

Gaussian Elimination & LU Decompositions

Square System of Equations

Consider

$$Ax = b$$

where

$$A = [a_{ij}] \longleftarrow n \times n \text{ matrix}$$

$$b \longleftarrow n \times 1 \text{ vector.}$$

In expanded form,

$$a_{11}x_1 + \cdots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + \cdots + a_{2n}x_n = b_2$$

$$\vdots$$

$$a_{n1}x_1 + \cdots + a_{nn}x_n = b_n$$

Gaussian Elimination



Carl Friedrich Gauss
(1777-1855)

A Summary of the Evolution of Gaussian Elimination

Gaussian Elimination With No Pivoting (GENP)

$A \longrightarrow A^{(1)} \longrightarrow \dots \longrightarrow A^{(n-1)} =: U$ (upper triangular).

$b \longrightarrow b^{(1)} \longrightarrow \dots \longrightarrow b^{(n-1)}.$

Gaussian Elimination With No Pivoting (GENP)

$$A \longrightarrow A^{(1)} \longrightarrow \dots \longrightarrow A^{(n-1)} =: U \text{ (upper triangular).}$$
$$b \longrightarrow b^{(1)} \longrightarrow \dots \longrightarrow b^{(n-1)}.$$

Step 1: Create zeros in the first column of A :

$$A \longrightarrow \underbrace{\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2}^{(1)} & \cdots & a_{nn}^{(1)} \end{bmatrix}}_{=:A^{(1)}}; \quad b \longrightarrow \underbrace{\begin{bmatrix} b_1 \\ b_2^{(1)} \\ \vdots \\ b_n^{(1)} \end{bmatrix}}_{=:b^{(1)}}$$

where

$$a_{ij}^{(1)} = a_{ij} - \underbrace{\frac{a_{i1}}{a_{11}}}_{=:m_{i1}} a_{1j}; \quad b_i^{(1)} = b_i - \frac{a_{i1}}{a_{11}} b_1; \quad i = 2 : n, j = 2 : n.$$

Here $a_{11} \leftarrow$ pivot (assumed non zero); $m_{i1} \leftarrow$ multipliers;

GENP

Step k: Create zeros in column k of $A^{(k-1)}$:

$$A^{(k-1)} = \left[\begin{array}{cccc|ccc} a_{11} & \cdots & \cdots & a_{1k} & a_{1,k+1} & \cdots & a_{1k}^{(1)} \\ & a_{22}^{(1)} & \cdots & a_{2k}^{(1)} & a_{2,k+1}^{(1)} & \cdots & a_{2n}^{(1)} \\ & & \ddots & \vdots & \vdots & \cdots & \vdots \\ & & & a_{kk}^{(k-1)} & a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \\ \hline & & & a_{k+1,k}^{(k-1)} & a_{k+1,k+1}^{(k-1)} & \cdots & a_{k+1,n}^{(k-1)} \\ & & & \vdots & \vdots & & \vdots \\ & & & a_{n,k}^{(k-1)} & a_{n,k+1}^{(k-1)} & \cdots & a_{nn}^{(k-1)} \end{array} \right]$$

$$\rightarrow \left[\begin{array}{cccc|ccc} a_{11} & \cdots & \cdots & a_{1k} & a_{1,k+1} & \cdots & a_{1k}^{(1)} \\ & a_{22}^{(1)} & \cdots & a_{2k}^{(1)} & a_{2,k+1}^{(1)} & \cdots & a_{2n}^{(1)} \\ & & \ddots & \vdots & \vdots & \cdots & \vdots \\ & & & a_{kk}^{(k-1)} & a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \\ \hline & & & & a_{k+1,k+1}^{(k)} & \cdots & a_{k+1,n}^{(k)} \\ & & & & \vdots & & \vdots \\ & & & & a_{n,k+1}^{(k)} & \cdots & a_{nn}^{(k)} \end{array} \right] =: A^{(k)};$$

GENP

The same operations are performed on $b^{(k-1)}$:

$$b^{(k-1)} \longrightarrow \begin{bmatrix} b_1 \\ b_2^{(1)} \\ \vdots \\ b_k^{(k-1)} \\ b_{k+1}^{(k)} \\ \vdots \\ b_n^{(k)} \end{bmatrix} =: b^{(k)}$$

where for $i = k + 1 : n, j = k + 1 : n$,

$$a_{ij}^{(k)} = a_{ij}^{(k-1)} - \underbrace{\frac{a_{ik}^{(k-1)}}{a_{kk}^{(k-1)}}}_{=: m_{ik}} a_{kj}^{(k-1)}; \quad b_i^{(k)} = b_i^{(k-1)} - \frac{a_{ik}^{(k-1)}}{a_{kk}^{(k-1)}} b_k^{(k-1)};$$

Here $a_{kk}^{(k-1)} \longleftarrow$ pivot (assumed non zero); $m_{ik} \longleftarrow$ multipliers;

Step $n - 1$: Create a zero in the $(n, n - 1)$ of $A^{(n-2)}$:

$$A^{(n-2)} \longrightarrow \underbrace{\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} \\ & & \ddots & \vdots \\ & & & a_{nn}^{(n-1)} \end{bmatrix}}_{=: A^{(n-1)} \text{ (also called } U)}; \quad b^{(n-2)} \longrightarrow b^{(n-1)};$$

where assuming pivot $a_{n-1,n-1}^{(n-2)} \neq 0$ and using multiplier

$$m_{n,n-1} := \frac{a_{n,n-1}^{(n-2)}}{a_{n-1,n-1}^{(n-2)}},$$

$$a_{nn}^{(n-1)} = a_{nn}^{(n-2)} - m_{n,n-1} a_{n-1,n}^{(n-2)}; \quad b_n^{(n-1)} = b_n^{(n-2)} - m_{n,n-1} b_{n-1}^{(n-2)}.$$

GENP

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- ▶ The system is transformed to $Ux = b^{(n-1)}$.
- ▶ The pivots at each step are on the diagonal of U !
- ▶ All steps have to be repeated to solve any new system $Ax = c$ if the multipliers used in the GENP are not saved.

GENP $\equiv LU$ decomposition of A

Let

$$L = \begin{bmatrix} 1 & & & & & & & & \\ m_{21} & 1 & & & & & & & \\ m_{31} & m_{32} & \ddots & & & & & & \\ \vdots & \vdots & & \ddots & & & & & \\ m_{k1} & m_{k2} & \cdots & \cdots & 1 & & & & \\ m_{k+1,1} & m_{k+1,2} & \cdots & \cdots & m_{k+1,k} & \ddots & & & \\ \vdots & \vdots & & & \vdots & & 1 & & \\ m_{n1} & m_{n2} & \cdots & \cdots & m_{nk} & \cdots & m_{n,n-1} & 1 \end{bmatrix}.$$

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Then $A = LU$!

LU decomposition: A square matrix A is said to have an LU decomposition if there exists a unit lower triangular matrix L and an upper triangular matrix U such that $A = LU$.

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This needs a proof!

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Proof: In step k of GENP

$$A^{(k)} = \left[\begin{array}{ccccccc} 1 & & & & & & \\ 0 & \ddots & & & & & \\ \vdots & \cdots & & 1 & & & \\ 0 & & -m_{k+1,k} & \ddots & & & \\ \vdots & & \vdots & & \ddots & & \\ 0 & \cdots & -m_{nk} & \cdots & & & 1 \end{array} \right] A^{(k-1)}$$

$\underbrace{\hspace{10em}}_{=:M_k}$

Then

$$U = A^{(n-1)} = M_{n-1}M_{n-2}\cdots M_k\cdots M_2M_1A$$

where M_k , $k = 1, \dots, n-1$ are the *multiplier* matrices or *Gauss transforms* of Gaussian Elimination.

Exercise: $b^{(n-1)} = M_{n-1}M_{n-2}\cdots M_1b$.

GENP $\equiv LU$ decomposition of A

Note that,

$$U = A^{(n-1)} = M_{n-1} \underbrace{\left(M_{n-2} \cdots \underbrace{\left(M_k \cdots \underbrace{\left(M_2 \underbrace{(M_1 A)}_{=A^{(1)}} \right)}_{=A^{(2)}} \right)}_{=A^{(k)}} \right)}_{=A^{(n-2)}}$$

and

$$M_k = I_n - \begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} e_k^T, \quad k = 1 : n-1,$$

are rank one updates of I_n . Here e_k is column k of I_n .

GENP $\equiv LU$ decomposition of A

Observe that

$$\blacktriangleright M_k^{-1} = I_n + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{kn} \end{bmatrix} e_k^T, \quad k = 1 : n-1, \text{ (Prove this!)}$$

\blacktriangleright For $i_1 < \dots < i_p$,

$$M_{i_1}^{-1} \dots M_{i_p}^{-1} = I_n + \sum_{i=i_1}^{i_p} \begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{i+1,i} \\ \vdots \\ m_{ni} \end{bmatrix} e_i^T, \text{ (Prove this!)}$$

GENP $\equiv LU$ decomposition of A

So $U = M_{n-1}M_{n-2} \cdots M_2M_1A$ implies,

$$A = M_1^{-1}M_2^{-1} \cdots M_{n-1}^{-1}U = \left(I_n + \sum_{k=1}^{n-1} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{pmatrix} e_k^T \right) U$$

$$= \begin{bmatrix} 1 & & & & & & & \\ m_{21} & 1 & & & & & & \\ m_{31} & m_{32} & \ddots & & & & & \\ \vdots & \vdots & & \ddots & & & & \\ m_{k1} & m_{k2} & \cdots & \cdots & 1 & & & \\ m_{k+1,1} & m_{k+1,2} & \cdots & \cdots & m_{k+1,k} & \ddots & & \\ \vdots & \vdots & & & \vdots & & 1 & \\ m_{n1} & m_{n2} & \cdots & \cdots & m_{nk} & \cdots & m_{n,n-1} & 1 \end{bmatrix} U = LU.$$

Rank one updates in GENP

In Step k ,

$$A^{(k)} = M_k A^{(k-1)}$$

$$= \left(I_n - \begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} e_k^T \right) A^{(k-1)} = A^{(k-1)} - \begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \underbrace{e_k^T A^{(k-1)}}_{\text{row } k \text{ of } A^{(k-1)}}$$

$$= A^{(k-1)} - \underbrace{\begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \begin{bmatrix} 0 & \dots & 0 & a_{kk}^{(k-1)} & \dots & a_{kn}^{(k-1)} \end{bmatrix}}_{\text{rank one update of } A^{(k-1)}}$$

Rank one updates in GENP

Now

$$\begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \begin{bmatrix} 0 & \dots & 0 & a_{kk}^{(k-1)} & \dots & a_{kn}^{(k-1)} \end{bmatrix} = \left[\begin{array}{c|c} \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \hat{M}_k \end{array} \right],$$

$$\text{where } \hat{M}_k = \begin{bmatrix} m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \begin{bmatrix} a_{kk}^{(k-1)} & \dots & a_{kn}^{(k-1)} \end{bmatrix}.$$

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As

$$m_{ik} a_{kk}^{(k-1)} = \left(a_{ik}^{(k-1)} / a_{kk}^{(k-1)} \right) a_{kk}^{(k-1)} = a_{ik}^{(k-1)}, \quad i = k+1 : n,$$

the first column of \widehat{M}_k is

$$\begin{bmatrix} a_{k+1,k}^{(k-1)} \\ \vdots \\ a_{nk}^{(k-1)} \end{bmatrix}.$$

Rank one updates in GENP

Therefore,

$$A^{(k)} = A^{(k-1)} - \left[\begin{array}{c|c} \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \widehat{M}_k \end{array} \right]$$

$$= \left[\begin{array}{c|c} A_{11}^{(k-1)} & A_{12}^{(k-1)} \\ \hline A_{21}^{(k-1)} & A_{22}^{(k-1)} \end{array} \right]$$

$$- \left[\begin{array}{cccc|cccc} 0 & & 0 & 0 & 0 & & \cdots & 0 \\ \vdots & \cdots & \vdots & \vdots & \vdots & & \ddots & \vdots \\ 0 & & 0 & 0 & 0 & & \cdots & 0 \\ \hline 0 & & 0 & a_{k+1,k}^{(k-1)} & \left[\begin{array}{c} m_{k+1,k} \\ \vdots \\ m_{nk} \end{array} \right] & \left[\begin{array}{ccc} a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \end{array} \right] \\ \vdots & \cdots & \vdots & \vdots & & & & \\ 0 & & 0 & a_{nk}^{(k-1)} & & & & \end{array} \right]$$

where

$$A_{11}^{(k-1)} \rightarrow k \times k; \quad A_{21}^{(k-1)} \rightarrow k \times (n-k);$$

$$A_{21}^{(k-1)} \rightarrow (n-k) \times k; \quad A_{22}^{(k-1)} \rightarrow (n-k) \times (n-k).$$

Rank one updates in GENP

$$\text{As } A_{21}^{(k-1)} = \begin{bmatrix} 0 & \cdots & 0 & a_{k+1,k}^{(k-1)} \\ \vdots & & \vdots & \vdots \\ 0 & & 0 & a_{nk}^{(k-1)} \end{bmatrix}, \text{ therefore,}$$

$$A^{(k)} = \left[\begin{array}{c|c} A_{11}^{(k-1)} & A_{12}^{(k-1)} \\ \hline & \textcolor{red}{A_{22}^{(k)}} \end{array} \right],$$

where

$$A_{22}^{(k)} = A_{22}^{(k-1)} - \underbrace{\begin{bmatrix} m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \begin{bmatrix} a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \end{bmatrix}}_{\text{rank one update of } A_{22}^{(k-1)}}$$

$$= \begin{bmatrix} a_{k+1,k+1}^{(k-1)} & \cdots & a_{k+1,n}^{(k-1)} \\ \vdots & \ddots & \vdots \\ a_{n,k+1}^{(k-1)} & \cdots & a_{nn}^{(k-1)} \end{bmatrix} - \begin{bmatrix} \frac{a_{k+1,k}^{(k-1)}}{a_{kk}^{(k-1)}} \\ \vdots \\ \frac{a_{nk}^{(k-1)}}{a_{kk}^{(k-1)}} \end{bmatrix} \begin{bmatrix} a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \end{bmatrix}$$

Algorithm for GENP/LU

```
for  $k = 1 : n - 1$ 
  if  $a_{kk} \neq 0$       (multiplier computation begins)
    for  $i = k + 1 : n$ 
       $a_{ik} = a_{ik} / a_{kk};$ 
    end
  else
    exit {'zero pivot encountered'}
  end      (multiplier computation ends)
  for  $i = k + 1 : n$  (matrix update begins)
    for  $j = k + 1 : n$ 
       $a_{ij} = a_{ij} - a_{ik} a_{kj}$ 
    end
  end      (matrix update ends)
end
end
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$L \longrightarrow I_n +$ strictly lower triangular part of output A .
 $U \longrightarrow$ upper triangular part of output A .

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Exercise: Show that the flop count of LU decomposition of an $n \times n$ matrix is $\frac{2}{3}n^3 + O(n^2)$ flops.

Algorithm for GENP/LU with higher level BLAS

```
for k = 1:n-1
    if A(k,k)  $\neq$  0      (multiplier computation begins)
        A(k+1:n,k) = A(k+1:n,k)/A(k,k);
    else
        exit {'zero pivot encountered'}
    end      (multiplier computation ends)

    (matrix update)
    A(k+1:n,k+1:n) = A(k+1:n,k+1:n) - A(k+1:n,k)*A(k,k+1:n);
end
```

GENP for solving systems of equations

Pseudocode for solving $n \times n$ system $Ax = b$:

1. Find LU decomposition of A . $(\frac{2}{3}n^3 + O(n^2)$ flops)
2. Solve $Ly = b$ for y . (n^2) flops)
3. Solve $Ux = y$ for x . (n^2) flops)

Total flops: $\frac{2}{3}n^3 + O(n^2)$ flops.

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Theorem: A nonsingular square matrix has an LU decomposition if and only if all its leading principal submatrices are nonsingular.

Additionally for such matrices, the LU decomposition is unique.

Gaussian Elimination With Partial Pivoting (GEPP)

1. Checking A for existence of LU decomposition is not possible in practice.
 - (i) Numerically it is only possible to ascertain how close A and its leading principal submatrices are to being singular.
 - (ii) Ascertaining the proximity of A and its leading principal submatrices to a singular matrix will cost more flops than finding the LU factors.

Gaussian Elimination With Partial Pivoting (GEPP)

1. Checking A for existence of LU decomposition is not possible in practice.
2. Even if A has an LU decomposition, computing it is a numerically unstable process.
 - ▶ Small pivots can lead to large multipliers and result in instability in finite precision arithmetic.

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For each $k = 1 : n - 1$

1. Find $a_{pk}^{(k-1)}$ such that $|a_{pk}^{(k-1)}| = \max_{k \leq j \leq n} |a_{jk}^{(k-1)}|$.
2. If $p \neq k$ interchange rows k and p .
3. Perform the usual GE steps to create zeros in column k .

$$A^{(k-1)} = \left[\begin{array}{cccc|ccc} a_{11} & \cdots & \cdots & a_{1k} & a_{1,k+1} & \cdots & a_{1n} \\ & a_{22}^{(1)} & \cdots & a_{2k}^{(1)} & a_{2,k+1}^{(1)} & \cdots & a_{2n}^{(1)} \\ & & \ddots & \vdots & \vdots & \cdots & \vdots \\ \hline & & & a_{kk}^{(k-1)} & a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \\ & & & a_{k+1,k}^{(k-1)} & a_{k+1,k+1}^{(k-1)} & \cdots & a_{k+1,n}^{(k-1)} \\ & & & \vdots & \vdots & \cdots & \vdots \\ & & & a_{n,k}^{(k-1)} & a_{n,k+1}^{(k-1)} & \cdots & a_{nn}^{(k-1)} \end{array} \right]$$

GEPP $\equiv LU$ decomposition of row permuted A

Permutation Matrices: An $n \times n$ permutation matrix P is obtained by interchanging rows and/or columns of I_n .

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Examples: $\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$, $\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$, $\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$.

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Transposition: A transposition is a permutation matrix obtained by interchanging only two rows or two columns of an identity matrix.

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1. Permutations are orthogonal matrices.

GEPP $\equiv LU$ decomposition of row permuted A

Permutation Matrices: An $n \times n$ permutation matrix P is obtained by interchanging rows and/or columns of I_n .

Examples: $\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$, $\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$, $\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$.

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Theorem Given any $n \times n$ matrix A , there exists a permutation P such that PA has an LU decomposition.