ESO 208A: Computational Methods in Engineering

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Recap

- Pitfalls of Gauss Elimination Method
- Gauss Jordan Method
- LU decomposition-Gauss Elimination, Dolittle, Crout

Today's lecture

- Thomas Algorithm
- Cholesky Decomposition
- Forward Error Analysis
- Indirect Methods-Gauss-Seidal, Jacobi iterative method

LU decomposition

Thomas Algorithm (Tri-diagonal Matrix)

Thomas Algorithm - Tri diagonal

$$\begin{bmatrix} d_1 & u_1 & & & \\ l_2 & d_2 & u_2 & & \\ & l_3 & d_3 & u_3 & \\ & & \ddots & \ddots & \ddots \\ & & & l_n & d_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

Define

$$\alpha_1 = d_1$$
$$\beta_1 = b_1$$

$$\lambda_2 = \frac{l_2}{\alpha_1}$$

$$R_1 - \alpha_1 x_1 + u_1 x_2 = \beta_1$$
$$R_2 - l_2 x_1 + d_2 x_2 + u_2 x_3 = b_2$$

$$R_2 \to R_2 - \lambda_2 R_1$$

$$x_2 (d_2 - \lambda_2 u_1) + u_2 x_3 = b_2 - \lambda_2 \beta_1$$

Define

$$\alpha_2 = d_2 - \lambda_2 u_1$$
$$\beta_2 = b_2 - \lambda_2 \beta_1$$

$$\Rightarrow \quad \alpha_2 x_2 + u_2 x_3 = \beta_2$$

$$\lambda_3 = \frac{l_3}{\alpha_2} \qquad l_3 x_2 + d_2 x_3 + u_3 x_4 = b_3$$

$$\lambda_i = \frac{l_i}{\alpha_{i-1}}$$
$$\alpha_i = d_i - \lambda_i u_{i-1}$$
$$\beta_i = b_i - \lambda_i \beta_{i-1}$$

$$x_i = \frac{\beta_i - u_i x_{i+1}}{\alpha_i}, \quad i = n-1, \dots, 1 \quad \leftarrow \quad \alpha_i x_i + u_i x_{i+1} = \beta_i$$

$i = n$: $$\alpha_n x_n = \beta_n \Rightarrow x_n = \beta_n / \alpha_n$$

LU decomposition

Thomas Algorithm (Tri-diagonal Matrix)

GE : $O(2/3\, n^3)$

Thomas : $O(n)$

Example

$$\begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 4 \\ 8 \\ 8 \end{bmatrix}$$

$\alpha_1 = d_1 \qquad \beta_1 = b_1 \qquad \lambda_i = \dfrac{l_i}{\alpha_{i-1}}$

$\alpha_i = d_i - \lambda_i u_{i-1}$

$\beta_i = b_i - \lambda_i \beta_{i-1}$

$x_n = \beta_n / \alpha_n$

$x_i = \dfrac{\beta_i - u_i x_{i+1}}{\alpha_i}$

i	l	d	u	b	λ	α	β	x
1		2	1	4		2	4	$x_1 = 1$
2	1	2	1	8	$\frac{l_2}{\alpha_1} = 0.5$	$2 - 0.5\times 1 = 1.5$	$8 - 0.5\times 4 = 6$	$x_2 = \frac{6 - 1\times 3}{3/2} = 2$
3	1	2		8	$\frac{l_3}{\alpha_2} = \frac{1}{1.5} = 2/3$	$4/3$	4	$x_3 = 4/\tfrac{4}{3} = 3$

LU decomposition

Cholesky Decomposition (for +ve definite matrix)

Diagonalization (*LDU* theorem):

Let $\boldsymbol{A}$ be a $n \times n$ invertible matrix then there exists a decomposition of the form $\boldsymbol{A} = \boldsymbol{LDU}$ where, $\boldsymbol{L}$ is a $n \times n$ lower triangular matrix with diagonal elements as 1, $\boldsymbol{U}$ is a $n \times n$ upper triangular matrix with diagonal elements as 1, and $\boldsymbol{D}$ is a $n \times n$ diagonal matrix.

Example of a 3×3 matrix:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} d_{11} = u_{11} & 0 & 0 \\ 0 & d_{22} = u_{22} & 0 \\ 0 & 0 & d_{33} = u_{33} \end{bmatrix} \begin{bmatrix} 1 & {}^{u_{12}}/_{u_{11}} & {}^{u_{13}}/_{u_{11}} \\ 0 & 1 & {}^{u_{23}}/_{u_{22}} \\ 0 & 0 & 1 \end{bmatrix}$$

LU decomposition

Cholesky Decomposition (for +ve definite matrix)

For a symmetric Marix

$$A^T = A$$

$$A = LDU$$

$$A = A^T = U^T D L^T$$

This implies,

$$L = U^T$$

$$U = L^T$$

For symmetric matrix: $\boldsymbol{U} = \boldsymbol{L}^T$ and $\boldsymbol{A} = \boldsymbol{L}\boldsymbol{D}\boldsymbol{L}^T$

Note that the entries of the diagonal matrix $\boldsymbol{D}$ are the *pivots*!

LU decomposition

Cholesky Decomposition (for +ve definite matrix)

- For positive definite matrices, *pivots* are positive!
- Therefore, a diagonal matrix $\boldsymbol{D}$ containing the *pivots* can be factorized as: $\boldsymbol{D} = \boldsymbol{D}^{1/2}\boldsymbol{D}^{1/2}$
- Example of a 3×3 matrix

$$\begin{bmatrix} d_{11} & 0 & 0 \\ 0 & d_{22} & 0 \\ 0 & 0 & d_{33} \end{bmatrix}$$

$$= \begin{bmatrix} \sqrt{d_{11}} & 0 & 0 \\ 0 & \sqrt{d_{22}} & 0 \\ 0 & 0 & \sqrt{d_{33}} \end{bmatrix} \begin{bmatrix} \sqrt{d_{11}} & 0 & 0 \\ 0 & \sqrt{d_{22}} & 0 \\ 0 & 0 & \sqrt{d_{33}} \end{bmatrix}$$

- For *positive definite* matrices: $\boldsymbol{A} = \boldsymbol{L}\boldsymbol{D}\boldsymbol{L}^T = \boldsymbol{L}\,\boldsymbol{D}^{1/2}\boldsymbol{D}^{1/2}\,\boldsymbol{L}^T$
- However, $\boldsymbol{D}^{1/2}\boldsymbol{L}^T = (\mathbf{L}\boldsymbol{D}^{1/2})^T$. Denote: $\boldsymbol{L}\,\boldsymbol{D}^{1/2} = \boldsymbol{L}_1$
- Therefore, $\boldsymbol{A} = \boldsymbol{L}_1\,\boldsymbol{L}_1{}^T$. This is also a *LU-Decomposition* where one needs to evaluate only one triangular matrix $\boldsymbol{L}_1$.

LU decomposition

Cholesky Decomposition (for +ve definite matrix)

$$
\begin{bmatrix}
a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\
a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\
a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\
\vdots & \vdots & \vdots & \ddots & \\
a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn}
\end{bmatrix}
=
\begin{bmatrix}
l_{11} & & & \\
l_{21} & l_{22} & & \\
l_{31} & l_{32} & l_{33} & \\
\vdots & & \ddots & \\
l_{n1} & l_{n2} & \cdots & l_{nn}
\end{bmatrix}
\begin{bmatrix}
l_{11} & l_{21} & \cdots & l_{n1} \\
 & l_{22} & l_{32} & \cdots \\
 & & \ddots & \\
 & & & l_{nn}
\end{bmatrix}
$$

$$a_{ij} = a_{ji}$$

$$l_{11}^2 = a_{11}$$

$$l_{11} = \sqrt{a_{11}}$$

$$l_{j1} = \frac{a_{j1}}{l_{11}}$$

$$l_{jj} = \sqrt{a_{jj} - \sum_{k=1}^{j-1} l_{jk}^2} \qquad j = 2, \ldots n$$

$$l_{kj} = \left(a_{kj} - \sum_{s=1}^{j-1} l_{js}\, l_{ks}\right) \Big/ l_{jj} \qquad k = j+1, \ldots n$$

LU decomposition

Cholesky Decomposition (for +ve definite matrix)

Example

$$\begin{bmatrix} 4 & 2 & 14 \\ 2 & 17 & -5 \\ 14 & -5 & 83 \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}$$

$$\Rightarrow \quad l_{11}^2 = a_{11} \quad \Rightarrow \quad \boxed{l_{11} = \sqrt{a_{11}}} = 2$$

$$l_{21}\, l_{11} = a_{21}$$

$$\Rightarrow \quad l_{21} = \frac{a_{21}}{l_{11}} \qquad \Rightarrow \quad l_{21} = \frac{2}{2} = 1$$

$$\boxed{l_{j1} = \frac{a_{j1}}{l_{11}}}$$

$$l_{31} = \frac{14}{2} = 7$$

$$L = \begin{bmatrix} 2 & 0 & 0 \\ 1 & 4 & 0 \\ 7 & -3 & 5 \end{bmatrix} \qquad L^T = \begin{bmatrix} 2 & 1 & 7 \\ 0 & 4 & -3 \\ 0 & 0 & 5 \end{bmatrix}$$

$$l_{21}^2 + l_{22}^2 = a_{22}$$

$$\Rightarrow \quad l_{22} = \sqrt{a_{22} - l_{21}^2} = \sqrt{17 - 1^2} = 4$$

$$\boxed{l_{jj} = \sqrt{a_{jj} - \sum_{k=1}^{j-1} l_{jk}^2}}$$

$$l_{31}\, l_{21} + l_{32} \cdot l_{22} = a_{32}$$

$$\Rightarrow \quad l_{32} = \frac{a_{32} - l_{31}\, l_{21}}{l_{22}} = \frac{-5 - 7 \times 1}{4} = -3$$

$$l_{kj} = \frac{a_{kj} - \sum_{s=1}^{j-1} l_{js}\, l_{ks}}{l_{jj}} \qquad k = j+1, \ldots, n$$

$$l_{33} = \sqrt{83 - 7^2 - 3^2} = 5$$

Summary

- Thomas Algorithm
- Cholesky Decompsition