

LU Decomposition

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LU Decomposition Methods

- Lower-Upper (LU) decomposition/factorization allows to factor a matrix as the product of a lower triangular matrix and an upper triangular matrix
- LU decomposition can be obtained using Gaussian elimination and can be seen as the matrix form of Gaussian elimination
- LU decomposition is typically used to solve systems of linear equations,
- LU decomposition can be used for computing the determinant of a matrix.

LU Decomposition Methods

- Any matrix A can be expressed as

$$PA = LU,$$

where L is a lower triangular matrix, U is an upper triangular matrix, and P is a permutation matrix.

- The process of computing L and U (and P) is called LU decomposition/factorization.

LU Decomposition Methods

- LU decomposition is not unique
- For example:

$$A = \begin{bmatrix} 1 & -1 \\ -1 & 5 \end{bmatrix}$$

has the following LU decompositions

$$\begin{aligned} A &= \begin{bmatrix} 1 & 0 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 0 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 0 & 4 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ -1 & 4 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \end{aligned}$$

LU Decomposition Methods

For example: Let us factorize the following 2-by-2 matrix:

$$\begin{bmatrix} 1 & -1 \\ -1 & 5 \end{bmatrix} = \begin{bmatrix} \ell_{00} & 0 \\ \ell_{10} & \ell_{11} \end{bmatrix} \begin{bmatrix} u_{00} & u_{01} \\ 0 & u_{11} \end{bmatrix}.$$

We can find the LU decomposition by solving a non-linear system of equations with 6 unknowns and 4 equations, ie, .

$$\ell_{00} \cdot u_{00} + 0 \cdot 0 = 1$$

$$\ell_{10} \cdot u_{00} + \ell_{11} \cdot 0 = -1$$

$$\ell_{00} \cdot u_{01} + 0 \cdot u_{11} = -1$$

$$\ell_{10} \cdot u_{01} + \ell_{11} \cdot u_{11} = 5.$$

This is an underdetermined system, then, to find a unique LU decomposition, it is necessary to put some restrictions.

LU Decomposition Methods

Some constraints should be considered to obtain unique decompositions:

- Doolittle's decomposition: $\ell_{ii} = 1, i = 0, 1, \dots, n - 1$

$$\begin{bmatrix} 1 & -1 \\ -1 & 5 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 0 & 4 \end{bmatrix}$$

- Crout's decomposition: $u_{ii} = 1, i = 0, 1, \dots, n - 1$

$$\begin{bmatrix} 1 & -1 \\ -1 & 5 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -1 & 4 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix}$$

- Cholesky's decomposition: $L = U^T$ and $\ell_{ii} = u_{ii} > 0, i = 0, 1, \dots, n - 1$

$$\begin{bmatrix} 1 & -1 \\ -1 & 5 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 0 & 2 \end{bmatrix}$$

LU Decomposition Methods

- The previous decompositions (Doolittle, Crout and Cholesky) do not always exist.
- If A is a square, invertible matrix and has an LU factorization with all diagonal entries of L or U equal to 1, then the factorization is unique.
- If A is a symmetric positive-definite matrix, the Cholesky decomposition always exists and is unique

LU Decomposition Methods

- For example: the following matrix A does not have Doolittle's, Crout's decomposition since $a_{0,0} = 0$.

$$A = \begin{bmatrix} 0 & 2 \\ 1 & 1 \end{bmatrix}$$

But we can find a permutation matrix such that $PA = LU$

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 2 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 2 \end{bmatrix}$$

LU Decomposition Methods

A square matrix could have infinitely many LU factorizations

- if two or more of any first $(n - 1)$ columns are linearly dependent
- or any of the first $(n - 1)$ columns are 0

For example: the matrix

$$\begin{bmatrix} 0 & 2 \\ 0 & 1 \end{bmatrix}$$

has LU factorizations of the form

$$\begin{bmatrix} 0 & 2 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ a & 1 \end{bmatrix} \begin{bmatrix} 0 & 2 \\ 0 & b \end{bmatrix}$$

for any a, b such that $2a + b = 1$

Solving a linear system using LU

If $A = LU$ the linear system

$$Ax = b$$

can be solved in two steps. From

$$LUx = b$$

$$L(Ux) = b$$

we can define $y = Ux$ and we solve the following two systems:

$$Ly = b, \text{ solve using } \mathbf{forward\ substitution}$$

$$Ux = y, \text{ solve using } \mathbf{backward\ substitution}$$

first w.r.t. y and then w.r.t. x

Computing the determinant using LU

Recall

- $\det(\mathbf{AB}) = \det(\mathbf{A}) \det(\mathbf{B})$
- If we swap two rows (columns) in \mathbf{A} , the determinant will change its sign.
- $\det(\mathbf{P}) = \pm 1$

From

$$\mathbf{PA} = \mathbf{LU},$$

and $\det(\mathbf{P}) = (-1)^k$, where k is the number of row exchanges in the previous decomposition, then

$$\det(\mathbf{A}) = (-1)^k \det(\mathbf{L}) \det(\mathbf{U}) = (-1)^k \prod \ell_{ii} \prod u_{ii}$$

Comment

If E_i is a permutation of two rows of the identity matrix (ie, a permutation of the form P_{ij}), then after k row exchanges.

$$\mathbf{P} = \mathbf{E}_k \mathbf{E}_{k-1} \cdots \mathbf{E}_1 \mathbf{I}$$

since $\det(\mathbf{E}_i) = -1$ then

$$\det(\mathbf{P}) = (-1)^k$$

Comment

Note also that $\mathbf{E}_i \mathbf{E}_i = \mathbf{I}$, $\mathbf{E}_i = \mathbf{E}_i^{-1} = \mathbf{E}_i^T$ these are properties of two-row permutation matrices of the form \mathbf{P}_{ij} , then

$$\mathbf{P} \mathbf{P}^T = \mathbf{E}_k \mathbf{E}_{k-1} \cdots \mathbf{E}_2 \mathbf{E}_1 \mathbf{E}_1^T \mathbf{E}_2^T \cdots \mathbf{E}_{k-1}^T \mathbf{E}_k^T = \mathbf{I}$$

and again

$$\begin{aligned} \det(\mathbf{P}) \det(\mathbf{P}^T) &= 1 \\ \det(\mathbf{P})^2 &= 1 \text{ since } \det(\mathbf{P}) = \det(\mathbf{P}^T) \\ \det(\mathbf{P}) &= \pm 1 \end{aligned}$$

Solve systems of linear equations using

We can use LU decomposition to solve **systems of linear equations** using:

$$AX = B$$

where X and B are matrices of the same size n-by-p.

We can rewrite the previous systems

$$LUX = B$$

Solve systems of linear equations using

We can also adapt the forward and backward substitutions methods to find the solution matrix X of the following systems of linear equations

$$L(UX) = B$$

by solving

$$LY = B$$

$$UX = Y$$

First, we solve for Y using forward substitution and then we solve for X using backward substitution.

Inverting a matrix

Inverting a matrix: In particular, if B is the identity matrix, then the solution X of

$$LUX = I$$

is the inverse of A (use forward-backward substitution).

Another alternative is to find both the inverse of L and U by solving

$$UX = I$$

$$LY = I$$

then $X = U^{-1}$ and $Y = L^{-1}$ therefore

$$A^{-1} = (LU)^{-1} = U^{-1}L^{-1} = XY$$

LU Decomposition Methods: Doolittle's Method

Doolittle's Decomposition Method 3×3 matrix

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ \ell_{1,0} & 1 & 0 \\ \ell_{2,0} & \ell_{2,1} & 1 \end{bmatrix}, \mathbf{U} = \begin{bmatrix} u_{0,0} & u_{0,1} & u_{0,2} \\ 0 & u_{1,1} & u_{1,2} \\ 0 & 0 & u_{2,2} \end{bmatrix}$$

LU Decomposition Methods: Doolittle's Method

Doolittle's Decomposition Method using a 3×3 matrix

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ \ell_{1,0} & 1 & 0 \\ \ell_{2,0} & \ell_{2,1} & 1 \end{bmatrix}, \mathbf{U} = \begin{bmatrix} u_{0,0} & u_{0,1} & u_{0,2} \\ 0 & u_{1,1} & u_{1,2} \\ 0 & 0 & u_{2,2} \end{bmatrix}$$

$$\mathbf{LU} = \begin{bmatrix} u_{0,0} & u_{0,1} & u_{0,2} \\ u_{0,0}\ell_{1,0} & u_{0,1}\ell_{1,0} + u_{1,1} & u_{0,2}\ell_{1,0} + u_{1,2} \\ u_{0,0}\ell_{2,0} & u_{0,1}\ell_{2,0} + u_{2,1} & u_{0,2}\ell_{2,0} + u_{2,2} \end{bmatrix}$$

LU Decomposition Methods: Doolittle's Method

Since $LU = A$, we obtain the following nonlinear system of equations

$$\begin{bmatrix} u_{0,0} & u_{0,1} & u_{0,2} \\ u_{0,0}\ell_{1,0} & u_{0,1}\ell_{1,0} + u_{1,1} & u_{0,2}\ell_{1,0} + u_{1,2} \\ u_{0,0}\ell_{2,0} & u_{0,1}\ell_{2,0} + u_{2,1} & u_{0,2}\ell_{2,0} + u_{2,2} \end{bmatrix} = \begin{bmatrix} a_{0,0} & a_{0,1} & a_{0,2} \\ a_{1,0} & a_{1,1} & a_{1,2} \\ a_{2,0} & a_{2,1} & a_{2,2} \end{bmatrix}$$

with 9 equations and 9 unknowns.

We can find a solution by solving this system. In this case, we observe that the entries of U corresponds to the Gaussian elimination process.

LU Decomposition Methods: Doolittle's Method

For example: $\mathbf{u}_{0,\cdot} = \mathbf{a}_{0,\cdot}$, ie, the first row of \mathbf{U} matches with the first row of \mathbf{A} . Note that: $u_{0,0}\ell_{1,0} = a_{1,0}$ and $u_{0,0}\ell_{2,0} = a_{2,0}$ then

$$\ell_{1,0} = \frac{a_{1,0}}{a_{0,0}}; \ell_{2,0} = \frac{a_{2,0}}{a_{0,0}}$$

and

$$\mathbf{u}_{1,\cdot} = \mathbf{a}_{1,\cdot} - \ell_{1,0}\mathbf{a}_{0,\cdot}$$

$$\mathbf{u}_{2,\cdot} = \mathbf{a}_{2,\cdot} - \ell_{2,0}\mathbf{a}_{0,\cdot}$$

this suggest to directly use Gaussian Elimination to compute the entries of \mathbf{L} and \mathbf{U}

LU Decomposition Methods: Doolittle's Method

Let us now apply Gauss elimination to the previous matrix

$$\begin{aligned} R_0 &: \begin{bmatrix} u_{0,0} & u_{0,1} & u_{0,2} \\ u_{0,0}\ell_{1,0} & u_{0,1}\ell_{1,0} + u_{1,1} & u_{0,2}\ell_{1,0} + u_{1,2} \\ u_{0,0}\ell_{2,0} & u_{0,1}\ell_{2,0} + u_{1,1}\ell_{2,1} & u_{0,2}\ell_{2,0} + u_{1,2}\ell_{2,1} + u_{2,2} \end{bmatrix} \\ R_1 &: \\ R_2 &: \end{aligned}$$

if $u_{0,0} \neq 0$ we can compute a **unique** $\ell_{1,0} = \frac{a_{1,0}}{a_{0,0}} = \frac{u_{0,0}\ell_{1,0}}{u_{0,0}}$,

$\ell_{2,0} = \frac{a_{2,0}}{a_{0,0}} = \frac{u_{0,0}\ell_{2,0}}{u_{0,0}}$ and apply the Gauss elimination that allows us to compute $u_{1,1}, u_{1,2}$

$$\begin{aligned} R_1 &\leftarrow R_1 - \ell_{1,0} R_0 \\ R_2 &\leftarrow R_2 - \ell_{2,0} R_0 \end{aligned}$$

$$\begin{aligned} R_0 &: \begin{bmatrix} u_{0,0} & u_{0,1} & u_{0,2} \\ \boxed{0} & \textcolor{red}{u_{1,1}} & \textcolor{red}{u_{1,2}} \\ \boxed{0} & u_{1,1}\ell_{2,1} & u_{1,2}\ell_{2,1} + u_{2,2} \end{bmatrix} \\ R_1 &: \\ R_2 &: \end{aligned}$$

LU Decomposition Methods: Doolittle's Method

if $u_{1,1} \neq 0$ then we can compute a **unique** $\ell_{2,1} = \frac{a_{2,1}}{a_{1,1}} = \frac{u_{1,1}\ell_{2,1}}{u_{1,1}}$,
and this allows us to compute $u_{2,2}$

$$\begin{bmatrix} u_{0,0} & u_{0,1} & u_{0,2} \\ \boxed{0} & u_{1,1} & u_{1,2} \\ \boxed{0} & u_{1,1}\ell_{2,1} & u_{1,2}\ell_{2,1} + u_{2,2} \end{bmatrix} \xrightarrow{R_2 - \ell_{2,1} R_1} \begin{bmatrix} u_{0,0} & u_{0,1} & u_{0,2} \\ \boxed{0} & u_{1,1} & u_{1,2} \\ \boxed{0} & \boxed{0} & \textcolor{red}{u_{2,2}} \end{bmatrix}$$

LU Decomposition Methods: Doolittle's Method

With the previous procedure, we obtain L and U

$$L = \begin{bmatrix} 1 & 0 & 0 \\ \ell_{1,0} & 1 & 0 \\ \ell_{2,0} & \ell_{2,1} & 1 \end{bmatrix}, \quad U = \begin{bmatrix} u_{0,0} & u_{0,1} & u_{0,2} \\ 0 & u_{1,1} & u_{1,2} \\ 0 & 0 & u_{2,2} \end{bmatrix}$$

Note that we can simply combine them in one matrix, ie,

$$\begin{bmatrix} u_{0,0} & u_{0,1} & u_{0,2} \\ \boxed{\ell_{1,0}} & u_{1,1} & u_{1,2} \\ \boxed{\ell_{2,0}} & \boxed{\ell_{2,1}} & u_{2,2} \end{bmatrix}$$

This algorithm requires $u_{i,i}^{(i)} \neq 0$ at each step $i = 0, 1$ in order to obtain a **unique** solution.

LU Decomposition Methods: Doolittle's Method

Two important features of Doolittle's decomposition:

- 1 The matrix U is identical to the upper triangular matrix that results from Gauss elimination.
- 2 The off-diagonal elements of L are the pivot equation multipliers used during Gauss elimination; ie, ℓ_{ij} is the multiplier that eliminated a_{ij} .
- 3 $\det(\mathbf{A}) = \det(\mathbf{U}) = \prod u_{ii}$

LU Decomposition Methods: Doolittle's Method

- 1 Doolittle's factorization without permutation exists if $u_{i,i}^i \neq 0$, $i = 0, 1, \dots, n-2$, where $u_{0,0}^0 = u_{0,0} = a_{0,0}$.
- 2 Note that $u_{n-1,n-1}^{n-1}$ can be any number. If $u_{n-1,n-1}^{n-1} = 0$ then the last row of \mathbf{U} is the null vector, ie, $\mathbf{u}_{n-1,\cdot} = \mathbf{0}$
- 3 For example: $\mathbf{A} = \mathbf{L}\mathbf{U}$ for

$$\mathbf{A} = \begin{bmatrix} 2 & 3 & 4 \\ 4 & 7 & 7 \\ 4 & 9 & 5 \end{bmatrix}$$
$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 2 & 3 & 1 \end{bmatrix}; \mathbf{U} = \begin{bmatrix} 2 & 3 & 4 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \end{bmatrix}$$

LU Decomposition Methods

Comments

① Crout's decomposition: $\det(\mathbf{A}) = \det(\mathbf{L}) = \prod \ell_{ii}$

② Cholesky's decomposition:

$$\det(\mathbf{A}) = \det(\mathbf{U}^T) \det(\mathbf{U}) = \prod u_{ii}^2$$

LU Decomposition

```
1 def LU(A): # without permutation
2     n = A.shape[0]
3     L = np.eye(n)
4     U = A.copy()
5     for j in range(n-1):
6         for i in range(j+1, n):
7             lij = U[i,j]/U[j,j]
8             U[i,:] = U[i,:] - lij*U[j,:]
9             L[i,j] = lij
10    return L, U
```

Note: $U[j, j] \neq 0, j = 0, 1, \dots, n-2$, ie $U[n-1, n-1]$ could be zero.

See: `scipy.linalg.lu`, `scipy.linalg.lu_factor`, `scipy.linalg.lu_solve`

LU Decomposition

```
1 def Lu_compact(A): # without permutation
2     n = A.shape[0]
3     L = np.eye(n)
4     U = A.copy()
5     for j in range(n-1):
6         for i in range(j+1, n):
7             lij = U[i,j]/U[j,j]
8             U[i,:] = U[i,:] - lij*U[j,:]
9             U[i,j] = lij
10    return U
```

Note: It only needs that $U[j,j] \neq 0, j = 0, 1, \dots, n-2$

LU Decomposition with permutation: Example 1

$$\begin{aligned} R_0 &: \begin{bmatrix} 2 & 1 & 5 \end{bmatrix} \\ R_1 &: \begin{bmatrix} 4 & 4 & -4 \end{bmatrix} \\ R_2 &: \begin{bmatrix} 1 & 3 & 1 \end{bmatrix} \end{aligned}$$

Permutation matrix $P = I$ or pivot index $p = [0, 1, 2]$

$$P$$

$$\begin{aligned} R_0 &: \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 2 & 1 & 5 \end{array} \right] \\ R_1 &: \left[\begin{array}{ccc|ccc} 0 & 1 & 0 & 4 & 4 & -4 \end{array} \right] \\ R_2 &: \left[\begin{array}{ccc|ccc} 0 & 0 & 1 & 1 & 3 & 1 \end{array} \right] \end{aligned}$$

LU Decomposition with permutation: Example 1

$$\begin{aligned} R_0 &: \begin{bmatrix} \textcircled{2} & 1 & 5 \end{bmatrix} \\ R_1 &: \begin{bmatrix} 4 & 4 & -4 \end{bmatrix} \\ R_2 &: \begin{bmatrix} 1 & 3 & 1 \end{bmatrix} \end{aligned}$$

Pivot: row = 0, column = 0, maximum absolute value: 4 in row 1. Then, permute $R_0 \leftrightarrow R_1$, P_{01} ; then $P = P_{01}P$ or $p = [1, 0, 2]$

P

$$\begin{aligned} R_0 &: \left[\begin{array}{ccc|ccc} 0 & 1 & 0 & \textcircled{4} & 4 & -4 \end{array} \right] \\ R_1 &: \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 2 & 1 & 5 \end{array} \right] \\ R_2 &: \left[\begin{array}{ccc|ccc} 0 & 0 & 1 & 1 & 3 & 1 \end{array} \right] \end{aligned}$$

LU Decomposition with permutation: Example 1

 P

$$\begin{array}{l} R_0 : \\ R_1 : \\ R_2 : \end{array} \left[\begin{array}{ccc|ccc} 0 & 1 & 0 & \textcircled{4} & 4 & -4 \\ 1 & 0 & 0 & 2 & 1 & 5 \\ 0 & 0 & 1 & 1 & 3 & 1 \end{array} \right]$$

Forward elimination: pivot column 0, pivot row 0.

$$\begin{aligned} R_1 &\leftarrow R_1 - \frac{2}{4}R_0 = R_1 - \frac{1}{2}R_0 \\ R_2 &\leftarrow R_2 - \frac{1}{4}R_0 \end{aligned}$$

LU Decomposition with permutation: Example 1

P

$$\begin{array}{l} R_0 : \\ R_1 : \\ R_2 : \end{array} \left[\begin{array}{ccc|ccc} 0 & 1 & 0 & \textcircled{4} & 4 & -4 \\ 1 & 0 & 0 & \boxed{0} & -1 & 7 \\ 0 & 0 & 1 & \boxed{0} & 2 & 2 \end{array} \right]$$

we can use the new entries with zeroes to set the entries of matrix ***L***

P

$$\begin{array}{l} R_0 : \\ R_1 : \\ R_2 : \end{array} \left[\begin{array}{ccc|ccc} 0 & 1 & 0 & \textcircled{4} & 4 & -4 \\ 1 & 0 & 0 & \boxed{1/2} & -1 & 7 \\ 0 & 0 & 1 & \boxed{1/4} & 2 & 2 \end{array} \right]$$

LU Decomposition with permutation: Example 1

Now we repeat the procedure

$$\begin{array}{c}
 \mathbf{P} \\
 R_0 : \left[\begin{array}{ccc|ccc} 0 & 1 & 0 & 4 & 4 & -4 \end{array} \right] \\
 R_1 : \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & \boxed{1/2} & \textcircled{-1} & 7 \end{array} \right] \\
 R_2 : \left[\begin{array}{ccc|ccc} 0 & 0 & 1 & \boxed{1/4} & 2 & 2 \end{array} \right]
 \end{array}$$

Pivot: row = 1, column = 1.

Maximum absolute value: 2 in row 2. Then, permute $R_1 \leftrightarrow R_2$, \mathbf{P}_{12} , then $\mathbf{P} = \mathbf{P}_{12}\mathbf{P}$ or $\mathbf{p} = [1, 2, 0]$

$$\begin{array}{c}
 \mathbf{P} \\
 R_0 : \left[\begin{array}{ccc|ccc} 0 & 1 & 0 & 4 & 4 & -4 \end{array} \right] \\
 R_1 : \left[\begin{array}{ccc|ccc} 0 & 0 & 1 & \boxed{1/4} & \textcircled{2} & 2 \end{array} \right] \\
 R_2 : \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & \boxed{1/2} & -1 & 7 \end{array} \right]
 \end{array}$$

LU Decomposition with permutation: Example 1

P

$$\begin{array}{l} R_0 : \\ R_1 : \\ R_2 : \end{array} \left[\begin{array}{ccc|ccc} 0 & 1 & 0 & 4 & 4 & -4 \\ 0 & 0 & 1 & \boxed{1/4} & \textcircled{2} & 2 \\ 1 & 0 & 0 & \boxed{1/2} & -1 & 7 \end{array} \right]$$

Forward elimination: Pivot row = 1, column = 1. Then

$$R_2 \leftarrow R_2 - \frac{-1}{2}R_1 = R_2 + \frac{1}{2}R_1$$

LU Decomposition with permutation: Example 1

Finally, we get: $\mathbf{p} = [1, 2, 0]$

$$\begin{array}{c}
 \mathbf{P} \qquad \qquad \mathbf{L} \backslash \mathbf{U} \\
 \begin{array}{l} R_0 : \\ R_1 : \\ R_2 : \end{array} \left[\begin{array}{ccc|ccc} 0 & 1 & 0 & 4 & 4 & -4 \\ 0 & 0 & 1 & \boxed{1/4} & 2 & 2 \\ 1 & 0 & 0 & \boxed{1/2} & \boxed{-1/2} & 8 \end{array} \right]
 \end{array}$$

where $\mathbf{PA} = \mathbf{LU}$ with

$$\mathbf{P} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ 1/4 & 1 & 0 \\ 1/2 & -1/2 & 1 \end{bmatrix}, \quad \mathbf{U} = \begin{bmatrix} 4 & 4 & -4 \\ 0 & 2 & 2 \\ 0 & 0 & 8 \end{bmatrix}$$

LU Decomposition with permutation: Example 1

$$\mathbf{PA} = \begin{bmatrix} 4 & 4 & -4 \\ 1 & 3 & 1 \\ 2 & 1 & 5 \end{bmatrix}$$
$$\mathbf{LU} = \begin{bmatrix} 4 & 4 & -4 \\ 1 & 3 & 1 \\ 2 & 1 & 5 \end{bmatrix}$$

LU Algorithm with permutation

```
1 def PLU(A): # LU with permutation
2     n=A.shape[0]
3     P,L,U=np.eye(n),np.eye(n),A.copy()
4     for j in range(n-1):
5         # Find arg max abs value, col 'j' and below row 'j-1'
6         k=argmax(U,j)
7         if k!=j: # permutes rows j and k
8             U,P=permute(U,P,j,k)
9         for i in range(j+1,n):
10             lij=U[i,j]/U[j,j]
11             U[i,:]=U[i,:]-lij*U[j,:]
12             L[i,j]=lij
13     return P,L,U
```

Note: It only needs that $U[j,j] \neq 0, j = 0, 1, \dots, n-2$

LU Decomposition with permutation: Example 2

Permutation matrix $P = I$ or $p = [0, 1, 2, 3, 4]$

P

$$\begin{array}{l} R_0 : \\ R_1 : \\ R_2 : \\ R_3 : \\ R_4 : \end{array} \left[\begin{array}{ccccc|ccccc} 1 & 0 & 0 & 0 & 0 & 3 & -8 & -7 & 6 & -4 \\ 0 & 1 & 0 & 0 & 0 & 6 & -18 & -12 & 12 & -6 \\ 0 & 0 & 1 & 0 & 0 & 2 & -5 & -5 & 5 & -8 \\ 0 & 0 & 0 & 1 & 0 & 3 & -7 & -10 & 8 & -9 \\ 0 & 0 & 0 & 0 & 1 & 2 & -5 & -3 & -1 & 4 \end{array} \right]$$

LU Decomposition with permutation: Example 2

Permute $R_0 \leftrightarrow R_1$, P_{01} ; then $P = P_{01}P$ or $p = [1, 0, 2, 3, 4]$

$$P$$

$$\begin{array}{l} R_0 : \\ R_1 : \\ R_2 : \\ R_3 : \\ R_4 : \end{array} \left[\begin{array}{ccccc|ccccc} 0 & 1 & 0 & 0 & 0 & 6 & -18 & -12 & 12 & -6 \\ 1 & 0 & 0 & 0 & 0 & 3 & -8 & -7 & 6 & -4 \\ 0 & 0 & 1 & 0 & 0 & 2 & -5 & -5 & 5 & -8 \\ 0 & 0 & 0 & 1 & 0 & 3 & -7 & -10 & 8 & -9 \\ 0 & 0 & 0 & 0 & 1 & 2 & -5 & -3 & -1 & 4 \end{array} \right]$$

LU Decomposition with permutation: Example 2

Forward elimination

 P

$$\begin{array}{l} R_0 : \\ R_1 : \\ R_2 : \\ R_3 : \\ R_4 : \end{array} \left[\begin{array}{ccccc|ccccc} 0 & 1 & 0 & 0 & 0 & 6 & -18 & -12 & 12 & -6 \\ 1 & 0 & 0 & 0 & 0 & \frac{1}{2} & 1 & -1 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & \frac{1}{3} & 1 & -1 & 1 & -6 \\ 0 & 0 & 0 & 1 & 0 & \frac{1}{2} & 2 & -4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & \frac{1}{3} & 1 & 1 & -5 & 6 \end{array} \right]$$

LU Decomposition with permutation: Example 2

Permute $R_1 \leftrightarrow R_3$, P_{13} ; then $P = P_{13}P$ or $p = [1, 3, 2, 1, 4]$

P

$$\begin{array}{l} R_0 : \\ R_1 : \\ R_2 : \\ R_3 : \\ R_4 : \end{array} \left[\begin{array}{ccccc|ccccc} 0 & 1 & 0 & 0 & 0 & 6 & -18 & -12 & 12 & -6 \\ 0 & 0 & 0 & 1 & 0 & \frac{1}{2} & 2 & -4 & 2 & -6 \\ 0 & 0 & 1 & 0 & 0 & \frac{1}{3} & 1 & -1 & 1 & -6 \\ 1 & 0 & 0 & 0 & 0 & \frac{1}{2} & 1 & -1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & \frac{1}{3} & 1 & 1 & -5 & 6 \end{array} \right]$$

LU Decomposition with permutation: Example 2

Forward elimination

P

$$\begin{array}{l} R_0 : \\ R_1 : \\ R_2 : \\ R_3 : \\ R_4 : \end{array} \left[\begin{array}{ccccc|ccccc} 0 & 1 & 0 & 0 & 0 & 6 & -18 & -12 & 12 & -6 \\ 0 & 0 & 0 & 1 & 0 & \frac{1}{2} & 2 & -4 & 2 & -6 \\ 0 & 0 & 1 & 0 & 0 & \frac{1}{3} & \frac{1}{2} & 1 & 0 & -3 \\ 1 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 1 & -1 & 2 \\ 0 & 0 & 0 & 0 & 1 & \frac{1}{3} & \frac{1}{2} & 3 & -6 & 9 \end{array} \right]$$

LU Decomposition with permutation: Example 2

Permute $R_2 \leftrightarrow R_4$, P_{24} ; then $P = P_{24}P$ or $p = [1, 3, 4, 1, 2]$

P

$$\begin{array}{l} R_0 : \\ R_1 : \\ R_2 : \\ R_3 : \\ R_4 : \end{array} \left[\begin{array}{ccccc|ccccc} 0 & 1 & 0 & 0 & 0 & 6 & -18 & -12 & 12 & -6 \\ 0 & 0 & 0 & 1 & 0 & \frac{1}{2} & 2 & -4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & \frac{1}{3} & \frac{1}{2} & 3 & -6 & 9 \\ 1 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 1 & -1 & 2 \\ 0 & 0 & 1 & 0 & 0 & \frac{1}{3} & \frac{1}{2} & 1 & 0 & -3 \end{array} \right]$$

LU Decomposition with permutation: Example 2

Forward elimination

P

$$\begin{array}{l}
 R_0 : \\
 R_1 : \\
 R_2 : \\
 R_3 : \\
 R_4 :
 \end{array}
 \left[\begin{array}{ccccc|ccccc}
 0 & 1 & 0 & 0 & 0 & 6 & -18 & -12 & 12 & -6 \\
 0 & 0 & 0 & 1 & 0 & \frac{1}{2} & 2 & -4 & 2 & -6 \\
 0 & 0 & 0 & 0 & 1 & \frac{1}{3} & \frac{1}{2} & 3 & -6 & 9 \\
 1 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{3} & 1 & -1 \\
 0 & 0 & 1 & 0 & 0 & \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & 2 & -6
 \end{array} \right]$$

LU Decomposition with permutation: Example 2

Permute $R_3 \leftrightarrow R_4$, P_{34} ; then $P = P_{34}P$ or $p = [1, 3, 4, 2, 1]$

P

$$\begin{array}{l}
 R_0 : \\
 R_1 : \\
 R_2 : \\
 R_3 : \\
 R_4 :
 \end{array}
 \left[\begin{array}{ccccc|ccccc}
 0 & 1 & 0 & 0 & 0 & 6 & -18 & -12 & 12 & -6 \\
 0 & 0 & 0 & 1 & 0 & \frac{1}{2} & 2 & -4 & 2 & -6 \\
 0 & 0 & 0 & 0 & 1 & \frac{1}{3} & \frac{1}{2} & 3 & -6 & 9 \\
 0 & 0 & 1 & 0 & 0 & \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & 2 & -6 \\
 1 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{3} & 1 & -1
 \end{array} \right]$$

LU Decomposition with permutation: Example 2

Forward elimination

P

$$\begin{array}{l}
 R_0 : \\
 R_1 : \\
 R_2 : \\
 R_3 : \\
 R_4 :
 \end{array}
 \left[\begin{array}{ccccc|ccccc}
 0 & 1 & 0 & 0 & 0 & 6 & -18 & -12 & 12 & -6 \\
 0 & 0 & 0 & 1 & 0 & \frac{1}{2} & 2 & -4 & 2 & -6 \\
 0 & 0 & 0 & 0 & 1 & \frac{1}{3} & \frac{1}{2} & 3 & -6 & 9 \\
 0 & 0 & 1 & 0 & 0 & \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & 2 & -6 \\
 1 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{3} & \frac{1}{2} & 2
 \end{array} \right]$$

LU Decomposition with permutation: Example 2

$PA = LU$ with

$$P = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$L = \begin{bmatrix} 6 & -18 & -12 & 12 & -6 \\ 0 & 2 & -4 & 2 & -6 \\ 0 & 0 & 3 & -6 & 9 \\ 0 & 0 & 0 & 2 & -6 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix}; U = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1/2 & 1 & 0 & 0 & 0 \\ 1/3 & 1/2 & 1 & 0 & 0 \\ 1/3 & 1/2 & 1/3 & 1 & 0 \\ 1/2 & 1/2 & 1/3 & 1/2 & 1 \end{bmatrix}$$

LU using Gaussian elimination: Let consider the following matrix

$$\mathbf{A}_j = \begin{bmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & a_{j+1,j} & & & \\ & & \vdots & & \ddots & \\ & & a_{n-1,j} & & & 1 \end{bmatrix}$$

ie, it is the $n \times n$ identity matrix with its j -th column replaced by the vector $[0 \ \cdots \ 0 \ 1 \ a_{j+1,j} \ \cdots \ a_{n,j}]^T$.

We can easily compute the inverse of A_j by

$$A_j^{-1} = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & -a_{j+1,j} & & \\ & & \vdots & \ddots & \\ & & -a_{n-1,j} & & 1 \end{bmatrix}$$

we just need to change the sign of the entries $a_{k,j}$

Column stacking

Column stacking

$$\mathbf{A}_{0 \rightarrow 1} := \mathbf{A}_0 \mathbf{A}_1 = \begin{bmatrix} 1 & & & & & & \\ a_{10} & 1 & & & & & \\ a_{20} & a_{21} & 1 & & & & \\ \vdots & \vdots & 0 & \ddots & & & \\ \vdots & \vdots & \vdots & & 1 & & \\ \vdots & \vdots & \vdots & & 0 & \ddots & \\ \vdots & \vdots & \vdots & & \vdots & & \ddots \\ a_{n-1,0} & a_{n-1,1} & 0 & 0 & \cdots & 0 & 1 \end{bmatrix}$$

Column stacking

$$\mathbf{A}_{0 \rightarrow j} := \mathbf{A}_0 \mathbf{A}_1 \cdots \mathbf{A}_j; \quad j = 0, \dots, n-2$$

$$= \begin{bmatrix} 1 & & & & & & & \\ a_{10} & 1 & & & & & & \\ a_{20} & a_{21} & 1 & & & & & \\ a_{30} & a_{31} & a_{32} & & & & & \\ \vdots & \vdots & \vdots & \ddots & & & & \\ \vdots & \vdots & \vdots & & & 1 & & \\ \vdots & \vdots & \vdots & \cdots & a_{j+1,j} & 1 & & \\ \vdots & \vdots & \vdots & & \vdots & 0 & \ddots & \\ a_{n-1,0} & a_{n-1,1} & a_{n-1,2} & \cdots & a_{n-1,j} & 0 & \cdots & 1 \end{bmatrix}$$

Recall: $(\alpha \mathbf{e}_i + \beta \mathbf{e}_j)^T \mathbf{A} = \alpha \mathbf{a}_{i,.} + \beta \mathbf{a}_{j,.}$, ie, premultiplying \mathbf{A} by

$$(\alpha \mathbf{e}_i + \beta \mathbf{e}_j)^T = [0, \dots, \alpha, \dots, \beta, \dots, 0]$$

obtains a linear combination of rows i, j of matrix \mathbf{A} . In particular, if $i = 0$, $\alpha = -\lambda_j$ and $\beta = 1$

$$(-\lambda_j \mathbf{e}_0 + \mathbf{e}_j)^T \mathbf{A} = [-\lambda_j, \dots, 1, \dots, 0] \mathbf{A} = \mathbf{a}_{j,.} - \lambda_j \mathbf{a}_{0,.}$$

Note that this corresponds to the transformation

$$(E_j - \lambda_j E_0) \rightarrow (E_j)$$

with $\lambda_j = \frac{a_{ji}}{a_{ii}}$ in the Gaussian elimination process

Now we can stack the previous operations, $j = 1, 2, \dots, n-1$, and at the top we use the row e_0^T , obtaining

$$M = \begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ -\lambda_1 & 1 & 0 & \cdots & 0 \\ -\lambda_2 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\lambda_{n-1} & 0 & 0 & \cdots & 1 \end{bmatrix}$$

Then

$$\begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ -\lambda_1 & 1 & 0 & \cdots & 0 \\ -\lambda_2 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\lambda_{n-1} & 0 & 0 & \cdots & 1 \end{bmatrix} \mathbf{A} \quad \begin{array}{l} E_0 \leftarrow E_0 \\ E_1 \leftarrow E_1 - \lambda_1 E_0 \\ E_2 \leftarrow E_2 - \lambda_2 E_0 \\ \cdots \\ E_{n-1} \leftarrow E_{n-1} - \lambda_{n-1} E_0 \end{array}$$

Note that, if

$$\lambda_j = \frac{a_{j,0}}{a_{0,0}}$$

then \mathbf{MA} corresponds to first step of the Gaussian elimination process and we call \mathbf{M} a Gaussian elimination matrix

So, after the first iteration we obtain

$$MA = \begin{bmatrix} a_{0,0}^{(0)} & a_{0,1}^{(0)} & \cdots & \cdots & a_{0,n-1}^{(0)} \\ 0 & a_{1,1}^{(0)} & & \cdots & a_{1,n-1}^{(0)} \\ 0 & a_{2,1}^{(0)} & & \cdots & a_{2,n-1}^{(0)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n-1,1}^{(0)} & & \cdots & a_{n-1,n-1}^{(0)} \end{bmatrix}$$

with $a_{i,0}^{(0)} = a_{i,0}$. Now, we can repeat the previous idea in order to obtain the next steps of the Gaussian elimination.

Let us define

$$\hat{\mathbf{L}}^{(k)} = \begin{bmatrix} 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & -\lambda_{k+1,k} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & -\lambda_{n-1,k} & 0 & \cdots & 1 \end{bmatrix}$$

with $k = 0, 1, \dots, n-2$ and

$$\lambda_{j,k} = \frac{a_{j,k}^{(k)}}{a_{k,k}^{(k)}}; \quad j = k+1, k+2, \dots, n-1$$

Then, the Gaussian elimination algorithm can be written as follows.

$$\begin{aligned}U^{(0)} &= A \\U^{(k+1)} &= \hat{L}^{(k)} U^{(k)}\end{aligned}$$

for $k = 0, 1, \dots, n-2$. The last step is

$$U^{(n-1)} = \hat{L}^{(n-2)} \hat{L}^{(n-3)} \dots \hat{L}^{(0)} A$$

where $U^{(n-1)}$ is an upper triangular matrix, which denoted by

$$U := U^{(n-1)}$$

In order to obtain the matrix factorization $A = LU$ we need to find L

$$A = LU = L\hat{L}^{(n-2)}\hat{L}^{(n-3)}\dots\hat{L}^{(0)}A$$

then we can simply define

$$\begin{aligned} L &:= \left(\hat{L}^{(n-2)}\hat{L}^{(n-3)}\dots\hat{L}^{(0)} \right)^{-1} \\ &= L^{(0)}\dots L^{(n-3)}L^{(n-2)} \end{aligned}$$

with $L^{(k)} := \left(\hat{L}^{(k)} \right)^{-1}$, ie, $L^{(k)}\hat{L}^{(k)} = I$

Note that

$$\mathbf{L}^{(k)} = \begin{bmatrix} 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \lambda_{k+1,k} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \lambda_{n-1,k} & 0 & \cdots & 1 \end{bmatrix}$$

with $k = 0, 1, \dots, n-2$. Then,

$$\mathbf{L} = \mathbf{L}^{(0)} \mathbf{L}^{(1)} \cdots \mathbf{L}^{(n-3)} \mathbf{L}^{(n-2)} = \mathbf{L}_{0 \rightarrow n-2}$$

$$\mathbf{L} = \begin{bmatrix}
 1 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 \\
 \lambda_{1,0} & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
 \vdots & \cdots & 1 & 0 & 0 & \cdots & 0 & 0 \\
 \lambda_{k,0} & \cdots & \lambda_{k,k-1} & 1 & 0 & \cdots & & 0 \\
 \lambda_{k+1,0} & \cdots & \lambda_{k+1,k-1} & \lambda_{k+1,k} & 1 & \cdots & 0 & 0 \\
 \vdots & \ddots & & \vdots & \vdots & \ddots & & \vdots \\
 \lambda_{n-2,0} & \cdots & \lambda_{n-2,k-1} & \lambda_{n-2,k} & \lambda_{n-2,k+1} & \cdots & 1 & 0 \\
 \lambda_{n-1,0} & \cdots & \lambda_{n-1,k-1} & \lambda_{n-1,k} & \lambda_{n-1,k+1} & \cdots & \lambda_{n-1,n-2} & 1
 \end{bmatrix}$$

Note that

$$\begin{aligned}
 LU &= \left(L^{(0)} L^{(1)} \dots L^{(n-3)} L^{(n-2)} \right) \left(\hat{L}^{(n-2)} \hat{L}^{(n-3)} \dots \hat{L}^{(0)} \right) A \\
 &= \left(L^{(0)} L^{(1)} \dots L^{(n-3)} \right) L^{(n-2)} \hat{L}^{(n-2)} \left(\hat{L}^{(n-3)} \dots \hat{L}^{(0)} \right) A \\
 &= \left(L^{(0)} L^{(1)} \dots L^{(n-3)} \right) \left(\hat{L}^{(n-3)} \dots \hat{L}^{(1)} \hat{L}^{(0)} \right) A \\
 &= \dots \\
 &= L^{(0)} \hat{L}^{(0)} A \\
 &= A
 \end{aligned}$$

or simply

$$LU = \left(\hat{L}^{(n-2)} \hat{L}^{(n-3)} \dots \hat{L}^{(0)} \right)^{-1} \left(\hat{L}^{(n-2)} \hat{L}^{(n-3)} \dots \hat{L}^{(0)} \right) A = A$$

Summary:

Doolittle's decomposition is obtained with a sequence of Gaussian elimination (U) and a sequence of column stacking (L)

$$\begin{aligned}U &= \left(\hat{L}^{(n-2)} \hat{L}^{(n-3)} \dots \hat{L}^{(0)} \right) A \\L &= L^{(0)} L^{(1)} \dots L^{(n-3)} L^{(n-2)} = L_{0 \rightarrow n-2}\end{aligned}$$

Preserving matrix form property

For matrices of the form $A_{0 \rightarrow k}$ and permutation matrix P_{ij}

$$A_{0 \rightarrow k} = \begin{pmatrix} \text{orange} & \text{red} \\ \text{purple} & \text{green} \end{pmatrix}$$

multiplying on both sides of $A_{0 \rightarrow k}$ by P_{ij} for $k + 1 \leq i < j$ preserves the matrix form.

Preserving matrix form property

Multiplying on both sides of $A_{0 \rightarrow k}$ by P_{ij} for $k + 1 \leq i < j$

$$P_{ij} A_{0 \rightarrow k} P_{ij} = \begin{pmatrix} \text{orange} & \text{pink} \\ \text{light blue} & \text{light green} \\ \text{light blue} & \text{light green} \\ \text{light blue} & \text{light green} \\ \text{pink} & \text{light green} \end{pmatrix}$$

only permutes the subrows $a_{i,0:k}$ and $a_{j,0:k}$ of the matrix $A_{0 \rightarrow k}$, therefore the result has the same form as $A_{0 \rightarrow k}$ (matrix form preservation)

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 & 0 & 0 \\ 3 & 4 & 1 & 0 & 0 & 0 \\ 5 & 6 & 0 & 1 & 0 & 0 \\ 7 & 8 & 0 & 0 & 1 & 0 \\ 9 & 10 & 0 & 0 & 0 & 1 \end{pmatrix}$$

we can see that for $2 \leq i < j$

$$P_{ij}AP_{ij} = \begin{pmatrix} \text{orange} & \text{red} \\ \text{blue} & \text{green} \\ \text{blue} & \text{green} \\ \text{blue} & \text{green} \\ \text{red} & \text{green} \end{pmatrix}$$

ie the matrix keeps the same structure and only permutes the subrows i, j in the submatrix in blue

Example

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 & 0 & 0 \\ 3 & 4 & 1 & 0 & 0 & 0 \\ 5 & 6 & 0 & 1 & 0 & 0 \\ 7 & 8 & 0 & 0 & 1 & 0 \\ 9 & 10 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\mathbf{P}_{35}\mathbf{A}\mathbf{P}_{35} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 & 0 & 0 \\ 3 & 4 & 1 & 0 & 0 & 0 \\ 9 & 10 & 0 & 1 & 0 & 0 \\ 7 & 8 & 0 & 0 & 1 & 0 \\ 5 & 6 & 0 & 0 & 0 & 1 \end{pmatrix}$$

ie permutes the subrows $i = 3$ and $j = 5$ in the submatrix in blue

The Gaussian elimination with permutation can be written as the following sequence of transformations (permutation and Gaussian elimination at each step)

$$\begin{aligned}U^{(0)} &= A \\U^{(k+1)} &= \hat{L}^{(k)} \hat{P}^{(k)} U^{(k)}\end{aligned}$$

for $k = 0, 1, \dots, n-2$, and $\hat{P}^{(k)}$ is a two-row permutation or the identity matrix, ie, it has the form P_{ij} , $P_{ij}P_{ij} = I$. The last step is

$$U^{(n-1)} = \left(\hat{L}^{(n-2)} \hat{P}^{(n-2)} \right) \left(\hat{L}^{(n-3)} \hat{P}^{(n-3)} \right) \dots \left(\hat{L}^{(0)} \hat{P}^{(0)} \right) A$$

where $U^{(n-1)}$ is an upper triangular matrix, which denoted by

$$U := U^{(n-1)}$$

We need to find P and L . Let us write

$$\begin{aligned} L^{-1}P &= \left(\hat{L}^{(n-2)} \hat{P}^{(n-2)} \right) \left(\hat{L}^{(n-3)} \hat{P}^{(n-3)} \right) \dots \left(\hat{L}^{(0)} \hat{P}^{(0)} \right) \\ L &= P \left[\left(\hat{L}^{(n-2)} \hat{P}^{(n-2)} \right) \left(\hat{L}^{(n-3)} \hat{P}^{(n-3)} \right) \dots \left(\hat{L}^{(0)} \hat{P}^{(0)} \right) \right]^{-1} \end{aligned}$$

the problem is to find L (a lower triangular matrix) and P (a permutation matrix). Then

$$\begin{aligned} U &= L^{-1}PA \\ PA &= LU \end{aligned}$$

Let us define

$$\begin{aligned} B &:= P^T L \\ &= P^T P \left[\left(\hat{L}^{(n-2)} \hat{P}^{(n-2)} \right) \left(\hat{L}^{(n-3)} \hat{P}^{(n-3)} \right) \dots \left(\hat{L}^{(0)} \hat{P}^{(0)} \right) \right]^{-1} \end{aligned}$$

then

$$\begin{aligned} B &= \left[\left(\hat{L}^{(n-2)} \hat{P}^{(n-2)} \right) \left(\hat{L}^{(n-3)} \hat{P}^{(n-3)} \right) \dots \left(\hat{L}^{(0)} \hat{P}^{(0)} \right) \right]^{-1} \\ &= P^{(0)} L^{(0)} \dots P^{(n-2)} L^{(n-2)} \end{aligned}$$

where $P^{(k)} = \left(\hat{P}^{(k)} \right)^{-1} = \left(P^{(k)} \right)^{-1}$ ($P_{ij} = P_{ij}^{-1}$, $P_{ij} P_{ij} = I$)

and $L^{(k)} = \left(\hat{L}^{(k)} \right)^{-1}$

Since $P^{(1)}P^{(1)} = I$ then

$$\begin{aligned} B &= P^{(0)}L^{(0)}P^{(1)}L^{(1)} \dots P^{(n-2)}L^{(n-2)} \\ &= P^{(0)}P^{(1)} \left(P^{(1)}L^{(0)}P^{(1)} \right) L^{(1)} \dots P^{(n-2)}L^{(n-2)} \end{aligned}$$

$L_0 := P^{(1)}L^{(0)}P^{(1)}$, where L_0 and $L^{(0)}$ have the same matrix form. Since the application of $P^{(1)}$ on both sides of $L^{(0)}$ only permutes subrows.

$$\begin{aligned} B &= P^{(0)} P^{(1)} L_0 L^{(1)} P^{(2)} L^{(2)} \dots P^{(n-2)} L^{(n-2)} \\ &= P^{(0)} P^{(1)} P^{(2)} \left(P^{(2)} L_{0 \rightarrow 1} P^{(2)} \right) L^{(2)} \dots P^{(n-2)} L^{(n-2)} \end{aligned}$$

since $L_0 L^{(1)}$ can be written as $L_{0 \rightarrow 1}$.

Note $L_1 := P^{(2)} L_{0 \rightarrow 1} P^{(2)}$ and $L_{0 \rightarrow 1}$ has the same matrix form, since the application of $P^{(2)}$ on both sides of $L_{0 \rightarrow 1}$ only permutes subrows.

$$\begin{aligned} B &= P^{(0)} P^{(1)} P^{(2)} \left(P^{(3)} L_1 L^{(2)} P^{(3)} \right) L^{(3)} \dots P^{(n-2)} L^{(n-2)} \\ &= P^{(0)} P^{(1)} P^{(2)} \left(P^{(3)} L_{0 \rightarrow 2} P^{(3)} \right) L^{(3)} \dots P^{(n-2)} L^{(n-2)} \end{aligned}$$

since $L_1 L^{(2)}$ can be written as $L_{0 \rightarrow 2}$.

Note $L_2 := P^{(3)} L_{0 \rightarrow 2} P^{(3)}$ and $L_{0 \rightarrow 2}$ has the same matrix form, since the application of $P^{(3)}$ on both sides of $L_{0 \rightarrow 2}$ only permutes subrows.

We can repeat the previous procedure,

$$B = P^{(0)} P^{(1)} P^{(2)} P^{(3)} \dots P^{(n-2)} L_{n-3} L^{(n-2)}$$

with $L_{n-3} := P^{(n-2)} L_{0 \rightarrow n-3} P^{(n-2)}$. Since

$$B = P^T L$$

we can define $P^T := P^{(0)} P^{(1)} P^{(2)} P^{(3)} \dots P^{(n-2)}$ and $L := L_{n-3} L^{(n-2)} = L_{0 \rightarrow n-2}$. Note that

$$P = P^{(n-2)} P^{(n-3)} \dots P^{(0)}$$

Note that P is an orthogonal and L is a lower triangular matrix. We can use the recurrence

$$\begin{aligned} P &= P^{(0)} \\ P &= P^{(k)} P \end{aligned}$$

to compute P

Summary

Matrix form of LU with permutation

$$U = \left(\hat{L}^{(n-2)} \hat{P}^{(n-2)} \right) \left(\hat{L}^{(n-3)} \hat{P}^{(n-3)} \right) \cdots \left(\hat{L}^{(0)} \hat{P}^{(0)} \right) A$$

$$P = P^{(n-2)} P^{(n-3)} \cdots P^{(0)}$$

$$L = L_{0 \rightarrow n-2}$$

with the following sequence of subrows permutation and column stacking to compute L

$$L_{0 \rightarrow 0} := L_0$$

$$L_{k-1} := P^{(k)} L_{0 \rightarrow k-1} P^{(k)} \text{ subrow permutation}$$

$$L_{0 \rightarrow k} := L_{k-1} L^{(k)} \text{ column stacking}$$

for $k = 1, 2, \dots, n-2$

Example

$$\mathbf{A} = \begin{pmatrix} 3 & -8 & -6 & 6 \\ 6 & -18 & -12 & 12 \\ 2 & -5 & -5 & 5 \\ 3 & -7 & -10 & 8 \end{pmatrix}$$

Permutation

$$\mathbf{P}_{01}\mathbf{A} = \begin{pmatrix} 6 & -18 & -12 & 12 \\ 3 & -8 & -6 & 6 \\ 2 & -5 & -5 & 5 \\ 3 & -7 & -10 & 8 \end{pmatrix}$$

Example

Gaussian Elimination

$$\hat{L}^0 P_{01} A = \begin{pmatrix} 6 & -18 & -12 & 12 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & -1 & 1 \\ 0 & 2 & -4 & 2 \end{pmatrix}$$

Permutation

$$P_{13} \hat{L}^0 P_{01} A = \begin{pmatrix} 6 & -18 & -12 & 12 \\ 0 & 2 & -4 & 2 \\ 0 & 1 & -1 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Example

Gaussian Elimination

$$\hat{L}^1 P_{13} \hat{L}^0 P_{01} \mathbf{A} = \begin{pmatrix} 6 & -18 & -12 & 12 \\ 0 & 2 & -4 & 2 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 2 & -1 \end{pmatrix}$$

Permutation

$$P_{23} \hat{L}^1 P_{13} \hat{L}^0 P_{01} \mathbf{A} = \begin{pmatrix} 6 & -18 & -12 & 12 \\ 0 & 2 & -4 & 2 \\ 0 & 0 & 2 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Example

Gaussian Elimination

$$\hat{L}^2 P_{23} \hat{L}^1 P_{13} \hat{L}^0 P_{01} A = \begin{pmatrix} 6 & -18 & -12 & 12 \\ 0 & 2 & -4 & 2 \\ 0 & 0 & 2 & -1 \\ 0 & 0 & 0 & 0.5 \end{pmatrix}$$

then we obtain $U := \hat{L}^2 P_{23} \hat{L}^1 P_{13} \hat{L}^0 P_{01} A$.

In order to find L and P , let us choose B such that $BU = A$

Example

Now, we are going to compute P and L ,

$$\begin{aligned}
 B &:= (\hat{L}^2 P_{23} \hat{L}^1 P_{13} \hat{L}^0 P_{01})^{-1} \\
 &= P_{01} L^0 P_{13} L^1 P_{23} L^2 \\
 &= P_{01} (\textcolor{red}{P}_{13} \textcolor{red}{P}_{13}) L^0 P_{13} L^1 P_{23} L^2 \\
 &= P_{01} P_{13} (\textcolor{blue}{P}_{13} L^0 \textcolor{blue}{P}_{13}) L^1 P_{23} L^2 \\
 &= P_{01} P_{13} \textcolor{brown}{L}_0 L^1 P_{23} L^2 \\
 &= P_{01} P_{13} \textcolor{brown}{L}_{0 \rightarrow 1} P_{23} L^2
 \end{aligned}$$

where $L_0 = P_{13} L^0 P_{13}$ and $L_{0 \rightarrow 1} = L_0 L^1$.

Example

$$\begin{aligned}
 B &= P_{01}P_{13}(\mathbf{P}_{23}\mathbf{P}_{23})L_{0\rightarrow 1}P_{23}L^2 \\
 &= P_{01}P_{13}P_{23}(\mathbf{P}_{23}L_{0\rightarrow 1}\mathbf{P}_{23})L^2 \\
 &= P_{01}P_{13}P_{23}\mathbf{L}_1L^2 \\
 &= P^T\mathbf{L}_{0\rightarrow 2} \\
 &= P^TL
 \end{aligned}$$

where

$$\begin{aligned}
 L_1 &= P_{23}L_{0\rightarrow 1}P_{23} \\
 P &= P_{23}P_{13}P_{01} \\
 L_{0\rightarrow 2} &= L_1L^2
 \end{aligned}$$

since $A = BU$ then $PA = LU$

Example

Inverse of the first Gaussian elimination matrix

$$\mathbf{L}^0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1/2 & 1 & 0 & 0 \\ 1/3 & 0 & 1 & 0 \\ 1/2 & 0 & 0 & 1 \end{bmatrix}$$

Preserving from property

$$\mathbf{L}_0 = \mathbf{P}_{13}\mathbf{L}^0\mathbf{P}_{13} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \textcolor{red}{1/2} & 1 & 0 & 0 \\ 1/3 & 0 & 1 & 0 \\ \textcolor{blue}{1/2} & 0 & 0 & 1 \end{bmatrix}$$

Example

Inverse of the second Gaussian elimination matrix

$$\mathbf{L}^1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1/2 & 1 & 0 \\ 0 & 1/2 & 0 & 1 \end{bmatrix}$$

Column stacking of Gaussian elimination matrices

$$\mathbf{L}_{0 \rightarrow 1} := \mathbf{L}_0 \mathbf{L}^1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1/2 & 1 & 0 & 0 \\ 1/3 & 1/2 & 1 & 0 \\ 1/2 & 1/2 & 0 & 1 \end{bmatrix}$$

Example

Preserving from property

$$\mathbf{L}_1 = \mathbf{P}_{23}\mathbf{L}_{0 \rightarrow 1}\mathbf{P}_{23} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1/2 & 1 & 0 & 0 \\ \textcolor{red}{1/2} & \textcolor{red}{1/2} & 1 & 0 \\ \textcolor{blue}{1/3} & \textcolor{blue}{1/2} & 0 & 1 \end{bmatrix}$$

Inverse of the third Gaussian elimination matrix

$$\mathbf{L}^2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1/2 & 1 \end{bmatrix}$$

Example

Column stacking of Gaussian elimination matrices

$$\mathbf{L}_1 \mathbf{L}^2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1/2 & 1 & 0 & 0 \\ 1/2 & 1/2 & 1 & 0 \\ 1/3 & 1/2 & 1/2 & 1 \end{bmatrix}$$

Matrix \mathbf{L} :

$$\mathbf{L} := \mathbf{L}_{0 \rightarrow 2} = \mathbf{L}_1 \mathbf{L}^2$$

Example

Permutation matrix P

$$\begin{aligned} P^T &= P_{01} P_{13} P_{23} \\ &= \begin{bmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix} \\ P &= \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \end{aligned}$$

Example

Finally,

$$U = \hat{L}_2 P_{23} \hat{L}_1 P_{13} \hat{L}_0 P_{01} A$$

$$P = P_{23} P_{13} P_{01}$$

$$L = L_{0 \rightarrow 2}$$

where

$$L_0 = P_{13} L^0 P_{13}$$

$$L_{0 \rightarrow 1} = L_0 L^1$$

$$L_1 = P_{23} L_{0 \rightarrow 1} P_{23}$$

$$L_{0 \rightarrow 2} = L_1 L^2$$

Example

the PLU (permutation, lower-, and upper-triangular matrices) decomposition (factorization) is

$$PA = LU$$

with

$$P = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}; A = \begin{bmatrix} 3 & -8 & -6 & 6 \\ 6 & -18 & -12 & 12 \\ 2 & -5 & -5 & 5 \\ 3 & -7 & -10 & 8 \end{bmatrix}$$
$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1/2 & 1 & 0 & 0 \\ 1/2 & 1/2 & 1 & 0 \\ 1/3 & 1/2 & 1/2 & 1 \end{bmatrix}; U = \begin{bmatrix} 6 & -18 & -12 & 12 \\ 0 & 2 & -4 & 2 \\ 0 & 0 & 2 & -1 \\ 0 & 0 & 0 & 0.5 \end{bmatrix}$$