MATH 3Q03: Differentiation with Finite Differences

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Agenda

- 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

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

- 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

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

- 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:

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

- 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

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

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 :

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

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

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

- Central difference formula for the second derivative:

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

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

- 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

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

- 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:

$$1.00000000000012345 - 1.0 \approx 1.2e - 12 \qquad (2.8\% \text{ error})$$

$$1.000000000000001234 - 1.0 \approx 1.0e - 13 \qquad (19.0\% \text{ error})$$

...

- 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

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

- 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)