CEE432/CEE532/MAE541

Developing Software for Engineering Applications

Lecture 11: Matrix Algebra (Chapter 10)

Terminology

- Types of arrays, $\mathbf{A}_{\mathbf{mxn}}$
  - One-dimensional, vector, $\mathbf{g}_{\mathbf{mx1}}$
  - Square matrix, $\mathbf{A}_{\mathbf{nxn}}$
  - Symmetric matrix, $A_{ij}=A_{ji}$
  - Diagonal matrix
  - Identity matrix, $\mathbf{I}_{\mathbf{nxn}}$
  - Upper Triangular Matrix, $A_{ij}=0$, $i > j$
  - Lower Triangular Matrix, $A_{ij}=0$, $i < j$

Terminology

- Matrix Operations
  - Addition and subtraction, $\mathbf{A}_{\mathbf{mxn}}=\mathbf{B}_{\mathbf{mxn}} \pm \mathbf{C}_{\mathbf{mxn}}$
  - Multiplication, $\mathbf{A}_{\mathbf{mxn}}=\mathbf{B}_{\mathbf{mxq}}\,\mathbf{C}_{\mathbf{qxn}}$
  - Inverse (Avoid!!),$\mathbf{A}^{-1}$
  - Transpose, $\mathbf{A}^{T}$
  - Determinant (Avoid!!), det($\mathbf{A}$)

Linear Algebraic Equations

$$\mathbf{A}_{m \times n} \mathbf{x}_{n \times 1} = \mathbf{b}_{m \times 1}$$

- Unique, non-trivial solution iff
  - m=n
  - det(**A**)≠0
  - **b** is not a null vector

Solution Strategies

- Direct Solver
  - Gaussian Elimination
  - LU Factorization
  - LDL^T (Cholesky) Factorization
- Iterative Solver
  - Preconditioned Conjugate Gradient Method

Important Issues

- How much storage space will be used?
- How can numerically accurate solution can be generated?
- How much time will be taken to obtain the solution?
- How much of additional effort is needed if a solution is to be generated for a new right-hand side vector?

Storage Scheme: Full

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix}$$

Storage requirement: 4^2=16 locations. In general, storage requirement = $\mathbf{n^2}$ locations

Double Precision

n=$10^4 \rightarrow$ 800,000,000 bytes

1 GB = 1,073,741,824 bytes

Rowwise storage

$$\{A_{11}, A_{12}, \ldots, A_{1n}, A_{21}, A_{22}, \ldots, A_{2n}, \ldots A_{n1}, A_{n2}, \ldots, A_{nn}\}$$

Columnwise storage

$$\{A_{11}, A_{21}, \ldots, A_{n1}, A_{12}, A_{22}, \ldots, A_{n2}, \ldots A_{1n}, A_{2n}, \ldots, A_{nn}\}$$

Storage Scheme: Symmetric, Banded

$$
\begin{bmatrix}
A_{11} & A_{12} & & & A_{15} & A_{16} & & & & \\
 & A_{22} & & & A_{25} & A_{26} & & & & \\
 & & A_{33} & A_{34} & A_{35} & A_{36} & & & & \\
 & & & A_{44} & A_{45} & A_{46} & & & & \\
 & & & & A_{55} & A_{56} & A_{57} & A_{58} & A_{59} & A_{5,10} \\
 & & & & & A_{66} & A_{67} & A_{68} & A_{69} & A_{6,10} \\
 & & & & & & A_{77} & A_{78} & & \\
 & & & & & & & A_{88} & & \\
 & & & & & & & & A_{99} & A_{9,10} \\
 & & & & & & & & & A_{10,10}
\end{bmatrix}
\quad
\begin{array}{|c|}
\hline
\boxed{6} \\ 5 \\ 4 \\ 3 \\ \boxed{6} \\ 5 \\ 2 \\ 1 \\ 2 \\ 1 \\
\hline
\end{array}
$$

$$\left(HBW\right)_i = c - i + 1 \qquad\qquad HBW = \max_i \left(HBW\right)_i$$

Storage Scheme: Symmetric, Banded

$$
\begin{bmatrix}
A_{11} & A_{12} & & & A_{15} & A_{16} & & & & \\
& A_{22} & & & A_{25} & A_{26} & & & & \\
& & A_{33} & A_{34} & A_{35} & A_{36} & & & & \\
& & & A_{44} & A_{45} & A_{46} & & & & \\
& & & & A_{55} & A_{56} & A_{57} & A_{58} & A_{59} & A_{5,10} \\
& & & & & A_{66} & A_{67} & A_{68} & A_{69} & A_{6,10} \\
& & & & & & A_{77} & A_{78} & & \\
& & & & & & & A_{88} & & \\
& & & & & & & & A_{99} & A_{9,10} \\
& & & & & & & & & A_{10,10}
\end{bmatrix}
$$

Storage Scheme: Symmetric, Banded

$$\mathbf{A}_{10\times 6}^{banded} = \begin{bmatrix} A_{11} & A_{12} & 0 & 0 & A_{15} & A_{16} \\ A_{22} & 0 & 0 & 0 & A_{25} & A_{26} \\ A_{33} & A_{34} & A_{35} & A_{36} & 0 & 0 \\ A_{44} & A_{45} & A_{46} & 0 & 0 & 0 \\ A_{55} & A_{56} & 0 & 0 & 0 & 0 \\ A_{66} & A_{67} & A_{68} & A_{69} & A_{6,10} & 0 \\ A_{77} & A_{78} & 0 & 0 & 0 & 0 \\ A_{88} & 0 & 0 & 0 & 0 & 0 \\ A_{99} & K_{9,10} & 0 & 0 & 0 & 0 \\ A_{10,10} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Storage Scheme: Symmetric, Banded

$$\begin{bmatrix} A_{11} & A_{12} & 0 & 0 & A_{15} & A_{16} \\ A_{22} & 0 & 0 & 0 & A_{25} & A_{26} \\ A_{33} & A_{34} & A_{35} & A_{36} & 0 & 0 \\ A_{44} & A_{45} & A_{46} & 0 & 0 & 0 \\ A_{55} & A_{56} & 0 & 0 & 0 & 0 \\ A_{66} & A_{67} & A_{68} & A_{69} & A_{6,10} & 0 \\ A_{77} & A_{78} & 0 & 0 & 0 & 0 \\ A_{88} & 0 & 0 & 0 & 0 & 0 \\ A_{99} & K_{9,10} & 0 & 0 & 0 & 0 \\ A_{10,10} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$A_{i,j} = 0 \text{ if } \left(j - i + 1 \right) > HBW$$

$$A_{i,j} = 0 \text{ if } \left(j < i \right)$$

$$A_{i,j} \Rightarrow A^{banded}_{i,j-i+1}$$

Storage Scheme: Symmetric, Skyline

$$
\begin{bmatrix}
A_{11} & A_{12} & & & A_{15} & A_{16} & & & & \\
 & A_{22} & & & A_{25} & A_{26} & & & & \\
 & & A_{33} & A_{34} & A_{35} & A_{36} & & & & \\
 & & & A_{44} & A_{45} & A_{46} & & & & \\
 & & & & A_{55} & A_{56} & A_{57} & A_{58} & A_{59} & A_{5} \\
 & & & & & A_{66} & A_{67} & A_{68} & A_{69} & A_{6} \\
 & & & & & & A_{77} & A_{78} & & \\
 & & & & & & & A_{88} & & \\
 & & & & & & & & A_{99} & A_{9} \\
 & & & & & & & & & A_{10,10}
\end{bmatrix}
$$

Storage Scheme: Symmetric, Skyline

$$\mathbf{A}_{35\times 1}^{skyline} = \left\{ A_{11}, A_{22}, A_{12}, A_{33}, A_{44}, A_{34}, \ldots, A_{10,10}, A_{9,10}, A_{8,10}, A_{7,10}, A_{6,10}, A_{5,10} \right\}$$

$$\mathbf{D}_{11}^{loc} = \{1,2,4,5,7,12,18,21,25,30,36\}$$

$$A_{i,j} = 0 \text{ if } \left(j - i \right) > \left(D_{j+1}^{loc} - D_{j}^{loc} \right)$$

$$A_{i,j} = 0 \text{ if } \left(j < i \right)$$

$$A_{i,j} \Rightarrow l = D_{j}^{loc} + j - i \Rightarrow A_{l}^{skyline}$$

Storage Scheme: Comparison

Storage Scheme	Storing	Equivalent Integer Words
Full	$\mathbf{A}_{n\times n}$	$2n^2$
Symmetric Banded	$\mathbf{A}_{n\times hbw}^{banded}$	$2nq$
Symmetric Skyline	$\mathbf{A}_{m}^{skyline}, \mathbf{D}_{n+1}^{loc}$	$2m+n+1$

Storage Scheme: Sparse

$$
\begin{bmatrix}
A_{11} & A_{12} & & & A_{15} & A_{16} & & & & \\
 & A_{22} & & & A_{25} & A_{26} & & & & \\
 & & A_{33} & A_{34} & A_{35} & A_{36} & & & & \\
 & & & A_{44} & A_{45} & A_{46} & & & & \\
 & & & & A_{55} & A_{56} & A_{57} & A_{58} & A_{59} & A_{5} \\
 & & & & & A_{66} & A_{67} & A_{68} & A_{69} & A_{6} \\
 & & & & & & A_{77} & A_{78} & & \\
 & & & & & & & A_{88} & & \\
 & & & & & & & & A_{99} & A_{9} \\
 & & & & & & & & & A_{10,10}
\end{bmatrix}
$$

$$\mathbf{A}^{sparse}_{31\times 1} = \left\{ A_{11}, A_{12}, A_{15}, A_{16}, A_{22}, A_{25}, A_{26}, \ldots, A_{88}, A_{99}, A_{9,10}, A_{10,10} \right\}$$

$$\mathbf{C}_{31\times 1} = \left\{1,2,5,6,2,5,6,3,4,5,6,\ldots,8,9,10,10\right\}$$

$$\mathbf{R}_{11\times 1} = \left\{1,5,8,12,15,21,26,28,29,31,32\right\}$$

Comparison w/ Example

Storage Scheme	**Equivalent Integer Words***
Full	$10 \times 10 \times 2 = 200$
Banded (HBW=6)	$10 \times 6 \times 2 = 120$
Skyline	$35 \times 2 + 11 = 81$
Sparse	$31 \times 2 + 31 + 10 = 103$

*Assuming elements of **A** are *double*.

Direct Solvers: Gaussian Elimination

- To obtain another equivalent **Ax=b**
  - **We can interchange two rows.**
  - **Multiply both sides by a constant.**
  - **Multiply one equation by a constant and add it to another equation.**

$$\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} \times \\ \times \\ \times \end{Bmatrix} \Rightarrow \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} \times \\ \times \\ \times \end{Bmatrix}$$

Example

$$\begin{bmatrix} 8 & -1 \\ 4 & 7 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 6 \\ 18 \end{Bmatrix} \Rightarrow \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1 \\ 2 \end{Bmatrix}$$

Multiply first equation by (-4/8) and add to second

$$\begin{bmatrix} 8 & -1 \\ 0 & 7.5 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 6 \\ 15 \end{Bmatrix} \Rightarrow \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1 \\ 2 \end{Bmatrix}$$

Gaussian Elimination

Forward Elimination

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{1i} & A_{1n} \\ A_{21} & A_{22} & A_{23} & A_{2i} & A_{2n} \\ A_{31} & A_{32} & A_{33} & A_{3i} & A_{3n} \\ & & & & \\ A_{i1} & A_{i2} & A_{i3} & A_{ii} & A_{in} \\ & & & & \\ A_{n1} & A_{n2} & A_{n3} & A_{ni} & A_{nn} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ \\ x_i \\ \\ x_n \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \\ \\ b_i \\ \\ b_n \end{Bmatrix}$$

$$\boxed{\begin{matrix} \det(\mathbf{A}) = 0 \\ \left| A_{ii}^{(i-1)} \right| \le \varepsilon \end{matrix}}$$

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{1i} & A_{1n} \\ 0 & A_{22}^{(1)} & A_{23}^{(1)} & A_{2i}^{(1)} & A_{2n}^{(1)} \\ 0 & 0 & A_{33}^{(2)} & A_{3i}^{(2)} & A_{3n}^{(2)} \\ & & & & \\ 0 & 0 & 0 & A_{ii}^{(i-1)} & A_{in}^{(i-1)} \\ & & & & \\ 0 & 0 & 0 & 0 & A_{nn}^{(n-1)} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ \\ x_i \\ \\ x_n \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2^{(1)} \\ b_3^{(2)} \\ \\ b_i^{(i-1)} \\ \\ b_n^{(n)} \end{Bmatrix}$$

Gaussian Elimination

Backward Substitution

$$
\begin{bmatrix}
A_{11} & A_{12} & A_{13} & A_{1i} & A_{1n} \\
0 & A_{22}^{(1)} & A_{23}^{(1)} & A_{2i}^{(1)} & A_{2n}^{(1)} \\
0 & 0 & A_{33}^{(2)} & A_{3i}^{(2)} & A_{3n}^{(2)} \\
 & & & & \\
0 & 0 & 0 & A_{ii}^{(i-1)} & A_{in}^{(i-1)} \\
 & & & & \\
0 & 0 & 0 & 0 & A_{nn}^{(n-1)}
\end{bmatrix}
\begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ \\ x_i \\ \\ x_n \end{Bmatrix}
=
\begin{Bmatrix} b_1 \\ b_2^{(1)} \\ b_3^{(2)} \\ \\ b_i^{(i-1)} \\ \\ b_n^{(n)} \end{Bmatrix}
$$

$$
x_n = \frac{b_n}{A_{nn}} \qquad\qquad x_i = \frac{b_i - \sum_{j=i+1}^{n} A_{ij} x_j}{A_{ii}} \quad i = n-1, n-2, \ldots, 1
$$

Matrix Toolbox

- Example Program 10.3.1
  - CMatrixToolBox class
  - Several matrix functionalities

Gaussian Elimination Method

```
template <class T>
bool CMatToolBox<T>::AxEqb (CMatrix<T>& A,
                            CVector<T>& x,
                            CVector<T>& b,
                            T TOL)
```

Client Code

```
   CMatToolBox<double> MTBDP;    // double precision version
…..
    const int NUMEQNS=3;
    const double TOL = 1.0e-6;
    CMatrix<double> dMA(NUMEQNS,NUMEQNS);
    CVector<double> dVx(NUMEQNS), dVb(NUMEQNS);
    dMA(1,1) = 10.0;   dMA(1,2) = -5.0;    dMA(1,3) = 2.0;
    dMA(2,1) =  3.0;   dMA(2,2) = 20.0;    dMA(2,3) = 5.0;
    dMA(3,1) = -2.0;   dMA(3,2) =  7.0;    dMA(3,3) = 15.0;

    dVb(1) = 6.0;      dVb(2) = 58.0;      dVb(3) = 57.0;
    if (MTBDP.AxEqb (dMA, dVx, dVb, TOL))
    {
        MTBDP.Display ("Vector x in Ax = b", dVx);
    }
    else
        std::cout << "Error in AxEqb.\n";
```

Error Analysis

- How good is the “numerical” solution?

Residual Vector

$$\mathbf{r} = \mathbf{A}\mathbf{x} - \mathbf{b} \neq \mathbf{0}$$

Absolute Error

$$\varepsilon_{abs} = \left\| \mathbf{r} \right\|$$

Residual Vector

$$\varepsilon_{rel} = \frac{\left\| \mathbf{r} \right\|}{\left\| \mathbf{b} \right\|}$$

Error magnitude is a function of the condition number of **A.**

$$cond(\mathbf{A}) = \frac{\lambda_{\max}}{\lambda_{\min}}$$

Improving the Solution

- Partial Pivoting
  - Locate the largest remaining element (in the current column) and switch rows.
- Full Pivoting
  - Locate the largest remaining element and switch rows and columns.
- Scaling
  - Multiply the equations by a constant so that the ratio of the largest to the smallest element in the matrix is reduced.

LU Factorization

For a general **A**

$$\mathbf{A} = \mathbf{LU}$$

L: lower triangular matrix

U: upper triangular matrix

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix} = \begin{bmatrix} 1 & & & \\ L_{21} & 1 & & \\ L_{31} & L_{32} & 1 & \\ L_{41} & L_{42} & L_{43} & 1 \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} & U_{13} & U_{14} \\ & U_{22} & U_{23} & U_{24} \\ & & U_{33} & U_{34} \\ & & & U_{44} \end{bmatrix}$$

Crout's Method

LU Factorization

$$\mathbf{A}_{n\times n}\mathbf{x}_{n\times 1} = \mathbf{b}_{n\times 1}$$

$$\mathbf{L}_{n\times n}\mathbf{U}_{n\times n}\mathbf{x}_{n\times 1} = \mathbf{b}_{n\times 1}$$

Factorization

$$\mathbf{A} = \mathbf{LU}$$

Forward Substitution

$$\mathbf{L}_{n\times n}\mathbf{y}_{n\times 1} = \mathbf{b}_{n\times 1} \Rightarrow \text{Solve for } \mathbf{y}$$

Backward Substitution

$$\mathbf{U}_{n\times n}\mathbf{x}_{n\times 1} = \mathbf{y}_{n\times 1} \Rightarrow \text{Solve for } \mathbf{x}$$

LU Factorization

Storage Scheme

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix} \Rightarrow \begin{bmatrix} U_{11} & U_{12} & U_{13} & U_{14} \\ L_{21} & U_{22} & U_{23} & U_{24} \\ L_{31} & L_{32} & U_{33} & U_{34} \\ L_{41} & L_{42} & L_{43} & U_{44} \end{bmatrix}$$

Note

$$j = 1, 2, 3, \ldots, n$$

$$i = 1, 2, .., j \Rightarrow U_{ij} = A_{ij} - \sum_{k=1}^{i-1} L_{ik} U_{kj}$$

$$i = j+1, j+2, .., n \Rightarrow L_{ij} = \frac{A_{ij} - \sum_{k=1}^{j-1} L_{ik} U_{kj}}{U_{jj}}$$

LU Factorization

Storage Scheme

$$\begin{Bmatrix} y_1 \\ y_2 \\ .. \\ .. \\ y_n \end{Bmatrix} \Rightarrow \begin{Bmatrix} x_1 \\ x_2 \\ .. \\ .. \\ x_n \end{Bmatrix} : x_i = \frac{y_i - \sum_{j=i+1}^{n} U_{ij} x_j}{U_{ii}} \quad i = n-1, n-2, \ldots, 1$$

LU Factorization: Advantages

- Clearly separates factorization from forward and backward substitutions (helps solve multiple RHS vectors).
- No additional storage required.
- Easy to compute determinant

$$\det(\mathbf{A}) = \det(\mathbf{U}) = U_{11} U_{22} \cdots U_{nn}$$

Example

$$\begin{bmatrix} 10 & -5 & 2 \\ 3 & 20 & 5 \\ -2 & 7 & 15 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 6 \\ 58 \\ 57 \end{Bmatrix}$$

Factorization

j=1

$$U_{11} = A_{11} = 10$$

$$L_{21} = \frac{A_{21}}{U_{11}} = \frac{3}{10} = 0.3$$

$$L_{31} = \frac{A_{31}}{U_{11}} = \frac{-2}{10} = -0.2$$

j=2

$$U_{12} = A_{12} = -5$$

$$U_{22} = A_{22} - L_{21} - U_{12} = 21.5$$

$$L_{32} = \frac{A_{32} - L_{31}U_{12}}{U_{22}} = 0.27907$$

j=3

$$U_{13} = A_{13} = 2$$

$$U_{23} = A_{23} - L_{21}U_{13} = 4.4$$

$$U_{33} = A_{33} - L_{31}U_{13} - L_{32}U_{23} = 14.1721$$

$$\mathbf{LU} = \begin{bmatrix} 10 & -5 & 2 \\ 0.3 & 21.5 & 4.4 \\ -0.2 & 0.27907 & 14.1721 \end{bmatrix}$$

Example

Forward Substitution

$$y_1 = \frac{b_1}{L_{11}} = 6$$

$$y_2 = \frac{b_2 - L_{21}y_1}{L_{22}} = 56.2$$

$$y_3 = \frac{b_3 - L_{31}y_1 - L_{32}y_2}{L_{33}} = 42.5163$$

Backward Substitution

$$x_3 = \frac{y_3}{U_{33}} = 3$$

$$x_2 = \frac{y_2 - U_{23}x_3}{U_{22}} = 2$$

$$x_1 = \frac{y_1 - U_{12}x_2 - U_{13}x_3}{U_{11}} = 1$$

$$\det(A) = U_{11}U_{22}U_{33} = (10)(21.5)(14.1721) = 3047$$

Cholesky Decomposition

For a symmetric, positive definite **A**

$$\mathbf{A} = \mathbf{LDL}^T$$

L: lower triangular matrix (1's on the diagonal)

D: diagonal matrix

$$\begin{bmatrix} K_{11} & K_{12} & . & K_{1n} \\ K_{12} & K_{22} & . & K_{2n} \\ . & . & . & . \\ K_{1n} & K_{2n} & . & K_{nn} \end{bmatrix} = \begin{bmatrix} 1 & 0 & . & 0 \\ L_{21} & 1 & . & 0 \\ . & . & . & . \\ L_{n1} & L_{n2} & . & 1 \end{bmatrix} \begin{bmatrix} D_1 & 0 & . & 0 \\ 0 & D_2 & . & 0 \\ . & . & . & . \\ 0 & 0 & . & D_n \end{bmatrix} \begin{bmatrix} 1 & L_{21} & . & L_{n1} \\ 0 & 1 & . & L_{n2} \\ . & . & . & . \\ 0 & 0 & . & 1 \end{bmatrix}$$

$$= \left[\begin{array}{c|c|c|c|c} D_1 & D_1L_{21} & D_1L_{31} & . & D_1L_{n1} \\ \hline & D_2L_{21}^2 & D_1L_{21}L_{31} + D_2L_{32} & . & D_1L_{21}L_{n1} + D_2L_{n2} \\ \hline & & D_1L_{31}^2 + D_2L_{32}^2 + D_3 & . & D_1L_{31}L_{n1} + D_2L_{32}L_{n2} + D_3L_{n3} \\ \hline & & & . & . \\ \hline sym & & & & D_1L_{n1}^2 + D_2L_{n2}^2 + \ldots + D_n \end{array}\right]$$

Cholesky Decomposition

$$\mathbf{A}_{n\times n}\mathbf{x}_{n\times 1} = \mathbf{b}_{n\times 1}$$

$$\mathbf{L}_{n\times n}\mathbf{D}_{n\times 1}\mathbf{L}^{\mathbf{T}}_{n\times n}\mathbf{x}_{n\times 1} = \mathbf{b}_{n\times 1}$$

Decomposition

$$\mathbf{A} = \mathbf{LDL}^{\mathbf{T}}$$

Forward Substitution

$$\mathbf{L}_{n\times n}\mathbf{y}_{n\times 1} = \mathbf{b}_{n\times 1} \Rightarrow \text{Solve for } \mathbf{y}$$

Backward Substitution

$$\mathbf{D}_{n\times n}\mathbf{L}^{\mathbf{T}}_{n\times n}\mathbf{x}_{n\times 1} = \mathbf{y}_{n\times 1} \Rightarrow \text{Solve for } \mathbf{x}$$

Note

$$\mathbf{DL}^{\mathbf{T}} = \begin{bmatrix} D_1 & D_1L_{12} & . & D_1L_{1n} \\ & D_2 & . & D_2L_{2n} \\ & & . & . \\ \mathbf{0} & & & D_n \end{bmatrix}$$

Cholesky Decomposition: Advantages

- Clearly separates factorization from forward and backward substitutions (helps solve multiple RHS vectors).
- Can store all required elements (**L** and **D**) in the upper (or lower) triangular portion of **A**. No additional storage required.

Example

$$\begin{bmatrix} 3.5120 & 0.7679 & 0 & 0 & 0 \\ 0.7679 & 3.1520 & 0 & -2 & 0 \\ 0 & 0 & 3.5120 & -0.7679 & 0.7679 \\ 0 & -2 & -0.7679 & 3.1520 & -1.1520 \\ 0 & 0 & 0.7679 & -1.1520 & 3.1520 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ -0.04 \\ 0 \end{Bmatrix}$$

Decomposition

i=1

$$D_1 = A_{11} = 3.5120$$

$$L_{21} = \frac{A_{21}}{D_1} = 0.21865$$

$$L_{31} = L_{41} = L_{51} = 0$$

i=2

$$D_2 = A_{22} - L_{21}^2 D_1 = 2.9841$$

$$L_{32} = \frac{A_{32} - L_{31} D_1 L_{21}}{D_2} = 0$$

$$L_{42} = \frac{A_{42} - L_{41} D_1 L_{21}}{D_2} = -0.670219$$

$$L_{52} = 0$$

Example

i=3

$$D_3 = A_{33} - L_{31}^2 D_1 - L_{32}^2 D_2 = 3.5120$$

$$L_{43} = \frac{A_{43} - L_{41} D_1 L_{31} - L_{42} D_2 L_{32}}{D_3} = -0.21865$$

$$L_{53} = \frac{A_{53} - L_{51} D_1 L_{31} - L_{52} D_2 L_{32}}{D_3} = 0.21865$$

i=4

$$D_4 = A_{44} - L_{41}^2 D_1 - L_{42}^2 D_2 - L_{43}^2 D_3 = 1.64366$$

$$L_{54} = \frac{A_{54} - L_{51} D_1 L_{41} - L_{52} D_2 L_{42} - L_{53} D_3 L_{43}}{D_4} = -0.598724$$

Example

i=5

$$D_5 = A_{55} - L_{51}^2 D_1 - L_{52}^2 D_2 - L_{53}^2 D_3 - L_{54}^2 D_4 = 2.3949$$

$$\mathbf{L} \,\&\, \mathbf{D} \Rightarrow \left(\begin{bmatrix} 3.5120 & 0 & 0 & 0 & 0 \\ 0.21865 & 2.9841 & 0 & 0 & 0 \\ 0 & 0 & 3.5120 & 0 & 0 \\ 0 & -0.670219 & -0.21865 & 1.64366 & 0 \\ 0 & 0 & 0.21865 & -0.598724 & 2.3949 \end{bmatrix} \right)$$

Forward Substitution

Ly = b

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0.21865 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -0.670219 & -0.21865 & 1 & 0 \\ 0 & 0 & 0.21865 & -0.598724 & 1 \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ -0.04 \\ 0 \end{Bmatrix}$$

$$y_1 = b_1 = 0$$

$$y_2 = b_2 - L_{21} y_1 = 0$$

$$y_3 = b_3 - L_{31} y_1 - L_{32} y_2 = 0$$

$$y_4 = b_4 - L_{41} y_1 - L_{42} y_2 - L_{43} y_3 = -0.04$$

$$y_5 = b_5 - L_{51} y_1 - L_{52} y_2 - L_{53} y_3 - L_{54} y_4 = -0.023949$$

Backward Substitution

$$\mathbf{DL^T D = y}$$

$$\begin{bmatrix} 3.5120 & 0.21865 & 0 & 0 & 0 \\ 0 & 2.9841 & 0 & -0.670219 & 0 \\ 0 & 0 & 3.5120 & -0.21865 & 0.21865 \\ 0 & 0 & 0 & 1.64366 & -0.598724 \\ 0 & 0 & 0 & 0 & 2.3949 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ -0.04 \\ -0.023949 \end{Bmatrix}$$

$$x_5 = \frac{y_5}{D_5} = -0.01$$

$$x_4 = \frac{y_4}{D_4} - L_{45} x_5 = -0.0303232$$

$$x_3 = \frac{y_3}{D_3} - L_{34} x_4 - L_{35} x_5 = -0.00444367$$

$$x_2 = \frac{y_2}{D_2} - L_{23} x_3 - L_{24} x_4 - L_{25} x_5$$

$$= -0.0203232$$

$$x_1 = \frac{y_1}{D_1} - L_{12} y_2 - L_{13} y_3 - L_{14} y_4 - L_{15} y_5$$

$$= 0.00444367$$

Handling Constraints

Solve equations with special conditions

$$\mathbf{Ax = b}$$

$$(a)\ x_i = c$$

$$(b)\ c_i x_i + c_j x_j = c$$

Case (a)

$$\text{Solve} \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \end{Bmatrix}$$

$$\text{with} \quad x_2 = c$$

Solution

$$\begin{aligned} A_{11}x_1 + A_{12}x_2 + A_{13}x_3 &= b_1 \\ A_{21}x_1 + A_{22}x_2 + A_{23}x_3 &= b_2 \\ A_{31}x_1 + A_{32}x_2 + A_{33}x_3 &= b_3 \end{aligned} \quad \Longrightarrow \quad \begin{aligned} A_{11}x_1 + (0)x_2 + A_{13}x_3 &= b_1 - A_{12}c \\ (0)x_1 + (1)x_2 + (0)x_3 &= c \\ A_{31}x_1 + (0)x_2 + A_{33}x_3 &= b_3 - A_{32}c \end{aligned}$$

Case (a)

$$\begin{bmatrix} A_{11} & 0 & A_{13} \\ 0 & 1 & 0 \\ A_{31} & 0 & A_{33} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} b_1 - A_{12}c \\ c \\ b_3 - A_{32}c \end{Bmatrix}$$

Algorithm $x_j = c$

1. Modify the right-hand side vector as $b_i = b_i - A_{ij}c,\ i = 1, \ldots, n$

2. Modify the coefficient matrix as $A_{ij} = 0,\ i = 1, \ldots n$

$$A_{ji} = 0,\ i = 1, \ldots n$$

3. Set $A_{jj} = 1$

Example

$$\begin{bmatrix} 10 & -5 & 2 \\ 3 & 20 & 5 \\ -2 & 7 & 15 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 6 \\ 58 \\ 57 \end{Bmatrix} \text{ with } x_2 = 3$$

Modified Equations

$$\begin{bmatrix} 10 & 0 & 2 \\ 0 & 1 & 0 \\ -2 & 0 & 15 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 6+5(3) \\ 3 \\ 57-7(3) \end{Bmatrix} = \begin{Bmatrix} 21 \\ 3 \\ 36 \end{Bmatrix}$$

Case (b)

Minimization Problem

$$\Pi(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\mathbf{T}}\mathbf{A}\mathbf{x} - \mathbf{x}^{\mathbf{T}}\mathbf{b}$$

leads to the solution to

$$\frac{\partial \Pi}{\partial \mathbf{x}} = 0 = \mathbf{A}\mathbf{x} - \mathbf{b}$$

Case (b)

$$\Pi(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} - \mathbf{x}^{\mathrm{T}}\mathbf{b} + \frac{1}{2}C\left(c_i x_i - c_j x_j - c\right)^2$$

Large number

Minimum is when $c_i D_i - c_j D_j - c = 0$

$$\frac{\partial \Pi}{\partial \mathbf{x}} = 0$$

$$C = 10^4 \max\left|A_{pq}\right|, 1 \le p, q \le n$$

Case (b)

$$
\begin{bmatrix}
A_{11} & & A_{1i} & & A_{1j} & A_{1n} \\
& .. & & & & \\
A_{i1} & & A_{ii} + Cc_i^2 & & A_{ij} + Cc_i c_j & A_{in} \\
& & & .. & & \\
A_{j1} & & A_{ji} + Cc_i c_j & & A_{jj} + Cc_j^2 & A_{jn} \\
& & & & .. & \\
A_{n1} & & A_{ni} & & A_{nj} & A_{nn}
\end{bmatrix}
\begin{Bmatrix} x_1 \\ \\ x_i \\ \\ x_j \\ \\ x_n \end{Bmatrix}
=
\begin{Bmatrix} b_1 \\ .. \\ b_i + Ccc_i \\ .. \\ b_j + Ccc_j \\ .. \\ b_n \end{Bmatrix}
$$

Example

$$\begin{bmatrix} 10 & -5 & 2 \\ -5 & 20 & 5 \\ 2 & 5 & 15 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 6 \\ 58 \\ 57 \end{Bmatrix} \text{ with } 2x_1 + x_3 = 3$$

Modified Equations

$$\begin{bmatrix} 10+20\left(10^4\right)2^2 & -5 & 2+20\left(10^4\right)(2)(1) \\ -5 & 20 & 5 \\ 2+20\left(10^4\right)(2)(1) & 5 & 15+20\left(10^4\right)1^2 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 6+20\left(10^4\right)(3)(2) \\ 58 \\ 57+20\left(10^4\right)(3)(1) \end{Bmatrix}$$

Matrix Toolbox

- Specifications