 \epsilon_0 + \frac{1}{3} \delta \hat{P}_0 + \delta \hat{P}_1$

$n=3$ $\epsilon_3 = \frac{1}{3} ((\frac{1}{3})^2 \epsilon_0 + \frac{1}{3} \delta \hat{P}_0 + \delta \hat{P}_1) + \delta \hat{P}_2 = (\frac{1}{3})^3 \epsilon_0 + (\frac{1}{3})^2 \delta \hat{P}_0 + (\frac{1}{3}) \delta \hat{P}_1 + \delta \hat{P}_2$

$$\epsilon_N = (\frac{1}{3})^N \epsilon_0 + n \delta \hat{P}_0 \quad \epsilon_N \leq (\frac{1}{3})^N \epsilon_0 + n \delta \hat{P}_0$$

\rightarrow ERRORS GROW LINEARLY

* FIXED POINT ROOT FINDING

WANT SOLUTION TO $f(x) = 0$, SOLVE BY SOLVING $p = g(p)$ INSTEAD
(FIXED POINT)

EX. $x^3 - 7x + 2 = 0$ WHERE $f(x) = x^3 - 7x + 2$

$$g(x) \text{ FORM} \rightarrow x = (x^3 + 2)/7 \rightarrow x_{n+1} = (x_n^3 + 2)/7$$

$$\rightarrow \text{ITERATE UNTIL } |x_{n+1} - x_n| < \epsilon \rightarrow x_{n+1} \equiv \text{ROOT OF } f(x)$$

CONVERGENCE CRITERIA:

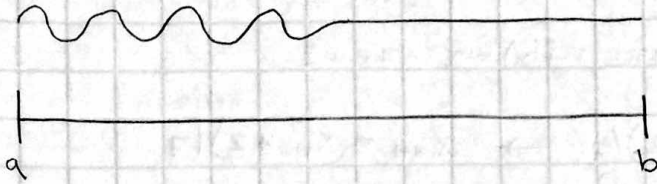
$$p_n = g(p_n) \rightarrow p_n - p_{n-1} = g(p_n) - g(p_{n-1}) \rightarrow \text{MVT} = g'(p_n) = \frac{g(p_n) - g(p_{n-1})}{p_n - p_{n-1}}$$

$$(p_n - p_{n-1}) g'(p_n) = g(p_n) - g(p_{n-1})$$

$$\hookrightarrow |g'(p_n)| < 1 \text{ FOR CONVERGENCE, } \epsilon_n = g'(p_n)(p_n - p_{n-1})$$

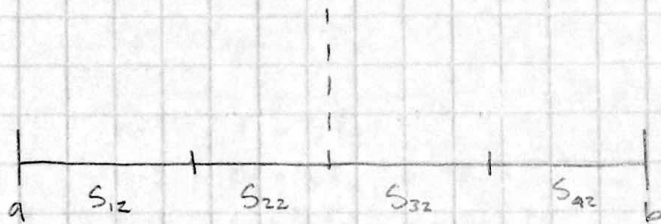
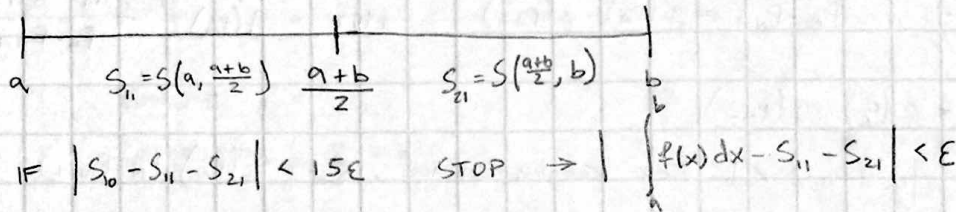
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* ADAPTIVE QUADRATURE



$$S(a,b) \equiv S_{1,0}$$

\nearrow SECTION \nwarrow REFINEMENT



IF $|S_{1,1} - S_{1,2} - S_{2,2}| < 15\left(\frac{\epsilon}{2}\right)$ IF $|S_{2,1} - S_{3,2} - S_{4,2}| < 15\left(\frac{\epsilon}{2}\right)$

$$\int_a^b f(x) dx \approx \text{SUM OF PIECES}$$

* GAUSSIAN QUADRATURE (SECTION 4.7)

- IS THERE AN OPTIMAL SET OF POINTS FOR APPROXIMATING $\int_a^b f(x) dx$
- OPTIMAL IN THE SENSE THAT WE CAN INTEGRATE THE MAX. ORDER POLYNOMIAL USING THE MINIMUM POSSIBLE POINTS.

$$\int_a^b f(x) dx \approx \sum_{i=1}^N a_i f(x_i)$$

\leftarrow "N" DEG. OF FREEDOM \rightarrow N-1 ORDER POLYNOMIAL
 2N DEG. OF 2N-1 ORDER POLYNOMIAL

THERE ARE 'SPECIAL' POINTS $\{x_i\}$ CALLED GAUSS POINTS WHICH ARE ROOTS OF THE LEGENDRE POLYNOMIALS

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BY USING THESE POINTS WE CAN INTEGRATE EXACTLY A POLYNOMIAL OF ORDER $2N+1$, WHERE $N = \#$ OF SAMPLE POINTS

TRAPEZOIDAL RULE: INTEGRATE A LINEAR FUNCTION EXACTLY

$$I(b) = \frac{h}{2}(f_1 + f_2) - \frac{h^2}{12} f''(\xi) \quad \xi \in [x_1, x_2]$$

$$I(b) = \sum_{i=1}^{N+1} a_i f(x_i) = a_1 f(x_1) + a_2 f(x_2)$$

WE SHOULD BE ABLE TO INTEGRATE A CUBIC EXACTLY: $P_{2N-1}(x) = P_3(x)$

$\hookrightarrow x^3, x^2, x, \text{CONSTANT}$

$$x^3: \int_{-1}^1 x^3 dx = 0 = a_1 x_1^3 + a_2 x_2^3$$

$$x^2: \int_{-1}^1 x^2 dx = \frac{x^3}{3} \Big|_{-1}^1 = \frac{2}{3} = a_1 x_1^2 + a_2 x_2^2$$

$$x: \int_{-1}^1 x dx = 0 = a_1 x_1 + a_2 x_2$$

$$1: \int_{-1}^1 dx = 2 = a_1 + a_2$$

4 EQUATIONS, 4 UNKNOWNNS
 $a_1 = a_2 = 1$ (HEIGHTS)
 $-x_1 = x_2 = \sqrt{1/3}$ (GAUSS POINTS)

\rightarrow MAP $[-1, 1]$ TO $[a, b]$

$$\int_a^b f(y) dy \quad \text{WHERE } y = \frac{a+b}{2} + \frac{b-a}{2} x, \quad dy = \frac{b-a}{2} dx$$

$$\int_{-1}^1 f(y) \frac{b-a}{2} dx \approx \frac{b-a}{2} \sum_{i=1}^N a_i f(y_i) \quad \text{WHERE } y_i = \frac{a+b}{2} + \frac{b-a}{2} x_i \quad \uparrow \text{ GAUSS POINTS}$$

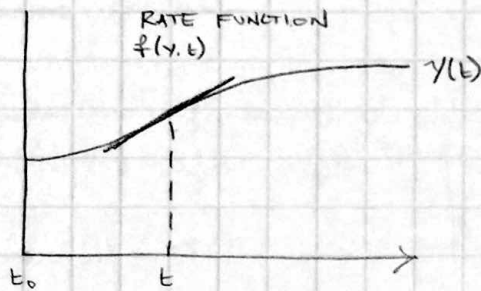
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* SOLUTIONS TO ODES

- ORDINARY: ONE IND. VARIABLE

"CLASSIC IVP"

$$\frac{d}{dt} y(t) = y'(t) = \underbrace{f(y, t)}_{\text{"RATE" FUNCTION}}; y(t_0) = y_0, \text{ WANT } y(t) \text{ GIVEN } f(y, t)$$



SOLUTION FAMILY IS AN INTRINSIC PROPERTY OF ODE

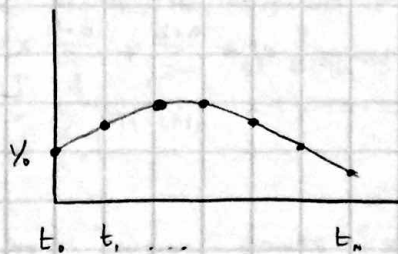
SIMPLEST CASE $f(y, t) = f(t)$



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- CLASSIC IVP: $\frac{dy(t)}{dt} = y' = f(y, t)$

FIND $y(t)$



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EULER'S METHOD:

- 3 DIFFERENT WAYS TO DERIVE

i.) SUBSTITUTE FINITE DIFFERENCE

$$y' = \left[\frac{y_{i+1} - y_i}{h} - f'(y_i, t) \right] = f(y, t) \quad \text{WHERE } y_i = y(t_i) \\ h = t_{i+1} - t_i$$

$$y_{i+1} = y_i + hf_i + \underbrace{\frac{h^2}{2} f''(y_i, t_i)}_{\text{TRUNCATION}}$$

TRUNCATE & SWITCH TO $w_i \approx y_i$

$$\boxed{w_{i+1} = w_i + hf_i} \quad \text{EULER'S METHOD}$$

ii.) INTEGRATE THE ODE

$$\int_{t_i}^{t_{i+1}} y' dt = \int_{t_i}^{t_{i+1}} f(y, t) dt \quad \rightarrow \quad y_{i+1} - y_i = \int_{t_i}^{t_{i+1}} f(y, t) dt$$

TAYLOR EXPAND
& EVALUATE @ t_{i+1}

$$I(t_{i+1}) = I(t_i) + hf_i + \frac{h^2 f''(s)}{2}$$

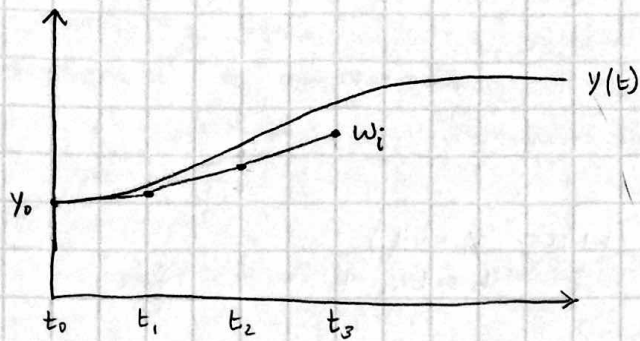
$$\boxed{y_{i+1} = y_i + hf_i + \frac{h^2 f''(s)}{2}}$$

iii.) TAYLOR EXPAND THE SOLUTION $y(t)$ AROUND t_i AND EVALUATE AT t_{i+1}

$$y(t) = y(t_i) + y'(t_i)(t-t_i) + \frac{y''(t_i)}{2!}(t-t_i)^2 + \dots$$

$$\boxed{y(t_{i+1}) = y(t_i) + hf_i + \frac{h^2}{2} f''(s)}$$

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$$w_{i+1} = w_i + h f_i$$

$w_i \neq y_i$ RATE FUNCTIONS WILL ONLY BE EQUAL IF $y_i = f(t)$ ONLY

- LOCAL TRUNCATION ERROR IS $O(h^2)$, AS t ADVANCES $\rightarrow O(h)$
'GLOBAL' ERROR
- ADDITIONAL ERROR COMPONENT DUE TO EVALUATION OF RATE FUNCTION AT WRONG PLACE

$$f(w_i, t_i) \neq f(y_i, t_i)$$

DEFINE TOTAL ERROR:

$$E_{i+1} = |y_{i+1} - w_{i+1}| \rightarrow y_{i+1} = y_i + h f_i + \frac{h^2}{2} f''(y_i, t_i)$$

EXACT: $f_i = f(y_i, t_i)$

COMP: $\bar{f}_i = f(w_i, t_i)$

$$y_{i+1} - w_{i+1} = y_i - w_i + h(f_i - \bar{f}_i) + \frac{h^2}{2} f''(y_i, t_i)$$

$$E_{i+1} = \epsilon_i \left[1 + \frac{h(f_i - \bar{f}_i)}{y_i - w_i} \right] + \frac{h^2}{2} f''(y_i, t_i)$$

ERROR COMPONENT FROM y DEPENDENCE
 $J_i = 0$ IF ONLY A FUNCTION OF t

$$J_i = \frac{\partial f}{\partial y}(\eta_i, t_i), \quad \eta_i \in [y_i, w_i]$$

\rightarrow JACOBIAN OF THE EQUATION

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DUE TO EVALUATION @ WRONG PLACE

$$\epsilon_{i+1} = \underbrace{\epsilon_i(1 + hJ_i)}_{\text{AMPLIFICATION FACTOR}} + \underbrace{\frac{h^2}{2} f''(y_i, t_i)}_{\text{TRUNCATION ERROR IN STEP } t_i \rightarrow t_{i+1} \text{ ASSUMING EXACT } \epsilon}$$

AMPLIFICATION FACTOR

TRUNCATION ERROR IN STEP $t_i \rightarrow t_{i+1}$ ASSUMING EXACT ϵ

- ERROR PROPAGATES AS TIME ADVANCES
- WANT J_i SMALL AND NEGATIVE, CERTAINLY NOT BIG.

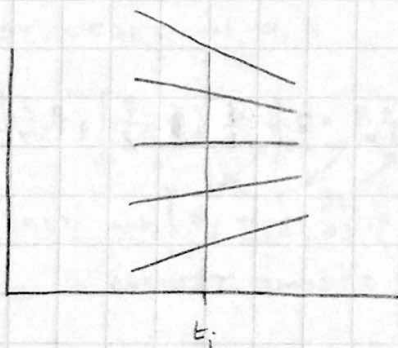
GE = GLOBAL ERROR

LTE = LOCAL TRUNCATION ERROR

$$GE_{i+1} = (1 + hJ_i) GE_i + LTE_i \rightarrow \text{FOR EULER'S METHOD, WE NEED}$$

$$|1 + J_i h| < 1 \text{ OTHERWISE GE BLOWS UP} \rightarrow J_i < 0$$

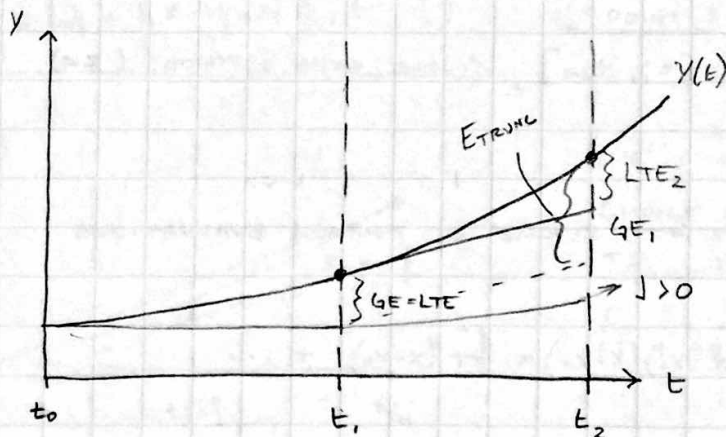
$$\frac{\partial f}{\partial y} < 0?$$



A STABLE ODE HAS $\frac{\partial f}{\partial y} < 0$

STABILITY CRITERION FOR EULER'S METHOD

$$h < \frac{2}{|J|}$$



FIRST STEP:

$$y_i = y_0 + h f_0 + \frac{h^2}{2} f''(s)$$

$$w_i = w_0 + h f_0 \quad \text{LTE}$$

2ND STEP:

$$y_2 = y_1 + h f(y_1, t_1) + LTE_2$$

$$w_2 = w_1 + h f(w_1, t_1)$$

$$GE_{i+1} = (1 + hJ_i) GE + LTE_{i+1}$$

- E_{TRUNC} IS GROWING
- IF $J = 0$, $E_{SLOPE} = 0$

$J < 0$, E_{SLOPE} CANCELS SOME OF E_{TRUNC} .

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EXAM:

- TESTED ON 'MATHEMATICAL' SIDE
- NO ODE'S

* EULER'S METHOD:

- NOT VERY ACCURATE
- STABILITY LIMITATIONS
- SUSCEPTIBLE TO EXPONENTIAL ERROR GROWTH
- WANT METHODS W/ HIGHER ORDER LTE

$$y_{i+h} = y_i + hf_i$$

EULER'S METHOD, $O(h^2)$ / STEP
 $O(h)$ / GLOBAL

$$\rightarrow y_{i+h} = y_i + hf_i + \frac{h^2}{2} f_i'$$

$O(h^2)$ / STEP
 $O(h^2)$ / GLOBAL

$$\rightarrow \text{BUT NEED } f_i' = \frac{d}{dt} f(y, t) = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} \frac{dy}{dt} = \frac{\partial f}{\partial t} + f \frac{\partial f}{\partial y}$$

$$y_{i+h} = y_i + hf_i + \frac{h^2}{2} f_i' + \frac{h^3}{3!} f_i''$$

$$\rightarrow f_i'' = \frac{d}{dt} [f_i'] = \frac{\partial}{\partial t} \left[\frac{\partial f}{\partial t} + f \frac{\partial f}{\partial y} \right] + f \frac{\partial}{\partial y} \left[\frac{\partial f}{\partial t} + f \frac{\partial f}{\partial y} \right]$$

- HIGHER ORDER TAYLOR METHOD'S QUICKLY BECOME TEDIOUS
- INSTEAD APPROXIMATE DERIVATIVES USING WEIGHTED FUNCTION EVALUATIONS OF f .
- RESTRICT EVALUATIONS TO $[t_i, t_{i+1}]$, SINGLE STEP METHODS (RK)

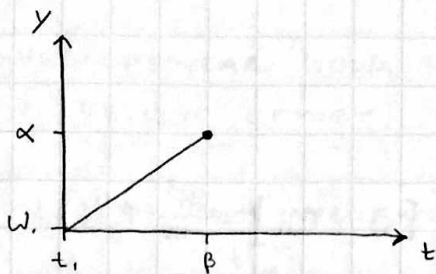
* RUNGE-KUTTA 2 (RK2)

$$w_{i+1} = w_i + hf_i + \frac{h^2}{2} f_i' \leftarrow \text{REPLACE W/ FUNCTION EVALUATIONS}$$

• BEFORE: $f(x) = f(x_0) + f'(x_0)(x-x_0) + \frac{f''}{2!}(x-x_0)^2 + \dots$

• NOW: $f(y, t) = ?$

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EXPAND $f(w, t)$ AROUND w_i, t_i
AND EVALUATE AT $w_i + \alpha, t_i + \beta$

$$f(w, t) = f(w_i, t_i) + \frac{\partial f_i}{\partial t} (t - t_i) + \frac{\partial f_i}{\partial y} (w - w_i) + \frac{\partial^2 f_i}{\partial t^2} \frac{(t - t_i)^2}{2} + \frac{\partial^2 f_i}{\partial y^2} \frac{(w - w_i)^2}{2} + \frac{\partial^2 f_i}{\partial t \partial y} (w - w_i)(t - t_i) \dots$$

→ EVALUATE @ α, β

$$f(w_i + \alpha, t_i + \beta) = f_i + \alpha \frac{\partial f_i}{\partial y} + \beta \frac{\partial f_i}{\partial t} + \frac{\beta^2}{2} \frac{\partial^2 f_i}{\partial t^2} + \frac{\alpha^2}{2} \frac{\partial^2 f_i}{\partial y^2} + \alpha \beta \frac{\partial^2 f_i}{\partial t \partial y} + \dots$$

TO FIRST ORDER IN α, β

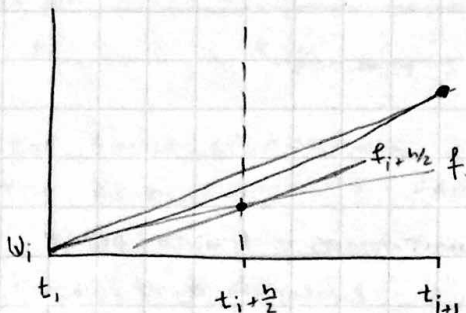
$$f(w_i + \alpha, t_i + \beta) = f_i + \beta \frac{\partial f_i}{\partial t} + \alpha \frac{\partial f_i}{\partial y}$$

$$w_{i+1} = w_i + h \left[f_i + \frac{h}{2} \frac{\partial f_i}{\partial t} + \frac{h}{2} \frac{\partial f_i}{\partial y} f_i \right]$$

IF WE LET $\beta = \frac{h}{2}$; $\alpha = \frac{h}{2} f_i$

$$w_{i+1} = w_i + h f \left(w_i + \frac{h}{2} f_i, t_i + \frac{h}{2} \right)$$

MIDPOINT RULE (RK2)



THE MIDPOINT RULE IS A PARTICULAR CHOICE OF A MORE GENERAL APPROX. TO

$$\left[f_i + \frac{h}{2} \left(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} f \right) \right] = a_1 f_i + a_2 f [w_i + \alpha, t_i + \beta]$$

→ MIDPOINT RULE:

$$a_1 = 0, a_2 = 1$$

$$\alpha = \frac{h}{2} f_i, \beta = \frac{h}{2}$$

↳ LEADS TO TRAPEZOIDAL RULE METHOD ; MODIFIED EULER'S METHOD.

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$$\int_{t_i}^{t_{i+1}} y' dt = \int_{t_i}^{t_{i+1}} f(v, \tau) d\tau$$

USE TRAPEZOIDAL RULE $\frac{h}{2} [f_i + f_{i+1}] - \frac{h^3}{12} f'(s)$

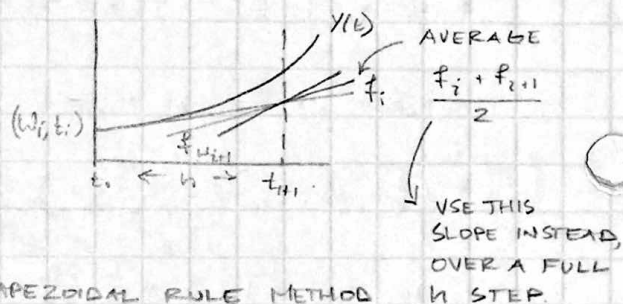
$$y_{i+1} - y_i = \frac{h}{2} [f_i + f_{i+1}] - \frac{h^3}{12} f'(s)$$

$$w_{i+1} = w_i + \frac{h}{2} [f_i + f(w_{i+1}, t_{i+1})]$$

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ODE SOLUTIONS

FIND $y(t_i)$ GIVEN $y' = f(v, t); y(t_0) = y_0$



$$w_{i+1} = w_i + \frac{h}{2} [f_i + f(w_{i+1}, t_{i+1})]$$

TRAPEZOIDAL RULE METHOD

↑ AVERAGE OF SLOPE @ i & $i+1$

HOW TO GET w_{i+1} IN $f(w_{i+1}, t_{i+1})$

GENERAL APPROXIMATION TO:

$$[f_i + \frac{h}{2} (\frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} f)] = a_1 f_i + a_2 f(w_i + \alpha, t_i + \beta)$$

MODIFIED
EULER'S
METHOD

$$w_{i+1} = w_i + \frac{h}{2} [f_i + f(w_i + hf_i, t_{i+1})]$$

HEUN'S
METHOD

$$w_{i+1} = w_i + \frac{h}{4} [f_i + 3f_{i+2/3}]$$

RK2 METHODS

4TH ORDER RUNGE-KUTTA BEGINS TO REACH A LIMITATIONS - HIGHER ORDER METHODS HAVE $\epsilon_{TRUNC} \sim O(\epsilon_{ROUND})$

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* RUNGE-KUTTA 4TH ORDER

- VERY POPULAR. GOOD TRADE-OFF BETWEEN TRUNC. ERROR REDUCTION
 & RELATIVE EFFORT.

- DERIVED FROM INTEGRATION OF ODE USING SIMPSON'S RULE

$$\int_{t_i}^{t_{i+1}} y_i' dt = \int_{t_i}^{t_{i+1}} f(y, t) dt = \frac{h}{6} [f_i + 4f_{i+1/2} + f_{i+1}] + O(h^5)$$

RUNGE-KUTTA
 4TH ORDER
 METHOD

$$W_{i+1} = W_i + \frac{h}{6} [f_i + 4f_{i+1/2} + f_{i+1}]$$

GENERAL FORMULA: WEIGHTED AVERAGE OF RATE FUNCTIONS EVALUATED
 AT $t_i, t_{i+1/2}, t_{i+1}$

- MANY POSSIBILITIES: MOST COMMON

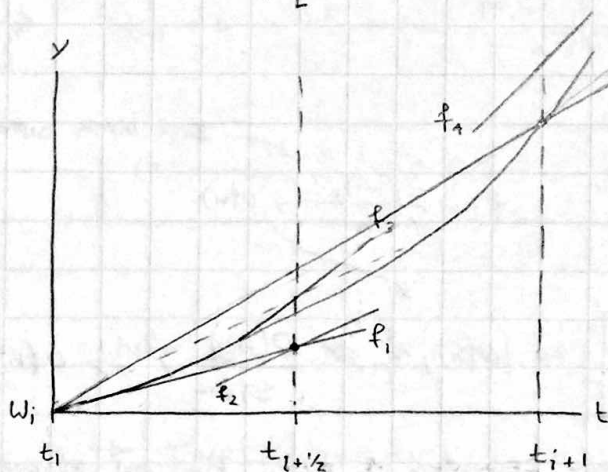
$$W_{i+1} = W_i + \frac{h}{6} [f_1 + 2(f_2 + f_3) + f_4]$$

WHERE $f_1 = f_i$

$$f_2 = f(W_i + \frac{h}{2}f_1, t_{i+1/2})$$

$$f_3 = f(W_i + \frac{h}{2}f_2, t_{i+1/2})$$

$$f_4 = f(W_i + hf_3, t_{i+1})$$



$$f_5 = \frac{f_1 + 2f_2 + 2f_3 + f_4}{6}$$

SAFE & STABLE METHOD (FOR
 SINGLE STEP)

- FOR SINGLE STEP METHODS, WE DO NOT USE ANY INFORMATION ABOUT
 THE RATE FUNCTION @ PREVIOUS STEPS: t_{i-1}, t_{i-2}, \dots

* MULTI-STEP METHODS:

- USE PAST INFORMATION ABOUT RATE FUNCTION
- MORE RISKY & LIKELY TO GO UNSTABLE

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INSTEAD USE f_i, f_{i-1}, f_{i-2} ETC. TO APPROX. f', f'' , ETC.

IF WE USE f_{i+1} (EQ. TRAPEZOIDAL METHOD) THEN WE HAVE TO FIGURE OUT w_{i+1} IN $f()$

THESE METHODS ARE NOT SELF STARTING \rightarrow MUST USE A SINGLE STEP METHOD TO GET STARTED.

FOR N STEP METHOD, MUST TAKE N-1 STEPS W/ A SINGLE STEP METHOD

* ADAMS METHODS

- ADAMS - BASHFORTH METHODS: "OPEN" OR EXPLICIT METHODS DO NOT INCLUDE f_{i+1}
- ADAMS - MOULTON METHOD: "CLOSED" OR IMPLICIT METHODS DO INCLUDE f_{i+1}

$$y_{i+1} = y_i + hf_i + \frac{h^2}{2} f'_i + \frac{h^3}{3!} f''_i + \dots$$

APPROXIMATE DERIVATIVES W/ $f_{i+1}, f_i, f_{i-1}, f_{i-2}$

A-B

A-M

- ADAMS - BASHWORTH 2-STEP

$$y_{i+1} = y_i + hf_i + \frac{h^2}{2} f'_i + \frac{h^3}{3!} f''_i$$

$$f'_i = \frac{f_i - f_{i-1}}{h} + O(h)$$

BACKWARDS DIFFERENCE

$$w_{i+1} = w_i + h \left[\frac{3}{2} f_i - \frac{1}{2} f_{i-1} \right]$$

$$[O(h)] h^2 \rightarrow \frac{O(h^3)}{\text{STEP}} \checkmark \rightarrow O(h^2) \text{ GLOBALY}$$

ONLY REQUIRES 1 RATE FUNCTION EVALUATION

$$w_{i+2} = w_{i+1} + h \left[\frac{3}{2} f_{i+1} - \frac{1}{2} f_i \right]$$

- A-B 3 STEP:

3 POINTS TO APPROXIMATE $\rightarrow \left. \begin{matrix} f' \sim O(h^2) \\ f'' \sim O(h) \end{matrix} \right\} \rightarrow \text{EXPECT } \frac{O(h^4)}{\text{STEP}} \Rightarrow \frac{O(h^3)}{\text{GLOBAL}}$

$$w_{i+1} = w_i + \frac{h}{12} [23f_i - 16f_{i-1} + 5f_{i-2}]$$

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$$y_{i+h} = y_i + hf_i + \frac{h^2}{2} f'_i + \frac{h^3}{3!} f'' + \dots$$

- ADAMS MOULTON METHODS INVOLVE f_{i+1} , SO WE CAN USE CENTERED DIFFERENCES TO APPROXIMATE THE DERIVATIVES

IE, f' TO $O(h^2)$ w/ ONLY TWO STEPS

- 2 STEP METHOD'S

t_{i-1} t_i t_{i+1} WE CAN DO CENTER DIFF. APPROXIMATIONS TO f' & f''

$$\frac{h^2}{2} f'_i \rightarrow \frac{h^2}{2} \left[\frac{f_{i+1} - f_{i-1}}{2h} + O(h^2) \right]$$

$$\frac{h^3}{3!} f''_i \rightarrow \frac{h^3}{6} \left[\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + O(h^2) \right]$$

EXPECT $O(h^4)$

$$w_{i+1} = w_i + hf_i + \frac{h^2}{2} \left[\frac{f_{i+1} - f_{i-1}}{2h} \right] + \frac{h^3}{6} \left[\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \right]$$

ADAMS MOULTON
2-STEP

$$w_{i+1} = w_i + \frac{h}{12} [5f_{i+1} + 8f_i - f_{i-1}]$$

$$\text{LTE} = -\frac{h^4}{24} f'''(y_i, \xi_i) \quad \xi \in [t_{i-1}, t_{i+1}]$$

WHAT ABOUT $f_{i+1} = f(w_{i+1}, t_{i+1})$?

→ TWO POSSIBILITIES:

1) y APPEARS LINEARLY IN $f(y, t)$

I.E. $y' = -y + t + 1 \rightarrow$ THEN y_{i+1} IS NO PROBLEM

USING A A-M 2 STEP

$$w_{i+1} = w_i + \frac{h}{12} [5(-w_{i+1} + t_{i+1} + 1) + 8(-w_i + t_i + 1) + (-w_{i-1} + t_{i-1} + 1)]$$

SOLVE FOR w_{i+1}

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$$\left(1 + \frac{5h}{12}\right) w_{i+1} = w_i + \frac{h}{12} \left[5(t_{i+1} + 1) + 8f_i - f_{i-1} \right]$$

↳ EXPLICIT SOLUTION

2. y APPEARS NON-LINEAR IN $f(y, t)$

IE. $y' = \cos(y) + t$

$$w_{i+1} = w_i + \frac{h}{12} \left[5(\cos(w_{i+1}) + t_{i+1}) + 8f_i - f_{i-1} \right]$$

↳ NOT POSSIBLE TO COMBINE w_{i+1} TO GET EXPLICIT SOLUTION

INSTEAD WE MUST PREDICT w_{i+1} AND CORRECT w / THE METHOD

WHICH LEADS TO THE "PREDICTOR / CORRECTOR" SCHEME

ACTUALLY DID THIS ALREADY W/ MODIFIED EULER METHOD.

$$w_{i+1} = w_i + \frac{h}{2} [f_i + f_{i+1}], \quad f_{i+1} = f(w_{i+1}, t_{i+1})$$

→ A-B/A-M 2 STEP P/C

ALL JUST
WEIGHTED AVERAGES
OF RATE FUNCTIONS

$$\hat{w}_{i+1} = w_i + \frac{h}{2} (3f_i - f_{i-1}) \quad (\text{PREDICTOR}) \rightarrow O(h^2) \text{ OVERALL}$$

$$w_{i+1} = w_i + \frac{h}{12} \left[5f(\hat{w}_{i+1}, t_{i+1}) + 8f_i - f_{i-1} \right]$$

↑ USE A PREDICTOR NO MORE THAN ONE
ORDER OF h LOWER

CAN CORRECT MORE THAN ONCE (ITERATE THE PROCESS)

ITERATION
INDEX

$$\rightarrow w_{i+1}^{k+1} = g(w_{i+1}^k) \quad \text{w/ } w_{i+1}^0 \text{ COMING FROM THE PREDICTOR}$$

$g(w_{i+1}^k)$ IS THE RHS OF w_{i+1}^{k+1} : THE CORRECTOR

- IN MOST CASES, ITERATION IS BETTER SPENT ON SMALLER
STEP SIZE.

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- IF WE DO ITERATE, THEN CONVERGENCE TO w_{i+1}

$$|g'(w_{i+1})| < 1$$

EG. 2-STEP A-B/A-M P/C:

$$|g'(w_{i+1})| = \left| \frac{\partial g}{\partial y} \right| = \left| \frac{5h}{12} \frac{\partial f}{\partial y} \right|_{w_{i+1}} < 1$$

J = JACOBIAN

PROBLEMS CAN OCCUR WHEN J IS LARGE, REQUIRES SMALL h

* KNOWN AS "STIFF" PROBLEMS.

→ NEWTON'S METHOD:

- REWRITE $g(w_{i+1}^k) = w_{i+1}^{k+1}$ AS $F(w_{i+1}) = 0$

$$F(w_{i+1}) = w_{i+1} - \left\{ w_i + \frac{h}{12} [5f(w_{i+1}, t_{i+1}) + 8f_i - f_{i-1}] \right\} = 0$$

$$F(z) = 0 \quad \text{WHERE } z = w_{i+1}$$

$$z^{k+1} = z^k - \frac{F(z^k)}{F'(z^k)}$$

$$w_{i+1}^{k+1} = w_{i+1}^k - \frac{w_{i+1}^k - \left\{ w_i + \frac{h}{12} [5f(w_{i+1}^k, t_{i+1}) + 8f_i - f_{i-1}] \right\}}{1 - \frac{5h}{12} \frac{\partial f}{\partial y} \Big|_{w_{i+1}^k}}$$

↳ CONVERGES QUADRATICALLY TO w_{i+1} , BUT REQUIRES A GOOD GUESS

$$y' = -ky \rightarrow y = y_0 e^{-kt}, \quad \frac{\partial f}{\partial y} = -k$$

SYSTEMS OF ODES

- M 1ST ORDER ODES IN M VARIABLES AND t

$$\frac{dz}{dt} = f(z, t) \quad \text{WHERE } z = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix}$$

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$$f(\underline{z}, t) = \begin{bmatrix} f_1(z_1, z_2, \dots, z_m, t) \\ f_2(z_1, z_2, \dots, z_m, t) \\ \vdots \\ f_m(z_1, z_2, \dots, z_m, t) \end{bmatrix}$$

M ELEMENT
COLUMN VECT.

$$\underline{z}_0 = \begin{bmatrix} z_1(0) \\ z_2(0) \\ \vdots \\ z_m(0) \end{bmatrix}$$

EXPLICIT METHODS ARE EASY

EQ. FOR $i=1:N$

$$t_i = t_0 + i \cdot h$$

$$w_i = w_{i-1} + h \cdot f(w_{i-1}, t_{i-1})$$

END.

FOR $j=1:M$

$$z_j(t_i) = z_j(t_{i-1}) + h \cdot f_j(\underline{z}(t_{i-1}), t_{i-1})$$

END

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* SYSTEMS OF ODE'S

- M 1ST ORDER ODE'S IN M VARIABLES & t

$$\frac{d\underline{z}}{dt} = \underline{f}(\underline{z}, t); \underline{z}_0 \rightarrow \text{WANT } \underline{z}(t_i)$$

→ EXPLICIT: EASY (LOOP)

→ IMPLICIT: PREDICT ALL THEN CORRECT ALL

HIGHER ORDER ODE'S:

$$y'' = f(y, y', t) \quad w/ \quad y'(0) = y_0' \quad ; \quad y(0) = y_0$$

↳ WRITE AS A SYS. OF FIRST ORDER ODE'S ; SOLVE USING ANY METHOD.

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WRITE AS A SYSTEM OF FIRST ORDER ODES

$$\begin{aligned} z_1(t) &= y(t) & z_2(t) &= y'(t) \\ z_1'(t) &= y'(t) & z_2'(t) &= y''(t) \end{aligned}$$

$$\begin{aligned} &\vdots \\ z_m(t) &= y^{(m)}(t) = z_{m-1}'(t) \rightarrow y^{(m)}(t) = z_m'(t) = f(z_1, z_2, \dots, z_{m-1}, t) \end{aligned}$$

w/ I.C.S:

$$z_1(0) = y_0$$

$$z_2(0) = y_0'$$

\vdots

$$z_m(0) = y_0^{m+1}$$

→ IN VECTOR NOTATION:

$$\begin{bmatrix} z_1'(t) \\ z_2'(t) \\ \vdots \\ z_m'(t) \end{bmatrix} = \begin{bmatrix} z_2(t) \\ z_3(t) \\ \vdots \\ f(z_1, z_2, \dots, z_m, t) \end{bmatrix} \quad \text{w/ I.C. } z_0 = \begin{bmatrix} z_1(0) \\ z_2(0) \\ \vdots \\ z_m(0) \end{bmatrix}$$

EX. FIND $y(t_i)$

$$\text{GIVEN } y'' + 4y' + 5y = 0; \quad y(0) = 3 \\ y'(0) = 5$$

$$\left. \begin{aligned} z_1(t) &= y(t) \\ z_2(t) &= y'(t) \end{aligned} \right\} \rightarrow \begin{cases} z_1'(t) = z_2(t) \\ z_2'(t) = -4z_2(t) - 5z_1(t) \\ z_1(0) = 3; \quad z_2(0) = 5 \end{cases} \quad \leftarrow \text{SOLVE USING EULER'S METHOD}$$

TIME STEP

$$z_1^{i+1} = z_2^i + h f_1^i = z_1^i + h z_2^i$$

$$z_2^{i+1} = z_2^i + h f_2^i = z_2^i + h(-4z_2^i - 5z_1^i)$$

$$\boxed{\begin{aligned} z_1^{i+1} &= z_1^i + h z_2^i \\ z_2^{i+1} &= z_2^i(1-4h) - 5h z_1^i \end{aligned}}$$

→ SOLUTION

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* STABILITY

- RECALL EULER'S METHOD:

$$\xi_{i+1} = \underbrace{(1 + hJ_i)}_{\text{STABILITY DEPENDS ON } J_i \text{ (AMPLIFICATION FACTOR)}} \xi_i + \frac{h^2}{2} f''(\xi)$$

ERROR HAS BOTH A TRUNCATION COMPONENT & A PROPAGATING COMPONENT

- ASSUME ODE IS ANALYTICALLY STABLE (SECTION 5.1) $\rightarrow J \leq 0$

- 3 IDEAS ABOUT SOLUTIONS

i. DOES THE DIFFERENCE EQUATION APPROACH THE ODE AS $h \rightarrow 0$? I.E. $\lim_{h \rightarrow 0} \text{LTE} = 0$ (CONSISTENCY)

- FOR ODE METHODS STUDIED, ALL ARE BASED ON TAYLOR EXPANSIONS, SO THIS IS ALWAYS THE CASE (h IN NUMERATOR) OF LOCAL TRUNCATION ERROR.

ii. DO ERRORS ONCE INTRODUCED REMAIN BOUNDED OR GROW EXPONENTIALLY? I.E. $|\lambda| \leq 1$? (STABILITY)

iii. DOES THE NUMERICAL SOLUTION APPROACH THE EXACT SOLUTION AS $h \rightarrow 0$? (CONVERGENCE)

- THIS IS REALLY WHAT WE WANT TO KNOW

- HARD TO PROVE THEORETICALLY.

EQUIVALENCE THEOREM: A NECESSARY & SUFFICIENT CONDITION FOR CONVERGENCE IS CONSISTENCY & STABILITY.

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- NOTE THAT STABILITY DOES NOT GUARENTEE ACCURACY.
- LOOK AT STABILITY OF VARIOUS METHODS
 - NOTE THAT STABILITY DEPENDS ON
 - STEP SIZE
 - SOLUTION FAMILY (J)
 - NUMERICAL METHOD (LTE)

BACKWARD EULER METHOD:

$$w_{i+1} = w_i + h f_{i+1}, \text{ COMES FROM EXPANDING } I(t) = \int_t^{t_{i+1}} f dt \text{ AROUND } t_{i+1}$$

$$E_{i+1} = (1 - hJ_{i+1})^{-1} E_i + O(h^2) \text{ (IMPLICIT)}$$

- GIVEN AN ANALYTICALLY STABLE ODE ($J \leq 0$), THE AMPLIFICATION FACTOR IS ≤ 1 FOR ANY $h > 0$

↳ UNCONDITIONALLY STABLE METHOD (GREAT FOR STIFF PROBLEM)

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TRAPEZOIDAL RULE METHOD:

- CAME FROM

$$\int_{t_i}^{t_{i+1}} f dt \approx \frac{h}{2} [f_i + f_{i+1}] + O(h^3)$$

- CAN SHOW:

$$E_{i+1} = \left(\frac{1 + \frac{h}{2} J_i}{1 - \frac{h}{2} J_{i+1}} \right) E_i + O(h^3)$$

IF $J \leq 0 \rightarrow$ ANALYTICALLY STABLE ODE

THEN THE AMPLIFICATION FACTOR IS ≤ 1 FOR ANY $h > 0$

↳ UNCONDITIONALLY STABLE

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ORDER (LTE) IS BETTER THAN BACKWARD EULER

BUT FOR STIFF PROBLEMS, AMPLIFICATION $\rightarrow 1$

- FOR OTHER METHODS IT GETS MORE DIFFICULT TO EXPRESS ϵ_{i+1} IN TERMS OF J .

- INSTEAD, CHOOSE A PROTOTYPE PROBLEM THAT CAN BE ANALYZED AND EXTRAPOLATE THE FINDINGS TO THE GENERAL CASE

"PROTOTYPE"

$$y' = -ky, \quad y(0) = y_0 \quad \rightarrow \quad \text{SOLUTION: } y(t) = y_0 e^{-kt}$$

$$\frac{\partial f}{\partial y} = -k = J$$

- TRAPEZOIDAL EULE

$$w_{i+1} = w_i + \frac{h}{2} [f_i + f_{i+1}]$$

\rightarrow EULER'S METHOD: $f_{i+1} = f(w_i + hf_i, t_{i+1})$

$$f_i = f(w_i, t_i) = -kw_i$$

$$f_{i+1} = f(w_{i+1}, t_{i+1}) = f(w_i + hf_i, t_{i+1}) = -k(w_i + hf_i) = -k(w_i + h(-kw_i))$$

$$w_{i+1} = w_i + \frac{h}{2} [-kw_i + -k(w_i + h(-kw_i))] = w_i - \frac{hk}{2} w_i - \frac{hk}{2} w_i + \frac{h^2 k^2}{2} w_i$$

$$w_{i+1} = w_i \left[1 - hk + \frac{(hk)^2}{2} \right]$$

NEED THIS TO BE < 1 . SINCE $w_{i+1} \rightarrow 0$ AS $t_{i+1} \rightarrow \infty$

A.) TURNS OUT TO BE THE AMPLIFICATION FACTOR

\rightarrow I.E. THIS ERROR PROPAGATES (BEHAVES) THE SAME WAY AS THE SOLUTION

B.) THIS TURNS OUT TO BE THE FIRST 3 TERMS IN THE T-EXPANSION OF THE EXACT SOLUTION TO THE PROTOTYPE PROBLEM. (RK 4 PRODUCES THE 1ST 5 TERMS)

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$$y_{i+h} = y_0 e^{-kt_{i+h}} = y_0 e^{-k(t_i+h)} = y_0 e^{-kt_i} e^{-kh}$$

$$y_i = y_0 e^{-kt_i}$$

$$\frac{y_{i+h}}{y_i} = e^{-kh} = \underbrace{1 - kh + \frac{(kh)^2}{2}}_{\text{RK2}} - \frac{(kh)^3}{3!} + \frac{(kh)^4}{4!} + \dots$$

RK4

$$\begin{aligned} y_{i+h} &= y_i + hf_i + \frac{h^2}{2} f_i' + \frac{h^3}{3} f_i''(s) \\ &= y_i + hf_i + \frac{h^2}{2} \left[\frac{\partial f_i}{\partial t} + \frac{\partial f_i}{\partial y} f_i \right] + \frac{h^3}{3!} f_i''(s) \end{aligned}$$

→ PROTOTYPE PROBLEM ←

$$\frac{\partial f}{\partial t} = 0; \quad \frac{\partial f}{\partial y} = -k; \quad f_i = -ky$$

$$y_{i+h} = y_i - hky_i + \frac{(hk)^2}{2} y_i + \frac{h^3}{3} f_i''(s)$$

$$w_{i+h} = w_i - hk w_i + \frac{(hk)^2}{2} w_i \rightarrow \varepsilon_{i+h} = \varepsilon_i - hk \varepsilon_i + \frac{(hk)^2}{2} \varepsilon_i + \text{LTE}$$

STABILITY OF MULTI-STEP METHODS

- APPLY TO PROTOTYPE PROBLEM → DIFFERENCE EQUATION W/ CONST. COEFF.

EG. 4-STEP A-B

$$w_{i+1} = w_i + \frac{h}{24} [55f_i - 59f_{i-1} + 37f_{i-2} - 9f_{i-3}]$$

$$f_i = -kw_i, \quad f_{i-1} = -kw_{i-1} \rightarrow \text{GROUP TERMS:}$$

$$w_{i+1} = -\left(1 - \frac{55hk}{24}\right) w_i - \frac{59hk}{24} w_{i-1} - \frac{37hk}{24} w_{i-2} + \frac{9hk}{24} w_{i-3} = 0$$

SINCE ε_i BEHAVES LIKE w_i , $w_i \sim \lambda^i$

$$\lambda^4 - \left(-\frac{55hk}{24}\right) \lambda^3 - \frac{39hk}{24} \lambda^2 - \frac{37hk}{24} \lambda + \frac{9hk}{24} = 0$$

↳ NEED ALL 4 ROOTS ≤ 1 FOR STABILITY

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FOR QUADRATICS,

$$A\lambda^2 + B\lambda + C = 0 \quad w/ \quad A > 0$$

$$|\lambda| < 1 \quad \text{IFF} \quad \frac{C}{A} < 1 \quad \& \quad |B| < A + C$$

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BOUNDARY VALUE PROBLEMS

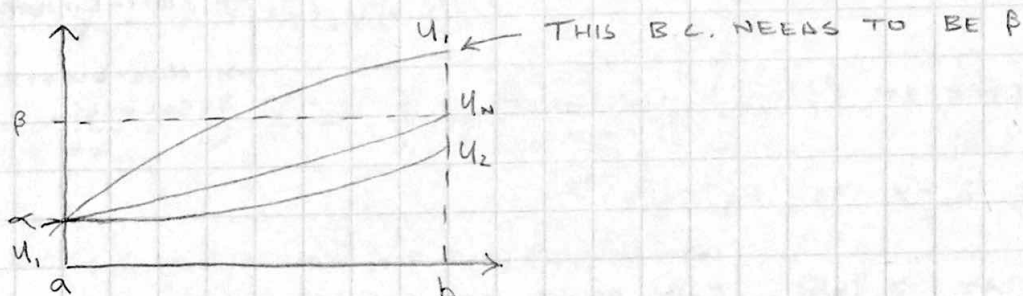
$y'' = f(x, y, y')$ \rightarrow WANT $y(x_i)$ FOR $a \leq x_i \leq b$

- GIVEN B.C.'S: $y(a) = \alpha$
 $y(b) = \beta$ } COULD SOLVE IF WE HAD $y'(a) = \gamma$

$\left. \begin{array}{l} z_1(x) = y \\ z_2(x) = y' \end{array} \right\} \rightarrow \begin{array}{l} z_1' = z_2 \\ z_2' = f(x, z_1, z_2) \end{array}$ w/ B.C.S $z_1(a) = \alpha, z_1(b) = \beta$
 $z_2(a) = ?$

SHOOTING METHOD:

- GUESS THE BOUNDARY CONDITION: $z_2(a) = \gamma$
- SOLVE FOR $z_1(x_i), z_2(x_i)$ ON $a \leq x_i \leq b$
- SEE IF $z_1(b) = \beta$, IF IT IS, THEN WE'RE DONE. IF NOT, THEN GUESS AGAIN



HOW TO UPDATE GUESS OF $\gamma = z_2(a) = y'(a)$?

- SIMPLE CASE

$f(x, y, y')$ IS LINEAR IN y, y' THEN WE ONLY NEED TWO GUESSES, WE CAN ALWAYS CONSTRUCT A LINEAR SOLUTION FROM A LINEAR COMBINATION OF LINEAR SOLUTIONS

$$z_1(x_i) = C_1 z_1(x_i, u_0) + C_2 z_1(x_i, u_1)$$

\rightarrow FIND C_1, C_2 AT B.C.S.

$$x=a: z_1(a) = \alpha = C_1 z_1(a, u_0) + C_2 z_1(a, u_1)$$

$$x=b: z_1(b) = \beta = C_1 z_1(b, u_0) + C_2 z_1(b, u_1)$$

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$$C_1 = \frac{\beta - z_1(b, u_1)}{z_1(b, u_0) - z_1(b, u_1)}$$

AND

$$C_2 = \frac{z_1(b, u_0) - \beta}{I(b, u_0) - z_1(b, u_0)}$$



$$\sum F_y = m\vec{a}_y = -m\vec{g}$$

$$m \frac{d^2y}{dt^2} = -mg$$

$$y'' = -g$$

LINEAR DIFF EQ

NON-LINEAR SOLUTION

$$\frac{d^2y}{dt^2} = g \Rightarrow \frac{dy}{dt} = gt + C_1$$

$$y = gt^2 + C_1t + C_2$$



$$\sum F_y = F_a - F_g = m\vec{a}$$

$$F_a = \frac{1}{2} \rho A v^2$$

$$F_g = m\vec{g}$$

$$\frac{1}{2} \rho A v^2 - m\vec{g} = m\vec{a}$$

$$\frac{1}{2} \rho A \left(\frac{dy}{dt}\right)^2 - m\vec{g} = m \frac{d^2y}{dt^2}$$

$$y'' = \frac{1}{2} \rho A y'^2 - mg$$

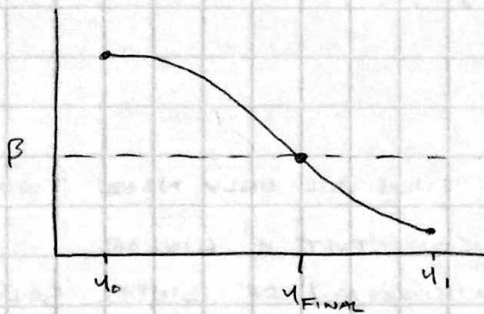
NON-LINEAR

NON-LINEAR SOLUTION

NOW LOOK AT $f(x, y, y')$ NON-LINEAR

WRITE $z_1 = y$ AS $z_1(x, u)$

LOOK AT $z_1(b, u)$; END POINT OF SOLUTION



THINK OF AS A ROOT FINDING PROBLEM

$$z_1(b, u) - \beta = 0$$

$$F(u) = 0$$

→ USE ANY OF THE ITERATIVE METHODS THAT WE KNOW TO FIND u_{FINAL}

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$u_1 = u_2 \rightarrow$
 $u_2 = u_3$

SECANT METHOD:



$$u_{N+1} = u_N - F(u_N) \left[\frac{u_N - u_{N-1}}{F(u_N) - F(u_{N-1})} \right]$$

- NEED TWO GUESSES, u_0, u_1
- CONVERGENCE IS SLOW, $\alpha = \frac{1+\sqrt{5}}{2}$
- FUNCTION EVALUATIONS COSTLY

NEWTON'S METHOD:

$$u_{N+1} = u_N - \frac{F(u_N)}{F'(u_N)} \leftarrow \frac{\partial}{\partial u}, \quad u_{N+1} = u_N - \frac{z_1(b, u_N) - \beta}{\frac{\partial z_1(b, u_N)}{\partial u}} \leftarrow \text{NEED THIS TERM}$$

\rightarrow DIFFERENTIATE ODE:

$$y'' = f(x, y(x, u), y'(x, u)) \rightarrow \frac{\partial}{\partial u}$$

$$\frac{\partial y''}{\partial u} = \frac{\partial f}{\partial x} \frac{dx}{du} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial u} + \frac{\partial f}{\partial y'} \frac{\partial y'}{\partial u}$$

\downarrow
 $= 0$

\rightarrow SWITCH ORDER OF DIFFERENTIATION

$$\left(\frac{\partial y}{\partial u} \right)' = \frac{\partial f}{\partial y} \frac{\partial y}{\partial u} + \frac{\partial f}{\partial y'} \left(\frac{\partial y}{\partial u} \right)' \quad \text{WHERE PRIME IS WITH RESPECT TO } x$$

RECALL,

$$z_1(x, u) = y, \text{ SO, } \frac{\partial y}{\partial u} = \frac{\partial z_1(x, u)}{\partial u} \leftarrow \text{WANT AT } x=b$$

$$g = g(x, u) = \frac{\partial z_1(x, u)}{\partial u}, \text{ WE WANT } g(b, u) = \frac{\partial z_1(b, u)}{\partial u}$$

$$g'' = \frac{\partial f}{\partial y} g + \frac{\partial f}{\partial y'} g'$$

10/30/2015

TO SOLVE FOR $g(b, u) = \frac{\partial z_1(b, u)}{\partial u}$ WE NEED $g(a)$; $g' \Rightarrow$ IVP

$$\text{SO } g(a, u) = \frac{\partial z_1(a, u)}{\partial u} = 0 ; z_1(a, u) = \alpha$$

$$g'(a, u) = \frac{\partial z_1'(a, u)}{\partial u} = 1 ; z_1'(a, u) = z_2(a) = \gamma$$

$$\left. \begin{array}{l} v_1 = g \\ v_2 = g' \end{array} \right\} \Rightarrow \begin{array}{l} v_1' = v_2 \\ v_2' = \frac{\partial f}{\partial y} v_1 + \frac{\partial f}{\partial y'} v_2 \end{array} \quad \begin{array}{l} v_1(a) = 0 \\ v_2(a) = 1 \end{array}$$

• SOLVE SYSTEM FOR $v_1(x_i)$, $v_2(x_i)$
 \hookrightarrow WANT $v_1(b) = g(b, u) = \frac{\partial z_1(b, u)}{\partial u}$

- PICK u_0

- SOLVE $y'' = f(x, y, y')$ w/ $y(a) = \alpha$
 $y'(a) = \gamma_0$

- SOLVE $g'' = \frac{\partial f}{\partial y} g + \frac{\partial f}{\partial y'} = g'$ w/ $g(a) = 0$
 $g'(a) = 0$

- REPEAT UNTIL $|z_1(b) - \beta| < \epsilon$

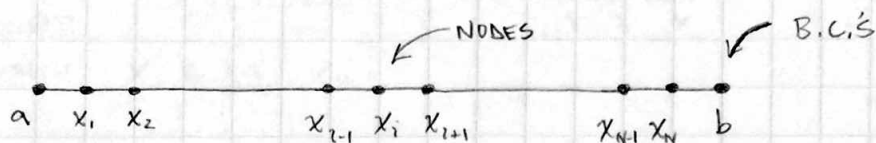
$$u_{N+1} = u_N - \frac{z_1(b, u_N) - \beta}{v_1(b, u_N)}$$

11/2/2015

* FINITE DIFFERENCE METHODS FOR BVP'S

IDEA: WRITE DOWN FINITE DIFFERENCE "APPROXIMATION" OF ODE AT SOME POINT x_i , WHERE $a \leq x_i \leq b$

- APPROXIMATE y' & y'' W/ FINITE DIFFERENCES
- MAKE APPROXIMATION AT AN INTERVAL OF NODES



LINEAR CASE.

$$y'' = f(x, y, y') = p(x)y'(x) + q(x)y(x) + r(x)$$

↑ LINEAR ↑

- WHERE $p(x), q(x), r(x)$ ARE KNOWN

- APPROXIMATE AT NODE i :

$$y_i'' = \frac{w_{i+1} - 2w_i + w_{i-1}}{h^2} \quad (\text{SECOND ORDER C.D. } O(h^2))$$

$$\frac{w_{i+1} - 2w_i + w_{i-1}}{h^2} - p(x) \left[\frac{w_{i+1} - w_{i-1}}{2h} \right] - q(x)w_i = r(x_i)$$

$$y_i'' - p(x)y_i' - q(x)y_i = r(x_i)$$

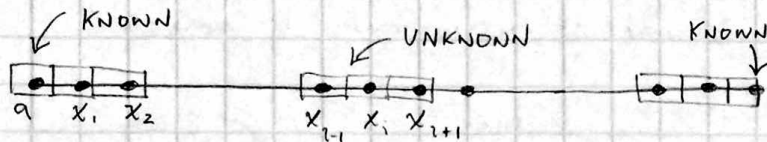
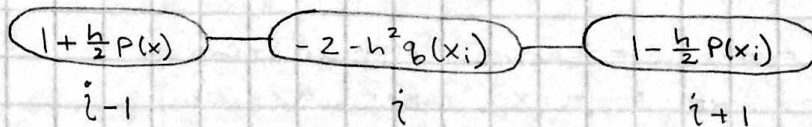
- GROUP TERMS:

$$\left[1 + \frac{h}{2} p(x_i) \right] w_{i-1} - \left[2 + h^2 q(x_i) \right] w_i + \left[1 - \frac{h}{2} p(x_i) \right] w_{i+1} = h^2 r(x_i)$$

↳ ONE EQUATION, 3 UNKNOWNNS → WRITE AS A FINITE DIFFERENCE MOLECULE

11/2/2015

- MOLECULE :



→ COUPLED SYSTEM OF N LINEAR EQUATIONS IN N UNKNOWN

→ WRITE IN MATRIX FORM :

$$\begin{bmatrix}
 -(2+h^2 q_0) & (1-\frac{h}{2} P_1) & 0 & 0 & \dots & 0 \\
 (1+\frac{h}{2} P_2) & -(2+h^2 q_2) & (1+\frac{h}{2} P_2) & 0 & \dots & 0 \\
 0 & (1+\frac{h}{2} P_3) & -(2+h^2 q_3) & (1+\frac{h}{2} P_3) & 0 & \dots & 0 \\
 0 & & & & & & \\
 \vdots & & & & & & \\
 \vdots & & & & & & \\
 \vdots & & & & & & \\
 0 & & & & & & (1+\frac{h}{2} P_N) & -2(h^2 q_N)
 \end{bmatrix}
 \begin{bmatrix}
 w_1 \\
 w_2 \\
 \\
 \\
 \\
 \\
 w_{N-1} \\
 w_N
 \end{bmatrix}
 = h^2
 \begin{bmatrix}
 r_1 \\
 r_2 \\
 \\
 \\
 \\
 \\
 r_{N-1} \\
 r_N
 \end{bmatrix}$$

↳ TRIAGONAL N X N SPARSE MATRIX

$$\begin{bmatrix}
 1 + \frac{h}{2} P_1 K \\
 0 \\
 \vdots \\
 0 \\
 (1 - \frac{h}{2} P_N) F
 \end{bmatrix}$$

SOLVE $y = w = A^{-1} b \rightarrow O(h^3)$
 $w = A b \rightarrow O(h)$

↳ NON-LINEAR CASE

11/2/2015

NON-LINEAR CASE:

- WRITE ODE AS $-y'' + f(x, y, y') = 0$

- APPROXIMATE:

$$-\left(\frac{w_{i+1} - 2w_i + w_{i-1}}{h^2}\right) + f\left(x_i, w_i, \frac{w_{i+1} - w_{i-1}}{2h}\right) = 0$$

FOR EACH $x_i \in [x_1, x_N]$

↳ SYSTEM OF NON-LINEAR EQUATIONS IN N UNKNOWN

$$-2w_1 - w_2 + h^2 f\left(x_1, w_1, \frac{w_2 - \alpha}{2h}\right) - \alpha = 0 ; F_1(x_1, \underline{w}) = 0$$

$$-w_1 + 2w_2 - w_3 + h^2 f\left(x_2, w_2, \frac{w_3 - w_1}{2h}\right) = 0 ; F_2(x_2, \underline{w}) = 0$$

\vdots

$$-w_{N-1} + 2w_N + h^2 f\left(x_N, w_N, \frac{\beta - w_{N-1}}{2h}\right) - \beta = 0 ; F_N(x_N, \underline{w}) = 0$$

↳ USE NEWTON'S METHOD FOR SYSTEMS OF EQUATIONS

- NEED \underline{w}_0

- AND $\underline{J}(x, \underline{w})$

* PARTIAL DIFFERENTIAL EQUATIONS:

- MORE THAN ONE VARIABLE (INDEPENDENT)

EQUATIONS:

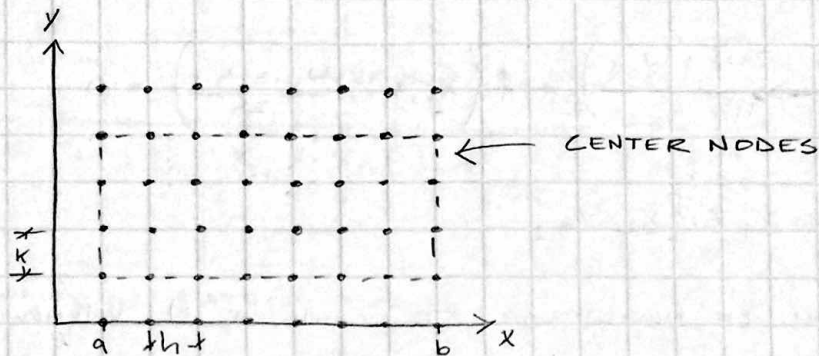
- $\nabla^2 u = f(x, y)$; POISSON'S EQUATION ← SOURCE TERM
- $\nabla^2 u = 0$; LAPLACE'S EQUATION

↳ IN 2D CARTESIAN $\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$

11/2/2015

- AS W/ ODE'S, APPROXIMATE DERIVATIVES W/ FINITE DIFFERENCES

USE i, j INDEXING



- SECOND CENTER DIFFERENCE

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} - \frac{h^2}{12} \frac{\partial^4 u}{\partial x^4}(x_i, y_j)$$

$$\frac{\partial^2 u}{\partial y^2} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} - \frac{k^2}{12} \frac{\partial^4 u}{\partial y^4}(x_i, y_j), \quad y \in [y_{j-1}, y_{j+1}]$$

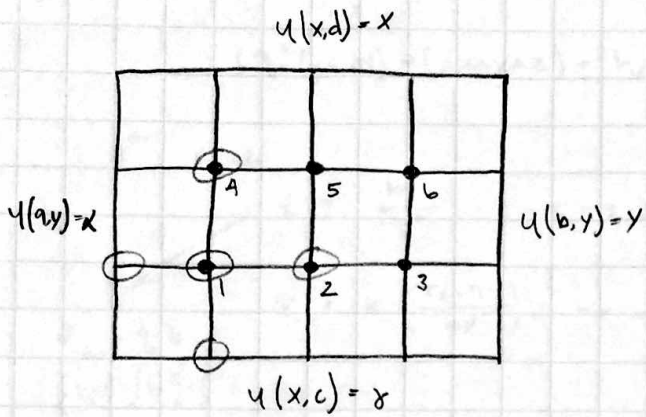
$$u_{i+1,j} + u_{i-1,j} + \beta(u_{i,j+1} + u_{i,j-1}) - (2 + 2\beta)u_{i,j} = 0 \quad (\text{LAPLACE EQ.})$$

$$\beta = \frac{h^2}{k^2}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} \quad ; \quad \frac{\partial^2 u}{\partial y^2} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2}$$

$$\beta = \frac{h^2}{k^2}$$

$$u_{i+1,j} + u_{i-1,j} + \beta(u_{i,j+1} + u_{i,j-1}) - 2(1 + \beta)u_{i,j} = 0 = h^2 f(x_i, y_j)$$



$$\begin{bmatrix}
 -4 & 1 & 0 & 1 & 0 & 0 \\
 1 & -4 & 1 & 0 & 1 & 0 \\
 0 & 1 & -4 & 0 & 0 & 1 \\
 1 & 0 & 0 & -4 & 1 & 0 \\
 0 & 1 & 0 & 1 & -4 & 1 \\
 0 & 0 & 1 & 0 & 1 & -4
 \end{bmatrix}
 \begin{bmatrix}
 u_1 \\
 u_2 \\
 u_3 \\
 u_4 \\
 u_5 \\
 u_6
 \end{bmatrix}
 =
 \begin{bmatrix}
 -x - x \\
 -x \\
 -x - (c+k) \\
 -x - (a+b) \\
 -(a+2h) \\
 -(a+3h) - (c+2k)
 \end{bmatrix}$$

TYPES OF PDES:

ELLIPTIC: LAPLACE, POISSONS

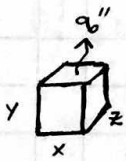
PROPAGATING: PARABOLIC, HYPERBOLIC

- DIFFUSION EQUATION

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} \quad \text{BVP w/ INITIAL CONDITIONS}$$

$$\frac{D \Delta t}{h^2} \leq \frac{1}{2}$$

STABILITY
CRITERIA



$$q'' A \Delta t = m h_f \rightarrow q'' A t = h_f$$

$$\left\{ \frac{W}{kg} m^2 \right\} = \{ \}$$

$$t q'' (\Delta x \Delta z) \rho (\Delta x \Delta y \Delta z) = h_f \rho (\Delta x \Delta y \Delta z) \rightarrow \underbrace{q'' \Delta x \Delta z t}_{L=1} = h_f$$

1ST CELL:

$$t = \frac{h_f}{q''} \quad \text{TIME TO FREEZE CELL}$$

$$Q_{out} = q'' t$$

$$\{KJ\} = \{W\} \{t\}$$

$$Q_{out} = -K \left(\frac{T_2 - T_1}{\Delta y} \right) t \rightarrow T_2 = \frac{q'' \Delta y}{-K t} + T_1$$

KNOWN (FREEZING TEMP)

+1 2ND CELL

$$T_3 = \frac{q'' \Delta y}{-K} + T_2, \quad T_2 =$$

$$Q_{COND} = \dot{q} t = h_f \rightarrow Q = q'' t = -K \left(\frac{T_2 - T_1}{\Delta y} \right) t \rightarrow \underline{T_2 = \text{KNOWN}}$$

$$Q_{COND} = -K \left(\frac{T_2 - T_1}{\Delta y} \right) t, \quad t_{FREEZE} = \frac{h_f}{q''_{COND}}$$

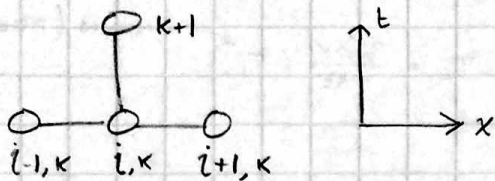
$$Q_{COND} = \frac{-K(T_2 - T_3)}{\Delta y} t \rightarrow T_3 = \text{KNOWN}$$

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* PDES

ELLIPTIC: $\nabla^2 u = 0$

PARABOLIC: $\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} \rightarrow$ FORWARD DIFFERENCE METHOD



$$u_i^{k+1} = u_i^k + \underbrace{\frac{D\Delta t}{h^2}}_{\lambda} (u_{i+1}^k - 2u_i^k + u_{i-1}^k) \rightarrow \text{EXPLICIT SOLUTION FOR I.V.P}$$

$u = Au + b$ WHERE,

DIFFERENT THAN LAPLACE EQ. SOLUTION

NOT AN IMPLICIT SOLUTION

$$A = \begin{bmatrix} 1-2\lambda & \lambda & 0 & 0 & 0 & \dots \\ \lambda & 1-2\lambda & \lambda & 0 & 0 & \dots \\ 0 & \lambda & 1-2\lambda & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \lambda & 1-2\lambda & 0 \end{bmatrix}$$

$$b = \begin{bmatrix} \lambda\alpha \\ 0 \\ 0 \\ 0 \\ \vdots \\ \lambda\beta \end{bmatrix}$$

STABILITY LIMIT:

$$\lambda \equiv \frac{D\Delta t}{h^2} \leq \frac{1}{2}$$

COMES FROM THE REQUIREMENT THAT THE SPECTRAL RADIUS OF A BE ≤ 1 , OR NORM OF THE LARGEST EIGENVALUE OF A , $|\lambda| \leq 1$

11/6/2015

HOW ABOUT A BACKWARD DIFFERENCE IN TIME

↳ FROM BACKWARD EULER INTEGRATION

$$w_{i+1} = w_i + h f_{i+1}$$

- RESULTS IN A FLIPPED TEMPLATE:

$$y_i^{k+1} - y_i^k = \frac{\Delta t}{h^2} (y_{i+1}^{k+1} - 2y_i^{k+1} + y_{i-1}^{k+1})$$

$$\left. \begin{matrix} -\lambda & & & \\ & 1+2\lambda & & \\ & & -\lambda & \\ & & & \lambda \end{matrix} \right\} \text{IMPLICIT SOLUTION}$$

$$\underline{Ay}^{k+1} = -y^k + b$$

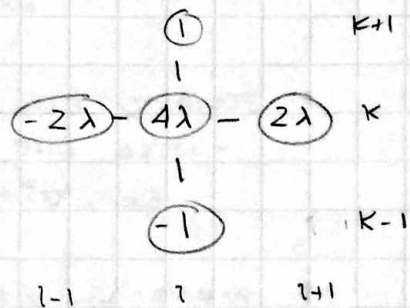
↑
N x N TRIAGONAL MATRIX

- SOLUTION IS "TIED" TOGETHER IN SPACIAL COORDINATES
- UNCONDITIONALLY STABLE METHOD, BUT STILL ONLY $O(\Delta t + h^2)$
- COMPUTATIONALLY EXPENSIVE → MUST SOLVE A LINEAR SYS. @ EACH TIME STEP.

TO MAKE TIME STEP MORE ACCURATE, TRY CENTER DIFF.

$$\frac{y_i^{k+1} - y_i^{k-1}}{2\Delta t} = \frac{D}{h^2} [y_{i+1}^k - 2y_i^k + y_{i-1}^k]$$

→ UNCONDITIONALLY UNSTABLE



- CALLED THE LEAPFROG SCHEME

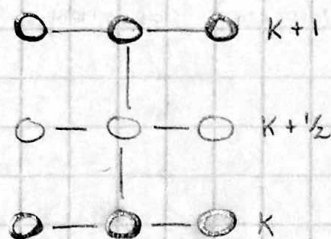
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INSTEAD APPROXIMATE PDE AT $x_i, t_{k+1/2}$: (PDE) ^{$k+1/2$}

$$\frac{u_i^{k+1} - u_i^k}{\Delta t} = D \frac{(u_{i+1}^{k+1/2} - 2u_i^{k+1/2} + u_{i-1}^{k+1/2}))}{h^2}$$

HOW TO GET $u^{k+1/2}$? \rightarrow AVERAGE $\Rightarrow u^{k+1/2} = \frac{u^k + u^{k+1}}{2}$

$$u_i^{k+1} - u_i^k = \frac{D \Delta t}{2h^2} \left\{ [u_{i+1}^k - 2u_i^k + u_{i-1}^k] + [u_{i+1}^{k+1} - 2u_i^{k+1} + u_{i-1}^{k+1}] \right\}$$



CRANK-NICHOLSON SCHEME

$$\rightarrow AU^{k+1} = BU^k + b$$

\rightarrow MATRIX SOLUTION @ EACH TIME STEP, BUT UNCOND. STABLE W/ $O((\Delta t)^2 + h^2)$

* BOUNDARY CONDITIONS

- TYPE 1, OR 'DIRICHLET' B.C'S. VALUE IS GIVEN $u(x) = \alpha$

- TYPE 2, OR 'NEUMANN' BC'S. DERIVATIVE IS GIVEN $\frac{\partial u(x)}{\partial x} = \alpha$

- TYPE 3, MIXED OR 'CAUCHEY'. LINEAR COMBO OF TYPE 1, 2'S

$$a u(x) + b \frac{\partial u}{\partial x} = \beta$$

• ELLIPTIC EQ'S

- NEED ONE B.C (I, II, III) EVERYWHERE ON CLOSED BOUNDARY

EG. $\nabla^2 = 0$

• PARABOLIC EQ

- NEED ONE I.C, TWO B.C'S (I, II, III)

EG. $\frac{\partial u}{\partial t} = D \nabla^2 u$

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* LINEAR ALGEBRA

CHAPTER 6, DIRECT SOLUTIONS TO LINEAR ALGEBRAIC SYSTEMS

LOOKING FOR DIRECT SOLUTIONS OF ALGEBRAIC SYSTEMS, EXACT ANSWERS (NOT ACCOUNTING FOR ROUND-OFF ERROR) IN A FINITE # OF STEPS

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

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

SOLUTION STRATEGY: MAKE AN UPPER TRIANGULAR MATRIX THEN SOLVE USING BACKSUBSTITUTION TO SOLVE FOR x .

$$\begin{bmatrix} \tilde{a}_{11} & \tilde{a}_{12} & \dots & \tilde{a}_{1n} \\ 0 & \tilde{a}_{22} & \dots & \tilde{a}_{2n} \\ 0 & 0 & \tilde{a}_{33} & \tilde{a}_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \tilde{a}_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} \tilde{b}_1 \\ \tilde{b}_2 \\ \tilde{b}_3 \\ \vdots \\ \tilde{b}_n \end{bmatrix} \quad \begin{array}{l} \text{EQUIVALENT SYSTEM} \\ \text{OF EQUATIONS} \end{array}$$

$$x_n = \frac{\tilde{b}_n}{\tilde{a}_{nn}}$$

$$x_{n-1} = \frac{(\tilde{b}_{n-1} - \tilde{a}_{n-1,n} x_n)}{\tilde{a}_{n-1,n-1}} \quad \text{JUST SOLVED FOR!}$$

$$x_i = \left(b_i - \sum_{j=i+1}^n \tilde{a}_{ij} x_j \right) / a_{ii} \quad \text{FOR EACH } i = n-1, n-2, \dots$$

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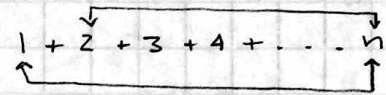
GAUSSIAN ELIMINATION W/ BACK SUBSTITUTION

STEP 1: ELIMINATION

STEP 2: BACK SUBSTITUTION

ON COMPUTERS:

$$T_{MULT} \sim T_{DIV} \gg T_{ADD}, T_{SUB}$$



$$(n+1)(n+1) \rightarrow \frac{n}{2}(n+1) \rightarrow O(n^2)$$

• DEFINE $R_j \equiv \text{ROW } j$ (E_j)

$$R_j - \frac{a_{ji}}{a_{ii}} R_i \rightarrow R_j$$

"PIVOT ELEMENT"

$j = \text{ROW}$
 $i = \text{COLUMN}$

FOR EACH $i = 1, 2, 3, \dots, N-1$ (EACH COLUMN)

$j = i+1, i+2, \dots, n$ (EACH ROW BELOW MASTER ROW)

↳ UPPER TRIANGULAR MATRIX (ASSUMING ALL PIVOTS $a_{ii} \neq 0$)

$i=1$: COLUMN 1

$$j=2: R_2 - \frac{a_{21}}{a_{11}} R_1 \rightarrow R_2: a_{21} = 0$$

$$j=3: R_3 - \frac{a_{31}}{a_{11}} R_1 \rightarrow R_3: a_{31} = 0$$

$A \rightarrow \tilde{A}$ WHERE \tilde{A} IS THE UPPER TRIANGULAR MATRIX.

EXAMPLE

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

$$3x_1 - 3x_2 + 9x_3 = 0$$

$$3x_1 + 3x_2 + 5x_3 = 4$$

$$\begin{bmatrix} 2 & -1 & 1 \\ 3 & 3 & 9 \\ 3 & 3 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 4 \end{bmatrix}$$

$$\underline{A} \quad \underline{x} = \underline{b}$$

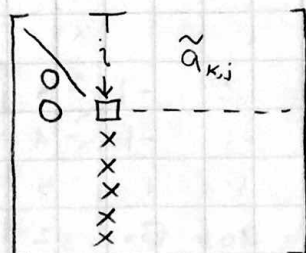
↳ FORM AUGMENTED MATRIX

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$$\left[\begin{array}{ccc|c} 2 & -1 & 1 & -1 \\ 3 & 3 & 9 & 0 \\ 3 & 3 & 5 & 4 \end{array} \right]$$

A b

ESTIMATE # OF OPERATIONS FOR GAUSSIAN ELIMINATION



$$R_j = \frac{a_{ji}}{a_{ii}} R_i \rightarrow R_j \quad \text{FOR } j = i+1 \dots n$$

NEED: $(n-i+1)$ MULTIPLIES PER M_j FOR $n-i$

$$\sum_{i=1}^{n-1} (n-i)(n-i+1) = \frac{2n^3 + 3n^2 - 5n}{6} \rightarrow O(n^3)$$

* PIVOTING STRATEGIES IN GAUSSIAN ELIMINATION

- IF THE PIVOT ELEMENT IS ZERO, THE ALGORITHM FAILS

$$M_{ji} = \infty$$

- THE 'FIX' IS TO INTERCHANGE "MASTER" ROW w | ANOTHER THAT DOESN'T HAVE $a_{ij} = 0$

$$\left[\begin{array}{cccc|c} 1 & -1 & 2 & -1 & -8 \\ 2 & -2 & 3 & -3 & -20 \\ 1 & 1 & 1 & 0 & -2 \\ 1 & 3 & 4 & 7 & -4 \end{array} \right] \xrightarrow{\text{AFTER 1st COL.}} \left[\begin{array}{cccc|c} 1 & -1 & 2 & -1 & -8 \\ 0 & 0 & -1 & -1 & -4 \\ 0 & 2 & -1 & 1 & 6 \\ 0 & 4 & 2 & 8 & 12 \end{array} \right]$$

↕ SWAP ALWAYS PICK A ROW BELOW

IN FINITE PRECISION COMPUTING, UNLIKELY TO HIT 0 EXACTLY, SO WE WATCH FOR SMALL NUMBERS

$$R_j - \frac{a_{ji}}{a_{ii}} R_i \rightarrow R_j$$

↖ SMALL

HOW TO DECIDE ON WHICH ROW TO EXCHANGE?

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* PRACTICAL PIVOTING - TAKE MAXIMUM

- COEFFICIENT IN COLUMN AS THE NEW POINT

$$\left[\begin{array}{cccc|c} 1 & -1 & 2 & -1 & -8 \\ 0 & \boxed{0} & -1 & -1 & -4 \\ 0 & 2 & -1 & 1 & 6 \\ 0 & \boxed{4} & 2 & 8 & 12 \end{array} \right]$$

ENSURES ALL $|m_{ji}| < 1 \rightarrow$ NO ERROR AMPLIFICATION
 \downarrow
 $O(h^2)$

11/11/2015

* MATRIX FACTORIZATION

\rightarrow $\underline{A} \underline{x} = \underline{b}$
 $N \times N$
 $\underline{A} = \underline{L} \cdot \underline{U}$

$\underline{L} = \begin{bmatrix} \text{shaded triangle} & 0 \\ 0 & \text{shaded triangle} \end{bmatrix}$ $\underline{U} = \begin{bmatrix} \text{shaded triangle} \\ 0 & \text{shaded triangle} \end{bmatrix}$

$\underline{L} \underline{U} \underline{x} = \underline{b}$

L U DECOMPOSITION

$\underline{y} \rightarrow \underline{L} \underline{y} = \underline{b}$ FS. $O(h^2)$
 $\underline{U} \underline{x} = \underline{y}$ BS. $O(h^2)$

$\sum_{k=i}^{\min(i,j)} l_{ik} u_{kj} = a_{ij}$

$\underline{L} \underline{U} = \underline{A}$

11/11/2015

* CROUT LU DECOMPOSITION

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

START W/ FIRST COLUMN OF \underline{L} , EVERY ROW OF \underline{L} BY COLUMN 1 OF \underline{U} $\rightarrow l_{i1} = a_{i1}$

THEN FIRST ROW OF \underline{U} * FIRST ROW OF \underline{L} TIMES COLUMNS THROUGH N OF \underline{U}

$$u_{1j} = \frac{a_{1j}}{l_{11}}$$

SECOND COLUMN OF \underline{L} :

- ROWS 2-N OF \underline{L} TIMES COLUMN 2 OF \underline{U}

$$- l_{i2} = a_{i2} - l_{i1} u_{12}$$

SECOND ROW OF \underline{U}

- ROW 2 OF \underline{L} BY COLUMNS 3-N OF \underline{U}

$$\rightarrow u_{2j} = (a_{2j} - l_{21} u_{1j}) / l_{22}$$

$$\underline{L}_{\text{DOOLITTLE}} = \underline{U}_{\text{CROUT}}^T, \quad \underline{U}_{\text{DOOLITTLE}} = \underline{L}_{\text{CROUT}}^T$$

* COMPUTING AN INVERSE OF A MATRIX: A^{-1}

TO $\underline{A}\underline{x} = \underline{b}$, $\underline{x} = \underline{A}^{-1}\underline{b}$ \rightarrow DO NOT DO THIS IF ONLY WANT SOLUTION

IN PRACTICE, A^{-1} IS DETERMINED BY SOLVING $\underline{A}\underline{x} = \underline{b}$ FOR MULTIPLE \underline{b} 'S, WHERE \underline{b} 'S ARE COLUMNS OF \underline{I}

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$$A = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & 0 \\ -1 & 1 & 2 \end{bmatrix}; \quad \text{SOLVE } \underline{Ax} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \underline{Ay} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \underline{Az} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\underline{A^{-1}} = \left[\begin{bmatrix} x \\ y \\ z \end{bmatrix} \right] \rightarrow \underline{Ay} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}; \quad \underline{y} = A^{-1} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} x \\ x \\ x \end{bmatrix}$$

BETTER TO USE LU DECOMPOSITION, ONLY DECOMPOSE ONCE, $O(n^3)$

* COMPUTING DETERMINATE OF A MATRIX

$$\text{DET}(A) = \text{DET}(LU) = \text{DET}(L) \cdot \text{DET}(U)$$

FOR UPPER ; LOWER TRIANGULAR MATRICES THE DET IS PRODUCT OF ELEMENTS ALONG THE DIAGONAL

$$\text{DET}(A) = \text{DET}(L) \cdot \text{DET}(U) = \prod_{i=1}^N l_{ii} \prod_{j=1}^N u_{jj}$$

$$= \prod_{i=1}^N l_{ii} \quad \text{CRUT}$$

$$= \prod_{i=1}^N u_{ij} \quad \text{DOOLITTLE}$$

$$= \prod_{i=1}^N u_{ij}^2 \quad \text{CHOLESKI}$$

* BANDED MATRICES

$(NB+1) \times (NB+1)$

$$\begin{bmatrix} x & x & x & 0 & 0 & 0 & 0 & \dots \\ x & x & x & x & 0 & 0 & 0 & \dots \\ x & x & x & x & x & 0 & 0 & \dots \\ x & x & x & x & x & x & 0 & \dots \\ 0 & x & x & x & x & x & x & \dots \\ 0 & 0 & & & & & & \dots \end{bmatrix}$$

N.B. = "HALF BANDWIDTH, EXCLUDES MAIN DIAGONAL"

→ MOST SITUATIONS LEAD TO BANDED MATRICES

- CUBIC SPLINE
- BVP, ETC.

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DIAGONALLY DOMINANT

$$|a_{ij}| > \sum_{\substack{j=1 \\ j \neq i}}^N |a_{ij}| \rightarrow \text{NO ZERO PIVOTS}$$

* STORAGE FOR Banded MATRICES

- NO SENSE IN STORING ALL THE ZERO'S
- INSTEAD PACK INTO A $N(2NB+1)$ MATRIX

FOR $NB \ll N$

$$\begin{array}{cccc} & & & \overbrace{\text{NB}} \\ 0 & 0 & 0 & X & X & X & X \\ 0 & 0 & X & X & X & X & X \\ 0 & X & X & X & & & \\ X & X & X & X & & & \\ & & & & & & X \end{array}$$

N ROWS, $2NB+1$ COLUMNS

* TRIDIAGONAL MATRIX - NB=1

↳ LOOK AT VIDEO

- 1.) GET ALL NON-ZERO OFF DIAGONAL TERMS IN L
- MULTIPLY ROW i IN L BY COLUMN $i-1$ IN U

→ $l_{i,i}$ → VIDEO

- IN A Banded MATRIX, THE # OF NON-ZERO BANDS OFF (AND EXCLUDING) THE MAIN DIAGONAL IS CALLED THE HALF BANDWIDTH

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* ITERATIVE MATRIX SOLUTIONS

- VERY USEFUL FOR SPARSE MATRICES

- IDEA: TO SOLVE $Ax = b$

- GUESS SOLUTION x^0
- UPDATE: $x^{k+1} = f(x^k)$
- CONTINUE UNTIL $x^k \rightarrow x$

- ISSUES:

- HOW TO UPDATE?
- DOES PROCESS CONVERGE?
- STOP CRITERIA

- TWO CLASSIC METHODS:

- JACOBIAN ITERATION
- GAUSS-SEIDEL ITERATION

* JACOBIAN ITERATION:

- SOLVE EQ. (OR ROW) i FOR x_i AND USE PREVIOUS GUESS OF SOLUTION TO COMPUTE UPDATED SOLUTION

$$x^{k+1} = \left(b_i - [a_{i2}x_2^k + a_{i3}x_3^k + \dots + a_{iN}x_N^k] \right) / a_{ii}$$

$$x^{k+1} = \left(b_2 - [a_{21}x_1^k + a_{23}x_3^k + \dots + a_{2N}x_N^k] \right) / a_{22}$$

JACOBI
ITERATION

$$x_i^{k+1} = \left(b_i - \sum_{\substack{j=1 \\ j \neq i}}^N a_{ij} x_j^k \right) / a_{ii}$$

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* GAUSS SEIDEL ITERATION

$$x_3^{k+1} = \left(b_3 - \left[a_{31} x_1^{k+1} + a_{32} x_2^{k+1} + a_{34} x_4^{k+1} + \dots + a_{3N} x_N^k \right] \right) / a_{33}$$

GAUSS-SEIDEL

$$x_i^{k+1} = \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{k+1} - \sum_{j=i+1}^N a_{ij} x_j^k \right) / a_{ii}$$

* ANALYSIS OF ITERATIVE SCHEMES

DEFINE: $\underline{A} = \underline{L} + \underline{U} + \underline{D}$

$$\underline{L} = \begin{bmatrix} 0 & & & \\ \text{shaded} & & & \\ & & & \\ & & & 0 \end{bmatrix}; \quad \underline{U} = \begin{bmatrix} 0 & \text{shaded} & & \\ & 0 & & \\ & & & \\ & & & 0 \end{bmatrix}; \quad \underline{D} = \begin{bmatrix} & & & 0 \\ & & & \\ 0 & & & \\ & & & \end{bmatrix}$$

• IN MATRIX FORM:

- JACOBI: $\underline{D} \underline{x}^{k+1} = \underline{b} - (\underline{L} + \underline{U}) \underline{x}^k$

$$\underline{x}^{k+1} = \underbrace{-\underline{D}^{-1}(\underline{L} + \underline{U})}_{\underline{T}_J} \underline{x}^k + \underbrace{\underline{D}^{-1} \underline{b}}_{\underline{c}_3}$$

↳ "ITERATION MATRIX FOR JACOBI"

$$\underline{x}^{k+1} = \underline{T}_J \underline{x}^k + \underline{c}_3$$

- GAUSS-SEIDEL

$$\underline{D} \underline{x}^{k+1} = \left(\underline{b} - \underline{L} \underline{x}^{k+1} - \underline{U} \underline{x}^k \right) \rightarrow (\underline{D} + \underline{L}) \underline{x}^{k+1} = \left(\underline{b} - \underline{U} \underline{x}^k \right)$$

$$\underline{x}^{k+1} = \underbrace{-\left(\underline{D} + \underline{L} \right)^{-1} \underline{U}}_{\underline{T}_G} \underline{x}^k + \underbrace{\left(\underline{D} + \underline{L} \right)^{-1} \underline{b}}_{\underline{c}_4} \rightarrow \underline{x}^{k+1} = \underline{T}_{GS} \underline{x}^k + \underline{c}_{GS}$$

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BOTH METHODS HAVE FORM

$$\underline{x}^{k+1} = \underline{T} \underline{x}^k + \underline{c}$$

$$\underline{x} = \underline{T} \underline{x} + \underline{c} \quad (\text{EXACT SOLUTION})$$

$$\underline{x}^{k+1} - \underline{x} = \underline{T} (\underline{x}^k - \underline{x}) \Rightarrow \underline{e}^{k+1} = \underline{T} \underline{e}^k$$

↳ WE WANT $\underline{e}^{k+1} = 0$
↑ ↑
VECTOR SCALAR

- NEED THE CONCEPT OF A "NORM"

- A MEASURE OF THE SIZE OF \underline{e} & \underline{T}

* NORM $\| \quad \|$

- VECTOR NORMS $\| \underline{x} \|$

- PROPERTIES

- $\| \underline{x} \| \geq 0$

- $\| \underline{x} \| = 0$, IFF $\underline{x} = 0$, $i = 1, \dots, N$

- $\| \alpha \underline{x} \| = |\alpha| \| \underline{x} \|$

- $\| \underline{x} + \underline{y} \| \leq \| \underline{x} \| + \| \underline{y} \|$

- MOST USEFUL L-NORM:

$$L_2 \text{ NORM} = \| \underline{x} \|_2 = \left[\sum_{j=1}^N x_j^2 \right]^{1/2}$$

$$L_\infty \text{ NORM} = \| \underline{x} \|_\infty = \max_{1 \leq j \leq N} |x_j|$$

IN GENERAL

$$\| \underline{x}_p \| \equiv \left[\sum_{j=1}^N |x_j|^p \right]^{1/p} \quad (\text{P-NORM})$$

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- RELATIVE NORM:

$$\frac{\|x^{k+1} - x^k\|}{\|x^{k+1}\|}$$

- MATRIX NORM $\|A\| \equiv \max \|Ax\|$

- TAKE ALL THE VECTORS x W NORM OF 1, MULTIPLY BY A TO GET NEW VECTORS Ax THEN PICK LARGEST IN TERMS OF THE NORM

- EG. $\|A\|_2 = \max_{\|x\|_2=1} \|Ax\|_2$

• x IS INPUT VECTOR

• FIND LONGEST Ax

- EG $\|A\|_\infty = \max_{\|x\|_\infty=1} \|Ax\|_\infty$

• LARGEST ROW SUM OF ABSOLUTE VALUES

$$= \max_{1 \leq j \leq n} \sum_{i=1}^n |a_{ij}|$$

WE HAVE,

$$e^{k+1} = T e^k \rightarrow \|e^{k+1}\| = \|T e^k\| \leq \|T\| \|e^k\|$$

FOR ITERATION TO CONVERGE, $\|T\| < 1$

- IT TURNS OUT THAT THE MATRIX NORM IS NOT VERY PRACTICAL

- INSTEAD USE THE "SPECTRAL RADIUS"

FOR ITERATION TO CONVERGE

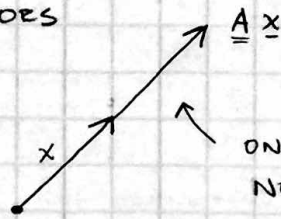
$\rho(T) < 1$, $\rho(T)$ IS THE SPECTRAL RADIUS OF T
↳ = THE LARGEST EIGENVALUE OF T

$\Rightarrow \max |\lambda_i| < 1$, $\{\lambda_i\}$ = EIGENVALUES OF T

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* EIGENVALUES / EIGENVECTORS

$$\underline{Ax} = \lambda x$$



ONLY A SCALAR TRANSFORMATION,
NO ROTATION

"PROOF"

$$\begin{aligned} \underline{x}^{k+1} &= \underline{T} \underline{x}^k + c \\ \underline{x}^k &= \underline{T} \underline{x}^{k-1} + c \end{aligned}$$

$$\rightarrow \underline{x}^{k+1} - \underline{x}^k = \underline{T}(\underline{x}^k - \underline{x}^{k-1})$$

$$\underline{\delta}^{k+1} = \underline{T} \underline{\delta}^k$$

↑
WRITE AS A LINEAR COMBINATION
OF N LINEARLY INDEPT.
EIGENVECTORS OF \underline{T}

$$\underline{T} \underline{v}_i = \lambda_i \underline{v}_i$$

$$\underline{\delta}^1 = \sum_{i=1}^N b_i \underline{v}_i$$

$$\begin{aligned} \underline{\delta}^2 &= \underline{T} \underline{\delta}^1 = \underline{T} \sum_{i=1}^N b_i \underline{v}_i = \sum_{i=1}^N b_i \underline{T} \underline{v}_i \\ &= \sum_{i=1}^N b_i \lambda_i \underline{v}_i \end{aligned}$$

$$\underline{\delta}^3 = \underline{T} \underline{\delta}^2 = \sum_{i=1}^N b_i \lambda_i^2 \underline{v}_i \rightarrow \underline{\delta}^N = \underline{T} \underline{\delta}^{N-1} = \dots \sum_{i=1}^N b_i \lambda_i^{N-1} \underline{v}_i$$

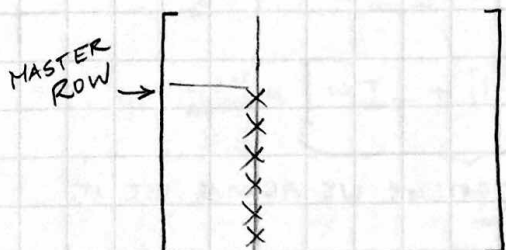
AS $N \rightarrow \infty$, FOR $\underline{\delta}^N \rightarrow 0$, IF ANY $|\lambda_i| > 1$, THEN $\underline{\delta}^N \rightarrow \infty$

$$|\lambda_i| = \frac{\|\underline{\delta}^{k+1}\|}{\|\underline{\delta}^k\|}$$

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* PIVOTING STRATEGIES

- PARTIAL PIVOTING, ORDER N^2 STEPS



$$R_j = \frac{a_{ji}}{a_{ii}} R_i \rightarrow R_j$$

$$\left[\begin{array}{cccc|c} 1 & -1 & 2 & -1 & -8 \\ 0 & 0 & -1 & -1 & -4 \\ 0 & 2 & -1 & 1 & 6 \\ 0 & 4 & 2 & 8 & 12 \end{array} \right]$$

- BETTER TO FIND THE PIVOT BASED ON ITS RELATIVE SIZE BASED ON OTHER ELEMENTS IN THE ROW

→ CALLED "SCALED" OR "COLUMN" PIVOTING.

- DETERMINE PIVOT ELEMENT BASED ON ITS SIZE RELATIVE TO OTHER COEFFICIENTS IN THE ROW.

- IN PRACTICE ITS TOO EXPENSIVE TO COMPUTE THE SCALE FACTORS FOR EVERY COLUMN

- INSTEAD, BASE SCALING ON SIZE RELATIVE TO ORIGINAL MATRIX COEFFICIENTS → GOES $O(N^2)$

→ LOOK AT ORIGINAL MATRIX, EQUAL TO MAX ABS. IN EACH ROW.

$$S_i = |a_{ij}| \rightarrow S_i = \begin{bmatrix} 2 \\ 3 \\ 1 \\ 7 \end{bmatrix}$$

COMPUTE ONCE & USE AT EACH STEP

11/10/2015

$$\rightarrow \left[\begin{array}{cccc|c} 1 & -1 & 2 & -1 & -8 \\ 0 & 0 & -1 & -1 & -4 \\ 0 & 2 & -1 & 1 & 6 \\ 0 & 4 & 2 & 8 & 12 \end{array} \right] \begin{array}{l} \leftarrow \text{MASTER ROW} \\ \downarrow \frac{1}{2} \\ \downarrow \frac{7}{4} \end{array}$$
$$S_i = \begin{bmatrix} 2 \\ 3 \\ 1 \\ 7 \end{bmatrix}$$

↑ CAN'T PROCEED DUE TO ZERO \rightarrow CALCULATE SCALE FACTORS

- IN PRACTICE, IF WE ARE USING A PIVOTING STRATEGY, WE ALWAYS USE IT.

23:09 IN VIDEO

11/16/2015 ITERATIVE MATRIX SOLUTIONS

$$\underline{x}^{k+1} = \underline{T} \underline{x}^k + \underline{c}, \rightarrow |\lambda_i| \approx \frac{\|\delta^{k+1}\|}{\|\delta^k\|}$$

BOTH JACOBI & GAUSS SEIDEL, GUARANTEED TO CONVERGE FOR \underline{x}^0

- IN GENERAL, $\rho(\underline{T}) \rightarrow 1$ AS RANK (SIZE) OF \underline{T} GETS LARGE

- CONVERGENCE SLOWS $\rho(\underline{T}) \rightarrow 1$

- STRATEGY: INTRODUCE A FACTOR, WHICH WE CONTROL, TO ALTER SPECTRAL RADIUS

↳ LEADS TO RELAXATION METHODS

IN GENERAL, $\tilde{\underline{x}}^{k+1} = \underline{T} \underline{x}^k + \underline{c}$

$$\underline{x}^{k+1} = w \tilde{\underline{x}}^{k+1} + (1-w) \underline{x}^k$$

$0 < w < 1 \rightarrow$ "UNDER RELAXATION": MORE WEIGHT ON OLD VALUE USED TO MAKE A NON-CONVERGENT PROCESS CONVERGE

↳ MORE "WEIGHT" ON NEW VALUE, SPEEDS CONVERGENCE

11/16/2015

LOOK @ JACOBI ITERATION

→ SUBSTITUTE FOR \tilde{x}^{k+1}

$$\underline{x}^{k+1} = w \underline{T} \underline{x}^k + (1-w) \underline{x}^k + w \underline{c}$$

$$\underline{x}^{k+1} = \underbrace{\left[w \underline{T} + (1-w) \underline{I} \right]}_{= \underline{T}_w} \underline{x}^k + w \underline{c}$$

$$\underline{x}^{k+1} = \underline{T}_w \underline{x}^k + w \underline{c}$$

• SUCCESSIVE OVER RELATION (SOR)

$$x_i^{k+1} = (1-w) x_i^k + w \tilde{x}_i^{k+1}$$

↑ COMPUTE USING GAUSS-SEIDEL

$$x_i^{k+1} = (1-w) x_i^k + w \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{k+1} - \sum_{j=i+1}^N a_{ij} x_j^k \right) / a_{ii}$$

- IN MATRIX FORM:

$$\left(\underline{D} + w \underline{L} \right) \underline{x}^{k+1} = \left[(1-w) \underline{D} - w \underline{U} \right] \underline{x}^k + w \underline{b}$$

$$\hookrightarrow \underline{x}^{k+1} = \underbrace{\left(\underline{D} + w \underline{L} \right)^{-1} \left[(1-w) \underline{D} - w \underline{U} \right]}_{\underline{I}_{SOR}} \underline{x}^k + w \left(\underline{D} + w \underline{L} \right)^{-1} \underline{b}$$

* EIGENVALUES & EIGENVECTORS (CHAPTER 9.1 - 9.4)

$$\underline{A} \underline{v}_i = \lambda_i \underline{v}_i \quad \rightarrow \quad (\underline{A} - \lambda_i \underline{I}) \underline{v}_i = 0$$

↳ SOLUTION REQUIRES $\det(\underline{A} - \lambda \underline{I}) = 0$

- FOR $N \times N$; \underline{A} , $\det(\underline{A} - \lambda \underline{I})$ IS AN N^{TH} DEG. POLYNOMIAL

11/16/2015

* POWER METHOD

- CONSIDER THE ITERATION

$$\underline{y}^{(k+1)} = \underline{A} \underline{y}^{(k)} \quad \text{EXPAND } \underline{y}^{(k)} \text{ IN TERMS OF EIGENVECTORS OF } \underline{A}$$

$$\underline{y}^0 = \sum_{i=1}^N b_i \underline{v}_i$$

$$\underline{y}^1 = \underline{A} \underline{y}^{(0)} = \underline{A} \sum_{i=1}^N b_i \underline{v}_i = \sum_{i=1}^N b_i \underline{A} \underline{v}_i$$

$$\underline{y}^2 = \underline{A} \underline{y}^{(1)} = \dots = \sum_{i=1}^N b_i \lambda_i^2 \underline{v}_i$$

⋮

$$\underline{y}^{(k)} = \underline{A} \underline{y}^{(k-1)} = \sum_{i=1}^N b_i \lambda_i^k \underline{v}_i \quad \rightarrow \text{ ASSUME } |\lambda_1| > |\lambda_2| > \dots > |\lambda_N|$$

$$\text{THEN, } \underline{y}^{(k)} = \lambda_1^k \left\{ b_1 \underline{v}_1 + \sum_{i=2}^N b_i \underbrace{\left(\frac{\lambda_i}{\lambda_1}\right)^k}_{< 1} \underline{v}_i \right\}$$

$$\lim_{k \rightarrow \infty} \underline{y}^{(k)} = b_1 \lambda_1^k \underline{v}_1 = \lambda_1 \underbrace{\left(b_1 \lambda_1^{k-1} \underline{v}_1 \right)}_{\underline{y}^{(k-1)}}$$

$$\underline{y}^{(k)} = \lambda_1 \underline{y}^{(k-1)}$$

IF $|\lambda_1| > 1$, THEN $\underline{y}^{(k)} \rightarrow \infty$ → TO KEEP $\underline{y}^{(k)}$ FINITE & BOUNDED
IF $|\lambda_1| < 1$, THEN $\underline{y}^{(k)} \rightarrow 0$ → NORMALIZE AT EACH STEP

$$\hookrightarrow \|\underline{y}^{(k)}\| = \|\lambda_1 \underline{y}^{(k-1)}\|$$

$$\|\underline{y}^{(k)}\| \cong |\lambda_1| \underbrace{\|\underline{y}^{(k-1)}\|}_{=1} \rightarrow |\lambda_1| \cong \|\underline{y}^{(k)}\|$$

"POWER METHOD" FINDS THE LARGEST EIGENVALUE & CORRESPONDING EIGENVECTOR, $\underline{y}^{(k)}$ OF \underline{A}

11/16/2015

• SHIFTING:

$$\underline{A}x = \lambda x - Sx + Sx \rightarrow (\underline{A} - S\underline{I})x = (\lambda - S)x$$

$$\underline{\bar{A}}x = \bar{\lambda}x$$

• INVERSE:

$$\underline{A}x = \lambda x \rightarrow x = \underline{A}^{-1}\lambda x \rightarrow \frac{1}{\lambda}x = \underline{A}^{-1}x$$