LU decomposition

The matrix form of the Gaussian elimination.

$$\mathbf{A}\mathbf{x} = \mathbf{b} \longrightarrow \mathbf{A}^{(1)}\mathbf{x} = \mathbf{b}^{(1)}$$

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ a_{31} & a_{32} & a_{33} & \dots & a_{3m} \\ & & \dots & & \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mm} \end{pmatrix} \begin{array}{c} \\ \gamma_{21} = a_{21}/a_{11} \\ \gamma_{31} = a_{31}/a_{11} \\ \dots \\ \gamma_{m1} = a_{m1}/a_{11} \end{array}$$

Elementary lower triangular matrices

Consider

$$\mathbf{\Lambda}_1 = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ -\gamma_{21} & 1 & 0 & \cdots & 0 \\ -\gamma_{31} & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & & \ddots & \\ -\gamma_{m1} & 0 & 0 & \cdots & 1 \end{pmatrix}$$

Transforming the first column is equivalent to

$$\mathbf{\Lambda}_1 \mathbf{A} \mathbf{x} = \mathbf{\Lambda}_1 \mathbf{b}$$

Elementary lower triangular matrices

Likewise

$$\mathbf{\Lambda}_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & -\gamma_{32} & 1 & 0 & \cdots & 0 \\ 0 & -\gamma_{42} & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \ddots & \\ 0 & -\gamma_{m2} & 0 & 0 & \cdots & 1 \end{pmatrix}$$

Transforming the second column is equivalent to

$$\mathbf{\Lambda}_2\mathbf{\Lambda}_1\mathbf{A}\mathbf{x} = \mathbf{\Lambda}_2\mathbf{\Lambda}_1\mathbf{b}$$

The forward sweep

The whole forward sweep is

$$\mathbf{\Lambda}_{m-1} \cdots \mathbf{\Lambda}_1 \mathbf{A}\,\mathbf{x} = \mathbf{\Lambda}_{m-1} \cdots \mathbf{\Lambda}_1\,\mathbf{b}$$

$$\begin{aligned} \mathbf{A} &= \left(\mathbf{\Lambda}_{m-1} \cdots \mathbf{\Lambda}_1\right)^{-1} \mathbf{U} \\ &= \mathbf{\Lambda}_1^{-1} \cdots \mathbf{\Lambda}_{m-1}^{-1} \mathbf{U} \end{aligned}$$

What is Λ_k^{-1}?

$$\mathbf{\Lambda}_1^{-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ \gamma_{21} & 1 & 0 & \cdots & 0 \\ \gamma_{31} & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & & \ddots & \\ \gamma_{m1} & 0 & 0 & \cdots & 1 \end{pmatrix}$$

What is Λ_k^{-1}?

$$\mathbf{\Lambda}_1^{-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ \gamma_{21} & 1 & 0 & \cdots & 0 \\ \gamma_{31} & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & & \ddots & \\ \gamma_{m1} & 0 & 0 & \cdots & 1 \end{pmatrix}$$

$$\mathbf{\Lambda}_2^{-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & \gamma_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & & \ddots & \\ 0 & \gamma_{m2} & 0 & \cdots & 1 \end{pmatrix}$$

What is the product of Λ_k^{-1}?

$$\mathbf{\Lambda}_1^{-1}\mathbf{\Lambda}_2^{-1}\cdots\mathbf{\Lambda}_{m-1}^{-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ \gamma_{21} & 1 & 0 & \cdots & 0 \\ \gamma_{31} & \gamma_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & & \ddots & \\ \gamma_{m1} & \gamma_{m2} & \gamma_{m3} & \cdots & 1 \end{pmatrix}$$

What is the product of Λ_k^{-1}?

$$\mathbf{\Lambda}_1^{-1}\mathbf{\Lambda}_2^{-1}\cdots\mathbf{\Lambda}_{m-1}^{-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ \gamma_{21} & 1 & 0 & \cdots & 0 \\ \gamma_{31} & \gamma_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & & \ddots & \\ \gamma_{m1} & \gamma_{m2} & \gamma_{m3} & \cdots & 1 \end{pmatrix}$$

So that

$$\mathbf{A} = \mathbf{L}\mathbf{U}$$

where L is a lower triangular matrix with a unit diagonal.

Using the LU factorization

Systems of linear equations: $\mathbf{A}\mathbf{x} = \mathbf{b}$

1. Decompose $\mathbf{A} = \mathbf{L}\mathbf{U}$
2. Transform the r.h.s.: compute $\mathbf{L}^{-1}\mathbf{b}$
3. Solve $\mathbf{U}\mathbf{x} = \mathbf{L}^{-1}\mathbf{b}$

Multiple right-hand sides: only perform the factorization once.

Pivoting

- Solution of $\mathbf{Ax} = \mathbf{b}$ exists and is unique iff $\det \mathbf{A} \neq 0$
- However, $\mathbf{LU}$ factorization requires all leading minors to be non zero.
- If a leading minor close to zero, it's also bad for stability.

The main idea: at each step, find a coefficient a_{ij} with the largest absolute value (*pivot*), and eliminate the corresponding unknown x_j.

Column pivoting

Column pivoting (or *partial pivoting*): look for a max element along columns of $\mathbf{A}$

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ a_{31} & a_{32} & a_{33} & \dots & a_{3m} \\ & & \dots & & \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mm} \end{pmatrix}$$

Complexity: $O(m)$ comparisons per column.

Full pivoting

Full pivoting: look for a max element in the whole matrix $\mathbf{A}$. Swap rows and relabel the unknowns.

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ a_{31} & a_{32} & a_{33} & \dots & a_{3m} \\ & & \dots & & \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mm} \end{pmatrix}$$

Complexity: $O(m^2)$ comparisons per column.

Column pivoting, the matrix form

Permutation matrices

An *elementary permutation matrix*, P_{kl}, is a square matrix obtained from an identity matrix by swapping rows k and l.

E.g., for $m = 3$

$$P_{12} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad P_{13} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad P_{23} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

Column pivoting, the matrix form

Permutation matrices

An *elementary permutation matrix*, P_{kl}, is a square matrix obtained from an identity matrix by swapping rows k and l.

$P_{kl}\mathbf{A}$ has rows k and l swapped

$\mathbf{A}P_{kl}$ has columns k and l swapped

LU factorization with column pivoting

For the k-th column, find a pivot (row i_k), left-multiply by $P_k \equiv P_{k,i_k}$, then left-multiply by $\mathbf{\Lambda}_k$. Proceed for $k = 1, \cdots, m-1$.

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$
$$\mathbf{\Lambda}_1 P_1 \mathbf{A}\mathbf{x} = \mathbf{\Lambda}_1 P_1 \mathbf{b}$$
$$\mathbf{\Lambda}_2 P_2 \mathbf{\Lambda}_1 P_1 \mathbf{A}\mathbf{x} = \mathbf{\Lambda}_2 P_2 \mathbf{\Lambda}_1 P_1 \mathbf{b}$$

$$\cdots$$

Finally,

$$\mathbf{A}^{(m-1)} = \mathbf{\Lambda}_{m-1} P_{m-1} \cdots \mathbf{\Lambda}_2 P_2 \mathbf{\Lambda}_1 P_1 \mathbf{A}$$

LU factorization with column pivoting

For any matrix $\mathbf{A}$ with $\det \mathbf{A} \neq 0$, factorization

$$\mathbf{A} = P\mathbf{L}\mathbf{U}$$

exists and is unique.

LU factorization with column pivoting

In practice, P is not constructed explicitly. Only need to store the permutation

$$\pi_m = \begin{pmatrix} 1 & 2 & \cdots & m-1 \\ i_1 & i_2 & \cdots & i_{m-1} \end{pmatrix}$$

LAPACK's `*getrf`

```
IPIV    (output) INTEGER array, dimension (min(M,N))
        The pivot indices; for 1 <= i <= min(M,N), row i
        of the matrix was interchanged with row IPIV(i).
```

Other applications of LU factorization

Computing determinants

$$\det \mathbf{A} = \det P \det \mathbf{L} \det \mathbf{U} = (-1)^S \prod_{k=1}^{m} u_{kk}$$

$$\log |\det \mathbf{A}| = \sum_{k=1}^{m} \log |u_{kk}|$$

Other applications of LU factorization

Computing $\mathbf{A}^{-1}$

$$\mathbf{A}\mathbf{X} = [\,\widehat{\mathbf{e}}_1 \,|\, \widehat{\mathbf{e}}_2 \,|\, \cdots \,|\, \widehat{\mathbf{e}}_m\,]$$

Computing $\cdots \mathbf{A}^{-1}\mathbf{B} \cdots$

$$\mathbf{X} = \mathbf{A}^{-1}\mathbf{B} \qquad \Longleftrightarrow \qquad \mathbf{A}\mathbf{X} = \mathbf{B}$$