## Linear equations: LU decomposition

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

$$A \cdot x = b \quad \to \quad A = L \cdot U$$

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

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

Looks formidable but very useful and not nearly as hard.
Multiplying

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

But without proper ordering, the factorization may fail!

## LU Decomposition

The matrix multiplication $L \cdot U$ yields

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

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.

Any of the decomposition of L and U can proceed iteratively.

$$\text{Dolittle :} \quad l_{11} = l_{22} = l_{33} = 1 \;\; \text{and} \;\; \text{Crout :} \quad u_{11} = u_{22} = u_{33} = 1$$

This straight away implies

$$
\begin{array}{ll}
\text{Doolittle :} & u_{11} = a_{11},\; u_{12} = a_{12},\; u_{13} = a_{13} \\
\text{Crout :} & l_{11} = a_{11},\; l_{21} = a_{21},\; l_{31} = a_{31}
\end{array}
$$

The rest of the $l_{ij}$ or $u_{ij}$ can be solved from the remaining equations to achieve LU 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

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

## LU storage

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 $a_{ij}$.
Hence memory requirement is half.

Storing Doolittle LU decomposed matrix

$$\mathrm{LU} = \begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ l_{21} & u_{22} & u_{23} & u_{24} \\ l_{31} & l_{32} & u_{33} & u_{34} \\ l_{41} & l_{42} & l_{43} & u_{44} \end{pmatrix} \rightarrow \mathrm{A}$$

No need to store $l_{ii} = 1$, modify loop over indices accordingly.

Otherwise, numerical cost of Gauss-Jordan and LU are same, $\mathcal{O}(N^3)$.

But, can LU be always done?

## Can we always LU decompose?

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

Solution : Row pivot

- Guaranteed if all *leading submatrices* have nonzero determinant

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

$\det[A_1] = 1,\ \det[A_2] = 1$ and $\det[A_3] = -3$

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

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

$\det[A_1] = 1,\ \det[A_2] = 0$ and $\det[A_3] = 4$

- 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

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

## 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

$$\mathsf{A}\cdot\mathsf{x}=\mathsf{b}\ \Rightarrow\ \mathsf{L}\cdot(\mathsf{U}\cdot\mathsf{x})=\mathsf{b}\ \Big|\ \mathsf{U}\cdot\mathsf{x}=\mathsf{y}\ \Rightarrow \mathsf{L}\cdot\mathsf{y}=\mathsf{b}$$

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

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 :

$$\begin{pmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

Starting from the last row *i.e.* moving backward to solve for $x_i$

$$\begin{aligned} u_{33}x_3 &= y_3 & \qquad x_3 &= y_3/u_{33} \\ u_{22}x_2 + u_{23}x_3 &= y_2 & \qquad x_2 &= \left(y_2 - u_{23}x_3\right)/u_{22} \\ u_{11}x_1 + u_{12}x_2 + u_{13}x_3 &= y_1 & \qquad x_1 &= \left(y_1 - u_{12}x_2 - u_{13}x_3\right)/u_{11} \end{aligned}$$

In generic form, the solutions for $y_i$ and subsequently $x_i$ are

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

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

⋆ Get determinant of A for free

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

⋆ 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 $L^T$

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

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.

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## 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) –

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

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