

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** :
 - $f : \Omega \rightarrow \mathbb{R}$ 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**

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

^aDetails 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**

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

- Rearrange the expansion

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

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:

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

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

- Subtracting the second from the first:

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

- Central Difference Formula**

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

- 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** :

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

DIFFERENTIATION VIA FINITE DIFFERENCES 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

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

- Central difference formula for the second derivative:

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

- The leading-order error is $\frac{h^2}{12}f^{(iv)}_j$, 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

$$\left(\frac{\delta f}{\delta x}\right)_j = \frac{-f_{j+2} + 8f_{j+1} - 8f_{j-1} + f_{j-2}}{12h}, \quad Err = \frac{h^4}{30} f^{(v)}$$
- 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 $\alpha_p, p = 0, 1, 2$ 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:

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

- 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**

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

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

DIFFERENTIATION VIA FINITE DIFFERENCES AN OPERATOR PERSPECTIVE (I)

- Quick review of **FUNCTIONAL ANALYSIS** background
 - NORMED SPACES** X : $\exists \|\cdot\| : X \rightarrow \mathbb{R}$ 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 (III)

- Using the fourth-order center difference formula we would obtain a **pentadiagonal system** \implies increased order of accuracy entails increased bandwidth of the differentiation matrix \mathbb{A}
- \mathbb{A} is a **TOEPLITZ MATRIX**, since it has constant entries along the diagonals; in fact, it is also a **CIRCULANT MATRIX** with entries a_{ij} depending only on $(i-j) \pmod N$
- 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

$$\left\| \frac{d}{dx} f(x) \right\|_X \leq C \|f\|_X, \quad \forall f \in X$$

For instance, $f(x) = e^{ikx}$, so that $|C| = k \rightarrow \infty$ for $k \rightarrow \infty \dots$

- 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 $N \rightarrow \infty$ (or, $h \rightarrow 0$) \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 $h \rightarrow 0$ —loss of precision due to finite-precision arithmetic (**SUBTRACTIVE CANCELLATION**), e.g., for double precision:

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

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

...

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

^aJ. 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.:

$$b_{-1}f'_{j-1} + f'_j + b_1f'_{j+1} - \sum_{p=-1}^1 \alpha_p f_{j+p} = \varepsilon$$

- Construct the **Taylor table** using the following expansions:

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

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

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	$f^{(iv)}_j$	$f^{(v)}_j$
$b_{-1}f'_{j-1}$	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
$b_1f'_{j+1}$	0	b_1	b_1h	$b_1\frac{h^2}{2}$	$b_1\frac{h^3}{6}$	$b_1\frac{h^4}{24}$
$-a_{-1}f_{j-1}$	$-a_{-1}$	$-a_{-1}(-h)$	$-a_{-1}\frac{(-h)^2}{2}$	$-a_{-1}\frac{(-h)^3}{6}$	$-a_{-1}\frac{(-h)^4}{24}$	$-a_{-1}\frac{(-h)^5}{120}$
$-a_0f_j$	$-a_0$	0	0	0	0	0
$-a_1f_{j+1}$	$-a_1$	$-a_1h$	$-a_1\frac{h^2}{2}$	$-a_1\frac{h^3}{6}$	$-a_1\frac{h^4}{24}$	$-a_1\frac{h^5}{120}$

- The algebraic system:

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

DIFFERENTIATION VIA FINITE DIFFERENCES PADÉ APPROXIMATION (III)

- The Padé approximation:

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

Leading-order error $\frac{h^4}{30}f^{(v)}_j$ (**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

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

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

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

where

- \mathbb{B} is a tri-diagonal matrix with $b_{i,i} = 1$ and $b_{i,i-1} = b_{i,i+1} = \frac{1}{4}$, $i = 1, \dots, N$
- \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 $f'(x) = ik e^{ikx}$
- 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

$$\begin{aligned} \left(\frac{\delta f}{\delta x}\right)_j &= \frac{-f_{j+2} + 8f_{j+1} - 8f_{j-1} + f_{j-2}}{12h} = \frac{2}{3h} (e^{ikh} - e^{-ikh}) f_j - \frac{1}{12h} (e^{ik2h} - e^{-ik2h}) f_j \\ &= i \left[\frac{4}{3h} \sin(hk) - \frac{1}{6h} \sin(2hk) \right] f_j = ik' f_j \end{aligned}$$

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

- Fourth-order Padé scheme:

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

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:

$$\begin{aligned} ik' \left(\frac{1}{4} e^{ikh} + 1 + \frac{1}{4} e^{-ikh} \right) f_j &= \frac{3}{4h} (e^{ikh} - e^{-ikh}) f_j \\ ik' \left(1 + \frac{1}{2} \cos(kh) \right) f_j &= i \frac{3}{2h} \sin(hk) f_j \implies k' \triangleq \frac{3 \sin(hk)}{2h + h \cos(hk)} \end{aligned}$$