Section 1.7. Gaussian Elimination and LU Decomposition.

Given a linear system $Ax = b$, where $A \in \mathbb{R}^{n \times n}$ is nonsingular, Gaussian elimination transforms the linear system to

$$Ux = y$$

where U is upper triangular, and then solves $Ux = y$ by back substitution.

Gaussian elimination performs three types of operations:

1) Add a multiple one equation to another.
2) Interchanges two equations.
3) Multiply an equation by a nonzero constant.

E.g. Solve the system:

$$x_1 - 2x_2 = 0$$
$$-3x_1 + 4x_2 = -2.$$

Multiplying the first row by 3 and adding the two rows, we obtain

$$x_1 - 2x_2 = 0$$
$$0 - 2x_2 = -2$$

$\Rightarrow$ use back substitution, $x_2 = 1 \Rightarrow x_1 = 2x_2 = 2$.

In the matrix form,

$$\begin{bmatrix} 1 & -2 \\ -3 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ -2 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} 1 & 0 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} 1 & -2 \\ -3 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ -2 \end{bmatrix}$$

$$\begin{bmatrix} 1 & -2 \\ 0 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ -2 \end{bmatrix}$$

Gaussian elimination can be represented as transformation of augmented matrix

$$[A|b] \rightarrow [U|y]$$

through operations are on rows of matrix.

(A is nonsingular if and only if U is nonsingular).

* <u>Gaussian Elimination and LU Factorization:</u>

- Gaussian elimination without row interchanges can be viewed as "triangular triangularization" of <u>nonsingular</u> $A \in \mathbb{R}^{n\times n}$.

$$\underbrace{L_{n-1} \cdots L_2 L_1}_{L^{-1}} A = U$$

Then $A = LU$. It is also called LU factorization.

For augmented matrix,

$$L^{-1}[A|b] = [U|y] \Rightarrow y = L^{-1}b.$$

Example of LU factorization of 4×4 matrix A:

$$\underbrace{\begin{bmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{bmatrix}}_{A} \xrightarrow{L_1} \underbrace{\begin{bmatrix} x & x & x & x \\ 0 & \otimes & \otimes & \otimes \\ 0 & \otimes & \otimes & \otimes \\ 0 & \otimes & \otimes & \otimes \end{bmatrix}}_{L_1 A} \xrightarrow{L_2} \underbrace{\begin{bmatrix} x & x & x & x \\ & \otimes & \otimes & \otimes \\ & 0 & \boxtimes & \boxtimes \\ & 0 & \boxtimes & \boxtimes \end{bmatrix}}_{L_2 L_1 A} \xrightarrow{L_3} \underbrace{\begin{bmatrix} x & x & x & x \\ & x & x & x \\ & & x & x \\ & & 0 & x \end{bmatrix}}_{L_3 L_2 L_1 A}.$$

<u>What is Matrix L_1?</u>

In Gaussian elimination, at first step A is transformed to $A^{(1)}$ by

$$l_{i1} = a_{i1}/a_{11}, \quad i = 2, \dots, n.$$

$$a_{ij}^{(1)} = a_{ij} - l_{i1}a_{1j}, \quad i = 2, \dots, n, \quad j = 2, \dots, n.$$

In matrix form, we have $A^{(1)} = L_1 A$, where

$$L_1 = \begin{bmatrix} 1 & & & & \\ -l_{2,1} & 1 & & & \\ -l_{3,1} & & 1 & & \\ \vdots & & & \ddots & \\ -l_{n,1} & & & & 1 \end{bmatrix}$$

What is Matrices L_k?

- At ~~k~~ step k, eliminates entries below $a_{kk}^{(k-1)}$:
- Let $a_{:,k}^{(k-1)}$ be the kth column of $L_{k-1} \cdots L_1 A$, then

$$a_{:,k}^{(k-1)} = \begin{bmatrix} a_{1k}^{(k-1)} \\ a_{2k}^{(k-1)} \\ \vdots \\ a_{kk}^{(k-1)} \\ a_{k+1,k}^{(k-1)} \\ \vdots \\ a_{n,k}^{(k-1)} \end{bmatrix}$$

$$\Rightarrow L_k a_{:,k}^{(k-1)} = \begin{bmatrix} a_{1k}^{(k-1)} \\ \vdots \\ a_{k,k}^{(k-1)} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

The multipliers $l_{jk} = \dfrac{a_{jk}^{(k-1)}}{a_{kk}^{(k-1)}}$ appear in L_k.

$$L_k = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & -\ell_{k+1,k} & 1 & \\ & & \vdots & & \ddots \\ & & -\ell_{n,k} & & & 1 \end{bmatrix}$$

* <u>Forming the L matrix</u>.

$$L = L_1^{-1} L_2^{-1} \cdots L_{n-1}^{-1}$$

has a simple form in terms of the multipliers

Observe that

$$L_1^{-1} L_2^{-1} = \begin{bmatrix} 1 & & & \\ \ell_{2,1} & 1 & & \\ \vdots & & \ddots & \\ \ell_{n,1} & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & \ell_{3,2} & \ddots & \\ & \vdots & & \\ & \ell_{n,2} & & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & & & \\ \ell_{2,1} & 1 & & \\ \ell_{31} & \ell_{32} & 1 & \\ \vdots & \vdots & & \ddots \\ \ell_{n1} & \ell_{n2} & & & 1 \end{bmatrix}$$

In general,

$$L = \begin{bmatrix} 1 & & & & & \\ \ell_{21} & 1 & & & & \\ \ell_{31} & \ell_{32} & 1 & & & \\ \vdots & \vdots & & \ddots & & \\ & & & & 1 & \\ \ell_{n1} & \ell_{n2} & \ell_{31} & & \ell_{n,n-1} & 1 \end{bmatrix}$$

E.g. Let $A = \begin{bmatrix} 2 & 1 & 1 \\ 2 & 2 & -1 \\ 4 & -1 & 6 \end{bmatrix}$ and $b = \begin{bmatrix} 9 \\ 9 \\ 16 \end{bmatrix}$

Solve $Ax = b$.

Sol. form the augmented matrix

$$[A \mid b] = \left[\begin{array}{ccc|c} 2 & 1 & 1 & 9 \\ 2 & 2 & -1 & 9 \\ 4 & -1 & 6 & 16 \end{array}\right]$$

$l_{21} = \frac{a_{21}}{a_{11}} = 1$

$l_{31} = \frac{a_{31}}{a_{11}} = 2$

$$\xrightarrow[R_3 - 2R_1]{R_2 - R_1,} \left[\begin{array}{ccc|c} 2 & 1 & 1 & 9 \\ 0 & 1 & -2 & 0 \\ 0 & -3 & 4 & -2 \end{array}\right]$$

$l_{32} = \frac{a_{32}^{(1)}}{a_{22}^{(1)}} = -3$

$$\xrightarrow{R_3 + 3R_2} \left[\begin{array}{ccc|c} 2 & 1 & 1 & 9 \\ 0 & 1 & -2 & 0 \\ 0 & 0 & -2 & -2 \end{array}\right]$$

Then solve

$$\begin{aligned} 2x_1 + x_2 + x_3 &= 9 \\ x_2 - 2x_3 &= 0 \\ -2x_3 &= -2 \end{aligned}$$

using back substitution,

$x_3 = 1$

$x_2 = 2x_3 = 2$

$x_1 = \frac{9 - x_2 - x_3}{2} = \frac{9-2-1}{2} = 3.$

Note that

$$A = LU$$

$$\begin{bmatrix} 2 & 1 & 1 \\ 2 & 2 & -1 \\ 4 & -1 & 6 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 2 & -3 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 \\ 0 & 1 & -2 \\ 0 & 0 & -2 \end{bmatrix}$$

* LU Factorization ~~and~~ (without Pivoting)

Factorize A into $A = LU$.

Pseudo-code

$U = A$, $L = I$

for $k = 1$ to $n-1$

  for $j = k+1$ to n

    $l_{jk} = u_{jk} / u_{kk}$

    $u_{j,k:n} = u_{j,k:n} - l_{jk} u_{k,k:n}$

Thm: Let A be an $n \times n$ matrix whose leading principal submatrices are all nonsingular. Then A can be factorized in exactly one way into a product $A = LU$, such that L is $\underbrace{\text{unit lower triangular}}_{\text{(lower triangular + diag. entries are 1)}}$ and U is upper triangular.

* Section 1.8 Gaussian Elimination with Pivoting

. At step k, we divide by u_{kk} (i.e., $a_{kk}^{(k-1)}$), which would break if u_{kk} is 0 (or close to 0).

$$\begin{bmatrix} x & x & x & x & x \\ & 0 & x & x & x \\ & 0 & x & x & x \\ & a_{ik}^{(k-1)} & x & x & x \\ & x & x & x & x \end{bmatrix}$$

$\Rightarrow$ other nonzero entry in kth column below diagonal can be pivoted, and we permute (interchange) row i with row k.

* Partial Pivoting:

$$\begin{bmatrix} x & x & x & x \\ & x & x & x \\ & \boxed{x_{ik} \quad x \quad x} \\ & x & x & x \end{bmatrix} \xrightarrow{P_k} \begin{bmatrix} x & x & x & x \\ & x_{kk} & x & x \\ & x & x & x \\ & x & x & x \end{bmatrix} \xrightarrow{L_k} \begin{bmatrix} x & x & x & x \\ & x_{kk} & x & x \\ & 0 & x & x \\ & 0 & x & x \end{bmatrix}$$

Pivot selection	Row interchange	Elimination
We Choose nonzero entry with largest magnitude as pivot.	we interchange row i with row k. . P_k is a permutation matrix, obtained by interchanging two rows of I.	

In terms of matrices, it becomes

$$L_{n-1}P_{n-1}\cdots L_2P_2L_1P_1A = U.$$

After $k-1$ steps of forward elimination, we have computed the reduced matrix.

$$A^{(k-1)} = \begin{bmatrix} a_{11} & a_{12} & \cdots & & \cdots & & a_{1n} \\ & a_{22}^{(1)} & \cdots & & \cdots & & a_{2n}^{(1)} \\ & & \ddots & & & & \vdots \\ & & & a_{k-1,k-1}^{(k-2)} & a_{k-1,k}^{(k-2)} & \cdots & a_{k-1,n}^{(k-2)} \\ & & & & a_{k,k}^{(k-1)} & \cdots & a_{k,n}^{(k-1)} \\ & & & & \vdots & & \\ & & & & a_{n,k}^{(k-1)} & \cdots & a_{n,n}^{(k-1)} \end{bmatrix}$$

- partial pivoting:
  - choose $a_{mk}^{(k-1)}$ as the <u>pivot</u> for step k, where
  $$|a_{mk}^{(k-1)}| = \max_{k\le i\le n} |a_{ik}^{(k-1)}|.$$
  - if $m \neq k$, then interchange rows m and k.
  - Matrix formulation of partial pivoting:
  $$A^{(1)} = L_1P_1A$$

where P_1 is a permutation matrix.

Then

$$A^{(2)} = L_2P_2A^{(1)}$$
$$= L_2P_2L_1P_1A.$$

$\Rightarrow$ after $n-1$ steps, we have

$$U = A^{(n-1)} = L_{n-1}P_{n-1}L_{n-2}P_{n-2}\cdots L_1P_1A.$$

E.g. Solve the system

$$\begin{bmatrix} 0 & 4 & 1 \\ 1 & 1 & 3 \\ 2 & -2 & 1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 9 \\ 6 \\ -1 \end{bmatrix}$$

by Gaussian elimination with partial pivoting.

Sol: $[A \mid b]$

$$\left[\begin{array}{ccc|c} 0 & 4 & 1 & 9 \\ 1 & 1 & 3 & 6 \\ 2 & -2 & 1 & -1 \end{array}\right] \xrightarrow[R_1 \leftrightarrow R_3]{P_1 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}} \left[\begin{array}{ccc|c} 2 & -2 & 1 & -1 \\ 1 & 1 & 3 & 6 \\ 0 & 4 & 1 & 9 \end{array}\right] \xrightarrow[R_2 - \frac{1}{2}R_1]{L_1 = \begin{bmatrix} 1 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}} \left[\begin{array}{ccc|c} 2 & -2 & 1 & -1 \\ 0 & 2 & \frac{5}{2} & \frac{13}{2} \\ 0 & 4 & 1 & 9 \end{array}\right]$$

$$P_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \xrightarrow[\substack{\cancel{R_3 - 2R_2} \\ R_3 \leftrightarrow R_2}]{} \left[\begin{array}{ccc|c} 2 & -2 & 1 & -1 \\ 0 & 4 & 1 & 9 \\ 0 & 2 & \frac{5}{2} & \frac{13}{2} \end{array}\right] \xrightarrow[R_3 - \frac{1}{2}R_2]{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{1}{2} & 1 \end{bmatrix} = L_2} \left[\begin{array}{ccc|c} 2 & -2 & 1 & -1 \\ 0 & 4 & 1 & 9 \\ 0 & 0 & 2 & 2 \end{array}\right]$$

$$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad U \qquad\quad y$$

$$Ux = y.$$

$$\Rightarrow \quad 2x_3 = \cancel{x}\,2 \quad \Rightarrow \quad x_3 = 1.$$

$$4x_2 + x_3 = 9 \quad \Rightarrow \quad x_2 = \frac{9 - x_3}{4} = \frac{8}{4} = 2$$

$$2x_1 - 2x_2 + x_3 = -1 \quad \Rightarrow \quad x_1 = \frac{-1 + 2x_2 - x_3}{2} = \frac{-1 + 4 - 1}{2} = 1.$$

$$\Rightarrow \quad x = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}.$$

* Complete pivoting: choose $a_{mp}^{(k-1)}$ as the pivot for step k, where

$$|a_{mp}^{(k-1)}| = \max_{\substack{k \le i \le n \\ k \le j \le n}} |a_{ij}^{(k-1)}|$$

If $m \ne n$, or $p \ne k$, then interchange rows m and k and columns p and k.

Matrix formulation of complete pivoting:

$$A^{(1)} = L_1 P_1 A Q_1$$

where P_1 and Q_1 are permutation matrices. Then

$$\begin{aligned} A^{(2)} &= L_2 P_2 A^{(1)} Q_2 \\ &= L_2 P_2 L_1 P_1 A Q_1 Q_2. \end{aligned}$$

and so on,

After $n-1$ steps,

$$\begin{aligned} A^{(n-1)} &= L_{n-1} P_{n-1} L_{n-2} P_{n-2} \cdots L_2 P_2 L_1 P_1 A Q_1 Q_2 \cdots Q_{n-1} \\ &= U. \end{aligned}$$

is upper triangular.

<u>Thm: 1.8.8</u>. For any $n \times n$ nonsingular matrix A, there exists a permutation matrix P such that PA has an LU factorization. That is,

$$PA = LU \quad \text{or} \quad A = P^T LU.$$