

LU decomposition

The matrix form of the Gaussian elimination.

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

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

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

$$\mathbf{\Lambda}_1 \mathbf{Ax} = \mathbf{\Lambda}_1 \mathbf{b}$$

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

$$\mathbf{\Lambda}_2 \mathbf{\Lambda}_1 \mathbf{Ax} = \mathbf{\Lambda}_2 \mathbf{\Lambda}_1 \mathbf{b}$$

The forward sweep

The whole forward sweep is

$$\Lambda_{m-1} \cdots \Lambda_1 \mathbf{A} \mathbf{x} = \Lambda_{m-1} \cdots \Lambda_1 \mathbf{b}$$

$$\begin{aligned} \mathbf{A} &= (\Lambda_{m-1} \cdots \Lambda_1)^{-1} \mathbf{U} \\ &= \Lambda_1^{-1} \cdots \Lambda_{m-1}^{-1} \mathbf{U} \end{aligned}$$

What is Λ_k^{-1} ?

$$\Lambda_1^{-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ \gamma_{21} & 1 & 0 & \cdots & 0 \\ \gamma_{31} & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & & \ddots & \\ \gamma_{m1} & 0 & 0 & \cdots & 1 \end{pmatrix}$$

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$$\Lambda_2^{-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & \gamma_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & & \ddots & \\ 0 & \gamma_{m2} & 0 & \cdots & 1 \end{pmatrix}$$

What is the product of Λ_k^{-1} ?

$$\Lambda_1^{-1} \Lambda_2^{-1} \cdots \Lambda_{m-1}^{-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ \gamma_{21} & 1 & 0 & \cdots & 0 \\ \gamma_{31} & \gamma_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & & \ddots & \\ \gamma_{m1} & \gamma_{m2} & \gamma_{m3} & \cdots & 1 \end{pmatrix}$$

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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: $\mathbf{Ax} = \mathbf{b}$

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

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, 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 $m = 3$

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

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 Λ_k . Proceed for $k = 1, \dots, m - 1$.

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

$$\Lambda_1 P_1 \mathbf{A}\mathbf{x} = \Lambda_1 P_1 \mathbf{b}$$

$$\Lambda_2 P_2 \Lambda_1 P_1 \mathbf{A}\mathbf{x} = \Lambda_2 P_2 \Lambda_1 P_1 \mathbf{b}$$

...

Finally,

$$\mathbf{A}^{(m-1)} = \Lambda_{m-1} P_{m-1} \cdots \Lambda_2 P_2 \Lambda_1 P_1 \mathbf{A}$$

LU factorization with column pivoting

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

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

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 $1 \leq i \leq \min(M,N)$, 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}

$$\mathbf{AX} = [\hat{\mathbf{e}}_1 \mid \hat{\mathbf{e}}_2 \mid \cdots \mid \hat{\mathbf{e}}_m]$$

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

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