Computational method and numerical algorithms

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Example 1. Consider the system

$$x + y = 3, \tag{1}$$
$$3x - 4y = 2. \tag{2}$$

How to solve this?

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$$x + y = 3, \quad (1)$$
$$3x - 4y = 2. \quad (2)$$

How to solve this? **Gaussian Elimination.**

2.1 Gaussian Elimination

Example 1. Consider the system

$$x + y = 3, \quad (1)$$
$$3x - 4y = 2. \quad (2)$$

How to solve this? **Gaussian Elimination.**

1. Elimination: $-3\times(1)+(2)$:

$$x + y = 3, \quad (3)$$
$$-7y = -7. \quad (4)$$

2. Back Substitution or backsolving: (4) gives:

$$y = 1.$$

   Then, back substitute $y = -1$ into (3) gives:

$$x + 1 = 3 \to x = 2.$$

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Operations in “Elimination”

1. Swap one equation for another.
2. Multiplying an equation by a nonzero constant.
3. Add or subtract a multiple of one equation from another.

An illustration in Matrix form

Example 2. Consider the following system of three equations:

$$
\begin{aligned}
x + 2y - z &= 3, \\
2x + y + z &= 3, \\
-3x + y + z &= -6.
\end{aligned}
$$

Sol. Elimination:

$$
\left[\begin{array}{ccc|c}
1 & 2 & -1 & 3 \\
2 & 1 & 1 & 3 \\
-3 & 1 & 1 & -6
\end{array}\right]
\xrightarrow{\text{Step 1}}
$$

An illustration in Matrix form

Example 2. Consider the following system of three equations:

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Sol. Elimination:

$$\left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ 2 & 1 & 1 & 3 \\ -3 & 1 & 1 & -6 \end{array}\right] \xrightarrow{\text{Step 1}} \left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ 0 & -3 & 3 & -3 \\ -3 & 1 & 1 & -6 \end{array}\right]$$

$$\xrightarrow{\text{Step 2}}$$

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An illustration in Matrix form

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$$\begin{aligned} x + 2y - z &= 3, \\ 2x + y + z &= 3, \\ -3x + y + z &= -6. \end{aligned}$$

Sol. Elimination:

$$\left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ 2 & 1 & 1 & 3 \\ -3 & 1 & 1 & -6 \end{array}\right] \xrightarrow{\text{Step 1}} \left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ \color{red}{0} & -3 & 3 & -3 \\ -3 & 1 & 1 & -6 \end{array}\right]$$

$$\xrightarrow{\text{Step 2}} \left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ \color{red}{0} & -3 & 3 & -3 \\ \color{red}{0} & 7 & -2 & 3 \end{array}\right] \xrightarrow{\text{Step 3}}$$

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An illustration in Matrix form

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\begin{aligned}
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$$

Sol. Elimination:

$$
\left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ 2 & 1 & 1 & 3 \\ -3 & 1 & 1 & -6 \end{array}\right]
\xrightarrow{\text{Step 1}}
\left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ 0 & -3 & 3 & -3 \\ -3 & 1 & 1 & -6 \end{array}\right]
$$

$$
\xrightarrow{\text{Step 2}}
\left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ 0 & -3 & 3 & -3 \\ 0 & 7 & -2 & 3 \end{array}\right]
\xrightarrow{\text{Step 3}}
\left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ 0 & -3 & 3 & -3 \\ 0 & 0 & 5 & -4 \end{array}\right]
$$

An illustration in Matrix form

Example 2. Consider the following system of three equations:

$$
\begin{aligned}
x + 2y - z &= 3, \\
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-3x + y + z &= -6.
\end{aligned}
$$

Sol. Elimination:

$$
\left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ 2 & 1 & 1 & 3 \\ -3 & 1 & 1 & -6 \end{array}\right] \xrightarrow{\text{Step } 1} \left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ 0 & -3 & 3 & -3 \\ -3 & 1 & 1 & -6 \end{array}\right]
$$

$$
\xrightarrow{\text{Step } 2} \left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ 0 & -3 & 3 & -3 \\ 0 & 7 & -2 & 3 \end{array}\right] \xrightarrow{\text{Step } 3} \left[\begin{array}{ccc|c} 1 & 2 & -1 & 3 \\ 0 & -3 & 3 & -3 \\ 0 & 0 & 5 & -4 \end{array}\right]
$$

Back substitution:

$$
\begin{aligned}
x &= 3 - 2y - z, \\
-3y &= -3 - 3z, \\
5z &= -4.
\end{aligned}
$$

The operation count in Elimination Step

For a general system of n linear equations in n variables:

$$\left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{array}\right]$$

$$\xrightarrow{\text{Step1:}} \left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ 0 & a_{22} - \frac{a_{21}a_{12}}{a_{11}} & \cdots & a_{2n} - \frac{a_{21}a_{1n}}{a_{11}} & b_2 - \frac{a_{21}b_1}{a_{11}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & a_{n2} - \frac{a_{n1}a_{12}}{a_{11}} & \cdots & a_{nn} - \frac{a_{n1}a_{1n}}{a_{11}} & b_n - \frac{a_{n1}b_1}{a_{11}} \end{array}\right]$$

- Number of multiplications/divisions in Step 1:
- Number of additions/subtractions in Step 1:

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The operation count in Elimination Step

For a general system of n linear equations in n variables:

$$\left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{array}\right]$$

$$\xrightarrow{\text{Step1:}{\color{red}a_{11}\neq 0}} \left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ {\color{red}0} & a_{22}-\frac{a_{21}a_{12}}{a_{11}} & \cdots & a_{2n}-\frac{a_{21}a_{1n}}{a_{11}} & b_2-\frac{a_{21}b_1}{a_{11}} \\ {\color{red}\vdots} & \vdots & \ddots & \vdots & \vdots \\ {\color{red}0} & a_{n2}-\frac{a_{n1}a_{12}}{a_{11}} & \cdots & a_{nn}-\frac{a_{n1}a_{1n}}{a_{11}} & b_n-\frac{a_{n1}b_1}{a_{11}} \end{array}\right]$$

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$$\left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{array}\right]$$

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- Number of multiplications/divisions in Step 1: $n(n-1)+n(n-1)$
- Number of additions/subtractions in Step 1:$n(n-1)$

The operation count in Elimination Step

For a general system of n linear equations in n variables:

$$\left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{array}\right]$$

$$\xrightarrow{\text{Step1:}{\color{red}a_{11}\neq 0}} \left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ {\color{red}0} & a_{22} - {\color{red}\frac{a_{21}}{a_{11}}}a_{12} & \cdots & a_{2n} - {\color{red}\frac{a_{21}}{a_{11}}}a_{1n} & b_2 - {\color{red}\frac{a_{21}}{a_{11}}}b_1 \\ {\color{red}\vdots} & \vdots & \ddots & \vdots & \vdots \\ {\color{red}0} & a_{n2} - {\color{red}\frac{a_{n1}}{a_{11}}}a_{12} & \cdots & a_{nn} - {\color{red}\frac{a_{n1}}{a_{11}}}a_{1n} & b_n - {\color{red}\frac{a_{n1}}{a_{11}}}b_1 \end{array}\right]$$

- Number of multiplications/divisions in Step 1: $n(n-1) + {\color{red}(n-1)}$
- Number of additions/subtractions in Step 1: $n(n-1)$

The operation count in Elimination Step

For a general system of n linear equations in n variables:

$$\left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{array}\right]$$

$$\xrightarrow{\text{Step1:}a_{11}\neq 0} \left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ 0 & a_{22} - \frac{a_{21}a_{12}}{a_{11}} & \cdots & a_{2n} - \frac{a_{21}a_{1n}}{a_{11}} & b_2 - \frac{a_{21}b_1}{a_{11}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & a_{n2} - \frac{a_{n1}a_{12}}{a_{11}} & \cdots & a_{nn} - \frac{a_{n1}a_{1n}}{a_{11}} & b_n - \frac{a_{n1}b_1}{a_{11}} \end{array}\right]$$

- Number of multiplications/divisions in Step 1: $n(n-1) + (n-1)$
- Number of additions/subtractions in Step 1:$n(n-1)$
- Number of multiplications/divisions in Step 2: $(n-1)(n-2) + (n-2)$,
- Number of additions/subtractions in Step 2: $(n-1)(n-2)$
- ...
- Number of multiplications/divisions in Step
- Number of additions/subtractions in Step

The operation count in Elimination Step

For a general system of n linear equations in n variables:

$$\left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{array}\right]$$

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- Number of multiplications/divisions in Step 1: $n(n-1) + (n-1)$
- Number of additions/subtractions in Step 1: $n(n-1)$
- Number of multiplications/divisions in Step 2: $(n-1)(n-2) + (n-2)$,
- Number of additions/subtractions in Step 2: $(n-1)(n-2)$
- ...
- Number of multiplications/divisions in Step $n-1$: $2 \times 1 + 1$
- Number of additions/subtractions in Step $n-1$: 2×1

The operation count in Elimination Step

For a general system of n linear equations in n variables:

$$\left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{array}\right]$$

$$\xrightarrow{\text{Step1}: a_{11}\neq 0} \left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ 0 & a_{22}-\frac{a_{21}a_{12}}{a_{11}} & \cdots & a_{2n}-\frac{a_{21}a_{1n}}{a_{11}} & b_2-\frac{a_{21}b_1}{a_{11}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & a_{n2}-\frac{a_{n1}a_{12}}{a_{11}} & \cdots & a_{nn}-\frac{a_{n1}a_{1n}}{a_{11}} & b_n-\frac{a_{n1}b_1}{a_{11}} \end{array}\right]$$

- Number of multiplications/divisions in Step 1: $n(n-1)+(n-1)$
- Number of additions/subtractions in Step 1: $n(n-1)$
- Number of multiplications/divisions in Step 2: $(n-1)(n-2)+(n-2)$, **Condition:** $a_{22}-a_{21}a_{12}/a_{11}\neq 0$.
- Number of additions/subtractions in Step 2: $(n-1)(n-2)$
- ...
- Number of multiplications/divisions in Step $n-1$: $2\times 1+1$
- Number of additions/subtractions in Step $n-1$: 2×1

Sum them up, we have

- Total Number of multiplications/divisions:

$$\sum_{j=2}^{n} j^2 - 1 = \frac{1}{6}n(n+1)(2n+1) - n$$

- Total Number of additions/subtractions:

$$\sum_{j=2}^{n} j(j-1) = \frac{1}{6}n(n+1)(2n+1) - \frac{n(n+1)}{2}$$

- Total Number of Operations:

$$\frac{1}{3}n(n+1)(2n+1) - \frac{n(n+1)}{2} - n = \frac{2}{3}n^3 + \frac{1}{2}n^2 - \frac{7}{6}n$$

The operation Count in Back-substitution Step

After the elimination, we get the following system of equations in matrix form:

$$\left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ 0 & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & a_{nn} & b_n \end{array}\right]$$

We easily get

$$\begin{aligned} x_1 &= \frac{b_1 - a_{12}x_2 - \cdots - a_{1n}x_n}{a_{11}} \\ x_2 &= \frac{b_2 - a_{23}x_3 - \cdots - a_{2n}x_n}{a_{22}} \\ &\vdots \\ x_n &= \frac{b_n}{a_{nn}}. \end{aligned}$$

The operation Count in Back-substitution Step

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We easily get

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- Number of Multiplications/Divisions: $n + \cdots + 1 = \frac{n(n+1)}{2}$
- Number of additions/subtractions: $(n-1) + \cdots + 0 = \frac{n(n-1)}{2}$
- Total Number of operations: n^2.

Computational Complexity of Gaussian Elimination Algorithm

The total number of operations is the sum of $\frac{2}{3}n^3 + \frac{1}{2}n^2 - \frac{7}{6}n$ operations in Elimination Step and n^2 operations in Back Substitution Step, i.e.,

$$\frac{2}{3}n^3 + \frac{3}{2}n^2 - \frac{7}{6}n = \mathcal{O}(n^3),$$

operations, which is defined as the **Computational Complexity** of Gaussian Elimination Algorithm.

Example 3. Estimate the time required to carry out back substitution on a system of 500 equations in 500 unknowns, on a computer where elimination takes 1 second.

Computational Complexity of Gaussian Elimination Algorithm

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$$\frac{2}{3}n^3 + \frac{3}{2}n^2 - \frac{7}{6}n = \mathcal{O}(n^3),$$

operations, which is defined as the **Computational Complexity** of Gaussian Elimination Algorithm.

Example 3. Estimate the time required to carry out back substitution on a system of 500 equations in 500 unknowns, on a computer where elimination takes 1 second.

Sol. First, each operation in elimination takes

$$\frac{1}{2/3 \times 500^3}.$$

Thus, back substitution takes

$$500^2/(2/3 \times 500^3) \approx 0.03\mathrm{sec}.$$

Totally, we see the Gaussian elimination takes

$$1 + 0.03 = 1.03\mathrm{sec}.$$

2.2 The LU Factorization

- An $m \times n$ matrix L is **Lower triangular matrix**: if $l_{ij} = 0$ for $i < j$.
- An $m \times n$ matrix U is **Upper triangular matrix**: if $u_{ij} = 0$ for $i > j$.

Theorem. If a linear system $Ax = b$ with $A \in \mathbb{R}^{n\times n}$ can be solved by the Gaussian elimination, then there exist a lower triangular matrix $L \in \mathbb{R}^{n\times n}$ and an upper triangular matrix $U \in \mathbb{R}^{n\times n}$ such that $A = LU$, and this decomposition is called the LU Factorization of A.

Example 1. Find the LU factorization of

$$A = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix}$$

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Example 1. Find the LU factorization of

$$A = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix} \xrightarrow{-2\times R1+R2} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ -3 & 1 & 1 \end{bmatrix}$$

$$\xrightarrow{-(-3)\times R1+R3} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 7 & -2 \end{bmatrix} \xrightarrow{-(-\frac{7}{3})\times R2+R3} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix} = U.$$

What we have done?

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & \frac{7}{3} & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} A = U.$$

Thus,

$$L = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & \frac{7}{3} & 1 \end{bmatrix}^{-1}$$

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Thus,

$$L = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{7}{3} & 1 \end{bmatrix}$$

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$$A = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix} \xrightarrow{-2\times R1+R2} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ -3 & 1 & 1 \end{bmatrix}$$

$$\xrightarrow{-(-3)\times R1+R3} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 7 & -2 \end{bmatrix} \xrightarrow{-(-\frac{7}{3})\times R2+R3} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix} = U.$$

What we have done?

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & \frac{7}{3} & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} A = U.$$

Thus,

$$L = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -3 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{7}{3} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -3 & -\frac{7}{3} & 1 \end{bmatrix}$$

Why L is computed in this way?

Prop.. Let $L_{ij}(c)$ be the lower triangular matrix whose only nonzero entries are 1's on the main diagonal and c in the (i, j) position. Then, $L_{ij}(c)A$ represents the operation "adding c times row j from row i". Clearly,

$$L_{ij}(c)L_{ij}(-c) = L_{ij}(-c)L_{ij}(c) = \quad .$$

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Prop.. Let $L_{ij}(c)$ be the lower triangular matrix whose only nonzero entries are 1's on the main diagonal and c in the (i, j) position. Then, $L_{ij}(c)A$ represents the operation "adding c times row j from row i". Clearly,

$$L_{ij}(c)L_{ij}(-c) = L_{ij}(-c)L_{ij}(c) = I.$$

Revisiting **Example 1.**The LU factorization:

$$A = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix} \xrightarrow{L_{21}(-2)} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ -3 & 1 & 1 \end{bmatrix}$$

$$\xrightarrow{L_{31}(3)} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 7 & -2 \end{bmatrix} \xrightarrow{L_{32}(7/3)} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix} = U.$$

$$L = (L_{32}(7/3)L_{31}(3)L_{21}(-2))^{-1} = L_{21}(2)L_{31}(-3)L_{32}(-7/3).$$

How to record L:Replace the resulting zero directly by the inverse of the multiplier in each elimination step.

$$A = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix} \xrightarrow{L_{21}(-2)} \begin{bmatrix} 1 & 2 & -1 \\ 2 & -3 & 0 \\ -3 & 1 & 1 \end{bmatrix}$$

$$\xrightarrow{L_{31}(-(-3))} \begin{bmatrix} 1 & 2 & -1 \\ 2 & -3 & 0 \\ -3 & 7 & -2 \end{bmatrix} \xrightarrow{L_{32}(-(-7/3))} \begin{bmatrix} 1 & 2 & -1 \\ 2 & -3 & 0 \\ -3 & -7/3 & -2 \end{bmatrix}.$$

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Forward and Backward substitutions with the LU factorization

How do we use LU factorization in solving $Ax = LUx = b$?
The substitution is a two-step procedure?

a. Forward substitution to solve $Lc = b$ for c;

b. Backward substitution to solve $Ux = c$ for x.

For example, let us solve

$$\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix} x = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -3 & -\frac{7}{3} & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix} x = \begin{bmatrix} 3 \\ 3 \\ -6 \end{bmatrix},$$

Firstly, forward solve

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -3 & -\frac{7}{3} & 1 \end{bmatrix} c = \begin{bmatrix} 3 \\ 3 \\ -6 \end{bmatrix} \to c = \begin{bmatrix} c_1 = 3 \\ c_2 = 3 - 2c_1 = -3 \\ c_3 = -6 + 3c_1 + \frac{7}{3}c_2 = -4 \end{bmatrix}$$

Secondly, backward solve

$$\begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix} x = \begin{bmatrix} 3 \\ -3 \\ -4 \end{bmatrix} \to x = \begin{bmatrix} x_1 = 3 - 2x_2 + x_3 = 3 \\ x_2 = 1 \\ x_3 = 2 \end{bmatrix}$$

Complexity of the LU factorization

Suppose now we need to solve k linear systems,

$$
\begin{aligned}
Ax &= b_1, \\
Ax &= b_2, \\
&\vdots, \\
Ax &= b_k.
\end{aligned}
$$

Computational Complexity of Gaussian Elimination:
Computational Complexity of LU factorization:

Complexity of the LU factorization

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$$
\begin{aligned}
Ax &= b_1, \\
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Computational Complexity of Gaussian Elimination: $O(\frac{2k}{3}n^3)$
Computational Complexity of LU factorization:

Complexity of the LU factorization

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Computational Complexity of Gaussian Elimination: $O(\frac{2k}{3}n^3)$
Computational Complexity of LU factorization: $\frac{2}{3}n^3 + 2kn^2$

Nonexistence of LU Factorization

Prove that

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

does not have an LU factorization.

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Nonexistence of LU Factorization

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Prove that

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

does not have an LU factorization.

Sol. Suppose otherwise, there exist L and U such that

$$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ l_{21} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} \\ 0 & u_{22} \end{bmatrix} = \begin{bmatrix} u_{11} & u_{12} \\ l_{21}u_{11} & l_{21}u_{12} + u_{22} \end{bmatrix}.$$

Then, we get

$$u_{11} = 0, \quad l_{21}u_{11} = 1,$$

which is impossible.

Some norms

Maximum or Infinity norm: $||x||_\infty = \max_{1\le i\le n} |x_i|$ for vector $x = (x_1, \ldots, x_n)$.
The **infinity norm** of an $n \times n$ matrix A is

$$||A||_\infty = \text{maximum absolute row sum},$$

The 1-norm of $x = (x_1, x_2, \ldots, x_n)$ is

$$||x||_1 = |x_1| + |x_2| + \cdots + |x_n|.$$

The 1-norm of an $n \times n$ matrix A is

$$||A||_1 = \text{maximum absolute column sum}.$$

One property of norm is

$$||Ax|| \le ||A|| \cdot ||x||.$$

Definition of Errors

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Let x_a be an approximate solution of the linear system $Ax = b$. Then,

- **Residual:** $r = b - Ax_a$;
- **Backward error:** $||r||_\infty = ||b - Ax_a||_\infty$.
- **Forward error:** $||x - x_a||_\infty$.
- **Relative Backward error:** $||r||_\infty / ||b||_\infty$.
- **Relative Forward error:** $||x - x_a||_\infty / ||x||_\infty$.

Example 1. Find the (relative) forward and (relative) backward errors for the approximation solution $[-1, 3.0001]$ of the system

$$x_1 + x_2 = 2,$$
$$1.0001x_1 + x_2 = 2.0001.$$

Sol. We can easily get the true solution $x = (1, 1)^T$: By definition, the backward error is

$$||b - Ax_a||_\infty = ||(-0.0001, 0.0001)^T||_\infty = 0.0001.$$

The forward error is

$$||x_a - x||_\infty = ||(0, 2.0001)^T||_\infty = 2.0001.$$

The relative backward error is

$$0.0001/||b||_\infty = 0.0001/2.0001 \approx 0.005\%.$$

The relative forward error is

$$2.0001/||x||_\infty = 200.01\%.$$

The error magnification factor then is $200.01\%/0.005\% = 40004.0001$.

Condition Number

The **condition number** of a square matrix A, $\mathrm{cond}(A)$, is the maximum possible error magnification factor for solving $Ax = b$, over all right-hand sides b.

Thoerem. The condition number of the $n \times n$ matrix A is

$$cond(A) = ||A|| \cdot ||A^{-1}||.$$

Proof. Let $r = Ax_a - b$ for $b = Ax$. Then,

$$\frac{||x - x_a||}{||x||} = \frac{||A^{-1}r||}{||x||} = \frac{||A^{-1}r|| \cdot ||A||}{||A|| \cdot ||x||} \leq \frac{||A^{-1}|| \cdot ||A|| \cdot ||r||}{||Ax||}$$

Thus, for any $b \in \mathbb{R}^n$

$$\frac{\frac{||x-x_a||}{||x||}}{\frac{||r||}{||b||}} \leq ||A^{-1}|| \cdot ||A||.$$

Thus,

$$cond(A) \leq ||A|| \cdot ||A^{-1}||.$$

Example 2. Evaluate the condition number of

$$A = \begin{bmatrix} 1 & 1 \\ 1.0001 & 1 \end{bmatrix}.$$

Sol. One easily gets

$$A^{-1} = \begin{bmatrix} -10000 & 10000 \\ 10001 & -10000 \end{bmatrix}.$$

Thus,

$$cond(A) = ||A||_\infty \cdot ||A^{-1}||_\infty = 2.0001 \times 20001 = 40004.0001.$$

Hilbert's Matrix

Example 3. Let H denote the $n \times n$ Hilbert matrix with $H_{ij} = 1/(i+j-1)$. Use MATLAB to show the condition number of H, and to solve the equation $Hx = H(1,\ldots,1)^T$ for $n = 6, 10$.

Sol. True solution is $x = (1,\ldots,1)$

When $n = 6$, one finds that $cond(A) \approx 2.91 \times 10^7$, and

$$x = \begin{bmatrix} 0.99999999999923 \\ 1.00000000002184 \\ 0.99999999985267 \\ 1.00000000038240 \\ 0.99999999957855 \\ 1.00000000016588 \end{bmatrix}.$$

When $n = 10$, one finds that $cond(A) \approx 3.54 \times 10^{13}$, and

$$x = \begin{bmatrix} 0.99999999875463 \\ 1.00000010746631 \\ 0.99999771299818 \\ 1.00002077769598 \\ 0.99990094548472 \\ 1.00027218303745 \\ 0.99955359665722 \\ 1.00043125589482 \\ 0.99977366058043 \\ 1.00004976229297 \end{bmatrix}.$$

Swamping: a typical example

$$
\begin{aligned}
10^{-20}x_1 + x_2 &= 1,\\
x_1 + 2x_2 &= 4.
\end{aligned}
$$

Sol1. Exact Gaussian Elimination:

$$
\begin{aligned}
10^{-20}x_1 + x_2 &= 1 & ,\\
(2-10^{20})x_2 &= 4-10^{20} \to x_2 = \frac{4-10^{20}}{2-10^{20}} \approx 1.
\end{aligned}
$$

Sol2. IEEE double precision:

$$
\begin{aligned}
10^{-20}x_1 + x_2 &= 1\\
-10^{20}x_2 &= -10^{20} \to x_2 = 1.
\end{aligned}
$$

Sol3. IEEE double precision after row exchange:

$$
\begin{aligned}
x_1 + 2x_2 &= 4,\\
10^{-20}x_1 + x_2 &= 1 \to (1 - 2\times 10^{-20})x_2 = 1 - 4\times 10^{-20} \to x_2 = 1.
\end{aligned}
$$

Swamping: a typical example

$$10^{-20}x_1 + x_2 = 1,$$
$$x_1 + 2x_2 = 4.$$

Sol1. Exact Gaussian Elimination:

$$10^{-20}x_1 + x_2 = 1 \to x_1 = \frac{-2 \times 10^{20}}{2 - 10^{20}} \approx 2,$$
$$(2 - 10^{20})x_2 = 4 - 10^{20} \to x_2 = \frac{4 - 10^{20}}{2 - 10^{20}} \approx 1.$$

Sol2. IEEE double precision:

$$10^{-20}x_1 + x_2 = 1$$
$$-10^{20}x_2 = -10^{20} \to x_2 = 1.$$

Sol3. IEEE double precision after row exchange:

$$x_1 + 2x_2 = 4,$$
$$10^{-20}x_1 + x_2 = 1 \to (1 - 2 \times 10^{-20})x_2 = 1 - 4 \times 10^{-20} \to x_2 = 1.$$

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$$10^{-20}x_1 + x_2 = 1,$$
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Sol1. Exact Gaussian Elimination:

$$10^{-20}x_1 + x_2 = 1 \to x_1 = \frac{-2\times 10^{20}}{2-10^{20}} \approx 2,$$
$$(2-10^{20})x_2 = 4 - 10^{20} \to x_2 = \frac{4-10^{20}}{2-10^{20}} \approx 1.$$

Sol2. IEEE double precision:

$$10^{-20}x_1 + x_2 = 1 \to x_1 = 0,$$
$$-10^{20}x_2 = -10^{20} \to x_2 = 1.$$

Sol3. IEEE double precision after row exchange:

$$x_1 + 2x_2 = 4, \to x_1 = 2$$
$$10^{-20}x_1 + x_2 = 1 \to (1-2\times 10^{-20})x_2 = 1 - 4\times 10^{-20} \to x_2 = 1.$$

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2.4 The $PA = LU$ Factorization

$$\left[\begin{array}{ccc|c} 1 & -1 & 3 & -3 \\ -1 & 0 & -2 & 1 \\ 2 & 2 & 4 & 0 \end{array}\right] \xrightarrow[\text{Exchange}]{\text{Pivoting.}} \left[\begin{array}{ccc|c} 2 & 2 & 4 & 0 \\ -1 & 0 & -2 & 1 \\ 1 & -1 & 3 & -3 \end{array}\right]$$

$$\xrightarrow{\text{Two Elim. Steps}} \left[\begin{array}{ccc|c} 2 & 2 & 4 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & -2 & 1 & -3 \end{array}\right] \xrightarrow[\text{Exchange}]{\text{Pivoting}} \left[\begin{array}{ccc|c} 2 & 2 & 4 & 0 \\ 0 & -2 & 1 & -3 \\ 0 & -1 & 0 & 1 \end{array}\right]$$

$$\xrightarrow{\text{One Elim. Step}} \left[\begin{array}{ccc|c} 2 & 2 & 4 & 0 \\ 0 & -2 & 1 & -3 \\ 0 & 0 & \frac{1}{2} & -\frac{1}{2} \end{array}\right] \xrightarrow{\text{Backsolver}} \left[\begin{array}{c} 1 \\ 1 \\ -1 \end{array}\right]$$

Partial pivoting

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Suppose in the i-th Elimination step, we encounter the following matrix

$$\begin{bmatrix} \ddots & \vdots & \vdots & \cdots \\ \cdots & a_{i-1,i-1} & \vdots & \cdots \\ \cdots & 0 & a_{ii} & \cdots \\ \cdots & 0 & a_{i+1,i} & \cdots \\ \cdots & \vdots & \vdots & \cdots \\ \cdots & 0 & a_{pi} & \cdots \\ \cdots & \vdots & \vdots & \cdots \\ \cdots & 0 & a_{ni} & \cdots \end{bmatrix}$$

In partial pivoting protocol:

1. determine which is the maximum number in $\{|a_{ji}|\}_{j=i}^{n}$. Suppose $|a_{pi}|$ is the maximum one.

Partial pivoting

Suppose in the i-th Elimination step, we encounter the following matrix

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In partial pivoting protocol:

1. determine which is the maximum number in $\{|a_{ji}|\}_{j=i}^n$. Suppose $|a_{pi}|$ is the maximum one.
2. exchange the p-th row and the i-th row

Partial pivoting

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Suppose in the i-th Elimination step, we encounter the following matrix

$$\begin{bmatrix} \ddots & \vdots & \vdots & \cdots \\ \cdots & a_{i-1,i-1} & \vdots & \cdots \\ \cdots & 0 & a_{pi} & \cdots \\ \cdots & 0 & a_{i+1,i} & \cdots \\ \cdots & \vdots & \vdots & \cdots \\ \cdots & 0 & a_{ii} & \cdots \\ \cdots & \vdots & \vdots & \cdots \\ \cdots & 0 & a_{ni} & \cdots \end{bmatrix}$$

In partial pivoting protocol:

1. determine which is the maximum number in $\{|a_{ji}|\}_{j=i}^{n}$. Suppose $|a_{pi}|$ is the maximum one.
2. exchange the p-th row and the i-th row
3. eliminate the rest elements in column i.

Permutation matrices

A permutation matrix is an $n \times n$ matrix consists of all zeros, except for a single 1 in every row and column.

Theorem. Fundamental Theorem of Permutation Matrices. Let P be the $n \times n$ permutation matrix formed by a particular set of row exchanges applied to the identity matrix. Then, for any $n \times n$ matrix A, PA is the matrix obtained by applying exactly the same set of row exchanges to A.

For example, the following permutation matrix

$$P_{132} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

performs an exchange of Row 2 and Row 3.

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performs an exchange of Row 2 and Row 3.

In general: suppose $\{a_1, a_2, \ldots, a_n\}$ is a rearrangement of $\{1, 2, \ldots, n\}$. Then, the following permutation matrix

$$P_{a_1 a_2 \cdots a_n},$$

is a rearrangement of rows of indentity matrix I_n, so that, the i-th row of $P_{a_1 a_2 \cdots a_n}$ is the **row of I_n.**

Permutation matrices

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$$P_{a_1 a_2 \cdots a_n},$$

is a rearrangement of rows of indentity matrix I_n, so that, the i-th row of $P_{a_1 a_2 \cdots a_n}$ is the **a_i-th row of I_n.**

How to get P and L?

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$$A = \begin{bmatrix} 1 & -1 & 3 \\ -1 & 0 & -2 \\ 2 & 2 & 4 \end{bmatrix} \xrightarrow[P_{321}]{\text{Swap}} \begin{bmatrix} 2 & 2 & 4 \\ -1 & 0 & -2 \\ 1 & -1 & 3 \end{bmatrix} \xrightarrow[L_{21}(1/2), L_{31}(-1/2)]{\text{2 Elims.}}$$

$$\begin{bmatrix} 2 & 2 & 4 \\ 0 & -1 & 0 \\ 0 & -2 & 1 \end{bmatrix} \xrightarrow[P_{132}]{\text{Swap}} \begin{bmatrix} 2 & 2 & 4 \\ 0 & -2 & 1 \\ 0 & -1 & 0 \end{bmatrix} \xrightarrow[L_{32}(-1/2)]{\text{1 Elim.}} \begin{bmatrix} 2 & 2 & 4 \\ 0 & -2 & 1 \\ 0 & 0 & \frac{1}{2} \end{bmatrix} = U.$$

How to get L and P?

$$L_{32}(-1/2) P_{132} L_{31}(-1/2) L_{21}(1/2) P_{321} A = U.$$

How to get P and L?

$$A = \begin{bmatrix} 1 & -1 & 3 \\ -1 & 0 & -2 \\ 2 & 2 & 4 \end{bmatrix} \xrightarrow[P_{321}]{\text{Swap}} \begin{bmatrix} 2 & 2 & 4 \\ -1 & 0 & -2 \\ 1 & -1 & 3 \end{bmatrix} \xrightarrow[L_{21}(1/2), L_{31}(-1/2)]{\text{2 Elims.}}$$

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How to get L and P?

$$L_{32}(-1/2) L_{21}(-1/2) P_{132} L_{21}(1/2) P_{321} A = U.$$

How to get P and L?

$$A = \begin{bmatrix} \color{red}{1} & -1 & 3 \\ \color{red}{-1} & 0 & -2 \\ \color{red}{2} & 2 & 4 \end{bmatrix} \xrightarrow[P_{321}]{\text{Swap}} \begin{bmatrix} 2 & 2 & 4 \\ -1 & 0 & -2 \\ 1 & -1 & 3 \end{bmatrix} \xrightarrow[L_{21}(1/2), L_{31}(-1/2)]{\text{2 Elims.}}$$

$$\begin{bmatrix} 2 & 2 & 4 \\ 0 & \color{red}{-1} & 0 \\ 0 & \color{red}{-2} & 1 \end{bmatrix} \xrightarrow[P_{132}]{\text{Swap}} \begin{bmatrix} 2 & 2 & 4 \\ 0 & -2 & 1 \\ 0 & -1 & 0 \end{bmatrix} \xrightarrow[L_{32}(-1/2)]{\text{1 Elim.}} \begin{bmatrix} 2 & 2 & 4 \\ 0 & -2 & 1 \\ 0 & 0 & \frac{1}{2} \end{bmatrix} = U.$$

How to get L and P?

$$L_{32}(-1/2)\color{red}{L_{21}(-1/2)L_{31}(1/2)}\color{black}{P_{132}P_{321}A = U.}$$

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How to get P and L?

$$A = \begin{bmatrix} 1 & -1 & 3 \\ -1 & 0 & -2 \\ 2 & 2 & 4 \end{bmatrix} \xrightarrow[P_{321}]{\text{Swap}} \begin{bmatrix} 2 & 2 & 4 \\ -1 & 0 & -2 \\ 1 & -1 & 3 \end{bmatrix} \xrightarrow[L_{21}(1/2), L_{31}(-1/2)]{\text{2 Elims.}}$$

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How to get L and P?

$$L_{32}(-1/2)L_{21}(-1/2)L_{31}(1/2)P_{132}P_{321}A = U.$$

Thus, we have:

$$P = P_{132}P_{321} = \qquad , \quad L = L_{31}(-1/2)L_{21}(1/2)L_{32}(1/2).$$

How to get P and L?

$$A = \begin{bmatrix} 1 & -1 & 3 \\ -1 & 0 & -2 \\ 2 & 2 & 4 \end{bmatrix} \xrightarrow[P_{321}]{\text{Swap}} \begin{bmatrix} 2 & 2 & 4 \\ -1 & 0 & -2 \\ 1 & -1 & 3 \end{bmatrix} \xrightarrow[L_{21}(1/2), L_{31}(-1/2)]{\text{2 Elims.}}$$

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How to get L and P?

$$L_{32}(-1/2) L_{21}(-1/2) L_{31}(1/2) P_{132} P_{321} A = U.$$

Thus, we have:

$$P = P_{132} P_{321} = P_{312}, \quad L = L_{31}(-1/2) L_{21}(1/2) L_{32}(1/2).$$

$$A = \begin{bmatrix} 1 & -1 & 3 \\ -1 & 0 & -2 \\ 2 & 2 & 4 \end{bmatrix} \xrightarrow[P = P_{321}]{\text{Swap}} \begin{bmatrix} 2 & 2 & 4 \\ -1 & 0 & -2 \\ 1 & -1 & 3 \end{bmatrix} \xrightarrow[L_{21}(1/2), L_{31}(-1/2)]{\text{2 Elims.}}$$

$$\begin{bmatrix} 2 & 2 & 4 \\ \frac{-1}{2} & -1 & 0 \\ \frac{1}{2} & -2 & 1 \end{bmatrix} \xrightarrow[P = P_{132} P]{\text{Swap}} \begin{bmatrix} 2 & 2 & 4 \\ ? & -2 & 1 \\ ? & -1 & 0 \end{bmatrix} \xrightarrow[L_{32}(-1/2)]{\text{1 Elim.}} \begin{bmatrix} 2 & 2 & 4 \\ ? & -2 & 1 \\ ? & ? & \frac{1}{2} \end{bmatrix}.$$

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How to get P and L?

$$A = \begin{bmatrix} 1 & -1 & 3 \\ -1 & 0 & -2 \\ 2 & 2 & 4 \end{bmatrix} \xrightarrow[P_{321}]{\text{Swap}} \begin{bmatrix} 2 & 2 & 4 \\ -1 & 0 & -2 \\ 1 & -1 & 3 \end{bmatrix} \xrightarrow[L_{21}(1/2), L_{31}(-1/2)]{\text{2 Elims.}}$$

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How to get L and P?

$$L_{32}(-1/2)L_{21}(-1/2)L_{31}(1/2)P_{132}P_{321}A = U.$$

Thus, we have:

$$P = P_{132}P_{321} = P_{312}, \quad L = L_{31}(-1/2)L_{21}(1/2)L_{32}(1/2).$$

$$A = \begin{bmatrix} 1 & -1 & 3 \\ -1 & 0 & -2 \\ 2 & 2 & 4 \end{bmatrix} \xrightarrow[P=P_{321}]{\text{Swap}} \begin{bmatrix} 2 & 2 & 4 \\ -1 & 0 & -2 \\ 1 & -1 & 3 \end{bmatrix} \xrightarrow[L_{21}(1/2), L_{31}(-1/2)]{\text{2 Elims.}}$$

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Solving $Ax = b$

Suppose we have found the PLU Factorization: $PA = LU$, then we can solve $Ax = b$ in the following way:

1. Find c such that $Lc = Pb$;
2. Find x such that $Ux = c$;
3. x solves $PAx = Pb$.

Complexity:

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Solving $Ax = b$

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Suppose we have found the PLU Factorization: $PA = LU$, then we can solve $Ax = b$ in the following way:

1. Find c such that $Lc = Pb$;
2. Find x such that $Ux = c$;
3. x solves $PAx = Pb$.

Complexity: the same as the usual LU Factorization,

$$\mathcal{O}(n^3).$$

Assignment II

Assignment II:
Page 79, 2.1, Computer Problems: 1.
P85, 2.2 Computer Problems: 1.
P94, 2.3 Computer Problems: 1.
P102, 2.4 Exercises: 2.
Due date: October 14, 2020.

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