Linear equations: LU decomposition

Consider solving a linear system of equations, say with 3 variables

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b} \quad \rightarrow \quad \mathbf{A} = \mathbf{L} \cdot \mathbf{U}$$

Matrix **A** is factorized or decomposed into a product of *lower triangular* **L** and *upper triangular* **U** matrices,

$$\mathbf{L} = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix} \qquad \mathbf{U} = \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}$$

Looks formidable but extremely useful and not nearly as hard. On multiplication,

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

A catch : $3 \times 3 = 9$ equations but $3 \times (3+1)$ variables!!

Trick : Either all three $l_{ii} = 1$, called *Doolittle* or all three $u_{ii} = 1$, called *Crout* decomposition.

Doolittle LU

Take Doolittle LU factorization,

1. Set $l_{ii} = 1 \;\; \forall i = 1, 2, \ldots, N$ implying

$$u_{11} = a_{11},\;\; u_{12} = a_{12} \text{ and } u_{13} = a_{13} \quad \Rightarrow \quad u_{1j} = a_{1j},\;\; (j = 1, 2, \ldots, N)$$

2. Do the calculation in the order they appear

$$\begin{array}{ll}
u_{21} = 0, & l_{21} = (a_{21})/u_{11} \\
u_{31} = 0, & l_{31} = (a_{31})/u_{11} \\
u_{22} = a_{22} - l_{21}u_{12}, & l_{22} = 1 \\
u_{32} = 0, & l_{32} = (a_{32} - l_{31}u_{31})/u_{22} \\
u_{23} = a_{23} - l_{21}u_{13}, & l_{23} = 0 \\
u_{33} = a_{33} - l_{31}u_{13} - l_{32}u_{23}, & l_{33} = 0
\end{array}$$

3. Generic form for each $j = 1, 2, \ldots, N$, in the order they appear

$$\begin{array}{lcll}
u_{ij} & = & a_{ij} - \sum_{k=1}^{i-1} l_{ik}u_{kj} & \text{for } i = 2, \ldots, j \\
l_{ij} & = & \left(a_{ij} - \sum_{k=1}^{j-1} l_{ik}u_{kj}\right)/u_{jj} & \text{for } i = j+1, j+2, \ldots, N
\end{array}$$

Important : Every a_{ij} is used only once and never again $\Rightarrow$ u_{ij}, l_{ij} can be stored in the same location / memory of a_{ij}.

Can we always LU decompose?

- If $a_{11} = 0$, then either $\mathbf{L}$ or $\mathbf{U}$ is singular $\rightarrow$ impossible if $\mathbf{A}$ is not.

Solution : Row pivot

- Guaranteed if all *leading submatrices* have nonzero determinant

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 2 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \Rightarrow \mathbf{A_1} = 1, \mathbf{A_2} = \begin{pmatrix} 1 & 0 \\ -2 & 1 \end{pmatrix} \text{ and } \mathbf{A_3} = \begin{pmatrix} 1 & 0 & 2 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

$$\det[\mathbf{A_1}] = 1,\ \det[\mathbf{A_2}] = 1 \text{ and } \det[\mathbf{A_3}] = -3$$

- Additional pivoting if determinant of any leading submatrix is zero but the matrix itself is invertible.

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 2 \\ 3 & 0 & 2 \\ -1 & 1 & 2 \end{pmatrix} \Rightarrow \mathbf{A_1} = 1, \mathbf{A_2} = \begin{pmatrix} 1 & 0 \\ 3 & 0 \end{pmatrix} \text{ and } \mathbf{A_3} = \begin{pmatrix} 1 & 0 & 2 \\ 3 & 0 & 2 \\ -1 & 1 & 2 \end{pmatrix}$$

$$\det[\mathbf{A_1}] = 1,\ \det[\mathbf{A_2}] = 0 \text{ and } \det[\mathbf{A_3}] = 4$$

- Otherwise, no solution exists and your are doomed!

U in Gauss-Jordan

Recall the **U** matrix needed for determinant calculation in Gauss-Jordan elimination

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \Rightarrow \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} \bar{b}_1 \\ \bar{b}_2 \\ \bar{b}_3 \end{pmatrix}$$

Solutions x_i starts from last row *i.e.* by *backward substitution*

$$\begin{aligned} u_{33}x_3 &= \bar{b}_3 & \qquad x_3 &= \frac{\bar{b}_3}{u_{33}} \\ u_{22}x_2 + u_{23}x_3 &= \bar{b}_2 & \qquad x_2 &= \frac{\bar{b}_2 - u_{23}x_3}{u_{22}} \\ u_{11}x_1 + u_{12}x_2 + u_{13}x_3 &= \bar{b}_1 & \qquad x_1 &= \frac{\bar{b}_1 - u_{12}x_2 - u_{13}x_3}{u_{11}} \end{aligned}$$

A generic solution for $N \times N$ matrix by backward substitution is

$$x_i = \frac{1}{u_{ii}} \left(\bar{b}_i - \sum_{j=i+1}^{N} u_{ij}x_j \right), \text{ where } x_N = \frac{\bar{b}_N}{u_{NN}} \text{ and } i = N-1, N-2, \ldots, 1$$

$\mathbf{LU}$ forward-backward

To solve linear system of equations using **LU** decomposition it is advisable to begin with partial pivoting.

⋆ In the next step, consider the following split up

$$\mathbf{A}\cdot\mathbf{x}=\mathbf{b} \;\rightarrow\; \mathbf{L}\cdot\mathbf{U}\cdot\mathbf{x}=\mathbf{b} \quad\Rightarrow\quad \mathbf{U}\cdot\mathbf{x}=\mathbf{y} \;\rightarrow\; \mathbf{L}\cdot\mathbf{y}=\mathbf{b}$$

⋆ First solve for $\mathbf{y}$ from $\mathbf{L}\cdot\mathbf{y}=\mathbf{b}$ using *forward substitution* and then use it to solve for $\mathbf{x}$ by *backward substitution* from $\mathbf{U}\cdot\mathbf{x}=\mathbf{y}$

$$y_i = b_i - \sum_{j=1}^{i-1} l_{ij} y_j, \qquad \text{where } y_1 = b_1 \text{ and } i = 2,3,\ldots,N$$

$$x_i = \frac{1}{u_{ii}}\left(y_i - \sum_{j=i+1}^{N} u_{ij} x_j\right), \quad \text{where } x_N = \frac{y_N}{u_{NN}} \text{ and } i = N-1, N-2, \ldots, 1$$

⋆ Get determinant of $\mathbf{A}$ for free

$$\det\mathbf{A} = \det\mathbf{LU} = \det\mathbf{L}\times\det\mathbf{U} = (-1)^n \prod_i u_{ii}$$

⋆ For inverse, iterate through each column of the identity matrix.

Cholesky decomposition

Cholesky decomposition : factorization of Hermitian, positive definite matrix (which often is the case in physics) into a product of **L** and $\mathbf{L}^T$

$$\mathbf{A} = \mathbf{L}\,\mathbf{L}^{\dagger} \xrightarrow{\text{real}} \mathbf{L}\,\mathbf{L}^{T} \Rightarrow \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix} \begin{pmatrix} l_{11} & l_{12} & l_{13} \\ 0 & l_{22} & l_{23} \\ 0 & 0 & l_{33} \end{pmatrix}$$

When **A** is real and positive definite,

$$\begin{aligned} l_{ii} &= \pm\sqrt{a_{ii} - \sum_{j=1}^{i-1} l_{ij}^2} \\ l_{ij} &= \frac{1}{l_{ii}}\left(a_{ij} - \sum_{k=1}^{i-1} l_{ik}\,l_{kj}\right) \quad \text{for } i < j \end{aligned}$$

Cholesky is about twice as efficient as the LU decomposition for solving system of linear equations.

Signs before square roots are inconsequential. DIY the decomposition for complex matrix.

An example of Cholesky decomposition of a real, symmetric matrix is (taken from Wikipedia),

$$\begin{pmatrix} 4 & 12 & -16 \\ 12 & 37 & -43 \\ -16 & -43 & 98 \end{pmatrix} = \begin{pmatrix} 2 & 0 & 0 \\ 6 & 1 & 0 \\ -8 & 5 & 3 \end{pmatrix} \begin{pmatrix} 2 & 6 & -8 \\ 0 & 1 & 5 \\ 0 & 0 & 3 \end{pmatrix}$$

Apart from being used for numerical solution of linear equations, Cholesky decomposition is also used in non-linear optimization for multiple variable, monte carlo simulation for decomposing covariance matrix, inversion of Hermitian matrices etc.

Forward substitution

$$\begin{pmatrix} 1 & 0 & 0 \\ l_{12} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

Starting from the first row *i.e.* moving forward we solve for y_i

$$\begin{aligned} y_1 &= b_1 & \qquad y_1 &= b_1 \\ l_{21} y_1 + y_2 &= b_2 & \qquad y_2 &= b_2 - l_{21} y_1 \\ l_{31} y_1 + l_{32} y_2 + y_3 &= b_3 & \qquad y_3 &= b_3 - l_{31} y_1 - l_{32} y_2 \end{aligned}$$

Backward substitution

Solve the following set of equations using Backward substitution using row echelon matrix **U** by Gauss-Jordon elimination (no need for fully reduced RREF) –

$$\begin{aligned} x + y + z &= 3 \\ 2x + 3y + 7z &= 0 \\ x + 3y - 2z &= 17 \end{aligned}$$

$x = 1,\ y = 4,\ z = -2$