CENG 216 - NUMERICAL COMPUTATION

Systems of Equations - Part II

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SLIDE CREDITS

Slides are based on material from the main textbook:

"Numerical Analysis", The new international edition, 2ed, by Timothy Sauer

Introduction

There are two primary sources of error when solving a system of equations using finite precision real numbers:

• Ill-conditioning: The system is not exactly singular, but it is nearly so.

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There are two primary sources of error when solving a system of equations using finite precision real numbers:

- Ill-conditioning: The system is not exactly singular, but it is nearly so. → There is not much to do, we should avoid such systems if we can.
- Swamping: The system is well-conditioned but the order of equations causes numerical problems.→ Solve by pivoting.

Sources of Error: Ill-conditioning

ERROR MAGNIFICATION AND THE CONDITION NUMBER

 For root finding, we defined forward and backward errors as the absolute value of the difference between two scalars (for example the estimated and the true values of the root). For a system of equations, we need the equivalent of absolute value for vectors.

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- Def: Infinity (maximum) norm of a vector $\mathbf{x} = [x_1, x_2, \dots, x_n]^{\mathsf{T}}$ is $\|\mathbf{x}\|_{\infty} = \max |x_i|, i = 1, \dots, n$.

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- Def: Infinity (maximum) norm of a vector $\mathbf{x} = [x_1, x_2, \dots, x_n]^{\top}$ is $\|\mathbf{x}\|_{\infty} = \max |x_i|, i = 1, \dots, n$.
- Def: Let \mathbf{x}_a be an approximate solution to $\mathbf{A}\mathbf{x} = \mathbf{b}$. Then the residual is $\mathbf{r} = \mathbf{b} \mathbf{A}\mathbf{x}_a$, the backward error is $\|\mathbf{r}\|_{\infty} = \|\mathbf{b} \mathbf{A}\mathbf{x}_a\|_{\infty}$, and the forward error is $\|\mathbf{x} \mathbf{x}_a\|_{\infty}$.

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

$$\begin{bmatrix} 1 & 1 \\ 3 & -4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$$
 with true solution $\mathbf{x} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$

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Backward Error
$$= \|\mathbf{b} - \mathbf{A}\mathbf{x}_a\|_{\infty} = \|\begin{bmatrix} 3 \\ 2 \end{bmatrix} - \begin{bmatrix} 1 & 1 \\ 3 & -4 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \|_{\infty}$$

$$= \|\begin{bmatrix} 3 \\ 2 \end{bmatrix} - \begin{bmatrix} 2 \\ -1 \end{bmatrix} \|_{\infty} = \|\begin{bmatrix} 1 \\ 3 \end{bmatrix} \|_{\infty} = 3$$

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$$= \|\begin{bmatrix} 3 \\ 2 \end{bmatrix} - \begin{bmatrix} 2 \\ -1 \end{bmatrix} \|_{\infty} = \|\begin{bmatrix} 1 \\ 3 \end{bmatrix} \|_{\infty} = 3$$
Forward Error $= \|\mathbf{x}_a - \mathbf{x}\|_{\infty} = \|\begin{bmatrix} 1 \\ 1 \end{bmatrix} - \begin{bmatrix} 2 \\ 1 \end{bmatrix} \|_{\infty} = \|\begin{bmatrix} -1 \\ 0 \end{bmatrix} \|_{\infty} = 1$

$$\begin{bmatrix} 1 & 1 \\ 1.0001 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 2.0001 \end{bmatrix}$$

Ex: Find the backward and forward errors for the approximate solution $\mathbf{x}_a = [-1, 3.0001]^{\mathsf{T}}$ of the system

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Backward Error
$$= \|\mathbf{r}\|_{\infty} = \|\begin{bmatrix} 2 \\ 2.0001 \end{bmatrix} - \begin{bmatrix} 1 & 1 \\ 1.0001 & 1 \end{bmatrix} \begin{bmatrix} -1 \\ 3.0001 \end{bmatrix} \|_{\infty}$$

 $= \|\begin{bmatrix} 2 \\ 2.0001 \end{bmatrix} - \begin{bmatrix} 2.0001 \\ 2 \end{bmatrix} \|_{\infty} = 0.0001$

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$$\begin{bmatrix} 1 & 1 \\ 1.0001 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 2.0001 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 1 \\ 0 & -0.0001 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ -0.0001 \end{bmatrix}$$

$$\rightarrow \begin{cases} x_1 = 1 \\ x_2 = 1 \end{cases}$$

Backward Error
$$= \|\mathbf{r}\|_{\infty} = \|\begin{bmatrix} 2 \\ 2.0001 \end{bmatrix} - \begin{bmatrix} 1 & 1 \\ 1.0001 & 1 \end{bmatrix} \begin{bmatrix} -1 \\ 3.0001 \end{bmatrix} \|_{\infty}$$

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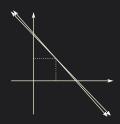
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Forward Error $= \|\mathbf{x}_a - \mathbf{x}\|_{\infty} = \|\begin{bmatrix} -1 \\ 3.0001 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \end{bmatrix} \|_{\infty} = 2.0001$

$$\begin{bmatrix} 1 & 1 \\ 1.0001 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 2.0001 \end{bmatrix}$$
 with true solution $\mathbf{x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

Backward Error
$$= \|\mathbf{r}\|_{\infty} = 0.0001$$

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Values for our example:

Relative Backward Error
$$=$$
 $\frac{0.0001}{2.0001} \approx 0.00005 = 0.005\%$

- · Def: Relative Backward Error= $\frac{\|\mathbf{r}\|_{\infty}}{\|\mathbf{b}\|_{\infty}}$.
- · Def: Relative Forward Error = $\frac{\|\mathbf{x} \mathbf{x}_a\|_{\infty}}{\|\mathbf{x}\|_{\infty}}$
- Def: Error Magnification Factor = $\frac{\| \mathbf{x} \|_{\infty}}{\| \mathbf{x} \|_{\infty}}$.

Values for our example:

Relative Backward Error
$$=$$
 $\frac{0.0001}{2.0001} \approx 0.00005 = 0.005\%$
Relative Forward Error $=$ $\frac{2.0001}{1} = 2.0001 \approx 200\%$

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- · Def: Relative Forward Error= $\frac{\|\mathbf{x} \mathbf{x}_a\|_{\infty}}{\|\mathbf{x}\|_{\infty}}$.
- Def: Error Magnification Factor = $\frac{\frac{\| \mathbf{x} \mathbf{x}_0 \|_{\infty}}{\| \mathbf{x} \|_{\infty}}}{\| \mathbf{x} \|_{\infty}}.$

Values for our example:

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$$=$$
 $\frac{0.0001}{2.0001} \approx 0.00005 = 0.005\%$
Relative Forward Error $=$ $\frac{2.0001}{1} = 2.0001 \approx 200\%$
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- Def: Error Magnification Factor= $\frac{\frac{\|\mathbf{x}\|_{\infty}}{\|\mathbf{x}\|_{\infty}}}{\frac{\|\mathbf{x}\|_{\infty}}{\|\mathbf{b}\|_{\infty}}}$

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Large error magnification factor → ill-conditioned system

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

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$$\mathbf{A} = \begin{bmatrix} 1 & 1 \\ 1.0001 & 1 \end{bmatrix} \rightarrow \|\mathbf{A}\|_{\infty} = 2.0001$$

- Def: The condition number of a square matrix A, cond (A), is the maximum possible error magnification factor for solving Ax = b for all right hand sides b.
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$$\|\mathtt{A}\|_{\infty} = \text{maximum absolute row sum}$$

• Thm: cond (A) = $\|A\|_{\infty} \|A^{-1}\|_{\infty}$ $A = \begin{bmatrix} 1 & 1 \\ 1.0001 & 1 \end{bmatrix} \rightarrow \|A\|_{\infty} = 2.0001$ $A^{-1} = \begin{bmatrix} -10000 & 10000 \\ 10001 & -10000 \end{bmatrix} \rightarrow \|A^{-1}\|_{\infty} = 20001$

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• Thm: cond (A) =
$$\|A\|_{\infty} \|A^{-1}\|_{\infty}$$

$$A = \begin{bmatrix} 1 & 1 \\ 1.0001 & 1 \end{bmatrix} \rightarrow \|A\|_{\infty} = 2.0001$$

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$$cond (A) = (2.0001)(20001) = 40004.1$$

Sources of Error: Swamping

SWAMPING EXAMPLE

Consider the system

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

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Exact Arithmetic:

$$\begin{bmatrix} 10^{-20} & 1 & 1 \\ 1 & 2 & 4 \end{bmatrix} \xrightarrow{\text{subtract } 10^{20} \times \text{ row } 1} \begin{bmatrix} 10^{-20} & 1 & 1 \\ 0 & 2 - 10^{20} & 4 - 10^{20} \end{bmatrix}$$

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$$x_2 = \frac{4 - 10^{20}}{2 - 10^{20}}$$
, and $x_1 = 10^{20} \left(1 - \frac{4 - 10^{20}}{2 - 10^{20}} \right) = \frac{-2 \times 10^{20}}{2 - 10^{20}} \approx 2$

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$$[x_1, x_2]^{\top} \approx [2, 1]^{\top}$$

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$$10^{-20}x_1 + x_2 = 1$$
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$$10^{-20}x_1 + x_2 = 1$$
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Exact Arithmetic: $[x_1, x_2]^{\top} \approx [2, 1]^{\top}$ IEEE double-precision:

$$\begin{bmatrix} 10^{-20} & 1 & 1 \\ 1 & 2 & 4 \end{bmatrix} \rightarrow \begin{bmatrix} 10^{-20} & 1 & 1 \\ 0 & \underbrace{2 - 10^{20}}_{\text{rounds to } -10^{20}} & \underbrace{4 - 10^{20}}_{\text{rounds to } -10^{20}} \end{bmatrix} \rightarrow \begin{cases} x_2 = 1 \\ x_1 = 0 \end{cases}$$

Consider the system

$$10^{-20}x_1 + x_2 = 1$$
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Exact Arithmetic: $[x_1, x_2]^{\top} \approx [2, 1]^{\top}$ IEEE double-precision: $[x_1, x_2]^{\top} \approx [0, 1]^{\top}$ IEEE double-precision with Row Exchange:

$$\begin{bmatrix} 1 & 2 & | & 4 \\ 10^{-20} & 1 & | & 1 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 \\ 1 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 4 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 & | & 2 & | & 2 & | & 2 \\ 0 & 1 & | & 1 &$$

Consider the system

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

Exact Arithmetic: $[x_1, x_2]^{\top} \approx [2, 1]^{\top}$ IEEE double-precision: $[x_1, x_2]^{\top} \approx [0, 1]^{\top}$

IEEE double-precision with Row Exchange: $[x_1, x_2]^{\top} \approx [2, 1]^{\top} \checkmark$

PARTIAL PIVOTING

Look for the biggest pivot in the column even when the pivot is not zero:

$$|a_{pj}| \geq |a_{ij}|$$
 , for $j \leq i \leq n \rightarrow \mbox{ exchange row } p$ and row i

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Partial pivoting solves both the problem with zero pivots and also the swamping problem.

$$\left[\begin{array}{ccc|ccc}
1 & -1 & 3 & -3 \\
-1 & 0 & -2 & 1 \\
2 & 2 & 4 & 0
\end{array}\right]$$

$$\begin{bmatrix} 1 & -1 & 3 & | & -3 \\ -1 & 0 & -2 & | & 1 \\ 2 & 2 & 4 & | & 0 \end{bmatrix} \xrightarrow{\text{Exchange rows 1 and 3}} \begin{bmatrix} 2 & 2 & 4 & | & 0 \\ -1 & 0 & -2 & | & 1 \\ 1 & -1 & 3 & | & -3 \end{bmatrix}$$

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$$\xrightarrow{\text{Subtract } -\frac{1}{2} \times \text{ row 1}} \begin{bmatrix} 2 & 2 & 4 & | & 0 \\ 0 & 1 & 0 & | & 1 \\ 1 & -1 & 3 & | & -3 \end{bmatrix}$$

$$\begin{bmatrix}
1 & -1 & 3 & | & -3 \\
-1 & 0 & -2 & | & 1 \\
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\end{bmatrix}
\xrightarrow{\text{Exchange rows 1 and 3}}
\begin{bmatrix}
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$$\underline{\text{Subtract } -\frac{1}{2} \times \text{row 1}}_{\text{from row 2}}
\begin{bmatrix}
2 & 2 & 4 & | & 0 \\
0 & 1 & 0 & | & 1 \\
1 & -1 & 3 & | & -3
\end{bmatrix}}_{\text{Subtract } \frac{1}{2} \times \text{row 1}}
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\end{bmatrix}$$

$$\xrightarrow{\text{Subtract } \frac{1}{2} \times \text{ row 1}}
\xrightarrow{\text{from row 3}}
\begin{bmatrix}
2 & 2 & 4 & | & 0 \\
0 & 1 & 0 & 1 \\
0 & -2 & 1 & | & -3
\end{bmatrix}
\xrightarrow{\text{Exchange rows 2 and 3}}
\begin{bmatrix}
2 & 2 & 4 & | & 0 \\
0 & -2 & 1 & | & -3 \\
0 & 1 & 0 & | & 1
\end{bmatrix}$$

$$\begin{bmatrix}
1 & -1 & 3 & | & -3 \\
-1 & 0 & -2 & | & 1 \\
2 & 2 & 4 & | & 0
\end{bmatrix}
\xrightarrow{\text{Exchange}}
\xrightarrow{\text{rows 1 and 3}}
\begin{bmatrix}
2 & 2 & 4 & | & 0 \\
-1 & 0 & -2 & | & 1 \\
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\end{bmatrix}$$

$$\xrightarrow{\text{Subtract } -\frac{1}{2} \times \text{ row 1}}
\xrightarrow{\text{from row 2}}
\begin{bmatrix}
2 & 2 & 4 & | & 0 \\
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\xrightarrow{\text{Exchange}}
\xrightarrow{\text{rows 2 and 3}}
\begin{bmatrix}
2 & 2 & 4 & | & 0 \\
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0 & -2 & 1 & | & -3 \\
0 & 0 & 2 & 1 & | & -3 \\
0 & 0 & \frac{1}{2} & | & -\frac{1}{2}
\end{bmatrix}$$

$$\xrightarrow{\text{Subtract } -\frac{1}{2} \times \text{ row 2}}
\xrightarrow{\text{from row 3}}
\begin{bmatrix}
2 & 2 & 4 & | & 0 \\
0 & 1 & 0 & | & 1 \\
0 & -2 & 1 & | & -3 \\
0 & 0 & \frac{1}{2} & | & -\frac{1}{2}
\end{bmatrix}$$

$$\begin{bmatrix}
1 & -1 & 3 & | & -3 \\
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\end{bmatrix}
\xrightarrow{\text{Exchange}}
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\begin{bmatrix}
2 & 2 & 4 & | & 0 \\
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\end{bmatrix}$$

$$\underbrace{\text{Subtract}}_{\text{from row 2}} \leftarrow \begin{bmatrix}
2 & 2 & 4 & | & 0 \\
0 & 1 & 0 & | & 1 \\
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\end{bmatrix}
\xrightarrow{\text{Exchange}}
\xrightarrow{\text{rows 2 and 3}}
\begin{bmatrix}
2 & 2 & 4 & | & 0 \\
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\end{bmatrix}
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\begin{bmatrix}
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0 & 1 & 0 & | & 1
\end{bmatrix}
\xrightarrow{\text{Subtract}}_{-\frac{1}{2} \times \text{ row 2}} \leftarrow \begin{bmatrix}
2 & 2 & 4 & | & 0 \\
0 & -2 & 1 & | & -3 \\
0 & 0 & \frac{1}{2} & | & -\frac{1}{2}
\end{bmatrix}
\xrightarrow{\text{Rom row 3}}
\xrightarrow{\text{Rom row 3}}
\begin{bmatrix}
2 & 2 & 4 & | & 0 \\
0 & -2 & 1 & | & -3 \\
0 & 0 & \frac{1}{2} & | & -\frac{1}{2}
\end{bmatrix}
\xrightarrow{\text{Rom row 3}}_{-\frac{1}{2}}
\xrightarrow{\text{Rom row 3}}
\xrightarrow{\text{Rom row 3}}
\begin{bmatrix}
3 & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3 & | & 3$$

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· All possible 3 × 3 permutation matrices:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

Thm: If P is an $n \times n$ permutation matrix that corresponds to a particular row exchange applied to the identity matrix, then PA is the matrix which is the result of applying the same row exchanges to A.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} = \begin{bmatrix} a & b & c \\ g & h & i \\ d & e & f \end{bmatrix}.$$

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- Since the position of the row multipliers that we put in L will be affected by row exchanges, we keep them in the position of the zeros of the A matrix that appear due to elimination. We circle them to remember that these are zeros of the A matrix.
- Every time we exchange rows, these multipliers will also change their position. See the example in the next slide to see how this works in practice.

Find the PA=LU factorization of
$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix}$$
. Set $\mathbf{P} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$.

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$$\begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix} \xrightarrow{\text{exchange } r_1 \text{ and } r_2} \begin{bmatrix} 4 & 4 & -4 \\ 2 & 1 & 5 \\ 1 & 3 & 1 \end{bmatrix}$$

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subtract
$$\begin{bmatrix} 4 & 4 & -4 \\ 4 & 4 & 4 \end{bmatrix}$$

$$\xrightarrow{\text{subtract}} \frac{1}{\frac{1}{4} \times r_1 \text{ from } r_3} \begin{cases} 4 & 4 & -4 \\ \frac{1}{2} & -1 & 7 \\ \frac{1}{4} & 2 & 2 \end{cases}$$

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$$\xrightarrow{\text{subtract}} \begin{bmatrix} 4 & 4 & -4 \\ \hline \vdots & -1 & 7 \\ \hline \frac{1}{4} \times r_1 \text{ from } r_3 \end{bmatrix} \xrightarrow{\text{exchange } r_2 \text{ and } r_3} \begin{bmatrix} 4 & 4 & -4 \\ \hline \vdots & 2 & 2 \end{bmatrix} \xrightarrow{\text{exchange } r_2 \text{ and } r_3} \begin{bmatrix} 4 & 4 & -4 \\ \hline \vdots & 2 & 2 \\ \hline \vdots & -1 & 7 \end{bmatrix}$$

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$$\xrightarrow[-\frac{1}{2} \times r_2 \text{ from } r_3]{\text{subtract}} \begin{bmatrix} 4 & 4 & -4 \\ \frac{1}{4} & 2 & 2 \\ \frac{1}{2} & -\frac{1}{2} & 8 \end{bmatrix}$$

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$$\xrightarrow{\text{subtract}} \xrightarrow{-\frac{1}{2} \times r_2 \text{ from } r_3} \begin{bmatrix} 4 & 4 & -4 \\ \frac{1}{4} & 2 & 2 \\ \frac{1}{2} & (-\frac{1}{2}) & 8 \end{bmatrix}$$

$$\begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix} \to \cdots$$

$$\xrightarrow{\text{exchange } r_2 \text{ and } r_3}$$

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

$$\begin{bmatrix} 4 & 4 & -4 \\ \frac{1}{4} & 2 & 2 \\ 1 & 7 & 1 \end{bmatrix}$$

$$\left(-\frac{1}{2}\right)$$
 8

$$\begin{bmatrix}
2 & 1 & 5 \\
4 & 4 & -4 \\
1 & 3 & 1
\end{bmatrix}$$

$$\begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix} \rightarrow \cdots$$

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

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\xrightarrow{\mathbf{P} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}}
\xrightarrow{\begin{bmatrix} 1 \\ 4 \end{bmatrix}}$$

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\underbrace{
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$$\xrightarrow{\text{exchange } r_2 \text{ and } r_3} \\
P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \xrightarrow{\begin{bmatrix} 4 & 4 & -4 \\ \frac{1}{4} & 2 & 2 \\ \frac{7}{2} & -1 & 7 \end{bmatrix}} \xrightarrow{\text{subtract}} \begin{bmatrix} 4 & 4 & -4 \\ \frac{1}{4} & 2 & 2 \\ \frac{7}{2} & -\frac{1}{2} \times r_2 \text{ from } r_3 \end{bmatrix}$$

$$\underbrace{\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}}_{\mathbf{P}} \underbrace{\begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix}}_{\mathbf{A}} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{4} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 1 \end{bmatrix}}_{\mathbf{I}} \underbrace{\begin{bmatrix} 4 & 4 & -4 \\ 0 & 2 & 2 \\ 0 & 0 & 8 \end{bmatrix}}_{\mathbf{I}}$$

SOLVING EQUATION SYSTEMS WITH PA=LU

To solve Ax = b, multiply both sides with P and use PA = LU:

$$\mathbf{A}\mathbf{x} = \mathbf{b} \longrightarrow \mathtt{P}\mathbf{A}\mathbf{x} = \mathtt{P}\mathbf{b}$$

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• First, solve L $\mathbf{c} = \mathtt{P}\mathbf{b}$ for \mathbf{c} .

SOLVING EQUATION SYSTEMS WITH PA=LU

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$$\longrightarrow LU\mathbf{x} = P\mathbf{b}$$

- First, solve Lc = Pb for c.
- Second, solve $\mathtt{U}\mathbf{x} = \mathbf{c}$ for \mathbf{x} .

So far, we have discussed only systems of linear equations in the form $a_1x_1 + a_2x_2 + \ldots + a_nx_n = b$. What if the equations are non-linear possibly involving powers of x_i ?

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- We can not have a closed form solution in general, so we will need iterative methods.
- We can extend iterative root-finding approaches to the simultaneous solution of multiple equations.

To derive the update rule for Newton's Method,

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} = x_k + \Delta_k$$

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we linearized the function f(x) around a guess for the root x_k :

$$f(\underbrace{x_k + \Delta_k}_{x_{k+1}}) \approx f(x_k) + \Delta_k f'(x_k) = 0.$$

We need to do a similar approximation to find a common root of the nonlinear system of equations,

$$f_1(x_1, x_2, \dots, x_N) = 0$$

 $f_2(x_1, x_2, \dots, x_N) = 0$
 \vdots
 $f_M(x_1, x_2, \dots, x_N) = 0$

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which we can write in vector form as

$$\mathbf{f}(\mathbf{x}) = \mathbf{0}_M$$

where $\mathbf{x} \in \mathbb{R}^N$, $\mathbf{f} : \mathbb{R}^N \to \mathbb{R}^M$ and $\mathbf{0}_M$ is a column vector of M zeros.

THE JACOBIAN

The analogue of the derivative for a vector function such as $\mathbf{f}(\mathbf{x})$ is the Jacobian matrix

$$\mathbf{J_f} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_2}{\partial x_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_M}{\partial x_1} & \frac{\partial f_M}{\partial x_2} & \dots & \frac{\partial f_M}{\partial x_N} \end{bmatrix},$$

which is an $M \times N$ matrix storing partial derivative of each component function w.r.t. each variable dimension.

The Jacobian for the system

$$x_2 - x_1^3 = 0$$
$$x_1^2 + x_2^2 - 1 = 0$$

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THE MULTIVARIATE NEWTON'S METHOD: THE STEP SIZE

Now, we can expand the nonlinear system around a given point \mathbf{x}_k

$$\mathbf{f}(\underbrace{\mathbf{x}_k + \mathbf{\Delta}_k}_{\mathbf{x}_{k+1}}) \approx \mathbf{f}(\mathbf{x}_k) + \mathbf{J}_{\mathbf{f}}\mathbf{\Delta}_k = \mathbf{0}_M$$

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$$J_{\mathbf{f}} \mathbf{\Delta}_k = -\mathbf{f}(\mathbf{x}_k)$$

and iterate with

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{\Delta}_k.$$

Make to steps of the Newton's Method to solve the system

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$$\mathbf{J}_{\mathbf{f}}(\mathbf{x}_0)\mathbf{\Delta}_0 = -\mathbf{f}(\mathbf{x}_0) \to \begin{bmatrix} -3 & 1 \\ 2 & 4 \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \end{bmatrix}$$

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$$\to \begin{bmatrix} \delta_1\\ \delta_2 \end{bmatrix} = \begin{bmatrix} 0\\ -1 \end{bmatrix}$$

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$$x_2 - x_1^3 = 0$$
$$x_1^2 + x_2^2 - 1 = 0$$

$$\mathbf{J}_{\mathbf{f}}(\mathbf{x}_{0})\boldsymbol{\Delta}_{0} = -\mathbf{f}(\mathbf{x}_{0}) \rightarrow \begin{bmatrix} -3 & 1\\ 2 & 4 \end{bmatrix} \begin{bmatrix} \delta_{1}\\ \delta_{2} \end{bmatrix} = -\begin{bmatrix} 1\\ 4 \end{bmatrix}$$
$$\rightarrow \begin{bmatrix} \delta_{1}\\ \delta_{2} \end{bmatrix} = \begin{bmatrix} 0\\ -1 \end{bmatrix}$$
$$\rightarrow \mathbf{x}_{1} = \begin{bmatrix} 1\\ 1 \end{bmatrix}$$

$$x_2 - x_1^3 = 0$$
$$x_1^2 + x_2^2 - 1 = 0$$

$$\mathbf{x}_1 = [1,1]^\top.$$

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$$J_{\mathbf{f}}(\mathbf{x}_1)\mathbf{\Delta}_1 = -\mathbf{f}(\mathbf{x}_1) \rightarrow$$

$$x_2 - x_1^3 = 0$$
$$x_1^2 + x_2^2 - 1 = 0$$

$$\mathbf{x}_1 = [1, 1]^\top.$$

$$\mathbf{J}_{\mathbf{f}}(\mathbf{x}_1)\mathbf{\Delta}_1 = -\mathbf{f}(\mathbf{x}_1) \rightarrow \begin{bmatrix} -3 & 1 \\ 2 & 2 \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \end{bmatrix}$$

$$x_2 - x_1^3 = 0$$
$$x_1^2 + x_2^2 - 1 = 0$$

$$\mathbf{x}_1 = [1, 1]^{\top}.$$

$$\mathbf{J}_{\mathbf{f}}(\mathbf{x}_1)\mathbf{\Delta}_1 = -\mathbf{f}(\mathbf{x}_1) \to \begin{bmatrix} -3 & 1 \\ 2 & 2 \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \end{bmatrix} = -\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

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$$\mathbf{J}_{\mathbf{f}}(\mathbf{x}_{1})\boldsymbol{\Delta}_{1} = -\mathbf{f}(\mathbf{x}_{1}) \rightarrow \begin{bmatrix} -3 & 1\\ 2 & 2 \end{bmatrix} \begin{bmatrix} \delta_{1}\\ \delta_{2} \end{bmatrix} = -\begin{bmatrix} 0\\ 1 \end{bmatrix}$$
$$\rightarrow \begin{bmatrix} \delta_{1}\\ \delta_{2} \end{bmatrix} = \begin{bmatrix} -\frac{1}{8}\\ -\frac{3}{8} \end{bmatrix}$$

$$x_2 - x_1^3 = 0$$
$$x_1^2 + x_2^2 - 1 = 0$$

$$\mathbf{x}_1 = [1, 1]^{\top}.$$

$$\mathbf{J_f}(\mathbf{x}_1)\mathbf{\Delta}_1 = -\mathbf{f}(\mathbf{x}_1) \to \begin{bmatrix} -3 & 1\\ 2 & 2 \end{bmatrix} \begin{bmatrix} \delta_1\\ \delta_2 \end{bmatrix} = -\begin{bmatrix} 0\\ 1 \end{bmatrix}$$
$$\to \begin{bmatrix} \delta_1\\ \delta_2 \end{bmatrix} = \begin{bmatrix} -\frac{1}{8}\\ -\frac{3}{8} \end{bmatrix}$$
$$\to \mathbf{x}_2 = \begin{bmatrix} \frac{7}{8}\\ \frac{5}{8} \end{bmatrix}$$