Lecture 3

MTH572/MTH472
Numerical Methods for PDEs

Alfa Heryudono

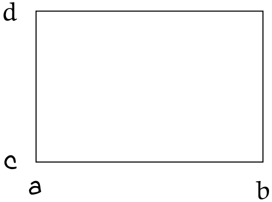
UMass Dartmouth

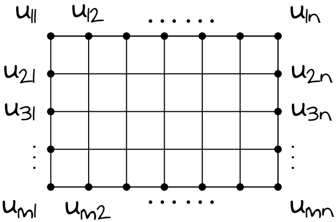
Main references (quotes):
Trefethen: NumPDE, ATAP, Spectral Methods in MATLAB
Fornberg: PS Guide
Leveque: NumPDE
Driscoll: Learning MATLAB

Rectangular Domain in 2-D

An example of a 2-D rectangular domain $a \le x \le b, c \le y \le d$.

Tensor Product Grid



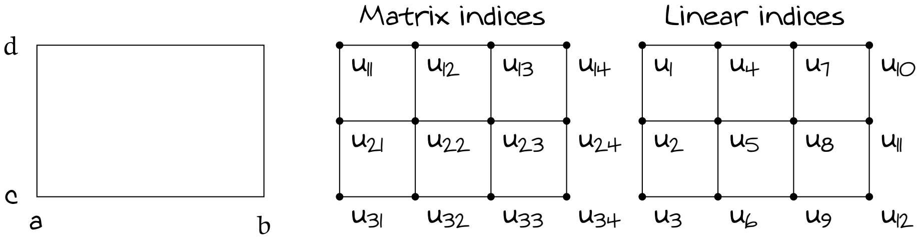


Solution values $\{u_{ij}\}$ can be stored in a matrix $\mathbf{U}$, which can also be "vectorized" by stacking the columns of $\mathbf{U}$ into a single column vector $\underline{u}$, i.e $\underline{u} = \mathrm{vec}(\mathbf{U})$.

$$\mathbf{U} = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ u_{21} & u_{22} & & u_{2n} \\ \vdots & & \ddots & \\ u_{m1} & u_{m2} & \cdots & u_{mn} \end{bmatrix}$$

In MATLAB, $\mathrm{vec}(\mathbf{U}) = \mathbf{U}(:)$

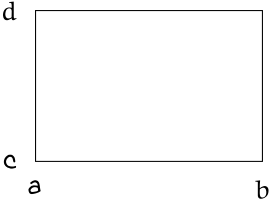
A Simple Example

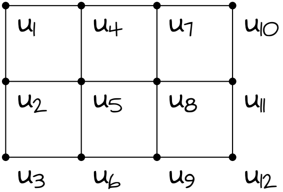


- Discretize x into $n = 4$ equally-spaced points with equal spacing $h_x = \frac{b-a}{n-1}$.
- Discretize y into $m = 3$ equally-spaced points with equal spacing h_y with equal spacing $h_y = \frac{d-c}{m-1}$.
- Entries of $\underline{u} = \text{vec}(\mathbf{U})$ is ordered using "lexicographic" ordering (linear index). Hence $\underline{u} = [u_1, \cdots, u_{12}]^T$.
- In MATLAB, conversion from linear index to "matrix indices" and vice versa can be done with the commands `ind2sub` and `sub2ind` respectively.

Differentiation Matrices

Differentiate x and y directions independently.





Derivatives with respect to y

Ex: 3-point stencil, 2-nd order accurate. Note that the prime $'$ here means partial derivative with respect to y.

$$\begin{bmatrix} u_1' & u_4' & u_7' & u_{10}' \\ u_2' & u_5' & u_8' & u_{11}' \\ u_3' & u_6' & u_9' & u_{12}' \end{bmatrix} \approx \frac{1}{2h_y} \begin{bmatrix} -3 & 4 & -1 \\ -1 & 0 & 1 \\ 1 & -4 & 3 \end{bmatrix} \begin{bmatrix} u_1 & u_4 & u_7 & u_{10} \\ u_2 & u_5 & u_8 & u_{11} \\ u_3 & u_6 & u_9 & u_{12} \end{bmatrix}$$

$$\mathbf{U}_y \approx D_y \mathbf{U}$$

$(\mathbf{D}_y)$: Differentiation Matrix with respect to y

In lexicographic ordering, the relation of $\underline{u}_y = \mathbf{D}_y \underline{u}$, where $\underline{u}_y = \texttt{vec}(\mathbf{U}_y)$ and $\underline{u} = \texttt{vec}(\mathbf{U})$, can be written as

$$\begin{bmatrix} u_1' \\ u_2' \\ u_3' \\ u_4' \\ u_5' \\ u_6' \\ u_7' \\ u_8' \\ u_9' \\ u_{10}' \\ u_{11}' \\ u_{12}' \end{bmatrix} = \frac{1}{2h_y} \left[\begin{array}{ccc|ccc|ccc|ccc} -3 & 4 & -1 & & & & & & & & & \\ -1 & 0 & 1 & & & & & & & & & \\ 1 & -4 & 3 & & & & & & & & & \\ \hline & & & -3 & 4 & -1 & & & & & & \\ & & & -1 & 0 & 1 & & & & & & \\ & & & 1 & -4 & 3 & & & & & & \\ \hline & & & & & & -3 & 4 & -1 & & & \\ & & & & & & -1 & 0 & 1 & & & \\ & & & & & & 1 & -4 & 3 & & & \\ \hline & & & & & & & & & -3 & 4 & -1 \\ & & & & & & & & & -1 & 0 & 1 \\ & & & & & & & & & 1 & -4 & 3 \end{array}\right] \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \\ u_{10} \\ u_{11} \\ u_{12} \end{bmatrix}$$

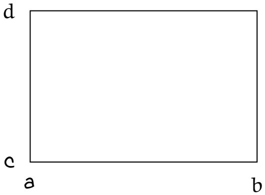
The differentiation matrix with respect to y can be concisely written using Kronecker product symbol as

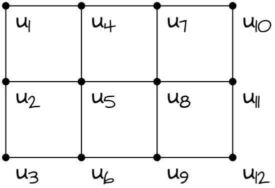
$$\mathbf{D}_y = I_n \otimes D_y = I_4 \otimes D_y$$

where,

$$I_4 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad D_y = \frac{1}{2h_y} \begin{bmatrix} -3 & 4 & -1 \\ -1 & 0 & 1 \\ 1 & -4 & 3 \end{bmatrix}$$

Derivatives with respect to x





An example using 3-point stencil (2-nd order accurate, see slides from the previous lecture). Note that the prime $'$ here means partial derivative with respect to x.

$$\begin{bmatrix} u_1' & u_2' & u_3' \\ u_4' & u_5' & u_6' \\ u_7' & u_8' & u_9' \\ u_{10}' & u_{11}' & u_{12}' \end{bmatrix} \approx \frac{1}{2h_x} \begin{bmatrix} -3 & 4 & -1 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 1 & -4 & 3 \end{bmatrix} \begin{bmatrix} u_1 & u_2 & u_3 \\ u_4 & u_5 & u_6 \\ u_7 & u_8 & u_9 \\ u_{10} & u_{11} & u_{12} \end{bmatrix}$$

Transposing the matrix gives

$$\begin{bmatrix} u_1' & u_4' & u_7' & u_{10}' \\ u_2' & u_5' & u_8' & u_{11}' \\ u_3' & u_6' & u_9' & u_{12}' \end{bmatrix} \approx \begin{bmatrix} u_1 & u_4 & u_7 & u_{10} \\ u_2 & u_5 & u_8 & u_{11} \\ u_3 & u_6 & u_9 & u_{12} \end{bmatrix} \begin{bmatrix} & & \\ & D_x & \\ & & \end{bmatrix}^T$$

$$U_x \approx U D_x^T$$

$(\mathbf{D}_x)$: Differentiation Matrix with respect to x

In lexicographic ordering, the relation of $\underline{u}_x = \mathbf{D}_x \underline{u}$, where $\underline{u}_x = \mathrm{vec}(\mathbf{U}_x)$ and $\underline{u} = \mathrm{vec}(\mathbf{U})$, can be written as

$$
\begin{bmatrix} u_1' \\ u_2' \\ u_3' \\ u_4' \\ u_5' \\ u_6' \\ u_7' \\ u_8' \\ u_9' \\ u_{10}' \\ u_{11}' \\ u_{12}' \end{bmatrix}
= \frac{1}{2h_x}
\left[\begin{array}{ccc|ccc|ccc|ccc}
-3 & & & 4 & & & -1 & & & 0 & & \\
 & -3 & & & 4 & & & -1 & & & 0 & \\
 & & -3 & & & 4 & & & -1 & & & 0 \\
\hline
-1 & & & 0 & & & 1 & & & 0 & & \\
 & -1 & & & 0 & & & 1 & & & 0 & \\
 & & -1 & & & 0 & & & 1 & & & 0 \\
\hline
0 & & & -1 & & & 0 & & & 1 & & \\
 & 0 & & & -1 & & & 0 & & & 1 & \\
 & & 0 & & & -1 & & & 0 & & & 1 \\
\hline
0 & & & 1 & & & -4 & & & 3 & & \\
 & 0 & & & 1 & & & -4 & & & 3 & \\
 & & 0 & & & 1 & & & -4 & & & 3
\end{array}\right]
\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \\ u_{10} \\ u_{11} \\ u_{12} \end{bmatrix}
$$

The differentiation matrix with respect to x can be concisely written using Kronecker product symbol as

$$\mathbf{D}_x = D_x \otimes I_m = D_x \otimes I_3$$

where,

$$
I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}
\qquad
D_x = \frac{1}{2h_x}\begin{bmatrix} -3 & 4 & -1 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 1 & -4 & 3 \end{bmatrix}
$$

Kronecker Product

- The Kronecker product $\otimes$ of two matrices A and B is computed in MATLAB by the command `kron(A,B)`.
- If A and B are of dimensions $p \times q$ and $r \times s$ respectively, then $A \otimes B$ is the matrix of dimension $pr \times qs$ with $p \times q$ block form, where the i, j block is $a_{ij}B$. For example:

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \otimes \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \left[\begin{array}{cc|cc} a & b & 2a & 2b \\ c & d & 2c & 2d \\ \hline 3a & 3b & 4a & 4b \\ 3c & 3d & 4c & 4d \end{array}\right]$$

- Useful properties:
  - $\mathrm{vec}(AXB) = (B^T \otimes A)\mathrm{vec}(X)$
  - If A is an $n \times n$ matrix and B is an $m \times m$ matrix, the Kronecker "sum" can be defined as

$$A \oplus B := A \otimes I_m + I_n \otimes B$$

- To vec or not to vec, that is your choice. Choose the one that makes implementation and analysis easier.

Things to do in class

1. With domain $[-1,1]\times[-1,1]$, $n = m = 11$, $h_x = h_y = h = 2/(n-1)$, create second-order accurate differentiation matrices that represent $\frac{\partial}{\partial x}$, $\frac{\partial}{\partial y}$, and Δ. i.e $\mathbf{D}_x$, $\mathbf{D}_y$, and Laplacian $\mathbf{L} = \mathbf{D}_{xx} + \mathbf{D}_{yy}$ respectively.
2. Test those operators to find the numerical derivatives of $u(x,y) = e^{-(x^2+\frac{1}{2}y^2)}$. Compute $\|\cdot\|_\infty$ to measure the error of numerical derivatives with respect the exact derivatives.
3. Using different values of $n = 10, 100, 1000$, redo problem 2 and plot the $\|\cdot\|_\infty$ vs h in log scale. Do you observe 2^{nd}-order convergence (i.e. $\mathcal{O}(h^2)$) ?
4. Redo (1)-(3) for periodic function $u(x,y) = \sin(\pi x)\cos(\pi y)$.

Tips: In MATLAB, 2D tensor product grid can be generated using the command `meshgrid`.