

MATH 3Q03: Differentiation with Finite Differences

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Agenda

Approach Based on Taylor Series

Interpolation-Based Approach

Complex Step Derivative

▶ **ASSUMPTIONS** :

- ▶ $f : \Omega \rightarrow \mathbb{R}$ is a **smooth** function, i.e. is continuously differentiable sufficiently many times,
- ▶ the domain $\Omega = [a, b]$ is discretized with a uniform grid $\{x_1 = a, \dots, x_N = b\}$, such that $x_{j+1} - x_j = h_j = h$ (extensions to nonuniform grids are straightforward)

- ▶ **PROBLEM** — given the nodal values of the function f , i.e., $f_j = f(x_j)$, $j = 1, \dots, N$ approximate the nodal values of the **function derivative**

$$\frac{df}{dx}(x_j) = f'(x_j) =: f'_j, \quad j = 1, \dots, N$$

- ▶ The symbol $\left(\frac{\delta f}{\delta x}\right)_j$ will denote the approximation of the derivative $f'(x)$ at $x = x_j$

- ▶ The simplest approach — Derivation of finite difference formulae via **TAYLOR-SERIES EXPANSIONS**

$$\begin{aligned} f_{j+1} &= f_j + (x_{j+1} - x_j)f'_j + \frac{(x_{j+1} - x_j)^2}{2!}f''_j + \frac{(x_{j+1} - x_j)^3}{3!}f'''_j + \dots \\ &= f_j + hf'_j + \frac{h^2}{2}f''_j + \frac{h^3}{6}f'''_j + \dots \end{aligned}$$

- ▶ Rearrange the expansion

$$f'_j = \frac{f_{j+1} - f_j}{h} - \frac{h}{2}f''_j + \dots = \frac{f_{j+1} - f_j}{h} + \mathcal{O}(h),$$

where $\mathcal{O}(h^\alpha)$ denotes the contribution from all terms with powers of h greater or equal α (here $\alpha = 1$).

- ▶ Neglecting $\mathcal{O}(h)$, we obtain a **FIRST ORDER FORWARD-DIFFERENCE FORMULA** :

$$\left(\frac{\delta f}{\delta x}\right)_j = \frac{f_{j+1} - f_j}{h}$$

- ▶ Backward difference formula is obtained by expanding f_{j-1} about x_j and proceeding as before:

$$f'_j = \frac{f_j - f_{j-1}}{h} - \frac{h}{2} f''_j + \dots \implies \left(\frac{\delta f}{\delta x} \right)_j = \frac{f_j - f_{j-1}}{h}$$

- ▶ Neglected term with the lowest power of h is the **LEADING-ORDER APPROXIMATION ERROR**, i.e., $Err = \left| f'(x_j) - \left(\frac{\delta f}{\delta x} \right)_j \right| \approx Ch^\alpha$
- ▶ The exponent α of h in the leading-order error represents the **ORDER OF ACCURACY OF THE METHOD** — it tells how quickly the approximation error vanishes when the resolution is refined
- ▶ The actual value of the approximation error depends on the constant C characterizing the function f
- ▶ In the examples above $Err = -\frac{h}{2} f''_j$, hence the methods are **FIRST-ORDER ACCURATE**

Higher-Order Formulas (I)

- ▶ Consider two expansions:

$$f_{j+1} = f_j + hf'_j + \frac{h^2}{2}f''_j + \frac{h^3}{6}f'''_j + \dots$$

$$f_{j-1} = f_j - hf'_j + \frac{h^2}{2}f''_j - \frac{h^3}{6}f'''_j + \dots$$

- ▶ Subtracting the second from the first:

$$f_{j+1} - f_{j-1} = 2hf'_j + \frac{h^3}{3}f'''_j + \dots$$

- ▶ **Central Difference Formula**

$$f'_j = \frac{f_{j+1} - f_{j-1}}{2h} - \frac{h^2}{6}f'''_j + \dots \implies \left(\frac{\delta f}{\delta x}\right)_j = \frac{f_{j+1} - f_{j-1}}{2h}$$

Higher-Order Formulas (II)

- ▶ The leading-order error is $\frac{h^2}{6} f_j'''$, thus the method is **SECOND-ORDER ACCURATE**
- ▶ Manipulating four different Taylor series expansions one can obtain a **fourth-order central difference formula** :

$$\left(\frac{\delta f}{\delta x}\right)_j = \frac{-f_{j+2} + 8f_{j+1} - 8f_{j-1} + f_{j-2}}{12h}, \quad \text{Err} = \frac{h^4}{30} f^{(v)}$$

Approximation of the Second Derivative

- ▶ Consider two expansions:

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

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

- ▶ Adding the two expansions

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

- ▶ Central difference formula for the second derivative:

$$f_j'' = \frac{f_{j+1} - 2f_j + f_{j-1}}{h^2} - \frac{h^2}{12}f_j^{(iv)} + \dots \implies \left(\frac{\delta^2 f}{\delta x^2}\right)_j = \frac{f_{j+1} - 2f_j + f_{j-1}}{h^2}$$

- ▶ The leading-order error is $\frac{h^2}{12}f_j^{(iv)}$, thus the method is

SECOND-ORDER ACCURATE

Taylor Table

- ▶ A general method for choosing the coefficients of a finite difference formula to ensure the highest possible order of accuracy
- ▶ Example: consider a one-sided finite difference formula $\sum_{p=0}^2 a_p f_{j+p}$, where the coefficients a_p , $p = 0, 1, 2$ are to be determined.
- ▶ Form an expression for the approximation error

$$f'_j - \sum_{p=0}^2 a_p f_{j+p} = \epsilon$$

and expand it about x_j in the powers of h

- ▶ Expansions can be collected in a Taylor table

	f_j	f_j'	f_j''	f_j'''
f_j'	0	1	0	0
$-a_0 f_j$	$-a_0$	0	0	0
$-a_1 f_{j+1}$	$-a_1$	$-a_1 h$	$-a_1 \frac{h^2}{2}$	$-a_1 \frac{h^3}{6}$
$-a_2 f_{j+2}$	$-a_2$	$-a_2(2h)$	$-a_2 \frac{(2h)^2}{2}$	$-a_2 \frac{(2h)^3}{6}$

- ▶ the leftmost column contains the terms present in the expression for the approximation error
 - ▶ the corresponding rows (multiplied by the top row) represent the terms obtained from expansions about x_j
 - ▶ columns represent terms with the same order in h — sums of columns are the contributions to the approximation error with the given order in h
- ▶ The coefficients a_p , $p = 0, 1, 2$ can now be chosen to cancel the contributions to the approximation error with the **lowest powers of h**

- ▶ Setting the coefficients of the first three terms to zero:

$$\begin{cases} -a_0 - a_1 - a_2 = 0 \\ -a_1 h - a_2(2h) = -1 \\ -a_1 \frac{h^2}{2} - a_2 \frac{(2h)^2}{2} = 0 \end{cases} \implies a_0 = -\frac{3}{2h}, \quad a_1 = \frac{2}{h}, \quad a_2 = -\frac{1}{2h}$$

- ▶ The resulting formula:

$$\left(\frac{\delta f}{\delta x}\right)_j = \frac{-f_{j+2} + 4f_{j+1} - 3f_j}{2h}$$

- ▶ The approximation error — determined the evaluating the first column with non-zero coefficient:

$$\left(-a_1 \frac{h^3}{6} - a_2 \frac{(2h)^3}{6}\right) f_j''' = \frac{h^2}{3} f_j'''$$

The formula is thus **SECOND-ORDER ACCURATE**

- ▶ An alternative derivation of a finite-difference scheme:
 - ▶ Find an N -th order accurate interpolating function $p(x)$ which interpolates the function $f(x)$ at the nodes x_j , $j = 1, \dots, N$, i.e., such that $p(x_j) = f(x_j)$, $j = 1, \dots, N$
 - ▶ Differentiate the interpolating function $p(x)$ and evaluate at the nodes to obtain an approximation of the derivative $p'(x_j) \approx f'(x_j)$, $j = 1, \dots, N$

- ▶ Example:
 - ▶ for $j = 2, \dots, N - 1$, let the interpolant have the form of a quadratic polynomial $p_j(x)$ on $[x_{j-1}, x_{j+1}]$ (Lagrange interpolating polynomial)

$$p_j(x) = \frac{(x - x_j)(x - x_{j+1})}{2h^2} f_{j-1} + \frac{-(x - x_{j-1})(x - x_{j+1})}{h^2} f_j + \frac{(x - x_{j-1})(x - x_j)}{2h^2} f_{j+1}$$

$$p'_j(x) = \frac{(2x - x_j - x_{j+1})}{2h^2} f_{j-1} + \frac{-(2x - x_{j-1} - x_{j+1})}{h^2} f_j + \frac{(2x - x_{j-1} - x_j)}{2h^2} f_{j+1}$$

- ▶ Evaluating at $x = x_j$ we obtain $f'(x_j) \approx p'_j(x_j) = \frac{f_{j+1} - f_{j-1}}{2h}$ (i.e., second-order accurate center-difference formula)

- ▶ Generalization to higher-orders straightforward
- ▶ Example:
 - ▶ for $j = 3, \dots, N - 2$, one can use a fourth-order polynomial as interpolant $p_j(x)$ on $[x_{j-2}, x_{j+2}]$
 - ▶ Differentiating with respect to x and evaluating at $x = x_j$ we arrive at the fourth-order accurate finite-difference formula

$$\left(\frac{\delta f}{\delta x}\right)_j = \frac{-f_{j+2} + 8f_{j+1} - 8f_{j-1} + f_{j-2}}{12h}, \quad \text{Err} = \frac{h^4}{30} f^{(v)}$$

- ▶ Order of accuracy of the finite-difference formula is **one less** than the order of the interpolating polynomial
- ▶ The set of grid points needed to evaluate a finite-difference formula is called **STENCIL**
- ▶ In general, higher-order formulas have larger stencils

Subtractive Cancellation Errors

- ▶ **SUBTRACTIVE CANCELLATION ERRORS** — when comparing two numbers which are almost the same using **finite-precision arithmetic**, the relative round-off error is proportional to the inverse of the difference between the two numbers
- ▶ Thus, if the difference between the two numbers is decreased by an order of magnitude, the relative accuracy with which this difference may be calculated using **finite-precision arithmetic** is also decreased by an order of magnitude.
- ▶ Problems with finite difference formulae when $h \rightarrow 0$ — loss of precision due to finite-precision arithmetic (**SUBTRACTIVE CANCELLATION**), e.g., for double precision:

$$1.0000000000012345 - 1.0 \approx 1.2e - 12 \quad (2.8\% \text{ error})$$

$$1.0000000000001234 - 1.0 \approx 1.0e - 13 \quad (19.0\% \text{ error})$$

...

- ▶ Consider the complex extension $f(z)$, where $z = x + iy$, of $f(x)$ and compute the complex Taylor series expansion

$$f(x_j + ih) = f_j + ihf'_j - \frac{h^2}{2}f''_j - i\frac{h^3}{6}f'''_j + \mathcal{O}(h^4)$$

Need to assume that $f(z)$ is **ANALYTIC** ! Then $f' = \frac{df(z)}{dz}$

- ▶ Take **imaginary** part and divide by h

$$f'_j = \frac{\Im(f(x_j + ih))}{h} + \frac{h^2}{6}f'''_j + \mathcal{O}(h^3) \implies \left(\frac{\delta f}{\delta x}\right)_j = \frac{\Im(f(x_j + ih))}{h}$$

- ▶ Note that the scheme is **second order accurate** — where is conservation of complexity?
- ▶ The method doesn't suffer from cancellation errors, is easy to implement and quite useful
- ▶ REFERENCE:
 - ▶ J. N. Lyness and C. B. Moler, "Numerical differentiation of analytical functions", *SIAM J. Numer. Anal.* **4**, 202-210, (1967)