Linear equations: LU decomposition

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

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

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

$$L = \begin{pmatrix} \ell_{00} & 0 & 0 \\ \ell_{10} & \ell_{11} & 0 \\ \ell_{20} & \ell_{21} & \ell_{22} \end{pmatrix} \qquad U = \begin{pmatrix} u_{00} & u_{01} & u_{02} \\ 0 & u_{11} & u_{12} \\ 0 & 0 & u_{22} \end{pmatrix}$$

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

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \\ a_{20} & a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} \ell_{00} u_{00} & \ell_{00} u_{01} & \ell_{00} u_{02} \\ \ell_{10} u_{00} & \ell_{10} u_{01} + \ell_{11} u_{11} & \ell_{10} u_{02} + \ell_{11} u_{12} \\ \ell_{20} u_{00} & \ell_{20} u_{01} + \ell_{21} u_{11} & \ell_{20} u_{02} + \ell_{21} u_{12} + \ell_{22} u_{22} \end{pmatrix}$$

But without proper ordering, the factorization may fail!

LU Decomposition

The matrix multiplication $L \cdot U$ yields

$$\begin{aligned}
\ell_{00} u_{00} &= a_{00} & \ell_{00} u_{01} &= a_{01} & \ell_{00} u_{02} &= a_{02} \\
\ell_{10} u_{00} &= a_{10} & \ell_{10} u_{01} + \ell_{11} u_{11} &= a_{11} & \ell_{10} u_{02} + \ell_{11} u_{12} &= a_{12} \\
\ell_{20} u_{00} &= a_{20} & \ell_{20} u_{01} + \ell_{21} u_{11} &= a_{21} & \ell_{20} u_{02} + \ell_{21} u_{12} + \ell_{22} u_{22} &= a_{22}
\end{aligned}$$

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

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

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

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

This straight away implies

$$\begin{aligned}
\text{Doolittle}: &\quad u_{00} = a_{00}, \; u_{01} = a_{01}, \; u_{02} = a_{02} \\
\text{Crout}: &\quad \ell_{00} = a_{11}, \; \ell_{10} = a_{10}, \; \ell_{20} = a_{20}
\end{aligned}$$

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 $\ell_{ii} = 1 \ \ \forall i = 0, 1, \ldots, N-1$ implying

   $u_{00} = a_{00},\ u_{01} = a_{01}$ and $u_{02} = a_{02} \ \ \Rightarrow \ \ u_{0j} = a_{0j},\ (j = 0, 1, \ldots, N-1)$

2. Do the calculation in the order they appear

$$
\begin{array}{ll}
u_{10} = 0, & \ell_{10} = (a_{10})/u_{00} \\
u_{20} = 0, & \ell_{20} = (a_{20})/u_{00} \\
u_{11} = a_{11} - \ell_{10} u_{01}, & \ell_{11} = 1 \\
u_{21} = 0, & \ell_{21} = (a_{21} - \ell_{20} u_{20})\,/u_{11} \\
u_{12} = a_{12} - \ell_{10} u_{02}, & \ell_{12} = 0 \\
u_{22} = a_{22} - \ell_{20} u_{02} - \ell_{21} u_{12}, & \ell_{22} = 0
\end{array}
$$

3. Generic form for each $j = 0, 2, \ldots, N-1$, in the order they appear

$$
\begin{array}{lcll}
u_{ij} & = & a_{ij} - \sum_{k=0}^{i-1} \ell_{ik} u_{kj} & \text{for } i = 2, \ldots, j \\
\ell_{ij} & = & \left(a_{ij} - \sum_{k=0}^{j-1} \ell_{ik} u_{kj}\right)/u_{jj} & \text{for } i = j+1, j+2, \ldots, N-1
\end{array}
$$

LU storage

Important : Every a_{ij} is used only once and never again.

$\Rightarrow \quad u_{ij}, \ell_{ij}$ can be stored in the same location / memory of a_{ij}.
Hence memory requirement is half.

Storing Doolittle LU decomposed matrix

$$\mathrm{LU} = \begin{pmatrix} u_{00} & u_{01} & u_{02} & u_{03} \\ \ell_{10} & u_{11} & u_{12} & u_{13} \\ \ell_{20} & \ell_{21} & u_{22} & u_{23} \\ \ell_{30} & \ell_{31} & \ell_{32} & u_{33} \end{pmatrix} \quad \rightarrow \quad \mathrm{A}$$

No need to store $\ell_{ii} = 1$, 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

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

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

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

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

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

- 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*

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

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

$$\mathrm{A}\cdot\mathrm{x}=\mathrm{b} \;\Rightarrow\; \mathrm{L}\cdot\left(\mathrm{U}\cdot\mathrm{x}\right)=\mathrm{b} \;\Big|\; \mathrm{U}\cdot\mathrm{x}=\mathrm{y} \;\Rightarrow \mathrm{L}\cdot\mathrm{y}=\mathrm{b}$$

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

Forward substitution :

$$\begin{pmatrix} 1 & 0 & 0 \\ \ell_{01} & 1 & 0 \\ \ell_{20} & \ell_{21} & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} b_0 \\ b_1 \\ b_2 \end{pmatrix}$$

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

$$\begin{aligned} y_0 &= b_0 & \qquad y_0 &= b_0 \\ \ell_{10}y_0 + y_1 &= b_1 & \qquad y_1 &= b_1 - \ell_{10}y_0 \\ \ell_{20}y_0 + \ell_{21}y_1 + y_2 &= b_2 & \qquad y_2 &= b_2 - \ell_{20}y_0 - \ell_{21}y_1 \end{aligned}$$

Backward substitution :

$$\begin{pmatrix} u_{00} & u_{01} & u_{02} \\ 0 & u_{11} & u_{12} \\ 0 & 0 & u_{22} \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ y_2 \end{pmatrix}$$

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

$$y_i = b_i - \sum_{j=0}^{i-1} \ell_{ij} y_j, \qquad \text{where } y_0 = b_0 \text{ and } i = 2, 3, \ldots, N$$

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

⋆ Get determinant of A for free

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

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

Cholesky decomposition

Properties and symmetries of A are often used to simplify the process of solving linear equations.

Cholesky decomposition : factorization of Hermitian, positive definite matrix (which often is the case in physics e.g. covariance matrix) into a product of L and L^T.

For a 3×3 system,

$$A = L\,L^\dagger \xrightarrow{\text{real}} L\,L^T \Rightarrow \begin{pmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \\ a_{20} & a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} \ell_{00} & 0 & 0 \\ \ell_{10} & \ell_{11} & 0 \\ \ell_{20} & \ell_{21} & \ell_{22} \end{pmatrix} \begin{pmatrix} \ell_{00} & \ell_{01} & \ell_{02} \\ 0 & \ell_{11} & \ell_{12} \\ 0 & 0 & \ell_{22} \end{pmatrix}$$

where $\ell_{ij} = \ell_{ji}$. When A is real and positive definite,

$$\ell_{ii} = \pm\sqrt{a_{ii} - \sum_{j=0}^{i-1} \ell_{ij}^2} \quad \text{and} \quad \ell_{ij} = \frac{1}{\ell_{ii}}\left(a_{ij} - \sum_{k=0}^{i-1} \ell_{ik}\ell_{kj}\right) \text{ for } i < j$$

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

Cholesky

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

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.