DS288: NUMERICAL METHODS

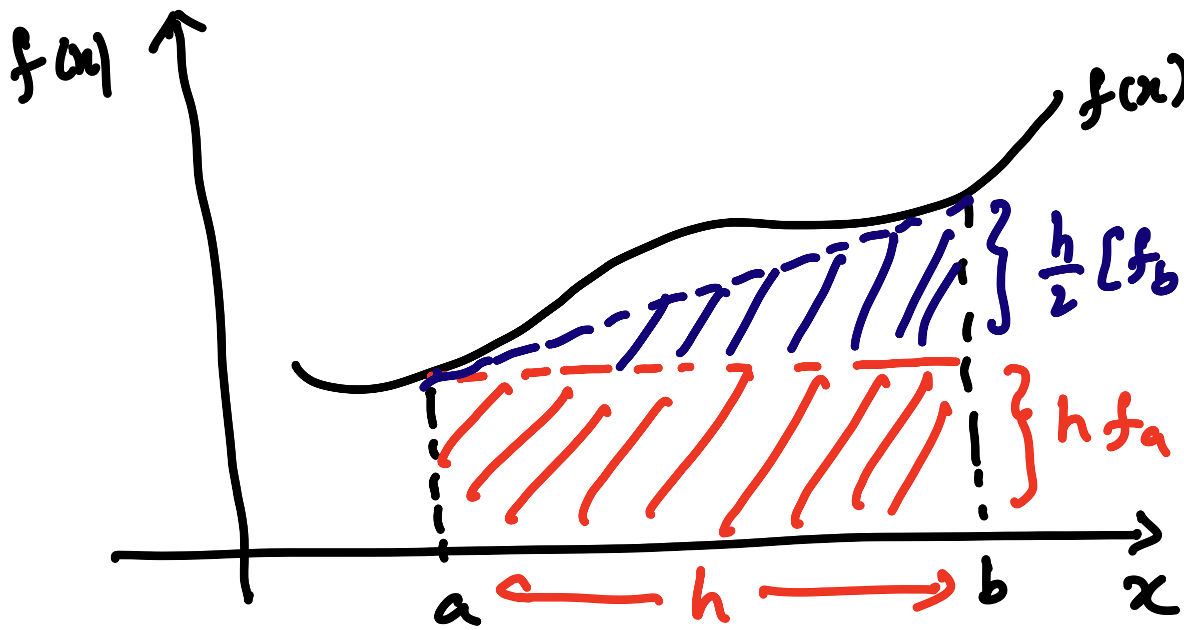
Sep-16-2021

Numerical Integration.

$$\boxed{I(b) = \frac{h}{2}\left[f_a + f_b\right] - \frac{h^3}{12} f''(\xi)}$$

TRAPEZOIDAL RULE

[$f''(\xi) = 0$ If f IS LINEAR]



REWRITE

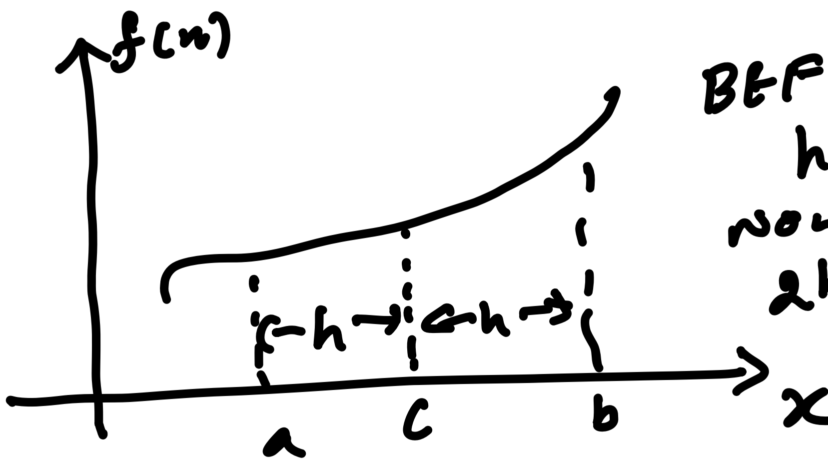
$$I(b) \cong \underbrace{h f_a} + \underbrace{\frac{h}{2}\left[f_b - f_a\right]}$$

* LOOK AT ORDER OF POLYNOMIAL THAT CAN BE EXACTLY INTEGRATED TO DETERMINE ORDER OF INTEGRATION ERROR

i.e. $p_N^{(N+1)}(x) = 0$

$\Rightarrow$ TRAPEZOIDAL RULE CAN INTEGRATE A LINEAR FUNCTION EXACTLY BECAUSE $p_1''(x) = 0$

- WHY NOT TRY A CENTERED DIFFERENCE SCHEME FOR f', f'' ... etc.



BEFORE:
$h = b - a$
NOW
$2h = b - a$

EXPAND $I(x)$ AROUND $x = c$

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

$$\cancelto{0}{I(a)} = I(c) - h f_c + \frac{h^2}{2!} f_c' - \frac{h^3}{3!} f_c'' + \cdots$$

$-$

$$I(b) = 2h f_c + \frac{2h^3}{3!} f_c'' + \frac{2h^5}{5!} f_c^{iv} + \cdots$$

USE A CENTERED SCHEME FOR f_c''

$$f_c'' = \frac{f_b - 2f_c + f_a}{h^2} - \frac{h^2}{12} f^{iv}(\xi)$$

SUBSTITUTE BACK.

$$I(b) = 2hf_c + \frac{h^3}{3}\left[\frac{f_a - 2f_c + f_b}{h^2}\right.$$

$$\left. - \frac{h^3}{3}\,\frac{h^2}{12} f^{iv}(\xi) + \frac{2h^5}{5!} f^{iv}(\xi)\right.$$

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

SIMPSON'S RULE $\quad \xi \in [a, b]$

- CAN DO A CUBIC FUNCTION EXACTLY

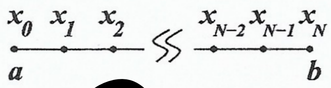
$P_3^{iv}(x) = 0$

Summary of Newton-Cotes Formulas

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

– Some integration rules for equally-spaced samples points.

"Closed" Formulas

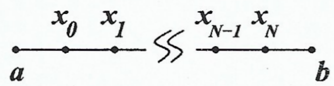


$a = x_0;\ b = x_N \Rightarrow Nh = b - a$

$N=1$	Trapezoidal Rule:	$I(b) = \frac{h}{2}(f_0 + f_1)$	$-\frac{h^3}{12}\, f''(\xi)$
$N=2$	Simpson's Rule:	$I(b) = \frac{h}{3}[f_0 + 4f_1 + f_2]$	$-\frac{h^5}{90}\, f^{iv}(\xi)$
$N=3$	Simpson's $\frac{3}{8}$ Rule:	$I(b) = \frac{3h}{8}[f_0 + 3f_1 + 3f_2 + f_3]$	$-\frac{3h^5}{80}\, f^{iv}(\xi)$
$N=4$	Boole's Rule:	$I(b) = \frac{2h}{45}[7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4]$	$-\frac{8h^7}{945}\, f^{vi}(\xi)$

→ VERIFY
→ NOT DONE

"Open" Formulas



Do not involve limits of integration
$\Rightarrow (N+2)h = b - a$

$N=0$	Midpoint Rule	$I(b) = 2hf_0$	$+\frac{h^3}{3}\, f''(\xi)$
$N=1$		$I(b) = \frac{3h}{2}[f_0 + f_1]$	$+\frac{3h^3}{4}\, f''(\xi)$
$N=2$		$I(b) = \frac{4h}{3}[2f_0 - f_1 + 2f_2]$	$+\frac{14h^5}{45}\, f^{iv}(\xi)$
$N=3$		$I(b) = \frac{5h}{24}[11f_0 + f_1 + f_2 + 11f_3]$	$+\frac{95h^5}{144}\, f^{iv}(\xi)$

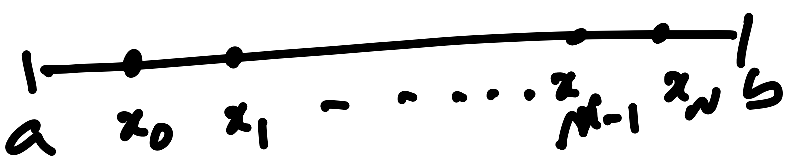
NEWTON- COTES CLOSED FORMULAS

- INCLUDE LIMITS OF INTEGRATION $a = x_0,\ b = x_n$

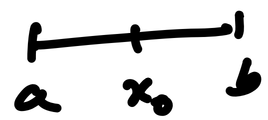
$b - a = nh$

ANTHOER CLASS OF FORMULAS THAT DO NOT INCLUDE LIMITS OF INTEGRATION

NEWTON-COTES "OPEN" FORMULAS



If $n = 0$



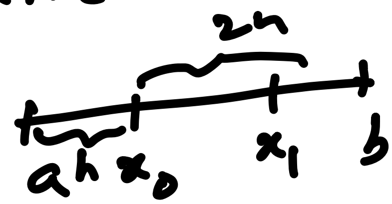
$$I(b) = I(x_0) + h f_0 + \frac{h^2}{2} f_0' + \frac{h^3}{3!} f_0'' + \cdots$$

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

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

CAN DO A LINEAR FUNCTION EXACTLY ($f''(x) = 0$)

<u>Ex:</u> $N = 1$



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

$$-\left(\cancel{I(a)}^{\,0} = I(x_0) - hf_0 + \frac{h^2}{2} f_0' - \frac{h^3}{3!} f_0'' + \dots\right)$$

$$I(b) = 3hf_0 + \frac{3}{2}h^2 \underbrace{\left[\frac{f_1 - f_0}{h} - \frac{h f_0''(\xi)}{2}\right]}_{f_0' \text{ FORWARD DIFF.}} + \frac{9h^3}{6} f_0''(\xi)$$

$$\boxed{I(b) = \frac{3h}{2}\left[f_1 + f_0\right] + \frac{3h^3}{4} f''(\xi)}$$

CAN STILL ONLY DO A LINER FUNCTION EXACTLY

- IF N IS EVEN, P_{N+1} CAN BE INTEGRATED EXACTLY
- IF N IS ODD, P_N CAN BE INTEGRATED EXACTLY
- WHEN N IS EVEN, ADDING A SINGLE POINT DOES <u>NOT</u> INCREASE THE POLYNOMIAL ORDER, IT DOES IMPROVE ACCURACY AS 'h' DECREASES.
- LARGER 'N' - NEWTON - COTES FORMULAS
  - * HARD TO DERIVE
  - * POSSIBLE POLYNOMIAL OSCILLATIONS FOR HIGHER ORDERS (UNIFORM SAMPLING)

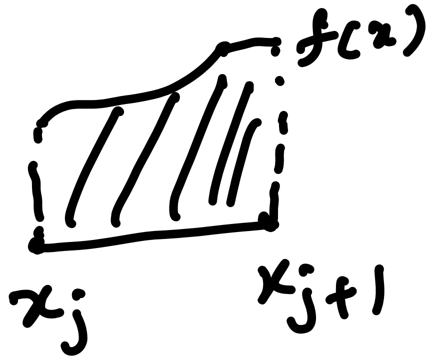
* INSTEAD OF HIGHER ORDER POLYNOMIAL (LARGE n), USE LOWER ORDER 'n' NEWTON-COTES FORMULAS SUCCESSIVELY ON SUB-INTERVALS

$\Rightarrow$ COMPOSITE INTEGRATION

[SIMILAR TO SPLINE CONCEPT]

COMPOSITE INTEGRATION

PANEL $\equiv$ BASIC UNIT OF INTEGRATION



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

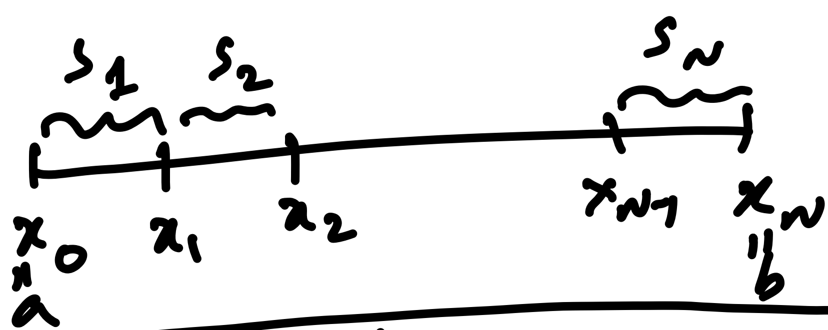
TRAPEZOIDAL RULE.

$$S_{j+1} = \frac{h}{2}\left[f_{j+1} + f_j\right] - \frac{h^3}{12} f''(\xi)$$

$$\xi \in [x_j, x_{j+1}]$$

COMPOSITE TRAPEZOIDAL RULE: $I(b) = \sum_{j=1}^{N-1} S_j$ CLOSED FORMULA

$$I(b) = \sum_{j=1}^{N} \frac{h}{2}\left(f_j + f_{j+1}\right) - \sum_{i=1}^{N-1} \frac{h^3}{12} f''(\xi_i)$$



$$\boxed{I(b) = \frac{h}{2}\left[2\sum_{i=1}^{N-1} f_i + f_0 + f_N\right]}$$

COMPOSITE TRAPEZOIDAL RULE.

FUNCTION EVALUATION:

COMPOSITE: $N+1$ → HIGHER COMPUTATIONAL COMPLEXITY

REGULAR: 2

ERROR BEHAVIOR

$$\text{ERROR} = \sum_{j=1}^{N} \frac{h^3}{12} f''(\xi_j) = \frac{h^3}{12} N \overline{f''(\xi)}$$

WHERE $\overline{f''(\xi)}$ IS AVERAGE VALUE OF $f''(\xi_i)$

$Nh = b-a$ (CLOSED FORMULAS)

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

$$\text{ERROR} = \left(\frac{b-a}{12}\right) h^2 f''(\xi)$$

ONE ORDER LOWER IN (h)

$O(h^3)$ IN TRAPEZOIDAL

$\Downarrow$

$O(h^2)$ IN COMPOSITE TRAPEZOIDAL

- APPLICATION OF METHOD N TIMES REDUCES ERROR BY

A FACTOR OF 'h' FOR ALL NEWTON-COTES METHODS

- CAN EXTEND ANY METHOD TO COMPOSITE INTEGRATION

<u>EX:</u> SIMPSON'S RULE

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

ONE APPLICATION OVER TWO PANELS

$$I(b) = \sum_{j=1,3,5}^{N-1} \left[S_j + S_{j+1}\right]$$

$$\boxed{I(b) = \frac{h}{3}\left\{f_0 + 2\sum_{j=1}^{\frac{N}{2}-1} f_{2j} + 4\sum_{j=1}^{N/2} f_{2j-1} + f_N\right\} - \frac{(b-a)h^4}{180} f^{iv}(\xi)}$$

PANEL ENDPOINTS

MID POINTS

x_{j-1} x_j x_{j+1}

COMPOSITE SIMPSON'S RULE.

ROUNDING ERRORS IN NUMERICAL INTEGRATION

RECALL: $$\int_a^b f(x)\,dx = \underbrace{\sum_{i=0}^{N}{}' a_i f_i}_{\text{QUDARATURE}} + E_{TRUNC}$$

E_{TRUNC} HAS 'h' IN NUMERATOR

AS $h \to 0 \Rightarrow E_{TRUNC} \to 0$

COMPOSITE $h = \frac{b-a}{N}$

$h \to 0$ $N \to \infty$ OR $b-a \to 0$

↳ COMPOSITE: 'N' INCREASES

REGULAR: $b-a \to$ DECREASE

ON COMPUTER

$$\hat{f}_i = \underset{\uparrow\ \text{EXACT}}{f_i} + \underset{\text{ROUND-OFF ERROR}}{\epsilon_i}$$

$$\underbrace{\sum_{i=0}^{N}{}' a_i \hat{f}_i}_{\text{COMPUTED}} = \underbrace{\sum_{i=0}^{N}{}' a_i f_i}_{\substack{\text{EXACT} \\ \text{(TRUE RESULT)}}} + \underbrace{\sum_{i=0}^{N}{}' a_i \epsilon_i}_{E_{\text{ROUNDOFF}}}$$

$$E_{\text{TOTAL}} = \left| I(b) - \sum_{i=0}^{N}{}' a_i \hat{f}_i \right|.$$

$$\left[I(b) = \int_a^b f(x)\,dx \right]$$

$$E_{\text{TOTAL}} = \left| \sum_{i=0}^{N}{}' a_i f_i + E_{\text{TRUNC}} - \sum_{i=0}^{N}{}' a_i \hat{f}_i \right|$$

$$= |E_{TRUNC} - E_{ROUND}|$$

$$E_{TOTAL} \leq |E_{TRUNC}| + |E_{ROUND}|$$

EXAMINE $E_{ROUND} = \sum_{i=0}^{N} a_i \epsilon_i$

WHAT ARE $\{a_i\}$

TRAPEZOIDAL RULE: $a_0 = a_1 = \frac{h}{2}$

$$\sum_{i=0}^{N=1} a_i f_i = \frac{h}{2}(f_0 + f_1)$$

CAN SAY THAT

$$E_{ROUND} = \sum_{i=0}^{N} a_i \epsilon_i \leq \epsilon \sum_{i=0}^{N} |a_i|$$

WHERE $\epsilon = \max|\epsilon_i|$

ALL NEWTON - COTES FORMULAS HAVE $\{a_i\}$'S AS A FACTOR OF 'h' IN THE NUMERATOR

AS $h \to 0$ $\quad a_i \to 0$ WE EXPECT $\varepsilon_{ROUND} \to 0$

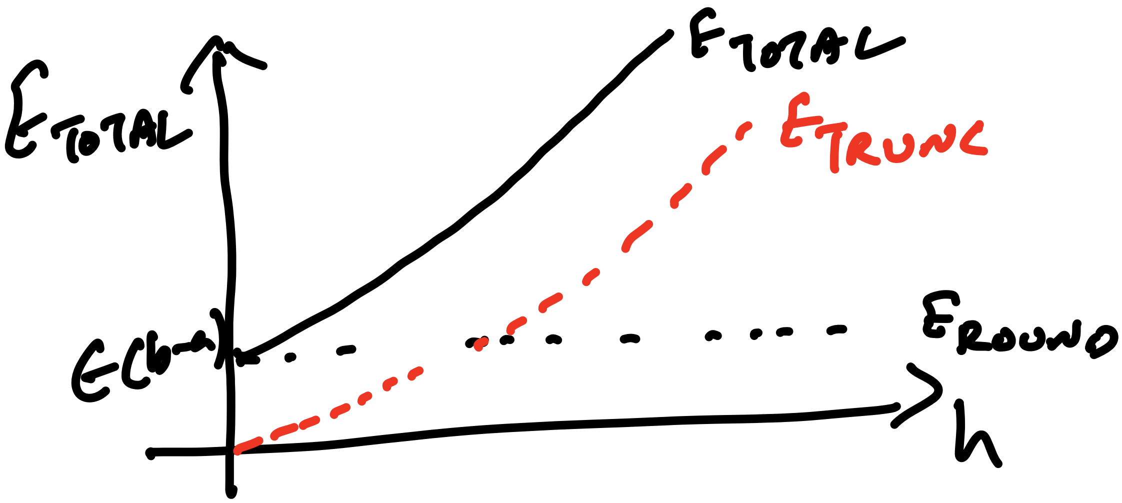
BUT: $\int_a^b dx = b - a = \sum_{i=0}^{n} a_i (1)$

$f(x) = 1.$

SO IF ALL $\{a_i\}$ ARE POSITIVE

THEN: $\varepsilon_{ROUND} \leq \epsilon (b-a)$

INDEPENDEN OF : DOES NOT GO AWAY IF $h \to 0$



[NUMERICAL DIFFERETIATION

E_{ROUNDOFF} DEPEDENT ON h

NUMICAL INTEGRATION

E_{ROUNDOFF} INDEPENDENT OF h]