Lecture 2

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Numerical Methods for PDEs

Outline of Lecture 2

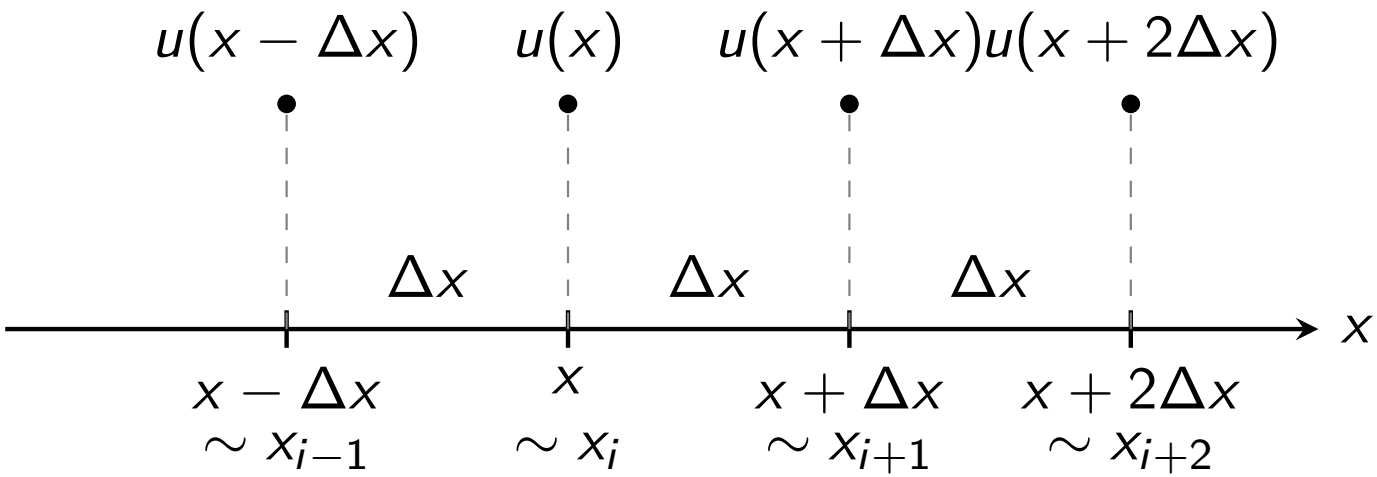
- exercises of Lecture 1
- finite difference approximations of derivatives
- shift matrices and their properties! (Laurent algebra)
- method of undetermined coefficients
- finite difference *matrices* and their *eigenvalues*
- non-uniform grids & transformations
- boundary-value models (stationary) $\Rightarrow$ exercises!
- outlook to Lecture 3

Finite differences [1]

Calculus of finite differences:

Grid Setup

Constant $\Delta x \implies$ **uniform grid**



Finite differences [2]

Forward Difference Operator

$$\Delta_+[u](x) = u(x + \Delta x) - u(x)$$

Forward difference approximation:

$$D_{1+}u(x) = \frac{u(x + \Delta x) - u(x)}{\Delta x} \approx u'(x)$$

Matrix representation:

$$D_{1+} = \frac{1}{\Delta x}\begin{pmatrix} \ddots & & & 0 \\ -1 & 1 & & \\ & -1 & 1 & \\ 0 & & & \ddots \end{pmatrix} \leftarrow \text{check diagonals}$$

Finite differences [3]

Backward Difference Operator

$$\Delta_-[u](x) = u(x) - u(x - \Delta x)$$

Backward difference approximation:

$$D_{1-}u(x) = \frac{u(x) - u(x - \Delta x)}{\Delta x} \approx u'(x)$$

Matrix representation:

$$D_{1-} = \frac{1}{\Delta x}\begin{pmatrix} \ddots & & & 0 \\ -1 & 1 & & \\ & -1 & 1 & \\ 0 & & & \ddots \end{pmatrix} \leftarrow \text{check diagonals}$$

Finite differences [4]

Central Difference Operator

$$\Delta_c[u](x) = u\left(x + \tfrac{1}{2}\Delta x\right) - u\left(x - \tfrac{1}{2}\Delta x\right)$$

Central difference approximation:

$$D_{1c}u(x) = \frac{u\left(x + \tfrac{1}{2}\Delta x\right) - u\left(x - \tfrac{1}{2}\Delta x\right)}{\Delta x} \approx u'(x)$$

$$\text{or} \qquad D_{1c}u(x) = \frac{u(x + \Delta x) - u(x - \Delta x)}{2\Delta x}$$

Matrix representation:

$$D_{1c} = \frac{1}{2\Delta x}\begin{pmatrix} \ddots & & & 0 \\ -1 & 0 & 1 & \\ & -1 & 0 & 1 \\ 0 & & & \ddots \end{pmatrix} \leftarrow \text{check diagonals}$$

Finite differences [5]

Central difference approximation for $u''(x)$:

$$u''(x) \approx \frac{\Delta_C^2[u](x)}{(\Delta x)^2} = \frac{\dfrac{u(x+\Delta x)-u(x)}{\Delta x} - \dfrac{u(x)-u(x-\Delta x)}{\Delta x}}{\Delta x}$$

$$= \frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{(\Delta x)^2}$$

Forward difference approximation for $u''(x)$:

$$u''(x) \approx \frac{\Delta_{1+}^2[u](x)}{(\Delta x)^2} = \frac{\dfrac{u(x+2\Delta x)-u(x+\Delta x)}{\Delta x} - \dfrac{u(x+\Delta x)-u(x)}{\Delta x}}{\Delta x}$$

$$= \frac{u(x+2\Delta x) - 2u(x+\Delta x) + u(x)}{(\Delta x)^2}$$

Backward difference approximation for $u''(x)$:

$$u''(x) \approx \frac{\Delta_{1-}^2[u](x)}{(\Delta x)^2} = \frac{u(x) - 2u(x-\Delta x) + u(x-2\Delta x)}{(\Delta x)^2}$$

Finite differences [6]

Operator Expansion

The second-order central difference operator is applied iteratively:

$$\begin{aligned}\Delta_C\big(\Delta_C[u]\big)(x) &= \Delta_C[u]\left(x+\tfrac{1}{2}\Delta x\right) - \Delta_C[u]\left(x-\tfrac{1}{2}\Delta x\right)\\ &= \Big(u(x+\Delta x)-u(x)\Big) - \Big(u(x)-u(x-\Delta x)\Big)\\ &= u(x+\Delta x) - 2u(x) + u(x-\Delta x)\end{aligned}$$

Finite differences [7]

General operator definitions:

$$\Delta_{1+}^{n}[u](x) = \sum_{i=0}^{n}(-1)^{i}\binom{n}{i}u\big(x+(n-i)\Delta x\big)$$

$$\Delta_{1-}^{n}[u](x) = \sum_{i=0}^{n}(-1)^{i}\binom{n}{i}u\big(x-i\Delta x\big)$$

$$\Delta_{1C}^{n}[u](x) = \sum_{i=0}^{n}(-1)^{i}\binom{n}{i}u\left(x+\left(\tfrac{n}{2}-i\right)\Delta x\right)$$

Derivative approximations and truncation errors:

$$u^{(n)}(x) = \frac{\Delta_{1+}^{n}[u](x)}{(\Delta x)^{n}} + \mathcal{O}(\Delta x) = \frac{\Delta_{1-}^{n}[u](x)}{(\Delta x)^{n}} + \mathcal{O}(\Delta x) = \frac{\Delta_{1C}^{n}[u](x)}{(\Delta x)^{n}} + \mathcal{O}\big((\Delta x)^{2}\big)$$

Finite differences [8]

Operator Mapping

The forward difference operator defines a mapping: $u \xrightarrow{\text{map}} \Delta_{1+}[u]$

Operational definition:

$$\Delta_{1+}[u] = \mathcal{S}_{\Delta x} - \mathcal{I}$$

Where $\mathcal{S}_{\Delta x} \triangleq u(x + \Delta x)$ is the **shift operator**, and $\mathcal{I}$ is the **identity operator**.

Powers of the operator:

$$\Delta_{1+}^n = \Delta_{1+}\left(\Delta_{1+}^{n-1}\right) \qquad \Longrightarrow \qquad \Delta_{1+}^n = (\mathcal{S}_{\Delta x} - \mathcal{I})^n$$

Algebraic properties:

- **Linearity:**
  $\Delta_{1+}[\alpha u + \beta v](x) = \alpha\, \Delta_{1+}[u](x) + \beta\, \Delta_{1+}[v](x)$
- **Leibniz rule (Product rule):**
  $\Delta_{1+}[uv](x) = \Delta_{1+}[u](x) \cdot v(x + \Delta x) + u(x) \cdot \Delta_{1+}[v](x)$

etcetera...

Finite differences [9]

Taylor series expansion for the operator:

$$\Delta_{1+} = \Delta x \cdot D + \frac{1}{2!}(\Delta x)^2 D^2 + \frac{1}{3!}(\Delta x)^3 D^3 + \cdots = e^{\Delta x \cdot D} - \mathcal{I}$$

(valid for sufficiently small Δx, where D is the derivative operator: $u \xrightarrow{D} u'$)

Resulting operator identities:

$$\Longrightarrow \quad \mathcal{S}_{\Delta x} = e^{\Delta x \cdot D} \qquad \text{and} \qquad \ln(\mathcal{I} + \Delta_{1+}) = \Delta_{1+} - \frac{1}{2}\Delta_{1+}^2 + \frac{1}{3}\Delta_{1+}^3 - \cdots$$

In a similar way for backward and central operators:

$$\Delta x \cdot D = -\ln(\mathcal{I} - \Delta_{1-}) \qquad \text{and} \qquad \Delta x \cdot D = 2\,\text{arcsinh}\left(\tfrac{1}{2}\Delta_{1C}\right)$$

Finite differences [10]

Basic Properties

- **Constant rule:** $\Delta_{1+} c = 0$
- **Linearity:** $\Delta_{1+}(\alpha u + \beta v) = \alpha \Delta_{1+} u + \beta \Delta_{1+} v$

Product and quotient rules:

Forward product rule: $\Delta_{1+}(uv) = u\Delta_{1+} v + v\Delta_{1+} u + \Delta_{1+} u \Delta_{1+} v$

Backward product rule: $\Delta_{1-}(uv) = u\Delta_{1-} v + v\Delta_{1-} u - \Delta_{1-} u \Delta_{1-} v$

Backward quotient rule: $\Delta_{1-}\left(\frac{u}{v}\right) = \frac{v\Delta_{1-} u - u\Delta_{1-} v}{v \cdot (v - \Delta_{1-} v)}$

etcetera...

Finite differences [11]

Method of undetermined coefficients:

Objective: Find a one-sided approximation for $u'(x_i)$ on the stencil $\{x_{i-2}, x_{i-1}, x_i\}$.

$$u'(x_i) \approx Au_i + Bu_{i-1} + Cu_{i-2} \qquad (*)$$

Where A, B, C are coefficients to be determined, and $u_i \triangleq u(x_i)$.

Taylor series expansions about x_i:

$$\begin{cases} u_{i-1} = u_i + (-\Delta x)u_x + \frac{(-\Delta x)^2}{2}u_{xx} + \frac{(-\Delta x)^3}{6}u_{xxx} + \dots \\ u_i \qquad = u_i + 0 \cdot \Delta x + 0 \cdot (\Delta x)^2 + \dots \\ u_{i-2} = u_i + (-2\Delta x)u_x + \frac{(-2\Delta x)^2}{2}u_{xx} + \frac{(-2\Delta x)^3}{6}u_{xxx} + \dots \end{cases}$$

Finite differences [12]

Substituting the expansions into $(*)$ yields:

$$\begin{aligned} Au_i + Bu_{i-1} + Cu_{i-2} = \; & Au_i \\ & + Bu_i - B\Delta x\, u_x + \frac{B}{2}(\Delta x)^2 u_{xx} - \frac{B}{6}(\Delta x)^3 u_{xxx} + \dots \\ & + Cu_i - 2C\Delta x\, u_x + 2C(\Delta x)^2 u_{xx} - \frac{4C}{3}(\Delta x)^3 u_{xxx} + \dots \end{aligned}$$

Matching coefficients to satisfy $u'(x_i) = 1 \cdot u_x + 0 \cdot u_i + 0 \cdot u_{xx}$:

$$\begin{cases} A + B + C = 0 \\ -B\Delta x - 2C\Delta x = 1 \\ \frac{B}{2}(\Delta x)^2 + 2C(\Delta x)^2 = 0 \end{cases} \xrightarrow{\text{solve}} \begin{cases} A = \frac{3}{2\Delta x} \\ B = \frac{-2}{\Delta x} \\ C = \frac{1}{2\Delta x} \end{cases}$$

Finite differences [13]

Resulting finite difference scheme:

$$\implies u_{x,i} = \frac{1}{2\Delta x}\left[3u_i - 4u_{i-1} + u_{i-2}\right]$$

Truncation error calculation:

$$\text{Error} = u_{x,i} - u'(x_i) = -B\frac{(\Delta x)^3}{6}u_{xxx} + C\frac{(-2\Delta x)^3}{6}u_{xxx} + \text{H.O.T.}$$

$$= -\frac{1}{3}(\Delta x)^2 u_{xxx} + \mathcal{O}\big((\Delta x)^3\big)$$

Conclusion

The leading error term is proportional to $(\Delta x)^2 \implies$ **second-order** accurate.

(H.O.T. $\equiv$ Higher Order Terms, which are $\mathcal{O}\big((\Delta x)^4\big)$ for the expansion)

Finite differences [14]

Objective

Find a **4th-order approximation** for the 1st derivative (u_x) using a 5-point central stencil:

$$\text{stencil: } \{x_{i-2}, x_{i-1}, x_i, x_{i+1}, x_{i+2}\}$$

Taylor series expansions about x_i:

$$\begin{cases} u_{i-2} = u_i + (-2\Delta x)u_x + \frac{(-2\Delta x)^2}{2}u_{xx} + \dots \\ u_{i-1} = u_i + (-\Delta x)u_x + \frac{(-\Delta x)^2}{2}u_{xx} + \dots \\ u_i \quad\quad = u_i + 0 \cdot \Delta x + 0 \cdot (\Delta x)^2 + \dots \\ u_{i+1} = u_i + (\Delta x)u_x + \frac{(\Delta x)^2}{2}u_{xx} + \dots \\ u_{i+2} = u_i + (2\Delta x)u_x + \frac{(2\Delta x)^2}{2}u_{xx} + \dots \end{cases}$$

Finite differences [15]

Setting up the scheme (assuming the coefficient for u_i is 0 due to symmetry):

$$u_{x,i} = Au_{i-2} + Bu_{i-1} + 0 \cdot u_i + Cu_{i+1} + Du_{i+2}$$

Resulting linear system of equations:

$$\Longrightarrow \begin{cases} -2A - B + C + 2D = \frac{1}{\Delta x} \\ 4A + B + C + 4D = 0 \quad \text{(eliminate 2nd order derivative terms)} \\ -8A - B + C + 8D = 0 \quad \text{(eliminate 3rd order derivative terms)} \\ 16A + B + C + 16D = 0 \quad \text{(eliminate 4th order derivative terms)} \end{cases}$$

Solution for the coefficients:

$$\Longrightarrow A = \frac{2}{4!\Delta x}, \quad B = \frac{-16}{4!\Delta x}, \quad C = \frac{16}{4!\Delta x}, \quad D = \frac{-2}{4!\Delta x}$$

Truncation error: $\mathcal{O}\left((\Delta x)^4\right)$

Finite differences [16]

Problem Definition

Given a small grid spacing Δx and an m-th order derivative, we want to achieve an accuracy of:

$$\text{Error} = \mathcal{O}\left((\Delta x)^p\right)$$

General finite difference scheme:

$$\frac{(\Delta x)^m}{m!} u_i^{(m)} = \sum_{i=i_{\min}}^{i_{\max}} C_i \, u_i$$

Terminology: The vector of coefficients:

$$\vec{C} = (C_{i_{\min}}, \ldots, C_{i_{\max}})$$

is called the **template** or **convolution mask** for the approximation.

Finite differences [17]

Procedure: Select m (derivative order) and p (order of accuracy), then find C_i.

Using the Taylor series expansion: $u_{i+1} = \sum_{n=0}^{\infty} \frac{i^n (\Delta x)^n}{n!} u_i^{(n)}$

Substitution into the general stencil yields:

$$\implies u^{(m)}(x_i) = \frac{m!}{(\Delta x)^m} \sum_{n=0}^{m+p-1} \left[\sum_{i=i_{\min}}^{i_{\max}} i^n C_i \right] \frac{(\Delta x)^n}{n!} u_i^{(n)} + \mathcal{O}\left((\Delta x)^p\right)$$

(where the double sum represents the approximation, and the remainder is the truncation error)

This implies the following algebraic conditions for accuracy:

$$\implies \sum_{i=i_{\min}}^{i_{\max}} i^n C_i = \begin{cases} 0\,, & 0 \leq n \leq m+p-1\,,\ n \neq m \\ 1\,, & n = m \end{cases}$$

Finite differences [18]

System Properties

The matching conditions yield a set of $m + p$ **linear equations** in $i_{\max} - i_{\min} + 1$ **unknowns**.

* If we restrict the number of unknowns to exactly $m + p$, then the resulting linear system has a **unique solution**.

Standard examples of unique stencils:

- **Forward Finite Differences (FDs):**

$$i_{\min} = 0\,, \quad i_{\max} = m + p - 1$$

- **Backward Finite Differences (FDs):**

$$i_{\max} = 0\,, \quad i_{\min} = -(m + p - 1)$$

- **Central Finite Differences (FDs):**

$$i_{\max} = -i_{\min} = \frac{m + p - 1}{2}$$

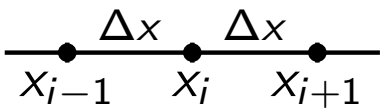
Finite differences [19]

m	p	Type	$i_{\min}$	$i_{\max}$	Formula	Truncation Error
1	1	Forward	0	1	$\frac{u_{i+1}-u_i}{\Delta x}$	$\mathcal{O}(\Delta x)$
1	1	Backward	-1	0	$\frac{u_i-u_{i-1}}{\Delta x}$	$\mathcal{O}(\Delta x)$
1	2	Central	-1	1	$\frac{u_{i+1}-u_{i-1}}{2\Delta x}$	$\mathcal{O}((\Delta x)^2)$
1	2	Forward	0	2	$\frac{-u_{i+2}+4u_{i+1}-3u_i}{2\Delta x}$	$\mathcal{O}((\Delta x)^2)$
1	2	Backward	-2	0	$\frac{3u_i-4u_{i-1}+u_{i-2}}{2\Delta x}$	$\mathcal{O}((\Delta x)^2)$
1	4	Central	-2	2	$\frac{-u_{i+2}+8u_{i+1}-8u_{i-1}+u_{i-2}}{12\Delta x}$	$\mathcal{O}((\Delta x)^4)$
2	1	Forward	0	2	$\frac{u_{i+2}-2u_{i+1}+u_i}{(\Delta x)^2}$	$\mathcal{O}(\Delta x)$
2	2	Central	-1	1	$\frac{u_{i+1}-2u_i+u_{i-1}}{(\Delta x)^2}$	$\mathcal{O}((\Delta x)^2)$
2	4	Central	-2	2	$\frac{-u_{i+2}+16u_{i+1}-30u_i+16u_{i-1}-u_{i-2}}{12(\Delta x)^2}$	$\mathcal{O}((\Delta x)^4)$

Finite difference matrices [1]

Objective: Approximate $\dfrac{\partial}{\partial x}$ on the stencil $\{x_{i-1}, x_i, x_{i+1}\}$ with a uniform Δx.

Define the matrix $D_{1C} = \frac{1}{2\Delta x}\begin{pmatrix} \ddots & & & 0 \\ -1 & 0 & 1 & \\ & -1 & 0 & 1 \\ 0 & & & \ddots \end{pmatrix}$



and the vector $\vec{u} = \left(\ldots, u_{i-1}, u_i, u_{i+1}, \ldots\right)^T$.

This corresponds to: $u_x(x_i) \approx u_{x,i} = \frac{u_{i+1} - u_{i-1}}{2\Delta x}$ $\left(\mathcal{O}((\Delta x)^2) \text{ error}\right)$

Boundary challenges at the edges of the domain:

- For $i = 2$: $u_{x,2} = \frac{u_3 - u_1}{2\Delta x}$ ✓
- For $i = 1$: $u_{x,1} = \frac{u_2 - u_0}{2\Delta x}$ → What is u_0?
- For $i = M$: $u_{x,M} = \frac{u_{M+1} - u_{M-1}}{2\Delta x}$ → What is u_{M+1}?

The boundaries of the matrix depend on the boundary conditions (BC) of the DE.

Finite difference matrices [2]

Periodic Boundary Conditions (BC)

We assume a periodic domain where the grid wraps around:

$$u_0 = u_M \qquad \text{and} \qquad u_{M+1} = u_1$$

Resulting boundary approximations:

$$\Longrightarrow \begin{cases} u_{x,1} = \frac{u_2 - u_M}{2\Delta x} \\ u_{x,M} = \frac{u_1 - u_{M-1}}{2\Delta x} \end{cases}$$

Resulting matrix structure:

$$\Longrightarrow D_{1C} = \frac{1}{2\Delta x} \begin{pmatrix} 0 & 1 & & & -1 \\ -1 & 0 & 1 & & \\ & -1 & 0 & 1 & \\ & & \ddots & \ddots & \ddots \\ 1 & & & -1 & 0 \end{pmatrix}$$

- This matrix is **skew-symmetric** (a **circulant matrix**).
- Its **eigenvalues lie strictly on the imaginary axis**.

Finite difference matrices [3]

Forward Finite Difference (FD) — "Upwind" style:

$$u_{x,i} = \frac{u_{i+1} - u_i}{\Delta x} \quad \Big(\mathcal{O}(\Delta x) \text{ error}\Big) \implies D_{1+} = \frac{1}{\Delta x} \begin{pmatrix} -1 & 1 & 0 & \dots & 0 \\ & & & & \vdots \\ 0 & -1 & 1 & \dots & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 0 \\ 0 & & -1 & 1 & 0 \\ 1 & \dots & & 0 & -1 \end{pmatrix}$$

Backward Finite Difference (FD) — "Downwind" style:

$$u_{x,i} = \frac{u_i - u_{i-1}}{\Delta x} \quad \Big(\mathcal{O}(\Delta x) \text{ error}\Big) \implies D_{1-} = \frac{1}{\Delta x} \begin{pmatrix} 1 & & & & -1 \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ 0 & \dots & & -1 & 1 \end{pmatrix}$$

Finite difference matrices [4]

FD matrix for $\dfrac{\partial^2 u}{\partial x^2}$ **at** $x = x_i$ **with periodic BCs:**

$$D_{2C} = D_{1+}D_{1-} = D_{1-}D_{1+} = \frac{1}{(\Delta x)^2}\begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ 1 & & & 1 & -2 \end{pmatrix}$$

Matrix Property:

This yields a **symmetric matrix** $\Longrightarrow$ **real eigenvalues**

Finite difference matrices [5]

Homogeneous Dirichlet Boundary Conditions: $u_0 = u_M = 0$

Approximation: $u_{xx,i} = \dfrac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}$ $\left(\mathcal{O}((\Delta x)^2) \text{ error}\right)$

Applying the boundary conditions at the edges:

- For $i = 1$: $u_{xx,1} = \dfrac{u_2 - 2u_1 + \overbrace{u_0}^{0}}{(\Delta x)^2} = \dfrac{u_2 - 2u_1}{(\Delta x)^2}$
- For $i = M - 1$: $u_{xx,M-1} = \dfrac{\overbrace{u_M}^{0} - 2u_{M-1} + u_{M-2}}{(\Delta x)^2} = \dfrac{-2u_{M-1} + u_{M-2}}{(\Delta x)^2}$

Resulting matrix structure (D_{2C}):

$$\Longrightarrow \frac{1}{\Delta x^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \end{pmatrix}$$

Finite difference matrices [6]

Fourth-order derivative matrix expression:

$$\frac{\partial^4 u}{\partial x^4} \quad \Longrightarrow \quad D_{4C} = (D_{2C})^2 = \frac{1}{(\Delta x)^4} \begin{pmatrix} \quad ? \quad \end{pmatrix} \quad \left(\mathcal{O}((\Delta x)^2) \text{ error}\right)$$

[Exercise]

Finite difference matrices [7]

Operator composition for the third derivative:

$$\frac{\partial^3 u}{\partial x^3} \quad \Longrightarrow \quad D_{3C} = \underset{\partial/\partial x}{D_{1+}} \; \underset{\partial/\partial x}{D_{1-}} \; \underset{\partial/\partial x}{D_{1C}} = \frac{1}{(\Delta x)^3} \begin{pmatrix} 0 & -\frac{1}{2} & 0 & \cdots & \frac{1}{2} \\ 1 & 0 & -\frac{1}{2} & & \\ -\frac{1}{2} & 1 & 0 & -\frac{1}{2} & \\ & \ddots & \ddots & \ddots & \ddots \\ -\frac{1}{2} & \cdots & & -\frac{1}{2} & 0 \end{pmatrix}$$

(Truncation error: $\mathcal{O}\left((\Delta x)^2\right)$)

Boundary blocks due to Periodic Bus:

- **Top-right corner block:** $\begin{pmatrix} -1 & 2 \\ 0 & -1 \end{pmatrix}$
- **Bottom-left corner block:** $\begin{pmatrix} 1 & 0 \\ -2 & 1 \end{pmatrix}$

etcetera...

Eigenvalues of FD matrices [1]

Tridiagonal Matrix A (Size: $(M-1)\times(M-1)$):

$$A = \begin{pmatrix} a & b & & & 0 \\ b & a & b & & \\ & b & a & b & \\ & & \ddots & \ddots & \ddots \\ 0 & & & b & a \end{pmatrix}$$

Eigenvalues: $\lambda_j(A) = a + 2b\cos\left(\frac{j\pi}{M}\right), \quad j = 1, 2, \ldots, M-1$

Eigenvectors: $\vec{v}_j(A) = \begin{pmatrix} v_j^1 \\ \vdots \\ v_j^{M-1} \end{pmatrix}$ with $v_j^k = \sin\left(\frac{kj\pi}{M}\right), \quad k, j \in \{1, \ldots, M-1\}$

Special Case: $A = D_{2C}$

Setting $a = \frac{-2}{(\Delta x)^2}, \quad b = \frac{1}{(\Delta x)^2}$

$$\Longrightarrow \lambda_j(D_{2C}) = \frac{2}{(\Delta x)^2}\left[\cos\left(\frac{j\pi}{M}\right) - 1\right], \quad j = 1, 2, \ldots, M-1$$

Eigenvalues of FD matrices [2]

Objective: Find the non-trivial solutions to the eigenvalue problem.

Define the normalized matrix $\tilde{A}$:

$$\tilde{A} = \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & -2 \end{pmatrix}$$

(Note: the factor $\dfrac{1}{(\Delta x)^2}$ can be added at the end of the calculation)

Eigenvalue equation to solve:

$$\tilde{A}\vec{y} = \lambda\vec{y}$$

Eigenvalues of FD matrices [3]

The matrix equation $\tilde{A}\vec{y} = \lambda\vec{y}$ can be written row by row as a system:

$$\begin{cases} y_{j-1} - (2+\lambda)y_j + y_{j+1} = 0\,, & j = 1, \ldots, M-1 \\ y_0 = y_M = 0 \end{cases}$$

The general solution of this **2nd-order linear recurrence relation** is obtained by substituting $y_j = z^j$:

$$y_j = \alpha w_1^j + \beta w_2^j$$

Where w_1 and w_2 are the roots of the characteristic equation:

$$z^2 - (2+\lambda)z + 1 = 0$$

Eigenvalues of FD matrices [4]

Using the boundary conditions to determine the coefficients α and β:

- From $y_0 = 0$ follows: $\alpha + \beta = 0 \implies \beta = -\alpha$
- From $y_M = 0$ follows: $\alpha w_1^M + \beta w_2^M = 0 \iff \alpha(w_1^M - w_2^M) = 0$

Assuming a non-trivial solution ($\alpha \neq 0$):

$$w_1^M = w_2^M \implies \left(\frac{w_1}{w_2}\right)^M = 1 \implies \frac{w_1}{w_2} = e^{\frac{2\pi ik}{M}}, \quad k = 1, \ldots, M-1$$

Consequently, the solution simplifies to: $y_j = \alpha\left(w_1^j - w_2^j\right)$

By symmetry, we can choose:

$$w_1 = e^{\frac{\pi ik}{M}} \quad \text{and} \quad w_2 = e^{-\frac{\pi ik}{M}} \quad \left(\text{note that } w_1 w_2 = 1\right)$$

Eigenvalues of FD matrices [5]

The number λ is an eigenvalue of $\tilde{A}$ if w_1, w_2 satisfy the characteristic equation:

$$(z - w_1)(z - w_2) = z^2 - (w_1 + w_2)z + w_1 w_2 = 0$$

Comparing this to $z^2 - (2 + \lambda)z + 1 = 0$, we find:

$$\begin{cases} w_1 + w_2 = 2 + \lambda \\ w_1 w_2 = 1 \end{cases}$$

Solving for λ using Euler's relation:

$$\lambda = w_1 + w_2 - 2 = e^{\frac{\pi ik}{M}} + e^{-\frac{\pi ik}{M}} - 2$$

$$= 2\cos\left(\frac{\pi k}{M}\right) - 2$$

Eigenvalues of FD matrices [6]

Using the trigonometric identity $2\cos(\theta) - 2 = -4\sin^2\left(\frac{\theta}{2}\right)$, we can rewrite the expression for λ:

$$\lambda = 2\cos\left(\frac{\pi k}{M}\right) - 2$$

$$= -4\sin^2\left(\frac{\pi k}{2M}\right)$$

$$= -4\sin^2\left(\frac{\pi k \Delta x}{2}\right)$$

(since $\Delta x = \frac{1}{M}$ for a normalized domain)

Eigenvalues of FD matrices [7]

Final step

Reintroducing the scaling factor $\frac{1}{(\Delta x)^2}$, the eigenvalues of the complete matrix A are:

$$\Longrightarrow \quad \lambda(A) = -\frac{4}{(\Delta x)^2} \sin^2\left(\frac{\pi k \Delta x}{2}\right)$$

The eigenvectors of A follow from:

$$y_j = \alpha\left(w_1^j - w_2^j\right)$$

$$= \ldots$$

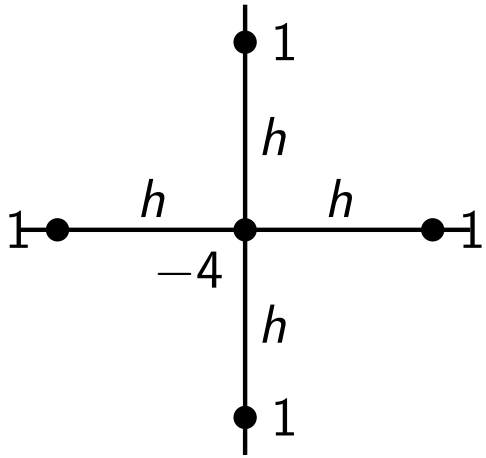
(See also the document on the webpage)

Higher dimensions [1]

Five-point stencil approximation:

$$\Delta u_{i,j} \approx \frac{1}{h^2}\left[u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}\right]$$

Truncation error: $\mathcal{O}(h^2)$



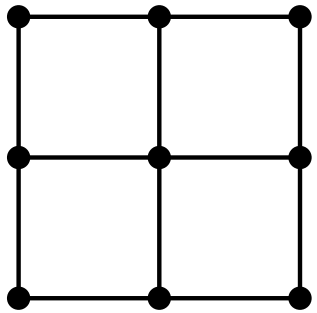
Derivation requires 2D Taylor expansions with two indices i, j:

$$\begin{cases} u_{i+1,j} = u_{i,j} + hu_x + \frac{h^2}{2}u_{xx} + \dots \\ u_{i,j-1} = u_{i,j} - hu_y + \frac{h^2}{2}u_{yy} - \dots \\ \text{etcetera...} \end{cases}$$

Higher dimensions [2]

Note on corner expansions:

$$u_{i+1,j+1} = u_{i,j} + hu_x + hu_y + \frac{h^2}{2}(u_{xx} + 2u_{xy} + u_{yy}) + \dots$$



Nine-point stencil approximation:

$$\begin{aligned}\Delta u_{i,j} \approx \frac{1}{6h^2}\Big[&4u_{i-1,j} + 4u_{i+1,j} + 4u_{i,j-1} + 4u_{i,j+1} \\ &+ u_{i-1,j-1} + u_{i-1,j+1} + u_{i+1,j-1} + u_{i+1,j+1} \\ &- 20u_{i,j}\Big]\end{aligned}$$

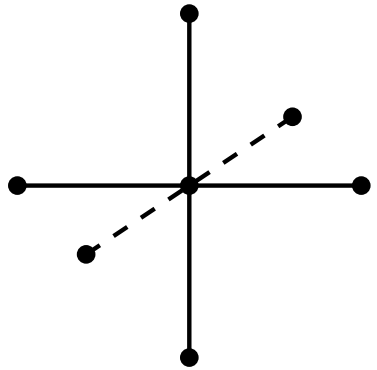
Show that the truncation error is $\mathcal{O}(h^2)$ $\rightarrow$ **exercise**

Higher dimensions [3]

3D: Seven-point stencil ($\Delta x = \Delta y = \Delta z = h$):

$$\Delta u_{i,j,k} \approx \frac{1}{h^2}\left[u_{i+1,j,k} + \cdots + u_{i,j,k-1} - 6u_{i,j,k}\right]$$

Error: $\mathcal{O}(h^2)$



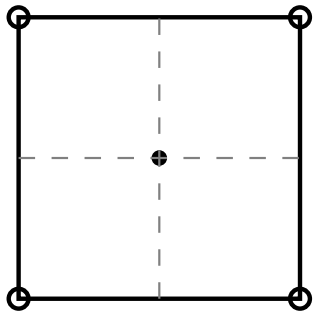
Generalization to d-dimensions (dD):

$$\Delta u_{i_1,i_2,\ldots,i_d} \approx \frac{1}{h^2}\Big[\underbrace{u_{i_1+1,i_2,\ldots,i_d} + \cdots + u_{i_1,i_2,\ldots,i_d-1}}_{2d \text{ terms}} - 2d \cdot u_{i_1,i_2,\ldots,i_d}\Big]$$

Higher dimensions [4]

Approximation for the mixed derivative:

$$\left.\frac{\partial^2 u}{\partial x \partial y}\right|_{i,j} \approx \frac{u_{i+1,j+1} + u_{i-1,j-1} - u_{i+1,j-1} - u_{i-1,j+1}}{4h^2}$$

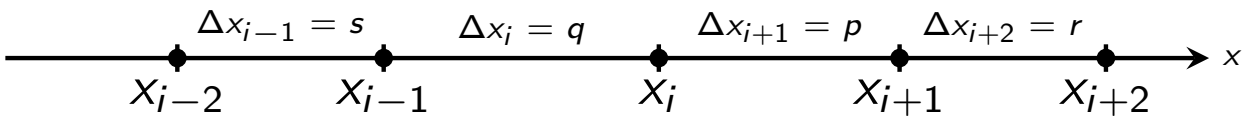


Note on the Stencil:

The mixed derivative approximation uses the four corner points of the 2D cell, omitting the central cross points.

Non-uniform grids [1]

Non-uniform grid structure:



If $p = q = r = s = \cdots = \Delta x$, then we have a **uniform grid**.

Example: Approximate $\dfrac{\partial u}{\partial x}$ at $x = x_i$ on the central stencil $\{x_{i-1}, x_i, x_{i+1}\}$:

$$\text{Taylor:} \quad \begin{cases} u_{i+1} = u_i + p\,u_x + \frac{p^2}{2}u_{xx} + \frac{p^3}{6}u_{xxx} + \dots \\ u_i \qquad = u_i + 0 + 0 + \dots \\ u_{i-1} = u_i - q\,u_x + \frac{q^2}{2}u_{xx} - \frac{q^3}{6}u_{xxx} + \dots \end{cases}$$

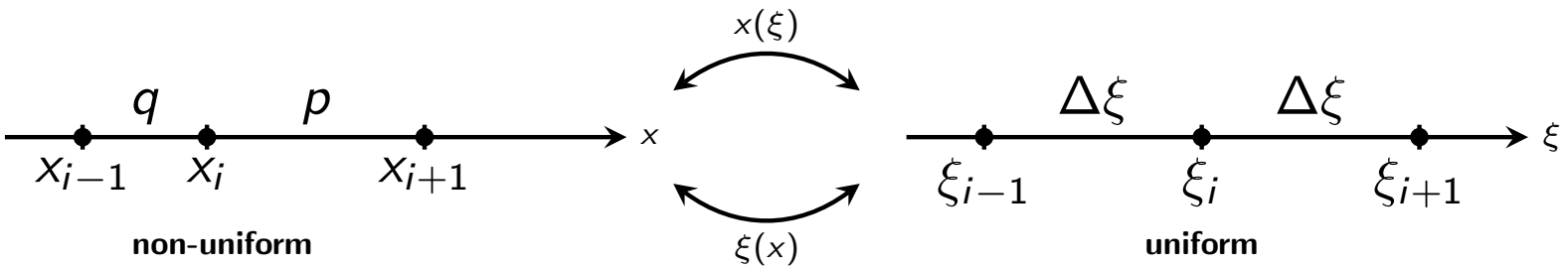
$$\implies u_{x,i} = \frac{u_{i+1} - u_{i-1}}{p+q} \quad \text{with error:} \quad -\frac{p^2 - q^2}{2(p+q)}u_{xx} - \frac{p^3 + q^3}{6(p+q)}u_{xxx} - \dots$$

$$\text{Leading error term:} \quad -\frac{p-q}{2}u_{xx} \implies \mathcal{O}(\Delta x) \text{ unless } p = q$$

Non-uniform grids [2]

Concept

Transform a non-uniform physical grid in x into a uniform computational grid in ξ using a mapping function $x(\xi)$ or $\xi(x)$.



Non-uniform grids [3]

Define the uniform computational grid spacing: $\Delta\xi = H = \dfrac{1}{M}$

(where M represents the number of grid points)

Taylor expansions for the physical step sizes p and q about ξ_i:

$$p = \Delta x_{i+1} = x_{i+1} - x_i = x(\xi_i + H) - x(\xi_i)$$
$$= H \cdot x_\xi + \frac{1}{2} H^2 \cdot x_{\xi\xi} + \mathcal{O}(H^3)$$

$$q = \Delta x_i \quad = x_i - x_{i-1} = x(\xi_i) - x(\xi_i - H)$$
$$= H \cdot x_\xi - \frac{1}{2} H^2 \cdot x_{\xi\xi} + \mathcal{O}(H^3)$$

Algebraic combinations (check!):

- $p - q = H^2 \cdot x_{\xi\xi} + \mathcal{O}(H^4)$
- $p \cdot q = H^2 \cdot x_\xi^2 + \mathcal{O}(H^4)$

Non-uniform grids [4]

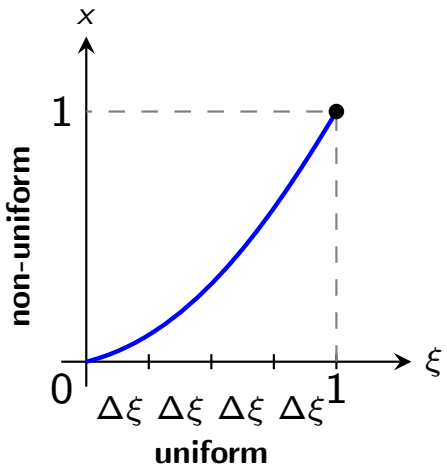
Resulting approximation for $u_{x,i}$:

$$u_{x,i} = \frac{u_{i+1} - u_{i-1}}{p + q}$$

with truncation error:

$$-\frac{H^2}{6}\left[3x_{\xi\xi}u_{xx} + x_\xi^2 u_{xxx}\right] + \mathcal{O}(H^4)$$

$\Longrightarrow$ This is **second-order** accurate ($\mathcal{O}(H^2)$)!



Properties of the mapping function $x(\xi)$:

- $x(\xi) = \xi \implies$ Uniform grid in x.
- $x_\xi > 0 \implies$ The mapping is non-singular.
- x_ξ and $x_{\xi\xi}$ play an important role in the properties of the non-uniform grid.

How to choose $x(\xi)$? $\Longrightarrow$ *See lecture on adaptive grids.*

Outlook to Lecture 3

- Prepare exercises of Lecture 2 (see webpage!)
- Method-of-Lines (horizontal vs vertical)
- Time-integration methods
- Stability regions