Lecture 2

MTH572/MTH472
Numerical Methods for PDEs
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Main references (quotes):
Trefethen: NumPDE, ATAP, Spectral Methods in MATLAB
Fornberg: PS Guide
Leveque: NumPDE
Driscoll: Learning MATLAB

Differentiating Lagrange Interpolant:

Goal: Compute FD weights by differentiating Lagrange interpolant (review your MTH361 course).

- interpolate data at stencil nodes
- differentiate the interpolant

Example: 3-point stencil

Data (function values) at stencil locations are interpolated by a polynomial of degree 2 (2-nd order accurate):

$$\boxed{u(x) = \ell_{j-1}(x)u_{j-1} + \ell_j(x)u_j + \ell_{j+1}(x)u_{j+1}.}$$

$\ell_k(x)$'s are Lagrange cardinal functions with conditions

$$\ell_k(x) = \begin{cases} 1 & x = x_k \\ 0 & x \neq x_m,\, m \neq k \end{cases},$$

at stencil nodes.

Construct and differentiate Lagrange cardinal functions

Construction:

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

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

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

Differentiation:

$$u'(x) = \ell'_{j-1}(x)u_{j-1} + \ell'_j(x)u_j + \ell'_{j+1}(x)u_{j+1}.$$

$$\ell'_{j-1}(x) = \frac{1}{2h^2}((x - x_j) + (x - x_{j+1}))$$

$$\ell'_j(x) = -\frac{1}{h^2}((x - x_{j-1}) + (x - x_{j+1}))$$

$$\ell'_{j+1}(x) = \frac{1}{2h^2}((x - x_{j-1}) + (x - x_j))$$

FD weights at stencil nodes

$$
\begin{aligned}
u'_{j-1} := u'(x_{j-1}) &= \ell'_{j-1}(x_{j-1})u_{j-1} + \ell'_j(x_{j-1})u_j + \ell'_{j+1}(x_{j-1})u_{j+1} \\
&= -\frac{3}{2h}u_{j-1} + \frac{2}{h}u_j - \frac{1}{2h}u_{j+1} \\
u'_j := u'(x_j) &= \ell'_{j-1}(x_j)u_{j-1} + \ell'_j(x_j)u_j + \ell'_{j+1}(x_j)u_{j+1} \\
&= -\frac{1}{2h}u_{j-1} + \frac{1}{2h}u_{j+1} \\
u'_{j+1} := u'(x_{j+1}) &= \ell'_{j-1}(x_{j+1})u_{j-1} + \ell'_j(x_{j+1})u_j + \ell'_{j+1}(x_{j+1})u_{j+1} \\
&= \frac{1}{2h}u_{j-1} - \frac{2}{h}u_j + \frac{3}{2h}u_{j+1}
\end{aligned}
$$

Assemble everything together in a matrix style

$$
\vec{u}' \approx \begin{bmatrix} u'_0 \\ u'_1 \\ u_2 \\ \vdots \\ u'_{n-1} \\ u'_n \end{bmatrix} = D\underline{u} = \frac{1}{2h}\begin{bmatrix} -3 & 4 & -1 & \cdots & 0 \\ -1 & 0 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 0 & 1 \\ 0 & \cdots & 1 & -4 & 3 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix}
$$

Fornberg (1988 MathComp, 1998 SIREV)

Weights (centered FD)

Order of derivative	Order of accuracy	−4	−3	−2	−1	0	1	2	3	4
		Approximations at $x = 0$; x-coordinates at nodes:								
0	∞					1				
1	2				$\frac{-1}{2}$	0	$\frac{1}{2}$			
	4			$\frac{1}{12}$	$\frac{-2}{3}$	0	$\frac{2}{3}$	$\frac{-1}{12}$		
	6		$\frac{-1}{60}$	$\frac{3}{20}$	$\frac{-3}{4}$	0	$\frac{3}{4}$	$\frac{-3}{20}$	$\frac{1}{60}$	
	8	$\frac{1}{280}$	$\frac{-4}{105}$	$\frac{1}{5}$	$\frac{-4}{5}$	0	$\frac{4}{5}$	$\frac{-1}{5}$	$\frac{4}{105}$	$\frac{-1}{280}$
2	2				1	−2	1			
	4			$\frac{-1}{12}$	$\frac{4}{3}$	$\frac{-5}{2}$	$\frac{4}{3}$	$\frac{-1}{12}$		
	6		$\frac{1}{90}$	$\frac{-3}{20}$	$\frac{3}{2}$	$\frac{-49}{18}$	$\frac{3}{2}$	$\frac{-3}{20}$	$\frac{1}{90}$	
	8	$\frac{-1}{560}$	$\frac{8}{315}$	$\frac{-1}{5}$	$\frac{8}{5}$	$\frac{-205}{72}$	$\frac{8}{5}$	$\frac{-1}{5}$	$\frac{8}{315}$	$\frac{-1}{560}$
3	2			$\frac{-1}{2}$	1	0	−1	$\frac{1}{2}$		
	4		$\frac{1}{8}$	−1	$\frac{13}{8}$	0	$\frac{-13}{8}$	1	$\frac{-1}{8}$	
	6	$\frac{-7}{240}$	$\frac{3}{10}$	$\frac{-169}{120}$	$\frac{61}{30}$	0	$\frac{-61}{30}$	$\frac{169}{120}$	$\frac{-3}{10}$	$\frac{7}{240}$
4	2			1	−4	6	−4	1		
	4		$\frac{-1}{6}$	2	$\frac{-13}{2}$	$\frac{28}{3}$	$\frac{-13}{2}$	2	$\frac{-1}{6}$	
	6	$\frac{7}{240}$	$\frac{-2}{5}$	$\frac{169}{60}$	$\frac{-122}{15}$	$\frac{91}{8}$	$\frac{-122}{15}$	$\frac{169}{60}$	$\frac{-2}{5}$	$\frac{7}{240}$

Weights (one-sided FD)

Order of derivative	Order of accuracy	0	1	2	3	4	5	6	7	8
		Approximations at $x = 0$; x-coordinates at nodes:								
0	∞	1								
1	1	−1	1							
	2	$\frac{-3}{2}$	2	$\frac{-1}{2}$						
	3	$\frac{-11}{6}$	3	$\frac{-3}{2}$	$\frac{1}{3}$					
	4	$\frac{-25}{12}$	4	−3	$\frac{4}{3}$	$\frac{-1}{4}$				
	5	$\frac{-137}{60}$	5	−5	$\frac{10}{3}$	$\frac{-5}{4}$	$\frac{1}{5}$			
	6	$\frac{-49}{20}$	6	$\frac{-15}{2}$	$\frac{20}{3}$	$\frac{-15}{4}$	$\frac{6}{5}$	$\frac{-1}{6}$		
	7	$\frac{-363}{140}$	7	$\frac{-21}{2}$	$\frac{35}{3}$	$\frac{-35}{4}$	$\frac{21}{5}$	$\frac{-7}{6}$	$\frac{1}{7}$	
	8	$\frac{-761}{280}$	8	−14	$\frac{56}{3}$	$\frac{-35}{2}$	$\frac{56}{5}$	$\frac{-14}{3}$	$\frac{8}{7}$	$\frac{-1}{8}$
2	1	1	−2	1						
	2	2	−5	4	−1					
	3	$\frac{35}{12}$	$\frac{-26}{3}$	$\frac{19}{2}$	$\frac{-14}{3}$	$\frac{11}{12}$				
	4	$\frac{15}{4}$	$\frac{-77}{6}$	$\frac{107}{6}$	−13	$\frac{61}{12}$	$\frac{-5}{6}$			
	5	$\frac{203}{45}$	$\frac{-87}{5}$	$\frac{117}{4}$	$\frac{-254}{9}$	$\frac{33}{2}$	$\frac{-27}{5}$	$\frac{137}{180}$		
	6	$\frac{469}{90}$	$\frac{-223}{10}$	$\frac{879}{20}$	$\frac{-949}{18}$	41	$\frac{-201}{10}$	$\frac{1019}{180}$	$\frac{-7}{10}$	
	7	$\frac{29531}{5040}$	$\frac{-962}{35}$	$\frac{621}{10}$	$\frac{-4006}{45}$	$\frac{691}{8}$	$\frac{-282}{5}$	$\frac{2143}{90}$	$\frac{-206}{35}$	$\frac{363}{560}$
3	1	−1	3	−3	1					
	2	$\frac{-5}{2}$	9	−12	7	$\frac{-3}{2}$				
	3	$\frac{-17}{4}$	$\frac{71}{4}$	$\frac{-59}{2}$	$\frac{49}{2}$	$\frac{-41}{4}$	$\frac{7}{4}$			
	4	$\frac{-49}{8}$	29	$\frac{-461}{8}$	62	$\frac{-307}{8}$	13	$\frac{-15}{8}$		
	5	$\frac{-967}{120}$	$\frac{638}{15}$	$\frac{-3929}{40}$	$\frac{389}{3}$	$\frac{-2545}{24}$	$\frac{268}{5}$	$\frac{-1849}{120}$	$\frac{29}{15}$	
	6	$\frac{-801}{80}$	$\frac{349}{6}$	$\frac{-18353}{120}$	$\frac{2391}{10}$	$\frac{-1457}{6}$	$\frac{4891}{30}$	$\frac{-561}{8}$	$\frac{527}{30}$	$\frac{-469}{240}$
4	1	1	−4	6	−4	1				
	2	3	−14	26	−24	11	−2			
	3	$\frac{35}{6}$	−31	$\frac{137}{2}$	$\frac{-242}{3}$	$\frac{107}{2}$	−19	$\frac{17}{6}$		
	4	$\frac{28}{3}$	$\frac{-111}{2}$	142	$\frac{-1219}{6}$	176	$\frac{-185}{2}$	$\frac{82}{3}$	$\frac{-7}{2}$	
	5	$\frac{1069}{80}$	$\frac{-1316}{15}$	$\frac{15289}{60}$	$\frac{-2144}{5}$	$\frac{10993}{24}$	$\frac{-4772}{15}$	$\frac{2803}{20}$	$\frac{-536}{15}$	$\frac{967}{240}$

MATLAB/Mathematica code to generate FD weights on 1-D arbitrarily spaced grids is available.

Infinite domain but not periodic case

Infinite dimensional matrix.

$$\vec{u}' \approx \begin{bmatrix} \vdots \\ u'_{j-2} \\ u'_{j-1} \\ u'_j \\ u'_{j+1} \\ u'_{j+2} \\ \vdots \end{bmatrix} = D\underline{u} = \frac{1}{2h} \begin{bmatrix} \ddots & \ddots & \ddots & \ddots & 0 \\ -1 & 0 & 1 & 0 & \ddots \\ \ddots & -1 & 0 & 1 & \ddots \\ \ddots & 0 & -1 & 0 & 1 \\ 0 & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ u_{j-2} \\ u_{j-1} \\ u_j \\ u_{j+1} \\ u_{j+2} \\ \vdots \end{bmatrix}$$

Note: Discretizing infinite domain with equally-spaced nodes gives DM with a special structure

- No one-sided weights
- Toeplitz matrix: having constant entries along diagonals.
- Convolution filter.

FD differentiation matrix as convolution filter

v(x): filter   u(x): signal (data)

	Continuous	Discrete
$(v * u)(x_m)$	$\int_{-\infty}^{\infty} v(x_m - y)u(y)dy$	$(v * u)_m = h \sum_{j=\infty}^{j=-\infty} v_{m-j}u_j$

assuming the integral exist.

Think the convolution as a weighted moving average of values u(x) with weights defined by v(x), or vice versa.

$$D\underline{u} := \frac{1}{h^2}(\cdots 0 \quad 0 \quad -\frac{1}{2} \quad 0 \quad \frac{1}{2} \quad 0 \quad 0 \cdots) * \underline{u}$$

In this case, data values $\underline{u}$ is a signal and the derivative operator is a convolution filter whose coefficients happen to be chosen so that it has the effect of differentiation.

Differentiation matrices for periodic cases

Infinite domain with periodic data values. Due to periodicity, x_0 coincides with x_n, no one sided weights.

$$\vec{u}' \approx \begin{bmatrix} u_0' \\ u_1' \\ u_2 \\ \vdots \\ u_{n-2}' \\ u_{n-1}' \end{bmatrix} = D\underline{u} = \frac{1}{2h} \begin{bmatrix} 0 & 1 & 0 & \cdots & -1 \\ -1 & 0 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 0 & 1 \\ 1 & \cdots & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{bmatrix}$$

Note: A special case of Toeplitz matrix

- Circulant matrix: entries d_{ij} depends on $(i-j)$ mod (n). In other words, the diagonals "wrap" around the matrix.
- PDE case: periodic boundary condition.

FD differentiation as Fourier multipliers

Circulant matrix decomposition

$$\frac{1}{2h}\begin{bmatrix} 0 & 1 & 0 & \cdots & -1 \\ -1 & 0 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 0 & 1 \\ 1 & \cdots & 0 & -1 & 0 \end{bmatrix} = \begin{bmatrix} d_0 & d_{n-1} & \cdots & d_2 & d_1 \\ d_1 & d_0 & d_{n-1} & & \vdots \\ \vdots & d_1 & d_0 & \ddots & \vdots \\ \vdots & & \ddots & \ddots & d_{n-1} \\ d_{n-1} & d_{n-2} & \cdots & d_1 & d_0 \end{bmatrix} = W^* F W$$

$$W = \frac{1}{\sqrt{n}}\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega & \omega^2 & \cdots & \omega^{n-1} \\ 1 & \omega^2 & \omega^4 & \cdots & \omega^{2(n-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{n-1} & \omega^{2(n-1)} & \cdots & \omega^{(n-1)(n-1)} \end{bmatrix}$$

$$F = \begin{bmatrix} f_0 & 0 & \cdots & 0 & 0 \\ 0 & f_1 & 0 & & 0 \\ \vdots & 0 & f_2 & \ddots & \vdots \\ 0 & & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & 0 & f_{n-1} \end{bmatrix}$$

$$\omega = e^{2\pi i/n}$$

$$f_j = \sum_{k=0}^{n-1} d_k \omega^{(k-1)(j-1)}$$

Solving BVP: Continuous - Discrete Analogy

A simple boundary value problem in 1-D

$$\frac{du}{dx} = f(x) \text{ for } x \in [a, b)$$
$$u(b) = g_n$$

Technique 1: Row Replacement

Step 1: Collocate the PDE all the way to the boundary

$$\frac{1}{2h}\begin{bmatrix} -3 & 4 & -1 & \cdots & 0 \\ -1 & 0 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 0 & 1 \\ 0 & \cdots & 1 & -4 & 3 \end{bmatrix}\begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_{n-1} \\ f_n \end{bmatrix}$$

Step 2: Replace/modify the corresponding row of boundary condition ($u_n = g_n$) at $x = b$.

Solving BVP: Continuous - Discrete Analogy

$$\frac{1}{2h}\begin{bmatrix} -3 & 4 & -1 & \cdots & 0 \\ -1 & 0 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 0 & 1 \\ 0 & \cdots & 0 & 0 & 2h \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_{n-1} \\ g_n \end{bmatrix}$$

Step 3: Solve the $(n+1) \times (n+1)$ system to obtain $u_0, u_1, \cdots, u_n$.

Technique 2: Strip rows and move over columns

Step 1: Collocate the PDE all the way to the boundaries as usual

$$-\frac{1}{2h}\begin{bmatrix} -3 & 4 & -1 & \cdots & 0 \\ -1 & 0 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 0 & 1 \\ 0 & \cdots & 1 & -4 & 3 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_{n-1} \\ f_n \end{bmatrix}$$

Solving BVP: Continuous - Discrete Analogy

Step 2: Strip the last row that corresponds to BC. Move the last column that is affected by BC value to the right hand side. Note that $u_n = g_n$.

$$\frac{1}{2h}\begin{bmatrix} -3 & 4 & -1 & \cdots & 0 \\ -1 & 0 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 0 & 1 \\ 0 & \cdots & 0 & -1 & 0 \end{bmatrix}\begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{bmatrix} = \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_{n-2} \\ f_{n-1} \end{bmatrix} - \frac{g_n}{2h}\begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}$$

Step 3: Solve the $n \times n$ system to obtain the unknowns $u_0, u_1, \cdots, u_{n-1}$.

> In some cases (depending on the problems and BCs), Strip Rows - Move Columns method gives a better structured system matrix due to the removal of weights corresponding to one-sided differences.

Things to do in class

1. Write the MATLAB code (with $n = 20$) to solve

$$\frac{du}{dx} = (\pi\cos(\pi x) - \sin(\pi x))e^{-x} \text{ for } x \in [-1, \tfrac{1}{2})$$
$$u(\tfrac{1}{2}) = e^{-\frac{1}{2}}$$

   using row replacement technique and strip row technique. Plot the numerical solution vs the exact solution $u(x) = e^{-x}\sin(\pi x)$ on the same figure. Compute $\|\cdot\|_\infty = |\underline{u} - \underline{u}_{exact}|_\infty$ to measure the error of numerical solution with respect the exact solution.

2. Using different values of $n = 10, 100, 1000, \cdots$, redo problem 1 and plot the $\|\cdot\|_\infty$ vs h in log scale. Do you observe 2^{nd}-order convergence (i.e. $\mathcal{O}(h^2)$ or $\mathcal{O}(n^{-2})$) ?

3. Use Fornberg's table to create the 2^{nd}-order convergence of 2^{nd} derivative differentiation matrix on an interval $[a, b]$ (discretized with equal spacing h). What is the size of the stencil ?