WELCOME TO MATH 745 – – TOPICS IN NUMERICAL ANALYSIS

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INTRODUCTION

- What is NUMERICAL ANALYSIS ?
  - Development of COMPUTATIONAL ALGORITHMS for solutions of problems in algebra and analysis
  - Use of methods of MATHEMATICAL ANALYSIS to determine a priori properties of these algorithms such as:
    * ACCURACY,
    * STABILITY,
    * CONVERGENCE
  - Application of these algorithms to solve actual problems arising in practice

PART I

Finite Differences

A Review

Differentiation via Finite Differences Basics[a] (I)

- Assumptions :
  - $f : \Omega \to \mathbb{R}$ 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 $\frac{df}{dx}(x_j) = f'(x_j)$, $j = 1, \dots, N$

[a] Details can be found in any standard textbook on elementary numerical analysis, e.g., K. Atkinson and W. Han, "Elementary Numerical Analysis", Wiley, (2004).

Differentiation via Finite Differences Basics (II)

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

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

- Rearrange the expansion

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

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

- Neglecting $O(h)$, we obtain a FIRST ORDER FORWARD–DIFFERENCE FORMULA :

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

DIFFERENTIATION VIA FINITE DIFFERENCES BASICS (III)

- 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

Differentiation via Finite Differences
Higher–Order Formula (I)

- 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

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

- 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 :

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

Differentiation via Finite Differences
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

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

- Central difference formula for the second derivative:

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

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

Differentiation via Finite Differences An alternative approach (I)

- 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)

Differentiation via Finite Differences An alternative approach (II)

- 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

DIFFERENTIATION VIA FINITE DIFFERENCES TAYLOR TABLE (I)

- 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

DIFFERENTIATION VIA FINITE DIFFERENCES
TAYLOR TABLE (II)

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

DIFFERENTIATION VIA FINITE DIFFERENCES
TAYLOR TABLE (III)

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

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

- 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

DIFFERENTIATION VIA FINITE DIFFERENCES AN OPERATOR PERSPECTIVE (I)

- Quick review of FUNCTIONAL ANALYSIS background
  - NORMED SPACES X: $\exists \|\cdot\| : X \to \mathbb{R}$ such that $\forall x, y \in X$

$$\begin{aligned} &\|x\| \geq 0, \\ &\|x+y\| \leq \|x\| + \|y\|, \\ &\|x\| = 0 \Leftrightarrow x \equiv 0 \end{aligned}$$

  - Banach spaces
  - vector spaces: finite–dimensional ($\mathbb{R}^N$) vs. infinite–dimensional (l_p)
  - function spaces (on $\Omega \subseteq \mathbb{R}^N$): Lebesgue spaces $L_p(\Omega)$, Sobolev spaces $W^{p,q}(\Omega)$
  - Hilbert spaces: inner products, orthogonality & projections, bases, etc.
  - Linear Operators: operator norms, functionals, Riesz' Theorem

DIFFERENTIATION VIA FINITE DIFFERENCES AN OPERATOR PERSPECTIVE (II)

- Assume that f and f' belong to a function space X; DIFFERENTIATION $\frac{d}{dx} : f \rightarrow f'$ can then be regarded as a LINEAR OPERATOR $\frac{d}{dx} : X \rightarrow X$
- When f and f' are approximated by their nodal values as $\mathbf{f} = [f_1 \; f_2 \; \dots \; f_N]^T$ and $\mathbf{f}' = [f'_1 \; f'_2 \; \dots \; f'_N]^T$, then the differential operator $\frac{d}{dx}$ can be approximated by a DIFFERENTIATION MATRIX $\mathbb{A} \in \mathbb{R}^{N \times N}$ such that $\mathbf{f}' = \mathbb{A}\mathbf{f}$; How can we determine this matrix?
- Assume for simplicity that the domain Ω is periodic, i.e., $f_0 = f_N$ and $f_1 = f_{N+1}$; then differentiation with the second–order center difference formula can be represented as the following matrix–vector product

$$\begin{bmatrix} f'_1 \\ \\ \vdots \\ \\ f'_N \end{bmatrix} = \frac{1}{h} \begin{bmatrix} 0 & \frac{1}{2} & & & -\frac{1}{2} \\ -\frac{1}{2} & 0 & & & \\ & \ddots & \ddots & \ddots & \\ & & & 0 & \frac{1}{2} \\ -\frac{1}{2} & & & -\frac{1}{2} & 0 \end{bmatrix} \begin{bmatrix} f_1 \\ \\ \vdots \\ \\ f_N \end{bmatrix}$$

DIFFERENTIATION VIA FINITE DIFFERENCES AN OPERATOR PERSPECTIVE (III)

- Using the fourth–order center difference formula we would obtain a pentadiagonal system $\Rightarrow$ increased order of accuracy entails increased bandwidth of the differentiation matrix $\mathbb{A}$
- $\mathbb{A}$ is a TOEPLITZ MATRIX , since is has constant entries along the the diagonals; in fact, it a also a CIRCULANT MATRIX with entries a_{ij} depending only on $(i-j)(\mathrm{mod}\,N)$
- Note that the matrix $\mathbb{A}$ defined above is SINGULAR (has a zero eigenvalue $\lambda = 0$) —Why?
- This property is in fact inherited from the original "continuous" operator $\frac{d}{dx}$ which is also singular and has a zero eigenvalue
- A singular matrix $\mathbb{A}$ does not have an inverse (at least, now in the classical sense); what can we do to get around this difficulty?

Differentiation via Finite Differences An operator perspective (IV)

- Matrix singularity $\Leftrightarrow$ linearly dependent rows $\Leftrightarrow$ the LHS vector does not contain enough information to determine UNIQUELY the RHS vector
- MATRIX DESINGULARIZATION —incorporating additional information into the matrix, so that its argument (the RHS vector) can be determined uniquely
- Example —desingularization of the second–order center difference differentiation matrix:
  - in a center difference formula, even and odd nodes are decoupled
  - knowing f'_j, $j = 1, \dots, N$ and f_1, one can recover f_j, $j = 3, 5, \dots$ (i.e., the odd nodes) only $\Rightarrow$ f_2 must also be provided
  - hence, the zero eigenvalue has multiplicity two
  - when desingularizing the differentiation matrix one must modify at least two rows (see, e.g., `sing_diff_mat_01.m`)

DIFFERENTIATION VIA FINITE DIFFERENCES AN OPERATOR PERSPECTIVE (V)

- What is WRONG with the differentiation operator?
- The differentiation operator $\frac{d}{dx}$ is UNBOUNDED !
  One usually cannot find a constant $C \in \mathbb{R}$ independent of f, such that
  $$\left\| \frac{d}{dx} f(x) \right\|_X \le C \|f\|_X, \quad \forall_{f \in X}$$
  For instance, $f(x) = e^{ikx}$, so that $|C| = k \rightarrow \infty$ for $k \rightarrow \infty$ ...
- Unfortunately, finite–dimensional emulations of the differentiation operator (the DIFFERENTIATION MATRICES) inherit this property
- OPERATOR NORM for matrices

$$\|\mathbb{A}\|_2^2 = \max_{\|\mathbf{x}\|=1} \|\mathbb{A}\mathbf{x}\|_2^2 = \max_{\mathbf{x}} \frac{(\mathbb{A}\mathbf{x}, \mathbb{A}\mathbf{x})}{(\mathbf{x}, \mathbf{x})} = \max_{\mathbf{x}} \frac{(\mathbf{x}, \mathbb{A}^T \mathbb{A}\mathbf{x})}{(\mathbf{x}, \mathbf{x})} = \lambda_{max}(\mathbb{A}^T \mathbb{A}) = \sigma_{max}^2(\mathbb{A})$$

Thus, the 2–norm of a matrix is given by the square root of its largest SINGULAR VALUE $\sigma_{max}(\mathbb{A})$

DIFFERENTIATION VIA FINITE DIFFERENCES AN OPERATOR PERSPECTIVE (VI)

- As can be rigorously proved in many specific cases, $\|\mathbb{A}\|_2$ grows without bound as $N \to \infty$ (or, $h \to 0$) $\Rightarrow$ this is a reflection of the unbounded nature of the underlying ∞–dim operator

- The loss of precision when solving the system $\mathbb{A}\mathbf{x} = \mathbf{b}$ is characterized by the CONDITION NUMBER (with respect to inversion) $\kappa_p(\mathbb{A}) = \|\mathbb{A}\|_p \|\mathbb{A}^{-1}\|_p$
  - for $p = 2$, $\kappa_2(\mathbb{A}) = \frac{\sigma_{max}(\mathbb{A})}{\sigma_{min}(\mathbb{A})}$
  - when the condition number is “large”, the matrix is said to be ILL–CONDITIONED —solution of the system $\mathbb{A}\mathbf{x} = \mathbf{b}$ is prone to round–off errors
  - if $\mathbb{A}$ is singular, $\kappa_p(\mathbb{A}) = +\infty$

Differentiation via Finite Differences
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 $h \to 0$ —loss of precision due to finite–precision arithmetic(SUBTRACTIVE CANCELLATION), e.g., for double precision:

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

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

$$\ldots$$

DIFFERENTIATION VIA FINITE DIFFERENCES 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)

DIFFERENTIATION VIA FINITE DIFFERENCES PADÉ APPROXIMATION (I)

- 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)

DIFFERENTIATION VIA FINITE DIFFERENCES
PADÉ APPROXIMATION (II)

- 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:

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

DIFFERENTIATION VIA FINITE DIFFERENCES PADÉ APPROXIMATION (III)

- 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

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

DIFFERENTIATION VIA FINITE DIFFERENCES PADÉ APPROXIMATION (IV)

- Closing the system at ENDPOINTS (where neighbors are not available) — use a lower–order one–sided (i.e., forward or backward) finite–difference formula

- The vector of derivatives can thus be obtained via solution of the following algebraic system

$$\mathbb{B}\,\mathbf{f}' = \frac{3}{2}\mathbb{A}\,\mathbf{f} \quad \Longrightarrow \quad \mathbf{f}' = \frac{3}{2}\mathbb{B}^{-1}\,\mathbb{A}\,\mathbf{f}$$

  where

  – $\mathbb{B}$ is a tri–diagonal matrix with $b_{i,i} = 1$ and $b_{i,i-1} = b_{i,i+1} = \frac{1}{4}$, $i = 1, \ldots, N$

  – $\mathbb{A}$ is a second–order accurate differentiation matrix

Differentiation via Finite Differences Modified Wavenumber Analysis (I)

- How do finite differences perform at different WAVELENGTHS ?
- 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

Differentiation via Finite Differences Modified Wavenumber Analysis (II)

- 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:

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

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