DS288: NUMERICAL METHODS

Sep-14-2021

- $f_j^{(n)} \rightarrow O(h)$ WE REQUIRE $(n+1)$ FUNCTION EVALUATIONS n TAYLOR EXPANSIONS

- IN SIMILAR MANNER, ONE CAN CONSTRUCT HIGHER ORDER APPROXIMATIONS TO A DERIVATIVE AT THE COST OF MORE TAYLOR EXPANSIONS & MORE FUNCTION EVALUATIONS.

  → HIGHER ORDER h MEANS HIGHER ACCURACY

Ex: $f_j' \rightarrow O(h)$ — FORWARD DIFFERENCE / BACKWARD DIFFERENCE

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

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

$$f_{j+2} - 4f_{j+1} = -3f_j - 2h f_j' + \frac{4h^3}{3!} f_j''' + \cdots$$

$$f_j' = \frac{-f_{j+2} + 4f_{j+1} - 3f_j}{2h} + \frac{2h^2}{6} f_j'''(\xi)$$

$$\xi \in [x_j \; x_{j+2}]$$

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

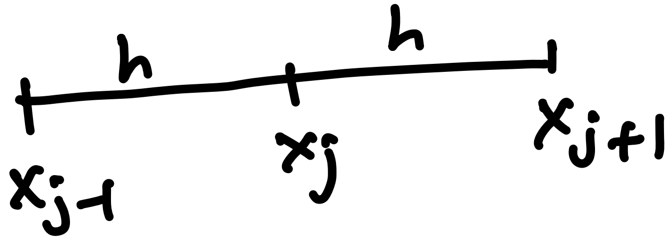
SO HIGHER ORDER OF ACCURACY WILL COST US ANOTHER FUNCTION EVALUATION (ANALOGY IS THAT WE ARE FITTING HIGHER ORDER POLYNOMIALS TO OUR FUNCTION AT x_i, SO WE NEED MORE POINTS)

FOR FORWARD OR BACKWARD DIFFERENCE:

N^{TH} ORDER DERIVATIVE TO ACCURACY $O(h^M)$ REQUIRES $N+M$ FUNCTION EVALUATIONS INVOLVING $N+M-1$ TAYLOR SERIES EXPANSIONS

CENTRAL DIFFERENCE APPROXIMATIONS

- COMBINE FORWARD & BACKWARD APPROXIMATIONS TO KILL HIGHER ORER TERMS RESULTING IN A SYMMETRIC SAMPLING AROUND x_j



$$f_{j+1} = f_j + f_j' h + f_j'' \frac{h^2}{2!} + f_j''' \frac{h^3}{3!} + f_j^{iv} \frac{h^4}{4!} + \cdots$$

$$f_{j-1} = f_j - f_j' h + f_j'' \frac{h^2}{2!} - f_j''' \frac{h^3}{3!} + f_j^{iv} \frac{h^4}{4!} - \cdots$$

$+$

$$f_{j+1} + f_{j-1} = 2 f_j + f_j'' h^2 + f_j^{iv} \frac{h^4}{12} + \cdots$$

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

ONLY 3 FUNCTION EVALUATIONS

(REQUIRES 4 FN EVALUATIONS FOR FORWARD OR BACKWARD)

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

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

TWO FUNCTION EVALUATIONS

- ERRORS CANCEL WHEN COMBINING FORWARD & BACKWARD SCHEMES.
- POSSIBLE IF WE SAMPLE UNIFORMLY 'h' IS FIXED THROUGHOUT [a, b]

WHILE $\Delta^n f_j = \underbrace{\Delta \Delta \Delta \ldots \Delta}_{n \text{ TIMES}} f_j = f_j^n$

& $\nabla^n f_j = \underbrace{\nabla \nabla \nabla \cdots \nabla}_{n \text{ TIMES}} f_j = f_j^n$

FOR CENTRAL DIFFERENCE.

$$\delta f_j = f_{j+1} - f_{j-1}$$

$$\delta^2 f_j = f_{j+1} - 2 f_j + f_{j-1}$$

$$\delta^2 f_j \neq \delta(\delta f_j)$$

Difference Tables: Forward, Backward, and Centered

Forward difference representations, $O(h)$.

	f_i	f_{i+1}	f_{i+2}	f_{i+3}	f_{i+4}
$hf'(x_i)$	-1	1			
$h^2f''(x_i)$	1	-2	1		
$h^3f'''(x_i)$	-1	3	-3	1	
$h^4f^{iv}(x_i)$	1	-4	6	-4	1

Backward difference representations, $O(h)$.

	f_{i-4}	f_{i-3}	f_{i-2}	f_{i-1}	f_i
$hf'(x_i)$				-1	1
$h^2f''(x_i)$			1	-2	1
$h^3f'''(x_i)$		-1	3	-3	1
$h^4f^{iv}(x_i)$	1	-4	6	-4	1

Forward difference representations, $O(h^2)$.

	f_i	f_{i+1}	f_{i+2}	f_{i+3}	f_{i+4}	f_{i+5}
$2hf'(x_i)$	-3	4	-1			
$h^2f''(x_i)$	2	-5	4	-1		
$2h^3f'''(x_i)$	-5	18	-24	14	-3	
$h^4f^{iv}(x_i)$	3	-14	26	-24	11	-2

Backward difference representations, $O(h^2)$.

	f_{i-5}	f_{i-4}	f_{i-3}	f_{i-2}	f_{i-1}	f_i
$2hf'(x_i)$				1	-4	3
$h^2f''(x_i)$			-1	4	-5	2
$2h^3f'''(x_i)$		3	-14	24	-18	5
$h^4f^{iv}(x_i)$	-2	11	-24	26	-14	3

Central difference representations, $O(h^2)$.

	f_{i-2}	f_{i-1}	f_i	f_{i+1}	f_{i+2}
$2hf'(x_i)$		-1	0	1	
$h^2f''(x_i)$		1	-2	1	
$2h^3f'''(x_i)$	-1	2	0	-2	1
$h^4f^4(x_i)$	1	-4	6	-4	1

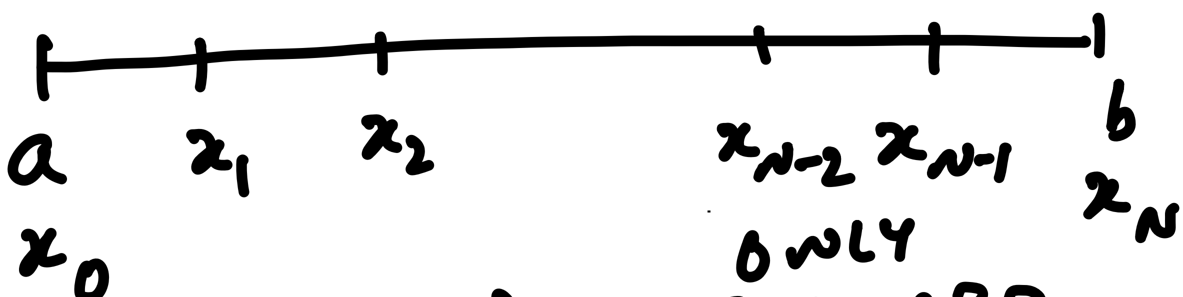
Central difference representations, $O(h^4)$.

	f_{i-3}	f_{i-2}	f_{i-1}	f_i	f_{i+1}	f_{i+2}	f_{i+3}
$12hf'(x_i)$		1	-8	0	8	-1	
$12h^2f''(x_i)$		-1	16	-30	16	-1	
$8h^3f'''(x_i)$	1	-8	13	0	-13	8	-1
$6h^4f^4(x_i)$	-1	12	-39	56	-39	12	-1

For the *centered* cases, we have extra accuracy for the same number of points:

$$
\begin{array}{lllll}
n^{th} \text{ derivative} & + & O(h^4) & \Rightarrow & n+3 \text{ pts.} \\
n^{th} \text{ derivative} & + & O(h^6) & \Rightarrow & n+5 \text{ pts.} \\
n^{th} \text{ derivative} & + & O(h^8) & \Rightarrow & n+7 \text{ pts.} \\
\vdots & \vdots & \vdots & \vdots & \vdots
\end{array}
$$

For the same number of points, the centered formulas always stay one order ahead of the uncentered formulas. Points are added alternately at the center of the formula, or in symmetric pairs.



ONLY

$f_0' \to O(h^2) \to$ FORWARD DIFFERENCE

$f_0 \longrightarrow$ CAN NOT APPLY CENTERED DIFF.

$f_N' \to O(h^2) \longrightarrow$ BACKWARD ONLY

Reference: Numerical Partial Differential Equations for Environmental Scientists and Engineers – A First Practical Course, Daniel R. Lynch – Springer, 2005. (Section: 2.1).

* NOTE ON INTERPRETATION OF ERROR $\underline{O(h^m)}$.

IF $E_h \rightarrow O(h^m)$

$h \rightarrow$ STEP-SIZE (SAMPLING DISTANCE)

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

VERIFY ORDER OF ACCURACY

$h \rightarrow x \rightarrow$ ERROR $\rightarrow f_j'$

$h/2 \rightarrow y \rightarrow$ ERROR $\rightarrow \tilde{f}_j'$

$$\frac{x}{y} \cong 2^m \qquad \frac{f_j'}{\tilde{f}_j} \sim 2^m$$

METHOD FOR US TO VERIFY THE $O(h^m)$ ACCURACY.

<u>NOTE</u>: NUMERICAL DIFFERENTIATION SCHEMES HAVE 'h' IN DENOMINATOR.

AS 'h' GETS SMALL, ROUND-OFF ERRORS CAN DESTROY ACCURACY

COMPUTED ERRORS IN NUMERICAL DIFFERENTIATION

Ex: CENTRAL DIFFERENCE SCHEME

$$f_j' = \frac{f_{j+1} - f_{j-1}}{2h} - \underbrace{\frac{f_j'''(\xi)\, h^2}{6}}_{= E_{TRUNC}} \quad \text{--- (1)}$$

E_{TRUNC} = TRUNCATION ERROR

COMPUTER: $\hat{f}_j = f_j + \epsilon_j$

$\hat{f}_j$ → COMPUTED VALUE

f_j → EXACT VALUE

ϵ_j → ROUND-OFF ERROR

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

$$= \underline{f_j' + E_{TRUNC}} \quad E_{ROUND}$$

$E_{ROUND} \sim O(1/h)$

REORDER TERMS

$$|\hat{f}_j' - f_j'| = |E_{TRUNC} + E_{ROUND}|$$

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

ASSUME $f_j'''(\xi)$ IS BOUNDED BY A NUMBER 'm'. & ϵ_{j+1} IS BOUNDED BY ϵ.

$$E_{TOTAL}(h) \leq \frac{mh^2}{6} + \frac{\epsilon}{h}$$

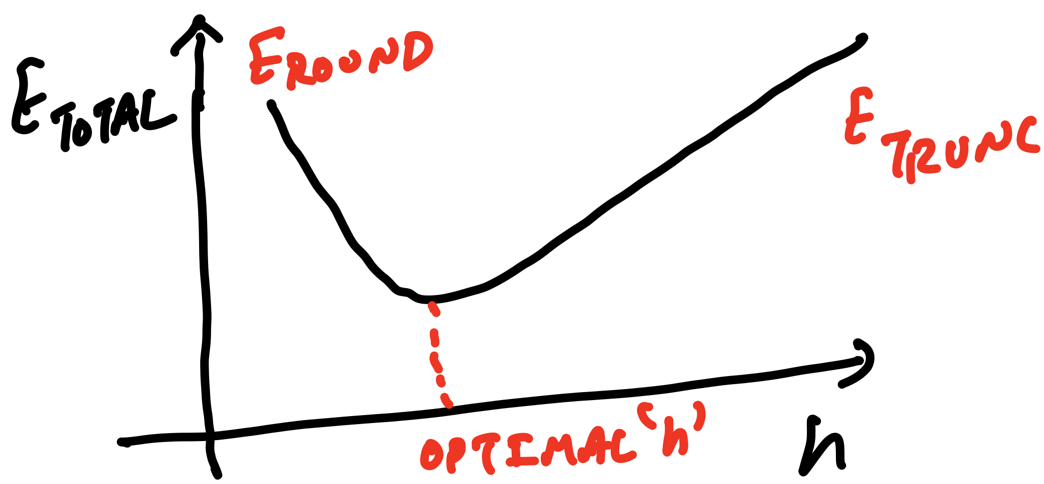
$h \to 0$ $\quad \left.\begin{array}{l} E_{TRUNC} \to 0 \\ E_{ROUND} \to \infty \end{array}\right\} E_{TOTAL} \to \infty$

↳ ROUND-OFF ERRORS DOMINATE

MINIMIZE $E_{TOTAL}(h)$

$$\left.\begin{array}{l} \dfrac{\partial E_{TOTAL}}{\partial h} = 0 \\ \dfrac{mh}{3} - \dfrac{\epsilon}{h^2} = 0 \end{array}\right\} \Rightarrow h = \left(\frac{3\epsilon}{m}\right)^{1/3}$$

OPTIMAL 'h'



TRADE OFF BETWEEN E_{TRUNC} & $E_{ROUND\,OFF}$ IN NUMERICAL DIFFERENTIATION

* HIGHER ORDER ACCURACY

↳ MAKING 'h' SMALL

ALTERNATIVE → HIGHER ORDER APPROXIMATION

<u>NUMERICAL INTEGRATION (OR)</u>

<u>NUMERICAL QUADRATURE</u>

(§4.3)

- NUMERICAL INTEGRATION IS MUCH MORE STABLE THAN NUMERICAL DIFFERENTIATION AS $h \to 0$.

<u>TEXT BOOK:</u> WRITES A POLYNOMIAL THROUGH f_j, f_{j+1} & INTEGRATES THE POLYNOMIAL

INCLASS: APPROACH IT USING TAYLOR SERIES

<u>TEXT</u>: APPROXIMATE

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

LAGRANGE INTERPOLATING POLYNOMIAL

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

$$\boxed{\int_a^b f(x)\,dx \cong \sum_{i=0}^{N} a_i f_i}$$

$a_i \rightarrow$ QUADRATURE

- APPROXIMAT THE INTEGRAL AS A SUM OF WEIGHTED FUNCTION VALUES

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

TEXT: USE ERROR FROM POLYNOMIAL APPROXIMATION

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

IN CLASS: TAYLOR SERIES

DEFINE:

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

WE WISH TO COMPUTE $I(b)$

EXPAND $I(x)$ AROUND 'a' USING TAYLOR SERIES

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

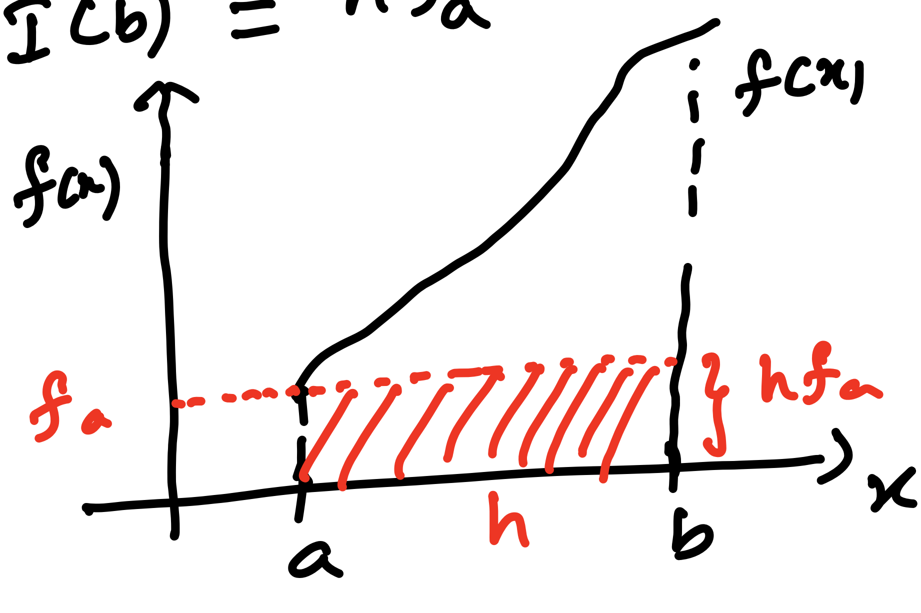
$$= 0 + f(a)(x-a) + \frac{f'(a)}{2}(x-a)^2 + \cdots$$

DEFINE $h = b - a$

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

LOWEST ORDER.:-

(i) $I(b) \simeq h f_a$



KEEP ANOTHER TERM

(ii) $I(b) = hf_a + \frac{h^2}{2} f_a' + \frac{h^3}{3!} f_a'' + \ldots$

FORWARD DIFFERENCE APPROX

$$f_a' = \frac{f_b - f_a}{h} - \frac{h}{2} f''(\xi)$$

$$I(b) = hf_a + \frac{h}{2}(f_b - f_a) + \frac{h^3 f_a''(\xi)}{3!} - \frac{h^3}{4} f''(\xi)$$

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

TRAPEZOIDAL RULE.

[ASSUMPTION ξ IS SAME IN BOTH FORWARD DIFFERENCE & TAYLOR SERIES TRUNCATION]