WELCOME TO MATH 745 –
– TOPICS IN NUMERICAL ANALYSIS

Instructor: Dr. Bartosz Protas

Department of Mathematics & Statistics

Email: bprotas@mcmaster.ca

Office HH 326, Ext. 24116

Course Webpage: http://www.math.mcmaster.ca/~bprotas/MATH745

REVIEW OF NUMERICAL DIFFERENTIATION — FINITE DIFFERENCE FORMULAE I

- Approximation of derivatives $\frac{df}{dx}$ on a discrete set of points $x_0, x_1, \dots, x_N$
- Definitions & Assumptions:
  - $f_j = f(x_j)$
  - uniform mesh with constant grid spacing $h = x_{j+1} - x_j$
    (extensions to nonuniform grids are straightforward)
- Derivation of finite difference formulae is based on Taylor–series expansions of the following form:

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

Finite Difference Formulae (II) — Forward–difference formula

- Rearrange the Taylor series expansion

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

$O(h^\alpha)$ denotes the contribution from all terms with powers of h greater or equal α.

- Neglecting $O(h)$, we obtain the first order forward–difference formula :

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

- Neglected term with the lowest power of h is the leading–order error
- Exponent of h in the leading–order error represents the order of accuracy of the method
- Here: $Err = -\frac{h}{2} f''_j$, hence this method is first order accurate

Finite Difference Formulae (III) — Backward Difference Formula

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

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

Finite Difference Formulae (IV) — Higher Order Formulae

- Consider two expansions:

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

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

- Subtracting the second from the first:

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

- Central Difference Formula

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

- 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 :

$$\left(\frac{\delta f}{\delta x}\right)_j = \frac{-f_{j+2} + 8 f_{j+1} - 8 f_{j-1} + f_{j-2}}{12h}$$

FINITE DIFFERENCE FORMULAE (V) — APPROXIMATION OF THE SECOND DERIVATIVE

- Consider two expansions:

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

- Adding the two expansions

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

- Central difference formula for the second derivative:

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

- Leading–order error is $\frac{h^2}{12} f^{iv}_j$, thus the method is second–order accurate

FINITE DIFFERENCE FORMULAE (VI) — 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 $\sum_{p=0}^{2} \alpha_p f_{j+p}$, where the coefficients $\alpha_p,\ p = 0,1,2$ are to be determined.
- Form an expression for the approximation error

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

and expand it about x_j in the powers of h

FINITE DIFFERENCE FORMULAE (VII) — TAYLOR TABLE

- 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 $\alpha_p,\ p = 0,1,2$ can now be chosen to cancel the contributions to the approximation error with the lowest powers of h

FINITE DIFFERENCE FORMULAE (VIII) — TAYLOR TABLE

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

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

- 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

FINITE DIFFERENCE FORMULAE (IX) — 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 $h \to 0$ — less of precision due to finite–precision arithmetic (subtractive cancellation), e.g., for double precision:

$$1.000000000000001 - 1 \sim 0$$

Finite Difference Formulae (X) — Complex Step Derivative[a]

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

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

- Take imaginary part and divide by h

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

- 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

---

[a] J. N. Lyness and C. B.Moler, "Numerical differentiation of analytical functions", *SIAM J. Numer Anal* **4**, 202-210, (1967)

Finite Difference Formulae (XI) — Padé Approximation

- General Idea — include in the finite–difference formula not only the function values , but also the values of the function derivative at the adjacent nodes, e.g.:

$$b_{-1} f'_{j-1} + f'_j + b_1 f'_{j+1} - \sum_{p=-1}^{1} \alpha_p f_{j+p} = \varepsilon$$

- Construct the Taylor table using the following expansions:

$$f_{j+1} = f_j + h f'_j + \frac{h^2}{2} f''_j + \frac{h^3}{6} f'''_j + \frac{h^4}{24} f^{(iv)}_j + \frac{h^5}{120} f^{(v)}_j + \dots$$

$$f'_{j+1} = f'_j + h f''_j + \frac{h^2}{2} f'''_j + \frac{h^3}{6} f^{(iv)}_j + \frac{h^4}{24} f^{(v)}_j + \dots$$

NOTE — need an expansion for the derivative and a higher order expansion for the function (more coefficient to determine)

Finite Difference Formulae (XII) — Padé Approximation

- The Taylor table

	f_j	f'_j	f''_j	f'''_j	$f_j^{(iv)}$	$f_j^{(v)}$
$b_{-1} f'_{j-1}$	0	b_{-1}	$b_{-1}(-h)$	$b_{-1}\frac{(-h)^2}{2}$	$b_{-1}\frac{(-h)^3}{6}$	$b_{-1}\frac{(-h)^4}{24}$
f'_j	0	1	0	0	0	0
$b_1 f'_{j+1}$	0	b_1	$b_1 h$	$b_1\frac{h^2}{2}$	$b_1\frac{h^3}{6}$	$b_1\frac{h^4}{24}$
$-a_{-1} f_{j-1}$	$-a_{-1}$	$-a_{-1}(-h)$	$-a_{-1}\frac{(-h)^2}{2}$	$-a_{-1}\frac{(-h)^3}{6}$	$-a_{-1}\frac{(-h)^4}{24}$	$-a_{-1}\frac{(-h)^5}{120}$
$-a_0 f_j$	$-a_0$	0	0	0	0	0
$-a_1 f_{j+1}$	$-a_1$	$-a_1 h$	$-a_1\frac{h^2}{2}$	$-a_1\frac{h^3}{6}$	$-a_1\frac{h^4}{24}$	$-a_1\frac{h^5}{120}$

- The algebraic system:

$$\begin{bmatrix} 0 & 0 & -1 & -1 & -1 \\ 1 & 1 & h & 0 & -h \\ -h & h & -h^2/2 & 0 & -h^2/2 \\ h^2/2 & h^2/2 & h^3/6 & 0 & -h^3/6 \\ -h^3/6 & h^3/6 & -h^4/24 & 0 & -h^4/24 \end{bmatrix} \begin{bmatrix} b_{-1} \\ b_1 \\ a_{-1} \\ a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \Longrightarrow \begin{bmatrix} b_{-1} \\ b_1 \\ a_{-1} \\ a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} 1/4 \\ 1/4 \\ 3/(4h) \\ 0 \\ -3/(4h) \end{bmatrix}$$

Finite Difference Formulae (XIII) — Padé Approximation

- The Padé approximation:

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

  Leading–order error $\frac{h^4}{30} f_j^{(v)}$ (fourth–order accurate)

- The approximation is nonlocal , in that it requires derivatives at the adjacent nodes which are also unknowns; Thus all derivatives must be determined at once via the solution of the following algebraic system

$$\begin{bmatrix} \ddots & \ddots & \ddots & & \\ 1/4 & 1 & 1/4 & & \\ & \ddots & \ddots & \ddots & \end{bmatrix} \begin{bmatrix} \vdots \\ \left(\frac{\delta f}{\delta x}\right)_{j-1} \\ \left(\frac{\delta f}{\delta x}\right)_{j} \\ \left(\frac{\delta f}{\delta x}\right)_{j+1} \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \vdots \\ \frac{3}{4h}\left(f_{j+1} - f\, j - 1\right) \\ \vdots \\ \vdots \end{bmatrix}$$

- Closing the system at endpoints — use a lower–order one–sided (i.e., forward or backward) finite–difference formula

Finite Difference Formulae (XIV) — Modified Wavenumber Analysis

- Finite–Difference formulae applied to the Fourier mode $f(x) = e^{ikx}$ with the (exact) derivative $f(x) = ike^{ikx}$
- Central–Difference formula:

$$\left(\frac{\delta f}{\delta x}\right)_j = \frac{f_{j+1} - f_{j-1}}{2h} = \frac{e^{ik(x_j+h)} - e^{ik(x_j-h)}}{2h} = \frac{e^{ikh} - e^{-ikh}}{2h} e^{ikx_j} = i\frac{\sin(hk)}{h} f_j = ik' f_j,$$

where the modified wavenumber $k' \triangleq \frac{\sin(hk)}{h}$

- Comparison of the modified wavenumber k' with the actual wavenumber k shows how numerical differentiation errors affect different Fourier components of a given function

Finite Difference Formulae (XV) — Modified Wavenumber Analysis

- Fourth-order central difference formula

$$\left(\frac{\delta f}{\delta x}\right)_j = \frac{-f_{j+2}+8f_{j+1}-8f_{j-1}+f_{j-2}}{12h} = \frac{2}{3h}\left(e^{ikh}-e^{-ikh}\right)f_j - \frac{1}{12h}\left(e^{ik2h}-e^{-ik2h}\right)f_j$$

$$= i\left[\frac{4}{3h}\sin(hk) - \frac{1}{6h}\sin(2hk)\right]f_j = ik' f_j$$

where the modified wavenumber $k' \triangleq \left[\frac{4}{3h}\sin(hk) - \frac{1}{6h}\sin(2hk)\right]$

- Fourth–order Padé scheme:

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

where $\left(\frac{\delta f}{\delta x}\right)_{j+1} = ik'e^{ikx_{j+1}} = ik'e^{ikh}f_j$ and $\left(\frac{\delta f}{\delta x}\right)_{j-1} = ik'e^{ikx_{j-1}} = ik'e^{-ikh}f_j$.

Thus

$$ik'\left(\frac{1}{4}e^{ikh}+1+\frac{1}{4}e^{-ikh}\right)f_j = \frac{3}{4h}\left(e^{ikh}-e^{-ikh}\right)f_j$$

$$ik'\left(1+\frac{1}{2}\cos(kh)\right)f_j = i\frac{3}{2h}\sin(hk)f_j \implies k' \triangleq \frac{3\sin(hk)}{2h+h\cos(hk)}$$