

# Gaussian Elimination

# Naïve Gaussian Elimination

A method to solve simultaneous linear equations of the form  $[A][X]=[C]$

Two steps

1. Forward Elimination
2. Back Substitution

# Forward Elimination

The goal of forward elimination is to transform the coefficient matrix into an upper triangular matrix

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$



$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.21 \\ 0.735 \end{bmatrix}$$

# Forward Elimination

A set of  $n$  equations and  $n$  unknowns

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \dots + a_{2n}x_n = b_2$$

$$\begin{array}{c} \cdot \\ \cdot \\ \cdot \end{array} \quad \begin{array}{c} \cdot \\ \cdot \\ \cdot \end{array}$$

$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \dots + a_{nn}x_n = b_n$$

( $n-1$ ) steps of forward elimination

# Forward Elimination

## Step 1

For Equation 2, divide Equation 1 by  $a_{11}$  and multiply by  $a_{21}$ .

$$\left[ \begin{array}{c} a_{21} \\ a_{11} \end{array} \right] (a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n = b_1)$$

$$a_{21}x_1 + \frac{a_{21}}{a_{11}}a_{12}x_2 + \dots + \frac{a_{21}}{a_{11}}a_{1n}x_n = \frac{a_{21}}{a_{11}}b_1$$

# Forward Elimination

Subtract the result from Equation 2.

$$\begin{array}{r} a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \dots + a_{2n}x_n = b_2 \\ - \quad a_{21}x_1 + \frac{a_{21}}{a_{11}}a_{12}x_2 + \dots + \frac{a_{21}}{a_{11}}a_{1n}x_n = \frac{a_{21}}{a_{11}}b_1 \\ \hline \left( a_{22} - \frac{a_{21}}{a_{11}}a_{12} \right) x_2 + \dots + \left( a_{2n} - \frac{a_{21}}{a_{11}}a_{1n} \right) x_n = b_2 - \frac{a_{21}}{a_{11}}b_1 \end{array}$$

$$\text{or} \quad a'_{22}x_2 + \dots + a'_{2n}x_n = b'_2$$

# Forward Elimination

Repeat this procedure for the remaining equations to reduce the set of equations as

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n = b_1$$

$$a'_{22}x_2 + a'_{23}x_3 + \dots + a'_{2n}x_n = b'_2$$

$$a'_{32}x_2 + a'_{33}x_3 + \dots + a'_{3n}x_n = b'_3$$

$$\vdots \quad \quad \quad \vdots \quad \quad \quad \vdots$$

$$a'_{n2}x_2 + a'_{n3}x_3 + \dots + a'_{nn}x_n = b'_n$$

**End of Step 1**

# Forward Elimination

## Step 2

Repeat the same procedure for the 3<sup>rd</sup> term of Equation 3.

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n = b_1$$

$$a'_{22}x_2 + a'_{23}x_3 + \dots + a'_{2n}x_n = b'_2$$

$$a''_{33}x_3 + \dots + a''_{3n}x_n = b''_3$$

$$\vdots \quad \vdots$$

$$a''_{n3}x_3 + \dots + a''_{nn}x_n = b''_n$$

**End of Step 2**



# Forward Elimination

At the end of (n-1) Forward Elimination steps, the system of equations will look like

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n = b_1$$

$$a'_{22}x_2 + a'_{23}x_3 + \dots + a'_{2n}x_n = b'_2$$

$$a''_{33}x_3 + \dots + a''_{3n}x_n = b''_3$$

$$\vdots$$

$$a^{(n-1)}_{nn}x_n = b^{(n-1)}_n$$

**End of Step (n-1)**

# Matrix Form at End of Forward Elimination

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a'_{22} & a'_{23} & \cdots & a'_{2n} \\ 0 & 0 & a''_{33} & \cdots & a''_{3n} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & 0 & a^{(n-1)}_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b'_2 \\ b''_3 \\ \vdots \\ b^{(n-1)}_n \end{bmatrix}$$

# Back Substitution

Solve each equation starting from the last equation

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.21 \\ 0.735 \end{bmatrix}$$

Example of a system of 3 equations

# Back Substitution Starting Eqns

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n = b_1$$

$$a'_{22}x_2 + a'_{23}x_3 + \dots + a'_{2n}x_n = b'_2$$

$$a''_{33}x_3 + \dots + a''_n x_n = b''_3$$

$$\vdots \quad \vdots$$

$$a^{(n-1)}_{nn}x_n = b^{(n-1)}_n$$

# Back Substitution

Start with the last equation because it has only one unknown

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

# Back Substitution

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

$$x_i = \frac{b_i^{(i-1)} - a_{i,i+1}^{(i-1)}x_{i+1} - a_{i,i+2}^{(i-1)}x_{i+2} - \dots - a_{i,n}^{(i-1)}x_n}{a_{ii}^{(i-1)}} \text{ for } i = n-1, \dots, 1$$

$$x_i = \frac{b_i^{(i-1)} - \sum_{j=i+1}^n a_{ij}^{(i-1)}x_j}{a_{ii}^{(i-1)}} \text{ for } i = n-1, \dots, 1$$

**THE END**

**Computational Physics**

# Additional Resources

For all resources on this topic such as digital audiovisual lectures, primers, textbook chapters, multiple-choice tests, worksheets in MATLAB, MATHEMATICA, MathCad and MAPLE, blogs, related physical problems, please visit

[Computational Physics /topics/gaussian\\_elimination.html](#)



# Naïve Gauss Elimination Example

Computational Physics

# Example 1

The upward velocity of a rocket is given at three different times

**Table 1** Velocity vs. time data.

<b>Time, <math>t</math> (s)</b>	<b>Velocity, <math>v</math> (m/s)</b>
5	106.8
8	177.2
12	279.2



The velocity data is approximated by a polynomial as:

$$v(t) = a_1 t^2 + a_2 t + a_3, \quad 5 \leq t \leq 12.$$

Find the velocity at  $t=6$  seconds .

# Example 1 Cont.

Assume

$$v(t) = a_1 t^2 + a_2 t + a_3, \quad 5 \leq t \leq 12.$$

Results in a matrix template of the form:

$$\begin{bmatrix} t_1^2 & t_1 & 1 \\ t_2^2 & t_2 & 1 \\ t_3^2 & t_3 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$$

Using data from Table 1, the matrix becomes:

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

# Example 1 Cont.

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix} \Rightarrow \begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix}$$

1. Forward Elimination
2. Back Substitution

# Forward Elimination

# Number of Steps of Forward Elimination

Number of steps of forward elimination is  
 $(n-1)=(3-1)=2$

# Forward Elimination: Step 1

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix}$$

Divide Equation 1 by 25 and multiply it by 64,  $\frac{64}{25} = 2.56$ .

$$[25 \quad 5 \quad 1 \quad \vdots \quad 106.8] \times 2.56 = [64 \quad 12.8 \quad 2.56 \quad \vdots \quad 273.408]$$

Subtract the result from Equation 2

$$\begin{array}{r} \begin{bmatrix} 64 & 8 & 1 & \vdots & 177.2 \\ -[64 & 12.8 & 2.56 & \vdots & 273.408] \end{bmatrix} \\ \hline \begin{bmatrix} 0 & -4.8 & -1.56 & \vdots & -96.208 \end{bmatrix} \end{array}$$

Substitute new equation for Equation 2

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix}$$

# Forward Elimination: Step 1 (cont.)

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix} \quad \begin{array}{l} \text{Divide Equation 1 by 25 and} \\ \text{multiply it by 144, } \frac{144}{25} = 5.76. \end{array}$$

$$[25 \quad 5 \quad 1 \quad \vdots \quad 106.8] \times 5.76 = [144 \quad 28.8 \quad 5.76 \quad \vdots \quad 615.168]$$

$$\begin{array}{l} \text{Subtract the result from} \\ \text{Equation 3} \end{array} \quad \begin{array}{r} [144 \quad 12 \quad 1 \quad \vdots \quad 279.2] \\ - [144 \quad 28.8 \quad 5.76 \quad \vdots \quad 615.168] \\ \hline [0 \quad -16.8 \quad -4.76 \quad \vdots \quad -335.968] \end{array}$$

$$\begin{array}{l} \text{Substitute new equation for} \\ \text{Equation 3} \end{array} \quad \begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 0 & -16.8 & -4.76 & \vdots & -335.968 \end{bmatrix}$$



# Forward Elimination: Step 2

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 0 & -16.8 & -4.76 & \vdots & -335.968 \end{bmatrix}$$

Divide Equation 2 by  $-4.8$   
and multiply it by  $-16.8$ ,  
 $\frac{-16.8}{-4.8} = 3.5$ .

$$[0 \quad -4.8 \quad -1.56 \quad \vdots \quad -96.208] \times 3.5 = [0 \quad -16.8 \quad -5.46 \quad \vdots \quad -336.728]$$

Subtract the result from  
Equation 3

$$\begin{array}{r} [0 \quad -16.8 \quad -4.76 \quad \vdots \quad 335.968] \\ - [0 \quad -16.8 \quad -5.46 \quad \vdots \quad -336.728] \\ \hline [0 \quad 0 \quad 0.7 \quad \vdots \quad 0.76] \end{array}$$

Substitute new equation for  
Equation 3

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 0 & 0 & 0.7 & \vdots & 0.76 \end{bmatrix}$$

# Back Substitution

# Back Substitution

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.2 \\ 0 & 0 & 0.7 & \vdots & 0.7 \end{bmatrix} \Rightarrow \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.208 \\ 0.76 \end{bmatrix}$$

Solving for  $a_3$

$$0.7a_3 = 0.76$$

$$a_3 = \frac{0.76}{0.7}$$

$$a_3 = 1.08571$$

# Back Substitution (cont.)

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.208 \\ 0.76 \end{bmatrix}$$

Solving for  $a_2$

$$-4.8a_2 - 1.56a_3 = -96.208$$

$$a_2 = \frac{-96.208 + 1.56a_3}{-4.8}$$

$$a_2 = \frac{-96.208 + 1.56 \times 1.08571}{-4.8}$$

$$a_2 = 19.6905$$

# Back Substitution (cont.)

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.2 \\ 0.76 \end{bmatrix}$$

Solving for  $a_1$

$$25a_1 + 5a_2 + a_3 = 106.8$$

$$a_1 = \frac{106.8 - 5a_2 - a_3}{25}$$

$$= \frac{106.8 - 5 \times 19.6905 - 1.08571}{25}$$

$$= 0.290472$$

# Naïve Gaussian Elimination Solution

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0.290472 \\ 19.6905 \\ 1.08571 \end{bmatrix}$$

# Example 1 Cont.

Solution

The solution vector is

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0.290472 \\ 19.6905 \\ 1.08571 \end{bmatrix}$$

The polynomial that passes through the three data points is then:

$$\begin{aligned} v(t) &= a_1 t^2 + a_2 t + a_3 \\ &= 0.290472 t^2 + 19.6905 t + 1.08571, \quad 5 \leq t \leq 12 \end{aligned}$$

$$\begin{aligned} v(6) &= 0.290472(6)^2 + 19.6905(6) + 1.08571 \\ &= 129.686 \text{ m/s.} \end{aligned}$$

**THE END**

**Computational Physics**



# Naïve Gauss Elimination Pitfalls

Computational Physics

# Pitfall#1. Division by zero

$$10x_2 - 7x_3 = 3$$

$$6x_1 + 2x_2 + 3x_3 = 11$$

$$5x_1 - x_2 + 5x_3 = 9$$

$$\begin{bmatrix} 0 & 10 & -7 \\ 6 & 2 & 3 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 11 \\ 9 \end{bmatrix}$$

Is division by zero an issue here?

$$12x_1 + 10x_2 - 7x_3 = 15$$

$$6x_1 + 5x_2 + 3x_3 = 14$$

$$5x_1 - x_2 + 5x_3 = 9$$

$$\begin{bmatrix} 12 & 10 & -7 \\ 6 & 5 & 3 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 15 \\ 14 \\ 9 \end{bmatrix}$$

# Is division by zero an issue here?

## YES

$$12x_1 + 10x_2 - 7x_3 = 15$$

$$6x_1 + 5x_2 + 3x_3 = 14$$

$$24x_1 - x_2 + 5x_3 = 28$$

$$\begin{bmatrix} 12 & 10 & -7 \\ 6 & 5 & 3 \\ 24 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 15 \\ 14 \\ 28 \end{bmatrix} \longrightarrow \begin{bmatrix} 12 & 10 & -7 \\ 0 & 0 & 6.5 \\ 12 & -21 & 19 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 15 \\ 6.5 \\ -2 \end{bmatrix}$$

Division by zero is a possibility at any step  
of forward elimination

# Pitfall#2. Large Round-off Errors

$$\begin{bmatrix} 20 & 15 & 10 \\ -3 & -2.249 & 7 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 1.751 \\ 9 \end{bmatrix}$$

Exact Solution

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

# Pitfall#2. Large Round-off Errors

$$\begin{bmatrix} 20 & 15 & 10 \\ -3 & -2.249 & 7 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 1.751 \\ 9 \end{bmatrix}$$

Solve it on a computer using **6** significant digits with chopping

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0.9625 \\ 1.05 \\ 0.999995 \end{bmatrix}$$

# Pitfall#2. Large Round-off Errors

$$\begin{bmatrix} 20 & 15 & 10 \\ -3 & -2.249 & 7 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 1.751 \\ 9 \end{bmatrix}$$

Solve it on a computer using **5** significant digits with chopping

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0.625 \\ 1.5 \\ 0.99995 \end{bmatrix}$$

Is there a way to reduce the round off error?

# Avoiding Pitfalls

Increase the number of significant digits

- Decreases round-off error
- Does not avoid division by zero



# Avoiding Pitfalls

## Gaussian Elimination with Partial Pivoting

- Avoids division by zero
- Reduces round off error

**THE END**

**Computational Physics**

# Gauss Elimination with Partial Pivoting

Computational Physics

# Pitfalls of Naïve Gauss Elimination

- Possible division by zero
- Large round-off errors

# Avoiding Pitfalls

Increase the number of significant digits

- Decreases round-off error
- Does not avoid division by zero

# Avoiding Pitfalls

## Gaussian Elimination with Partial Pivoting

- Avoids division by zero
- Reduces round off error

# What is Different About Partial Pivoting?

At the beginning of the  $k^{\text{th}}$  step of forward elimination, find the maximum of

$$|a_{kk}|, |a_{k+1,k}|, \dots, |a_{nk}|$$

If the maximum of the values is  $|a_{pk}|$

in the  $p^{\text{th}}$  row,  $k \leq p \leq n$ , then switch rows  $p$  and  $k$ .

# Matrix Form at Beginning of 2<sup>nd</sup> Step of Forward Elimination

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a'_{22} & a'_{23} & \cdots & a'_{2n} \\ 0 & a'_{32} & a'_{33} & \cdots & a'_{3n} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & a'_{n2} & a'_{n3} & a'_{n4} & a'_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix}$$



## Example (2<sup>nd</sup> step of FE)

$$\begin{bmatrix} 6 & 14 & 5.1 & 3.7 & 6 \\ 0 & -7 & 6 & 1 & 2 \\ 0 & 4 & 12 & 1 & 11 \\ 0 & 9 & 23 & 6 & 8 \\ 0 & -17 & 12 & 11 & 43 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 5 \\ -6 \\ 8 \\ 9 \\ 3 \end{bmatrix}$$

Which two rows would you switch?

## Example (2<sup>nd</sup> step of FE)

$$\begin{bmatrix} 6 & 14 & 5.1 & 3.7 & 6 \\ 0 & -17 & 12 & 11 & 43 \\ 0 & 4 & 12 & 1 & 11 \\ 0 & 9 & 23 & 6 & 8 \\ 0 & -7 & 6 & 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 5 \\ 3 \\ 8 \\ 9 \\ -6 \end{bmatrix}$$

Switched Rows

# Gaussian Elimination with Partial Pivoting

A method to solve simultaneous linear equations of the form  $[A][X]=[C]$

Two steps

1. Forward Elimination
2. Back Substitution

# Forward Elimination

Same as naïve Gauss elimination method except that we switch rows before **each** of the  $(n-1)$  steps of forward elimination.

# Example: Matrix Form at Beginning of 2<sup>nd</sup> Step of Forward Elimination

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a'_{22} & a'_{23} & \cdots & a'_{2n} \\ 0 & a'_{32} & a'_{33} & \cdots & a'_{3n} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & a'_{n2} & a'_{n3} & a'_{n4} & a'_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b'_2 \\ b'_3 \\ \vdots \\ b'_n \end{bmatrix}$$

# Matrix Form at End of Forward Elimination

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a'_{22} & a'_{23} & \cdots & a'_{2n} \\ 0 & 0 & a''_{33} & \cdots & a''_{3n} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & 0 & a^{(n-1)}_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b'_2 \\ b''_3 \\ \vdots \\ b^{(n-1)}_n \end{bmatrix}$$

# Back Substitution Starting Eqns

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n = b_1$$

$$a'_{22}x_2 + a'_{23}x_3 + \dots + a'_{2n}x_n = b'_2$$

$$a''_{33}x_3 + \dots + a''_n x_n = b''_3$$

$$\vdots \quad \vdots$$

$$a^{(n-1)}_{nn}x_n = b^{(n-1)}_n$$

# Back Substitution

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

$$x_i = \frac{b_i^{(i-1)} - \sum_{j=i+1}^n a_{ij}^{(i-1)} x_j}{a_{ii}^{(i-1)}} \text{ for } i = n-1, \dots, 1$$



**THE END**

**Computational Physics**

# Gauss Elimination with Partial Pivoting Example

Computational Physics

## Example 2

Solve the following set of equations by Gaussian elimination with partial pivoting

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

## Example 2 Cont.

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix} \Rightarrow \begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix}$$

1. Forward Elimination
2. Back Substitution

# Forward Elimination

# Number of Steps of Forward Elimination

Number of steps of forward elimination is  
 $(n-1)=(3-1)=2$

# Forward Elimination: Step 1

- Examine absolute values of first column, first row and below.

$$|25|, |64|, |144|$$

- Largest absolute value is 144 and exists in row 3.
- Switch row 1 and row 3.

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix} \Rightarrow \begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 25 & 5 & 1 & \vdots & 106.8 \end{bmatrix}$$

# Forward Elimination: Step 1 (cont.)

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 25 & 5 & 1 & \vdots & 106.8 \end{bmatrix}$$

Divide Equation 1 by 144 and multiply it by 64,  $\frac{64}{144} = 0.4444$ .

$$[144 \ 12 \ 1 \ \vdots \ 279.2] \times 0.4444 = [63.99 \ 5.333 \ 0.4444 \ \vdots \ 124.1]$$

Subtract the result from Equation 2

$$\begin{array}{r} \begin{bmatrix} 64 & 8 & 1 & \vdots & 177.2 \\ 63.99 & 5.333 & 0.4444 & \vdots & 124.1 \end{bmatrix} \\ - \\ \hline \begin{bmatrix} 0 & 2.667 & 0.5556 & \vdots & 53.10 \end{bmatrix} \end{array}$$

Substitute new equation for Equation 2

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.667 & 0.5556 & \vdots & 53.10 \\ 25 & 5 & 1 & \vdots & 106.8 \end{bmatrix}$$



# Forward Elimination: Step 1 (cont.)

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.667 & 0.5556 & \vdots & 53.10 \\ 25 & 5 & 1 & \vdots & 106.8 \end{bmatrix} \quad \begin{array}{l} \text{Divide Equation 1 by 144 and} \\ \text{multiply it by 25, } \frac{25}{144} = 0.1736. \end{array}$$

$$[144 \ 12 \ 1 \ \vdots \ 279.2] \times 0.1736 = [25.00 \ 2.083 \ 0.1736 \ \vdots \ 48.47]$$

Subtract the result from  
Equation 3

$$\begin{array}{r} \begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 25 & 2.083 & 0.1736 & \vdots & 48.47 \end{bmatrix} \\ - \\ \hline \begin{bmatrix} 0 & 2.917 & 0.8264 & \vdots & 58.33 \end{bmatrix} \end{array}$$

Substitute new equation for  
Equation 3

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.667 & 0.5556 & \vdots & 53.10 \\ 0 & 2.917 & 0.8264 & \vdots & 58.33 \end{bmatrix}$$

# Forward Elimination: Step 2

- Examine absolute values of second column, second row and below.

$$|2.667|, |2.917|$$

- Largest absolute value is 2.917 and exists in row 3.
- Switch row 2 and row 3.

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.667 & 0.5556 & \vdots & 53.10 \\ 0 & 2.917 & 0.8264 & \vdots & 58.33 \end{bmatrix} \Rightarrow \begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.917 & 0.8264 & \vdots & 58.33 \\ 0 & 2.667 & 0.5556 & \vdots & 53.10 \end{bmatrix}$$

# Forward Elimination: Step 2 (cont.)

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.917 & 0.8264 & \vdots & 58.33 \\ 0 & 2.667 & 0.5556 & \vdots & 53.10 \end{bmatrix}$$

Divide Equation 2 by 2.917 and multiply it by 2.667,  
 $\frac{2.667}{2.917} = 0.9143$ .

$$[0 \quad 2.917 \quad 0.8264 \quad \vdots \quad 58.33] \times 0.9143 = [0 \quad 2.667 \quad 0.7556 \quad \vdots \quad 53.33]$$

Subtract the result from  
Equation 3

$$\begin{array}{r} [0 \quad 2.667 \quad 0.5556 \quad \vdots \quad 53.10] \\ - [0 \quad 2.667 \quad 0.7556 \quad \vdots \quad 53.33] \\ \hline [0 \quad 0 \quad -0.2 \quad \vdots \quad -0.23] \end{array}$$

Substitute new equation for  
Equation 3

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.917 & 0.8264 & \vdots & 58.33 \\ 0 & 0 & -0.2 & \vdots & -0.23 \end{bmatrix}$$

# Back Substitution

# Back Substitution

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.917 & 0.8264 & \vdots & 58.33 \\ 0 & 0 & -0.2 & \vdots & -0.23 \end{bmatrix} \Rightarrow \begin{bmatrix} 144 & 12 & 1 \\ 0 & 2.917 & 0.8264 \\ 0 & 0 & -0.2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 279.2 \\ 58.33 \\ -0.23 \end{bmatrix}$$

Solving for  $a_3$

$$\begin{aligned} -0.2a_3 &= -0.23 \\ a_3 &= \frac{-0.23}{-0.2} \\ &= 1.15 \end{aligned}$$

# Back Substitution (cont.)

$$\begin{bmatrix} 144 & 12 & 1 \\ 0 & 2.917 & 0.8264 \\ 0 & 0 & -0.2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 279.2 \\ 58.33 \\ -0.23 \end{bmatrix}$$

Solving for  $a_2$

$$2.917a_2 + 0.8264a_3 = 58.33$$

$$\begin{aligned} a_2 &= \frac{58.33 - 0.8264a_3}{2.917} \\ &= \frac{58.33 - 0.8264 \times 1.15}{2.917} \\ &= 19.67 \end{aligned}$$

# Back Substitution (cont.)

$$\begin{bmatrix} 144 & 12 & 1 \\ 0 & 2.917 & 0.8264 \\ 0 & 0 & -0.2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 279.2 \\ 58.33 \\ -0.23 \end{bmatrix}$$

Solving for  $a_1$

$$144a_1 + 12a_2 + a_3 = 279.2$$

$$a_1 = \frac{279.2 - 12a_2 - a_3}{144}$$

$$= \frac{279.2 - 12 \times 19.67 - 1.15}{144}$$

$$= 0.2917$$

# Gaussian Elimination with Partial Pivoting Solution

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0.2917 \\ 19.67 \\ 1.15 \end{bmatrix}$$



# Gauss Elimination with Partial Pivoting Another Example

Computational Physics

# Partial Pivoting: Example

Consider the system of equations

$$10x_1 - 7x_2 = 7$$

$$-3x_1 + 2.099x_2 + 6x_3 = 3.901$$

$$5x_1 - x_2 + 5x_3 = 6$$

In matrix form

$$\begin{bmatrix} 10 & -7 & 0 \\ -3 & 2.099 & 6 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 3.901 \\ 6 \end{bmatrix}$$

Solve using Gaussian Elimination with Partial Pivoting using five significant digits with chopping

# Partial Pivoting: Example

Forward Elimination: Step 1

Examining the values of the first column

$|10|$ ,  $|-3|$ , and  $|5|$  or 10, 3, and 5

The largest absolute value is 10, which means, to follow the rules of Partial Pivoting, we switch row1 with row1.

Performing Forward Elimination

$$\begin{bmatrix} 10 & -7 & 0 \\ -3 & 2.099 & 6 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 3.901 \\ 6 \end{bmatrix} \Rightarrow \begin{bmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 2.5 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 6.001 \\ 2.5 \end{bmatrix}$$

# Partial Pivoting: Example

Forward Elimination: Step 2

Examining the values of the first column

$|-0.001|$  and  $|2.5|$  or  $0.0001$  and  $2.5$

The largest absolute value is 2.5, so row 2 is switched with row 3

Performing the row swap

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 2.5 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 6.001 \\ 2.5 \end{bmatrix} \Rightarrow \begin{bmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & -0.001 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 2.5 \\ 6.001 \end{bmatrix}$$

# Partial Pivoting: Example

Forward Elimination: Step 2

Performing the Forward Elimination results in:

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & 0 & 6.002 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 2.5 \\ 6.002 \end{bmatrix}$$

# Partial Pivoting: Example

Back Substitution

Solving the equations through back substitution

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & 0 & 6.002 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 2.5 \\ 6.002 \end{bmatrix}$$

$$x_3 = \frac{6.002}{6.002} = 1$$

$$x_2 = \frac{2.5 - 5x_3}{2.5} = -1$$

$$x_1 = \frac{7 + 7x_2 - 0x_3}{10} = 0$$

# Partial Pivoting: Example

Compare the calculated and exact solution

The fact that they are equal is coincidence, but it does illustrate the advantage of Partial Pivoting

$$[X]_{\text{calculated}} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \quad [X]_{\text{exact}} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix}$$

**THE END**

**Computational Physics**



# Determinant of a Square Matrix Using Naïve Gauss Elimination Example

Computational Physics

# Theorem of Determinants

If a multiple of one row of  $[A]_{n \times n}$  is added or subtracted to another row of  $[A]_{n \times n}$  to result in  $[B]_{n \times n}$  then  $\det(A) = \det(B)$

# Theorem of Determinants

The determinant of an upper triangular matrix  $[A]_{n \times n}$  is given by

$$\begin{aligned}\det(A) &= a_{11} \times a_{22} \times \dots \times a_{ii} \times \dots \times a_{nn} \\ &= \prod_{i=1}^n a_{ii}\end{aligned}$$

# Forward Elimination of a Square Matrix

Using forward elimination to transform  $[A]_{n \times n}$  to an upper triangular matrix,  $[U]_{n \times n}$ .

$$[A]_{n \times n} \rightarrow [U]_{n \times n}$$

$$\det(A) = \det(U)$$

# Example

Using naïve Gaussian elimination find the determinant of the following square matrix.

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix}$$

# Forward Elimination

# Forward Elimination: Step 1

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix}$$

Divide Equation 1 by 25 and multiply it by 64,  $\frac{64}{25} = 2.56$ .

$$[25 \quad 5 \quad 1] \times 2.56 = [64 \quad 12.8 \quad 2.56]$$

Subtract the result from Equation 2

$$\begin{array}{r} [64 \quad 8 \quad 1] \\ - [64 \quad 12.8 \quad 2.56] \\ \hline \end{array}$$

$$[0 \quad -4.8 \quad -1.56]$$

Substitute new equation for Equation 2

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 144 & 12 & 1 \end{bmatrix}$$

# Forward Elimination: Step 1 (cont.)

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 144 & 12 & 1 \end{bmatrix}$$

Divide Equation 1 by 25 and multiply it by 144,  $\frac{144}{25} = 5.76$ .

$$[25 \ 5 \ 1] \times 5.76 = [144 \ 28.8 \ 5.76]$$

Subtract the result from  
Equation 3

$$\begin{array}{r} [144 \quad 12 \quad 1] \\ - [144 \quad 28.8 \quad 5.76] \\ \hline [0 \quad -16.8 \quad -4.76] \end{array}$$

Substitute new equation for  
Equation 3

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & -16.8 & -4.76 \end{bmatrix}$$



# Forward Elimination: Step 2

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & -16.8 & -4.76 \end{bmatrix}$$

Divide Equation 2 by  $-4.8$   
and multiply it by  $-16.8$ ,  
 $\frac{-16.8}{-4.8} = 3.5$ .

$$([0 \quad -4.8 \quad -1.56]) \times 3.5 = [0 \quad -16.8 \quad -5.46]$$

Subtract the result from  
Equation 3

$$\begin{array}{r} [0 \quad -16.8 \quad -4.76] \\ - [0 \quad -16.8 \quad -5.46] \\ \hline [0 \quad 0 \quad 0.7] \end{array}$$

Substitute new equation for  
Equation 3

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix}$$

# Finding the Determinant

After forward elimination

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \rightarrow \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix}$$

$$\begin{aligned} \det(\mathbf{A}) &= u_{11} \times u_{22} \times u_{33} \\ &= 25 \times (-4.8) \times 0.7 \\ &= -84.00 \end{aligned}$$

# Summary

- Forward Elimination
- Back Substitution
- Pitfalls
- Improvements
- Partial Pivoting
- Determinant of a Matrix

**THE END**

**Computational Physics**