Scientific Computing

Lecture 3

Delft University of Technology

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Recap Last Week

- Transform continuous model to discrete numerical model
  - Transform domain Ω into discrete domain/grid G_h with grid points, i.e. from (x, y) to (x_i, y_j)
  - Discretize solution function $u(x, y)$ to $u(x_i, y_j)$ on the grid points
  - Discretize derivatives of the PDE at grid points using Finite Differences
  - Rewrite system of equations into matrix-vector format $\mathbf{Au} = \mathbf{f}$
    - Without elimination boundary nodes
    - With elimination boundary nodes

Today

- Properties of matrix $\mathbf{A}$
  - Symmetric
  - Positive-Definite
  - Irreducible
  - M-matrix
  - Sparse
- Relation to numerical solver choice
  - $\mathbf{u} = \mathbf{A}^{-1}\mathbf{f}$

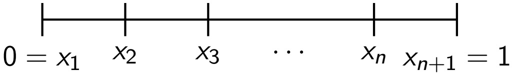
```
C:\ProgramData\Anaconda3\lib\site-packages\numpy\linalg\linalg.py in
     89
     90 def _raise_linalgerror_nonposdef(err, flag):
---> 91     raise LinAlgError("Matrix is not positive definite")
     92
     93 def _raise_linalgerror_eigenvalues_nonconvergence(err, flag):

LinAlgError: Matrix is not positive definite
```

1D Poisson - with elimination

$-\frac{d^2u}{dx^2} = f$ on $\Omega = (0,1), u(0) = \alpha, u(1) = \beta$

1. Define $G_h := \left\{ x_i | x_i = (i-1)h, i = 1, \dots, N+1, h = \frac{1}{N} \right\}$



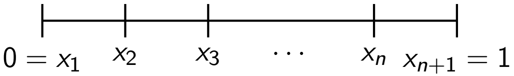
2. Define $u_i = u(x_i), f_i = f(x_i)$ for $i = 1, 2, \dots N+1$
3. Apply FD: $-\frac{d^2u}{dx^2} \approx \frac{-u_{i-1}+2u_i-u_{i+1}}{h^2} = f_i$, for $i = 2, \dots, N$.
4. Linear System Formulation ($\mathbf{Au} = \mathbf{f}, \mathbf{A} \in \mathbb{R}^{n \times n}$)

$$\frac{1}{h^2} \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & \cdots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} u_2 \\ u_3 \\ \vdots \\ u_{n-1} \\ u_n \end{pmatrix} = \begin{pmatrix} f_2 + \frac{\alpha}{h^2} \\ f_3 \\ \vdots \\ f_{n-1} \\ f_n + \frac{\beta}{h^2} \end{pmatrix}$$

1D Poisson - without elimination

$-\frac{d^2u}{dx^2} = f$ on $\Omega = (0,1), u(0) = \alpha, u(1) = \beta$

1. Define $G_h := \left\{ x_i | x_i = (i-1)h, i = 1, \ldots, N+1, h = \frac{1}{N} \right\}$



2. Define $u_i = u(x_i), f_i = f(x_i)$ for $i = 1, 2, \ldots N+1$
3. Apply FD: $-\frac{d^2u}{dx^2} \approx \frac{-u_{i-1}+2u_i-u_{i+1}}{h^2} = f_i$, for $i = 2, \ldots, N$.
4. Linear System Formulation ($\mathbf{Au} = \mathbf{f}, \mathbf{A} \in \mathbb{R}^{n+1 \times n+1}$)

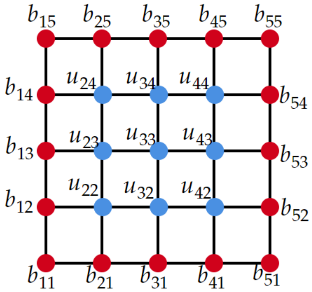
$$\frac{1}{h^2} \begin{pmatrix} h^2 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & \cdots & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & h^2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \\ u_{n+1} \end{pmatrix} = \begin{pmatrix} \alpha \\ f_2 \\ \vdots \\ f_n \\ \beta \end{pmatrix}$$

2D Poisson - with elimination

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f \text{ on } \Omega = (0,1) \times (0,1)$$

$$u(x,y) = b(x,y) \text{ on } \Gamma$$

1. $G_h := \{(x_i, y_j) \mid x_i = (i-1)h, y_j = (j-1)h; 1 \leq i,j \leq N+1\}$
2. Define $u_{i,j} = u(x_i, y_j)$, $f_{i,j} = f(x_i, y_j)$ and $b_{i,j} = u(x_i, y_j)$ for (x_i, y_j) on the boundary



2D Poisson - with elimination cont'd

1. Apply FD: $-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} \approx \frac{-u_{i,j-1} - u_{i-1,j} + 4u_{i,j} - u_{i+1,j} - u_{i,j+1}}{h^2} = f_{i,j}$ for $2 \leq i, j \leq N$
2. Linear System Formulation ($\mathbf{Au} = \mathbf{f}, \mathbf{A} \in \mathbb{R}^{(n-1)^2 \times (n-1)^2}$)

$$\frac{1}{h^2} \begin{pmatrix} 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 4 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 \end{pmatrix} \begin{bmatrix} u_{22} \\ u_{32} \\ u_{42} \\ u_{23} \\ u_{33} \\ u_{43} \\ u_{24} \\ u_{34} \\ u_{44} \end{bmatrix} =$$

2D Poisson - with elimination cont'd

Linear System Formulation ($\mathbf{Au} = \mathbf{f}, \mathbf{A} \in \mathbb{R}^{(n-1)^2 \times (n-1)^2}$)

$$= \begin{bmatrix} f_{22} + \frac{b_{21}+b_{12}}{h^2} \\ f_{32} + \frac{b_{23}}{h^2} \\ f_{42} + \frac{b_{41}+b_{52}}{h^2} \\ f_{23} + \frac{b_{13}}{h^2} \\ f_{33} \\ f_{43} + \frac{b_{53}}{h^2} \\ f_{24} + \frac{b_{14}+b_{25}}{h^2} \\ f_{34} + \frac{b_{35}}{h^2} \\ f_{44} + \frac{b_{45}+b_{54}}{h^2} \end{bmatrix} = \mathbf{f}$$

2D Poisson - without elimination

Linear System Formulation ($\mathbf{Au} = \mathbf{f}, \mathbf{A} \in \mathbb{R}^{(n+1)^2 \times (n+1)^2}$)

$$
\frac{1}{h^2}
\begin{pmatrix}
h^2 \\
& h^2 \\
& & h^2 \\
& & & h^2 \\
& & & & h^2 \\
& & & & & h^2 \\
& -1 & & & & -1 & 4 & -1 & & & & -1 \\
& & -1 & & & & -1 & 4 & -1 & & & & -1 \\
& & & -1 & & & & -1 & 4 & -1 & & & & -1 \\
& & & & & & & & & h^2 \\
& & & & & & & & & & h^2 \\
& & & & & & -1 & & & & -1 & 4 & -1 & & & & -1 \\
& & & & & & & -1 & & & & -1 & 4 & -1 & & & & -1 \\
& & & & & & & & -1 & & & & -1 & 4 & -1 & & & & -1 \\
& & & & & & & & & & & & & & h^2 \\
& & & & & & & & & & & & & & & h^2 \\
& & & & & & & & & & & -1 & & & & -1 & 4 & -1 & & & & -1 \\
& & & & & & & & & & & & -1 & & & & -1 & 4 & -1 & & & & -1 \\
& & & & & & & & & & & & & -1 & & & & -1 & 4 & -1 & & & & -1 \\
& & & & & & & & & & & & & & & & & & & h^2 \\
& & & & & & & & & & & & & & & & & & & & h^2 \\
& & & & & & & & & & & & & & & & & & & & & h^2 \\
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& & & & & & & & & & & & & & & & & & & & & & & h^2 \\
& & & & & & & & & & & & & & & & & & & & & & & & h^2
\end{pmatrix}
\begin{pmatrix}
u_{11} \\ u_{21} \\ u_{31} \\ u_{41} \\ u_{51} \\ u_{12} \\ u_{22} \\ u_{32} \\ u_{42} \\ u_{52} \\ u_{12} \\ u_{23} \\ u_{33} \\ u_{43} \\ u_{53} \\ u_{14} \\ u_{24} \\ u_{34} \\ u_{44} \\ u_{54} \\ u_{15} \\ u_{25} \\ u_{35} \\ u_{45} \\ u_{55}
\end{pmatrix}
=
\begin{pmatrix}
b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \\ b_{51} \\ b_{12} \\ f_{22} \\ f_{32} \\ f_{42} \\ b_{52} \\ b_{12} \\ f_{23} \\ f_{33} \\ f_{43} \\ b_{53} \\ b_{14} \\ f_{24} \\ f_{34} \\ f_{44} \\ b_{54} \\ b_{15} \\ b_{25} \\ b_{35} \\ b_{45} \\ b_{55}
\end{pmatrix}
$$

§ 2.1-2.2, 2.5: Preliminaries

- Eigenvector: $\mathbf{v}^{[k]} \in \mathbb{C}^n \backslash \{\mathbf{0}\}$ corresponding to eigenvalue $\lambda_k \in \mathbb{C}$ iff $A\mathbf{v}^{[k]} = \lambda_k \mathbf{v}^{[k]}$.
- Algebraic multiplicity: multiplicity of the root of λ_k of the characteristic equation $\det(A - \lambda I) = 0$.
- Geometric multiplicity: dimension of the space spanned by the eigenvectors.
- Spectrum: set of all eigenvalues of A denoted by $\sigma(A)$.
- Similarity: $n \times n$ matrices A_1 and A_2 are similar if and only if a non-singular $n \times n$ matrix V exists such that $A_2 = V^{-1} A_1 V$.
- Diagonalizability: set of eigenvectors has dimension n and $A = V^{-1} D V$ for some matrix V and diagonal matrix D.

§ 2.3: Symmetry

- The transpose of A, denoted by A^T, is an $n \times n$ matrix with components $a_{ij}^T = a_{ji}$.
- The matrix A is symmetric if and only if $A^T = A$.

Theorem 2.3.1

The eigenvalues of a symmetric matrix A are real, i.e., $A = A^T \Rightarrow \sigma(A) \subset \mathbb{R}$.

Theorem 2.3.2

A symmetric matrix A is orthogonally diagonalisable, i.e., there exists an orthogonal matrix Q and a diagonal matrix D such that $A = Q^T DQ$. The entries of D are the eigenvalues of A and the columns of Q span the eigenspaces of A.

§ 2.4: Positive-Definiteness

- A is called positive definite (positive semi-definite) if and only if

$$\forall \mathbf{u} \in \mathbb{R}^N \backslash \{\mathbf{0}\} : \mathbf{u}^T A \mathbf{u} > 0 \left(\mathbf{u}^T A \mathbf{u} \geq 0 \right)$$

Theorem 2.4.1

The spectrum of a symmetric positive definite (positive semi-definite) matrix A are strictly positive (positive), i.e.,
$ASPD \Rightarrow \sigma(A) \subset \mathbb{R}^+ \left(ASPSD \Rightarrow \sigma(A) \subset \mathbb{R}^+_0 \right)$.

SPD Systems

A matrix **A** which is SPD (symmetric positive-definite) has:

- Real, strictly positive eigenvalues
- Orthonormal eigenvectors which form a basis for diagonalization

Can we verify these properties for the resulting discretized Poisson matrices?

Example: 1D Poisson

$$-\frac{d^2u}{dx^2} = f \text{ on } \Omega = (0,1), \quad u(0) = u(1) = 0$$

§ 3.7: Discrete Spectrum

Recall (Lecture 2, book eq. 3.18) that the continuous eigenvalues and eigenfunctions are given by

$$\lambda_k = (k\pi)^2, \quad u^k(x) = \sin(k\pi x), k = 1, 2, \ldots$$

Theorem 3.7.1

With elimination, the 1D matrix $A \in \mathbb{R}^{(N-1)\times(N-1)}$ has eigenvalues and eigenvectors

$$A^h \mathbf{v}^{h,[k]} = \lambda_k^h \mathbf{v}^{h,[k]}$$

$$\mathbf{v}^{h,[k]} = \frac{1}{\sqrt{N-1}} \begin{pmatrix} \sin(\pi k x_1) \\ \vdots \\ \sin(\pi k x_{N-1}) \end{pmatrix} = \frac{1}{\sqrt{N-1}} \begin{pmatrix} \sin(\pi k h) \\ \vdots \\ \sin(\pi k (N-1) h) \end{pmatrix}$$

and

$$\lambda_k^h \left(A^h\right) = \frac{2}{h^2}[1 - \cos(\pi h k)] = \frac{2}{h^2} 2 \sin^2\left(\frac{\pi h k}{2}\right)$$

§ 3.7: Discrete Spectrum

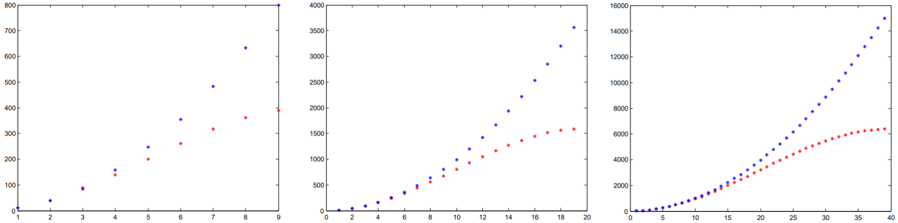


Figure: 1D continuous and discrete eigenvalues for 10, 20 and 40 gridpoints

§ 3.7: Discrete Spectrum (2D, theorem 3.7.2)

$$A^h \mathbf{v}^{h,[k\ell]} = \lambda^h_{k\ell} \mathbf{v}^{h,[k\ell]}, \quad k, \ell = 1, \ldots, N-1$$

$$\mathbf{v}^{h,[k\ell]} = \frac{1}{(N-1)} \begin{pmatrix} \sin(\pi kh)\sin(\pi \ell h) \\ \vdots \\ \sin(\pi k(N-1)h)\sin(\pi \ell h) \\ \sin(\pi kh)\sin(\pi \ell 2h) \\ \vdots \\ \sin(\pi k(N-1)h)\sin(\pi \ell 2h) \\ \vdots \\ \sin(\pi kh)\sin(\pi \ell (N-1)h) \\ \vdots \\ \sin(\pi k(N-1)h)\sin(\pi \ell (N-1)h) \end{pmatrix}$$

$$\lambda_{k\ell}\left(A^h\right) = \frac{4}{h^2}\left[1 - \frac{1}{2}\cos(\pi hk) - \frac{1}{2}\cos(\pi h\ell)\right] = \frac{4}{h^2}\left[\sin^2\left(\frac{\pi hk}{2}\right) + \sin^2\left(\frac{\pi h\ell}{2}\right.\right.$$

§ 2.8: Irreducibility and Diagonal Dominance

- Irreducibility: A is called irreducible iff no permutation matrix P exists such that PAP^T is block upper triangular.
- Row Diagonal Dominance: A is row diagonal dominant iff

$$|a_{ii}| \geq \sum_{j=1, j\neq i}^{n} |a_{ij}| \quad i = 1, \ldots, n$$

- Strict Diagonal Dominance: A is row strictly diagonal dominant iff

$$|a_{ii}| > \sum_{j=1, j\neq i}^{n} |a_{ij}| \quad i = 1, \ldots, n$$

- A is irreducibly strictly diagonal dominant iff A is irreducible and diagonally dominant.

§ 2.8: Irreducibility and Diagonal Dominance

Diagonal dominance of A and its spectrum can be related through the Gershgorin theorem

Theorem 2.8.1 (Gershgorin)

If $\lambda \in \sigma(A)$, then λ is located in one of the n closed disks in the complex plane that has center a_{ii} and radius

$$\rho_i = \sum_{j=1, j\neq i}^{n} |a_{ij}|$$

i.e.,

$$\lambda \in \sigma(A) \Rightarrow \exists i \text{ such that } |a_{ii} - \lambda| \leq \rho_i,$$

Gershgorin

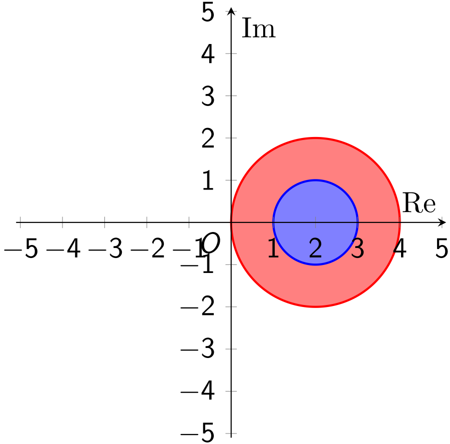
Example: 1D Poisson

$$-\frac{d^2u}{dx^2} = f \text{ on } \Omega = (0,1), \quad u(0) = u(1) = 0$$

$$\text{with discretized matrix } \mathbf{A} = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}$$

Gershgorin

Example: 1D Poisson



$$A = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$$

§ 2.8: M-matrix

- K-matrix: A is a K-matrix if:
  1. $a_{ii} > 0$ for $i = 1, \ldots, n$ (Diagonal Dominance);
  2. $a_{ij} \leq 0$ for $i \neq j, i, j = 1, \ldots, n$ (Z-matrix).
- M-matrix: A is an M-matrix if A is a Z-Matrix and $\left(A^{-1}\right)_{ij} \geq 0 \quad i, j = 1, \ldots, n$

Theorem 2.9.1

If matrix A is a K-matrix and irreducibly diagonally dominant, then A is an M-matrix.

§ 2.6: Condition Number

- Condition Number: in p-norm $\kappa_p(A)$ of an invertible $n \times n$ matrix A is defined as

$$\kappa_p(A) = \|A\|_p \left\|A^{-1}\right\|_p$$

  - 2-norm:

$$\kappa_2(A) = \frac{\sqrt{\lambda_{\text{max}}\left(A^T A\right)}}{\sqrt{\lambda_{\text{min}}\left(A^T A\right)}}$$

  - Symmetric or SPD A:

$$\kappa_2(A) = \frac{\lambda_{\text{max}}(A)}{\lambda_{\text{min}}(A)}$$

$$\lambda_{\text{max}}(A) = \max_{i=1,\dots,n} \{|\lambda_i| : \lambda_i \in \sigma(A)\}$$

$$\lambda_{\text{min}}(A) = \min_{i=1,\dots,n} \{|\lambda_i| : \lambda_i \in \sigma(A)\}$$

Condition Number

Example: 1D Poisson

$$-\frac{d^2u}{dx^2} = f \text{ on } \Omega = (0,1), \quad u(0) = u(1) = 0$$

with discretized matrix $\mathbf{A} = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}$

A is SPD so all eigenvalues real and positive.

$\lambda_{\max}(A) = \frac{2}{h^2} 2\sin^2\left(\frac{\pi h(\mathbf{n-1})}{2}\right) \approx \frac{4}{h^2}$

$\lambda_{\min}(A) = \frac{2}{h^2} 2\sin^2\left(\frac{\pi h(\mathbf{1})}{2}\right) \approx \pi^2$

$\kappa_2(A) = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} = \frac{\lambda_{(n-1)}(A)}{\lambda_{(1)}(A)} \approx \frac{4}{\pi^2 h^2}$

Condition Number

Example: 2D Poisson (corollary 3.7.2)

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f \text{ on } \Omega = (0,1)\times(0,1), u(x,y) = 0 \text{ on } \Gamma$$

with discretized matrix $\mathbf{A} = \frac{1}{h^2}\begin{bmatrix} 4 & -1 & 0 & -1 & 0 \\ -1 & 4 & -1 & 0 & -1 \\ 0 & -1 & 4 & 0 & 0 \\ -1 & 0 & 0 & 4 & -1 \\ 0 & -1 & 0 & -1 & 4 \end{bmatrix}$

$$\begin{aligned} \frac{\lambda_{(N-1)(N-1)}}{\lambda_{11}} &= \frac{1 - \frac{1}{2}\cos(\pi h(N-1)) - \frac{1}{2}\cos(\pi h(N-1))}{1 - \frac{1}{2}\cos(\pi h) - \frac{1}{2}\cos(\pi h)} \\ &= \frac{\pi^2 h^2 (N-1)^2 + \mathcal{O}\left(h^4\right)}{\pi^2 h^2 + \mathcal{O}\left(h^4\right)} = (N-1)^2 + \mathcal{O}\left(h^2\right) \\ &= \mathcal{O}\left(h^{-2}\right) \end{aligned}$$

Summary and Next Week

- Defined and analyzed matrix properties
  - Symmetry
  - Positive Definiteness
  - Conditioning (remember round-off error example first week!)
  - M-matrix
  - Sparsity
- Next week: iterative methods to solve $\mathbf{Au} = \mathbf{f}$
  - Pick solver based on properties of $\mathbf{A}$
  - Define convergence
  - Matrix norms