18-660: Numerical Methods for Engineering Design and Optimization

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Overview

- Linear Equation Solver
  - LU decomposition
  - Cholesky decomposition

Linear Equation Solver

- Gaussian elimination solves a linear equation

$$\begin{bmatrix} \quad A \quad \end{bmatrix} \cdot \begin{bmatrix} X \end{bmatrix} = \begin{bmatrix} B \end{bmatrix}$$

- Sometimes we want to repeatedly calculate the solutions for different right-hand-side vectors

$$\begin{bmatrix} \quad A \quad \end{bmatrix} \cdot \begin{bmatrix} X_1 \end{bmatrix} = \begin{bmatrix} B_1 \end{bmatrix}$$

Case 1

$$\begin{bmatrix} \quad A \quad \end{bmatrix} \cdot \begin{bmatrix} X_2 \end{bmatrix} = \begin{bmatrix} B_2 \end{bmatrix}$$

Case 2

Ordinary Differential Equation Example

- Backward Euler integration for linear ordinary differential equation with constant time step Δt

$$\dot{x}(t) = A \cdot x(t) + B \cdot u(t) \quad x(0) = 0$$

$$x(t_{n+1}) = \underbrace{(I - \Delta t \cdot A)^{-1}}_{\text{Identical @ all } t_n\text{'s}} \cdot \underbrace{[x(t_n) + \Delta t \cdot B \cdot u(t_{n+1})]}_{\text{Different @ all } t_n\text{'s}} \quad x(t_0) = 0$$

Identical
@ all t_n's

Different
@ all t_n's

LU Factorization

- It would be expensive to repeatedly run Gaussian elimination for many times
  - How can we save and re-use the intermediate results?
  - LU factorization is to address this problem

$$\begin{bmatrix} & A & \end{bmatrix} \cdot \begin{bmatrix} X_1 \end{bmatrix} = \begin{bmatrix} B_1 \end{bmatrix}$$

Case 1

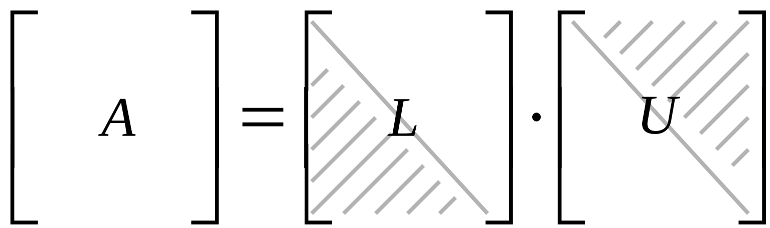
$$\begin{bmatrix} & A & \end{bmatrix} \cdot \begin{bmatrix} X_2 \end{bmatrix} = \begin{bmatrix} B_2 \end{bmatrix}$$

Case 2

LU Factorization

- Key idea:
  - Represent A as the product of L (lower triangular) and U (upper triangular) via Gaussian-elimination-like steps
  - All diagonal elements in U are set to 1 by proper scaling

$$\begin{bmatrix} & A & \end{bmatrix} \cdot \begin{bmatrix} X \end{bmatrix} = \begin{bmatrix} B \end{bmatrix}$$



LU factorization is unchanged as long as A is unchanged (i.e., independent of the right-hand-side vector B)

LU Factorization

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & \cdots & a_{2N} \\ \vdots & \vdots & \vdots & \vdots \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{bmatrix} = \begin{bmatrix} l_{11} & & & \\ l_{21} & l_{22} & & \\ \vdots & \vdots & \ddots & \\ l_{N1} & l_{N2} & \cdots & l_{NN} \end{bmatrix} \cdot \begin{bmatrix} 1 & u_{12} & \cdots & u_{1N} \\ & 1 & \cdots & u_{2N} \\ & & \ddots & \vdots \\ & & & 1 \end{bmatrix}$$

$$l_{i1} \cdot 1 = a_{i1} \quad \left(i = 1, 2, \cdots, N\right)$$

LU Factorization

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & \cdots & a_{2N} \\ \vdots & \vdots & \vdots & \vdots \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{bmatrix} = \begin{bmatrix} l_{11} & & & \\ l_{21} & l_{22} & & \\ \vdots & \vdots & \ddots & \\ l_{N1} & l_{N2} & \cdots & l_{NN} \end{bmatrix} \cdot \begin{bmatrix} 1 & u_{12} & \cdots & u_{1N} \\ & 1 & \cdots & u_{2N} \\ & & \ddots & \vdots \\ & & & 1 \end{bmatrix}$$

$$l_{11} \cdot u_{1i} = a_{1i} \quad \left(i = 2,3,\cdots,N\right)$$

LU Factorization

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & \cdots & a_{2N} \\ \vdots & \vdots & \vdots & \vdots \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{bmatrix} = \begin{bmatrix} l_{11} & & & \\ l_{21} & l_{22} & & \\ \vdots & \vdots & \ddots & \\ l_{N1} & l_{N2} & \cdots & l_{NN} \end{bmatrix} \cdot \begin{bmatrix} 1 & u_{12} & \cdots & u_{1N} \\ & 1 & \cdots & u_{2N} \\ & & \ddots & \vdots \\ & & & 1 \end{bmatrix}$$

$$l_{i1} \cdot u_{12} + l_{i2} \cdot 1 = a_{i2} \quad (i = 2,3,\cdots,N)$$

Continue iteration until all elements in L and U are solved

Memory Storage

- The matrix A can be iteratively replaced by L and U
  - No additional memory is required

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & \cdots & a_{2N} \\ \vdots & \vdots & \vdots & \vdots \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{bmatrix}$$

$$\Downarrow$$

$$\begin{bmatrix} l_{11} & u_{12} & \cdots & u_{1N} \\ l_{21} & l_{22} & \ddots & \vdots \\ \vdots & \vdots & \ddots & u_{N-1,N} \\ l_{N1} & l_{N2} & \cdots & l_{NN} \end{bmatrix}$$

A Simple LU Example

$$\begin{bmatrix} 2 & 1 & -1 \\ -3 & -1 & 2 \\ -2 & 1 & 2 \end{bmatrix} = \begin{bmatrix} l_{11} & & \\ l_{21} & l_{22} & \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \cdot \begin{bmatrix} 1 & u_{12} & u_{13} \\ & 1 & u_{23} \\ & & 1 \end{bmatrix}$$

$$l_{11} \cdot 1 = a_{11} \quad l_{21} \cdot 1 = a_{21} \quad l_{31} \cdot 1 = a_{31}$$

$$\begin{bmatrix} 2 & 1 & -1 \\ -3 & -1 & 2 \\ -2 & 1 & 2 \end{bmatrix}$$

A Simple LU Example

$$\begin{bmatrix} 2 & 1 & -1 \\ -3 & -1 & 2 \\ -2 & 1 & 2 \end{bmatrix} \quad \begin{bmatrix} l_{11} & & \\ l_{21} & l_{22} & \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \cdot \begin{bmatrix} 1 & u_{12} & u_{13} \\ & 1 & u_{23} \\ & & 1 \end{bmatrix}$$

$$l_{11} \cdot u_{12} = a_{12} \quad l_{11} \cdot u_{13} = a_{13}$$

$$\begin{bmatrix} 2 & 1/2 & -1/2 \\ -3 & -1 & 2 \\ -2 & 1 & 2 \end{bmatrix}$$

A Simple LU Example

$$\begin{bmatrix} 2 & 1/2 & -1/2 \\ -3 & -1 & 2 \\ -2 & 1 & 2 \end{bmatrix} \quad \begin{bmatrix} l_{11} & & \\ l_{21} & l_{22} & \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \cdot \begin{bmatrix} 1 & u_{12} & u_{13} \\ & 1 & u_{23} \\ & & 1 \end{bmatrix}$$

$$l_{21} \cdot u_{12} + l_{22} = a_{22} \qquad l_{31} \cdot u_{12} + l_{32} = a_{32}$$

$$\begin{bmatrix} 2 & 1/2 & -1/2 \\ -3 & 1/2 & 2 \\ -2 & 2 & 2 \end{bmatrix}$$

A Simple LU Example

$$\begin{bmatrix} 2 & 1/2 & -1/2 \\ -3 & 1/2 & 2 \\ -2 & 2 & 2 \end{bmatrix} \begin{bmatrix} l_{11} & & \\ l_{21} & l_{22} & \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \cdot \begin{bmatrix} 1 & u_{12} & u_{13} \\ & 1 & u_{23} \\ & & 1 \end{bmatrix}$$

$$l_{21} \cdot u_{13} + l_{22} \cdot u_{23} = a_{23}$$

$$\begin{bmatrix} 2 & 1/2 & -1/2 \\ -3 & 1/2 & 1 \\ -2 & 2 & 2 \end{bmatrix}$$

A Simple LU Example

$$\begin{bmatrix} 2 & 1/2 & -1/2 \\ -3 & 1/2 & 1 \\ -2 & 2 & 2 \end{bmatrix} \quad \begin{bmatrix} l_{11} & & \\ l_{21} & l_{22} & \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \cdot \begin{bmatrix} 1 & u_{12} & u_{13} \\ & 1 & u_{23} \\ & & 1 \end{bmatrix}$$

$$l_{31} \cdot u_{13} + l_{32} \cdot u_{23} + l_{33} = a_{33}$$

$$\begin{bmatrix} 2 & 1/2 & -1/2 \\ -3 & 1/2 & 1 \\ -2 & 2 & -1 \end{bmatrix}$$

LU Factorization

- Given L and U, solve linear equation via two steps

$$A \cdot X = B$$

$$\Downarrow \quad A = LU$$

$$L \cdot \underbrace{U \cdot X}_{V} = B$$

$$\Downarrow$$

$$L \cdot V = B$$

$$U \cdot X = V$$

LU Factorization

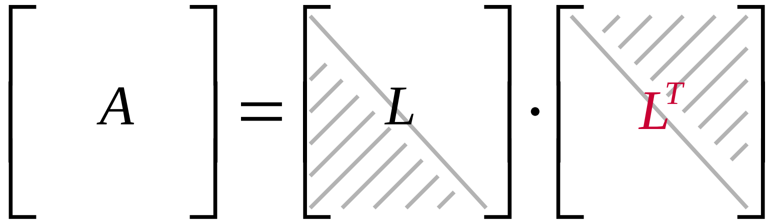
$$[L] \cdot [V] = [B] \quad \Rightarrow \quad [U] \cdot [X] = [V]$$

Forward substitution — Backward substitution

- Only the above two steps are repeated if the right-hand-side vector B is changed
  - LU factorization is not repeated
  - More efficient than Gaussian elimination

Cholesky Factorization

- If the matrix A is symmetric and positive definite, Cholesky factorization is preferred over LU factorization



- Cholesky factorization is cheaper than LU
  - Only needs to find a single triangular matrix L (instead of two different matrices L and U)

Cholesky Factorization

- A must be symmetric and positive definite to make Cholesky factorization applicable

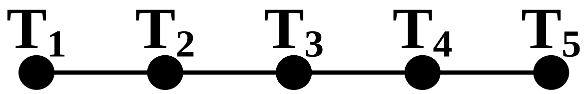
- A symmetric matrix A is positive definite if

$$P^T \cdot A \cdot P > 0 \quad \text{for any real-valued vector } P \neq 0$$

- Sufficient and necessary condition for a symmetric matrix A to be positive definite:
  - All eigenvalues of A are positive

Partial Differential Equation Example

- 1-D rod discretized into 4 segments



$$\kappa \cdot \frac{\partial^2 T(x,t)}{\partial x^2} = 0$$

$$T_1 = 30 \quad T_5 = 100$$

$$\kappa \cdot (-T_{i-1} + 2T_i - T_{i+1}) = 0 \quad (2 \le i \le 4)$$

$$-30 + 2T_2 - T_3 = 0$$

$$-T_2 + 2T_3 - T_4 = 0$$

$$-T_3 + 2T_4 - 100 = 0$$

Partial Differential Equation Example

$$-30 + 2T_2 - T_3 = 0$$
$$-T_2 + 2T_3 - T_4 = 0$$
$$-T_3 + 2T_4 - 100 = 0$$

⇒

$$\underbrace{\begin{bmatrix} 2 & -1 & \\ -1 & 2 & -1 \\ & -1 & 2 \end{bmatrix}}_{A} \cdot \begin{bmatrix} T_2 \\ T_3 \\ T_4 \end{bmatrix} = \begin{bmatrix} 30 \\ 0 \\ 100 \end{bmatrix}$$

- Eigenvalues of A

$$\lambda_1 = 3.41$$
$$\lambda_2 = 2.00$$
$$\lambda_3 = 0.58$$

(A is positive definite)

Partial Differential Equation Example

- In practice, we never calculate eigenvalues to check if a matrix is positive definite or not
  - Eigenvalue decomposition is much more expensive than solving a linear equation
- If we apply finite difference to discretize steady-state heat equation, the resulting linear equation is positive definite

Partial Differential Equation Example

$$\begin{bmatrix} 2 & -1 & \\ -1 & 2 & -1 \\ & -1 & 2 \end{bmatrix} = \begin{bmatrix} l_{11} & & \\ l_{21} & l_{22} & \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \cdot \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ & l_{22} & l_{32} \\ & & l_{33} \end{bmatrix}$$

$$l_{11} \cdot l_{11} = a_{11} \quad l_{21} \cdot l_{11} = a_{21} \quad l_{31} \cdot l_{11} = a_{31}$$

$$\begin{bmatrix} \sqrt{2} & -1 & \\ -\sqrt{1/2} & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$$

Partial Differential Equation Example

$$\begin{bmatrix} \sqrt{2} & -1 & \\ -\sqrt{1/2} & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \quad \begin{bmatrix} l_{11} & & \\ l_{21} & l_{22} & \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \cdot \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ & l_{22} & l_{32} \\ & & l_{33} \end{bmatrix}$$

$$l_{21} \cdot l_{21} + l_{22} \cdot l_{22} = a_{22} \qquad l_{21} \cdot l_{31} + l_{22} \cdot l_{32} = a_{23}$$

$$\begin{bmatrix} \sqrt{2} & -1 & \\ -\sqrt{1/2} & \sqrt{3/2} & -1 \\ 0 & -\sqrt{2/3} & 2 \end{bmatrix}$$

Partial Differential Equation Example

$$\begin{bmatrix} \sqrt{2} & -1 & \\ -\sqrt{1/2} & \sqrt{3/2} & -1 \\ 0 & -\sqrt{2/3} & 2 \end{bmatrix} \quad \begin{bmatrix} l_{11} & & \\ l_{21} & l_{22} & \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \cdot \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ & l_{22} & l_{32} \\ & & l_{33} \end{bmatrix}$$

$$l_{31} \cdot l_{31} + l_{32} \cdot l_{32} + l_{33} \cdot l_{33} = a_{33}$$

$$\begin{bmatrix} \sqrt{2} & -1 & \\ -\sqrt{1/2} & \sqrt{3/2} & -1 \\ 0 & -\sqrt{2/3} & \sqrt{4/3} \end{bmatrix}$$

Summary

- Linear equation solver
  - LU decomposition
  - Cholesky decomposition