NUMERICAL METHODS

$$U^{n+1} = U^n + \Delta t\, f(U^n)$$

$$\frac{\partial v}{\partial t} + V \cdot \nabla v = \nabla \cdot (k \nabla v) + g(v)$$

$$(\lambda + \mu)\nabla(\nabla \cdot u) + \mu \nabla^2 u = \alpha(3\lambda + 2\mu)\nabla T - \rho b$$

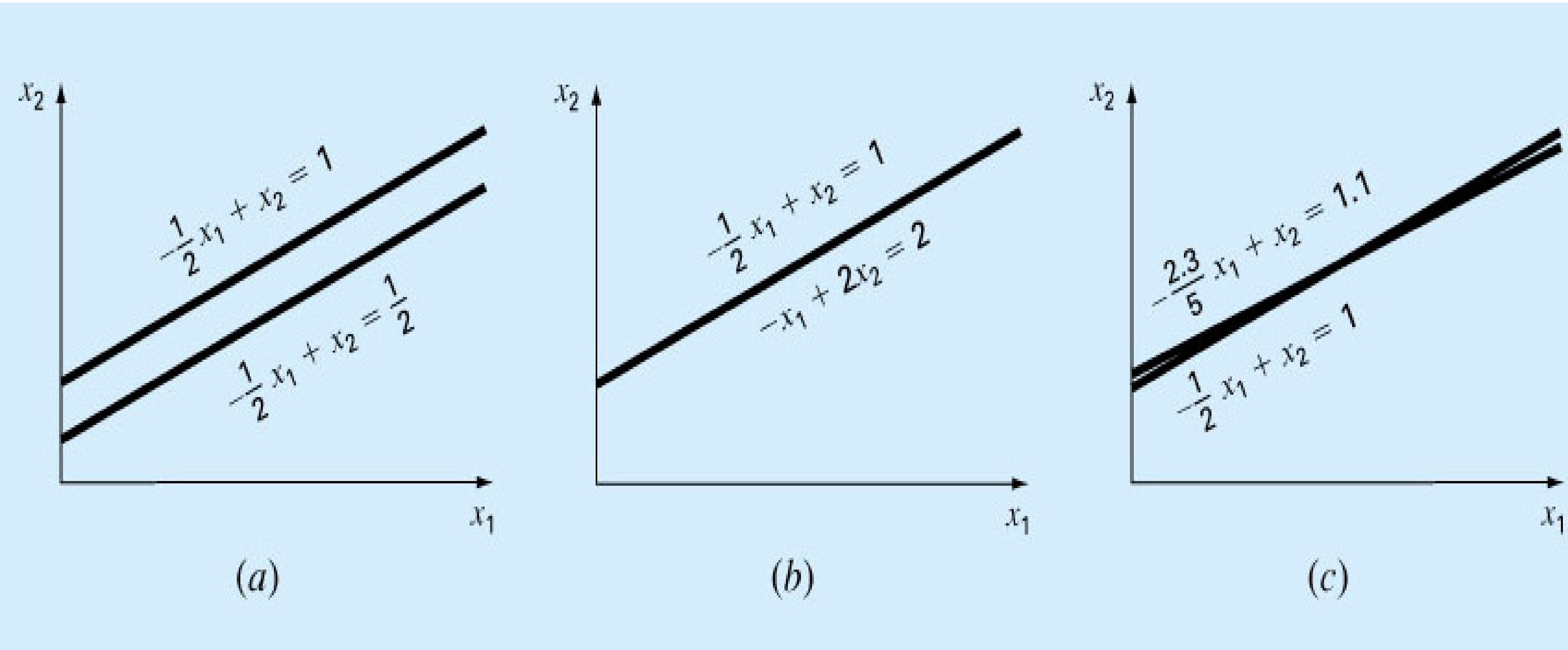
Lecture 4

$$\rho\left(\frac{\partial u}{\partial t} + V \cdot \nabla u\right) = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + \rho f_x$$

$$\nabla^2 u = f$$

Dr. P V Ramana

Graphical Method



No solution **Infinite solution** **ill condition**

(sensitive to round-off errors)

Algorithm for Gauss elimination

- **1. Forward elimination**
- **for each equation j, $j = 1$ to $n-1$**

  for all equations k greater than j

  (a) multiply equation j by a_{kj}/a_{jj}

  (b) subtract the result from equation k
- **This leads to an upper triangular matrix**
- **2. Back-Substitution**

  (a) determine x_n from $x_n = b_n^{(n-1)} / a_{nn}^{(n-1)}$

  (b) put x_n into (n-1)th equation, solve for x_{n-1}

  (c) repeat from (b), moving back to n-2, n-3, etc. until all equations are solved

Partial Pivoting

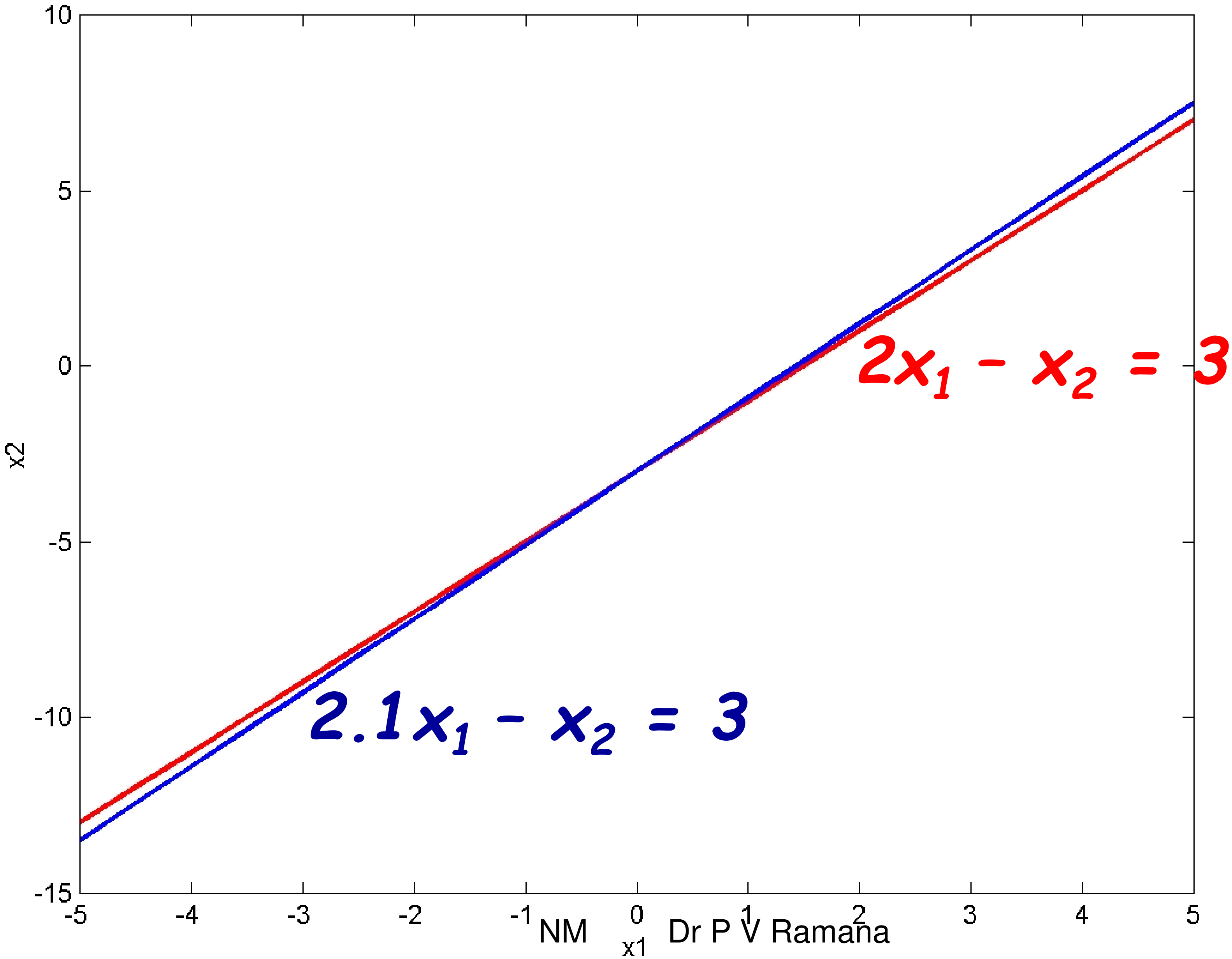
Problems with Gauss elimination

- division by zero
- round off errors
- ill conditioned systems

Use “Pivoting” to avoid this

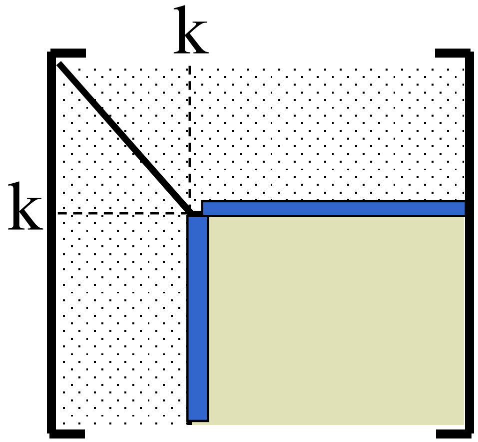
- Find the row with largest absolute coefficient below the pivot element
- Switch rows (“partial pivoting”)
- complete pivoting switch columns also (rarely used)

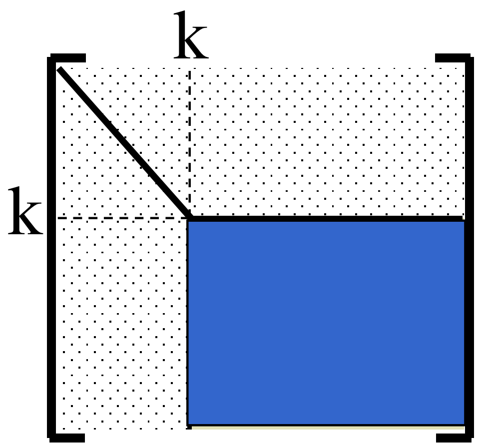
Ill-conditioned System



Pivoting strategies

- Partial Pivoting:
  - Only row interchange
- Complete (Full) Pivoting
  - Row and Column interchange
- Threshold Pivoting
  - Only if prospective pivot is found to be smaller than a certain threshold





Pitfalls

-Division by zero: May occur in the forward elimination steps. Consider the set of equations:

Two Potential Pitfalls

$$10x_1 - 7x_2 = 7$$

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

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

- Round-off error: Prone to round-off errors.

Pitfalls: Example

$$10x_1 - 7x_2 = 7$$
$$-3x_1 + 2.099x_2 + 6x_3 = 3.901$$
$$5x_1 - x_2 + 5x_3 = 6$$

Consider the system of equations: Use five significant figures with chopping

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

At the end of Forward Elimination

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 0 & 15005 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 6.001 \\ 15004 \end{bmatrix}$$

Pitfalls: Example

$$10x_1 - 7x_2 = 7$$
$$-3x_1 + 2.099x_2 + 6x_3 = 3.901$$
$$5x_1 - x_2 + 5x_3 = 6$$

Back Substitution

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 0 & 15005 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 6.001 \\ 15004 \end{bmatrix}$$

$$x_3 = \frac{15004}{15005} = 0.99993$$

$$x_2 = \frac{6.001 - 6x_3}{-0.001} = -1.5$$

$$x_1 = \frac{7 + 7x_2 - 0x_3}{10} = -0.3500$$

Pitfalls: Example

$$10x_1 - 7x_2 = 7$$
$$-3x_1 + 2.099x_2 + 6x_3 = 3.901$$
$$5x_1 - x_2 + 5x_3 = 6$$

Compare the calculated values with the exact solution

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

$$[X]_{calculated} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -0.35 \\ -1.5 \\ 0.99993 \end{bmatrix}$$

Improvements

Increase the number of significant digits

Decreases round off error

Does not avoid division by zero

Gaussian Elimination with Partial Pivoting

Avoids division by zero

Reduces round off error

Partial Pivoting

Gaussian Elimination with partial pivoting applies row switching to normal Gaussian Elimination.

How?

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

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

If the maximum of the values is $|a_{pk}|$ In the p^{th} row, $k \le p \le n$,

then switch rows p and k.

Partial Pivoting

What does it Mean?

Gaussian Elimination with Partial Pivoting ensures that each step of Forward Elimination is performed with the pivoting element $|a_{kk}|$ having the largest absolute value.

$$10x_1 - 7x_2 = 7$$
$$-3x_1 + 2.099x_2 + 6x_3 = 3.901$$
$$5x_1 - x_2 + 5x_3 = 6$$

Partial Pivoting: Example

Consider the system of equations

$$10x_1 - 7x_2 = 7$$
$$-3x_1 + 2.099x_2 + 3x_3 = 3.901$$
$$5x_1 - x_2 + 5x_3 = 6$$

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

$$10x_1 - 7x_2 = 7$$
$$-3x_1 + 2.099x_2 + 6x_3 = 3.901$$
$$5x_1 - x_2 + 5x_3 = 6$$

Forward Elimination: Step 1

Examining the values of the first colu

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

The largest absolute value is 10, which means, to follow the rules of Partial Pivoting, 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

$$10x_1 - 7x_2 = 7$$
$$-3x_1 + 2.099x_2 + 6x_3 = 3.901$$
$$5x_1 - x_2 + 5x_3 = 6$$

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

$$10x_1 - 7x_2 = 7$$
$$-3x_1 + 2.099x_2 + 6x_3 = 3.901$$
$$5x_1 - x_2 + 5x_3 = 6$$

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

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

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

$$10x_1 - 7x_2 = 7$$
$$-3x_1 + 2.099x_2 + 6x_3 = 3.901$$
$$5x_1 - x_2 + 5x_3 = 6$$

Compare the calculated and exact solution

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

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

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

Example 2

Solve using Naive Gaussian Eliminatio n :

Part 1 : Forward Eliminatio n ___ Step1 : Eliminate x_1 from equations 2, 3

$$x_1 + 2x_2 + 3x_3 = 8 \qquad eq1 \ \ unchanged \ \ (pivot \ equation)$$

$$2x_1 + 3x_2 + 2x_3 = 10 \qquad eq2 \leftarrow eq2 - \left(\frac{2}{1}\right) eq1$$

$$3x_1 + x_2 + 2x_3 = 7 \qquad eq3 \leftarrow eq3 - \left(\frac{3}{1}\right) eq1$$

$$x_1 + 2x_2 + 3x_3 = 8$$

$$x_2 + 4x_3 = 6$$

$$-5x_2 - 7x_3 = -17$$

Example 2

$$x_1 + 2x_2 + 3x_3 = 8$$
$$x_2 + 4x_3 = 6$$
$$-5x_2 - 7x_3 = -17$$

$\text{Part 1: Forward Elimination Step2 : Eliminate } x_2 \text{ from equation 3}$

$$x_1 + 2x_2 + 3x_3 = 8 \qquad eq\,1 \quad unchanged$$
$$-\ x_2 - 4x_3 = -6 \qquad eq\,2 \quad unchanged \quad (pivot \quad equation)$$
$$-5x_2 - 7x_3 = -17 \qquad eq\,3 \leftarrow eq\,3 - \left(\frac{-5}{-1}\right) eq\,2$$

$$\Rightarrow \begin{cases} x_1 + 2x_2 + 3x_3 = 8 \\ x_2 + 4x_3 = 6 \\ x_3 = \dfrac{13}{13} \end{cases}$$

Example 2
Backward Substitution

$$\begin{cases} x_1 + 2x_2 + 3x_3 = 8 \\ x_2 + 4x_3 = 6 \\ x_3 = \dfrac{13}{13} \end{cases}$$

$$x_3 = \frac{b_3}{a_{3,3}} = \frac{13}{13} = 1$$

$$x_2 = \frac{b_2 - a_{2,3}x_3}{a_{2,2}} = \frac{6 - 4x_3}{1} = 2$$

$$x_1 = \frac{b_1 - a_{1,2}x_2 - a_{1,3}x_3}{a_{1,1}} = \frac{8 - 2x_2 - 3x_3}{a_{1,1}} = 1$$

The solution is $\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}$

Determinant

$$x_1 + 2x_2 + 3x_3 = 8$$
$$x_2 + 4x_3 = 6$$
$$-5x_2 - 7x_3 = -17$$

$$\begin{cases} x_1 + 2x_2 + 3x_3 = 8 \\ x_2 + 4x_3 = 6 \\ 13x_3 = 13 \end{cases}$$

The elementary operations do not affect the determinant

Example:

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 2 \\ 3 & 1 & 2 \end{bmatrix} \xrightarrow{\text{Elementary operations}} A' = \begin{bmatrix} 1 & 2 & 3 \\ 0 & -1 & -4 \\ 0 & 0 & 13 \end{bmatrix}$$

$$\det(A) = \det(A') = -13$$

How Many Solutions Does a System of Equations AX=B Have?

Unique	No solution	Infinite
$\det(A) \neq 0$	$\det(A) = 0$	$\det(A) = 0$
reduced matrix has no zero rows	reduced matrix has one or more zero rows, corresponding B elements $\neq 0$	reduced matrix has one or more zero rows, corresponding B elements $= 0$
Unique	No solution	infinte # of solutions
$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} X = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$	$\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} X = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$	$\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} X = \begin{bmatrix} 2 \\ 4 \end{bmatrix}$

Examples

Unique

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} X = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

$$\downarrow$$

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

solution :

$$X = \begin{bmatrix} 0 \\ 0.5 \end{bmatrix}$$

No solution

$$\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} X = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$$

$$\downarrow$$

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

No solution

$$0 = -1 \; impossible!$$

infinte # of solutions

$$\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} X = \begin{bmatrix} 2 \\ 4 \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} 1 & 2 \\ 0 & 0 \end{bmatrix} X = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$$

Infinite # solutions

$$X = \begin{bmatrix} \alpha \\ 1 - .5\,\alpha \end{bmatrix}$$

Pseudo-Code: Forward Elimination

Do k = 1 to n-1

  Do i = k+1 to n

    factor = $a_{i,k}$ / $a_{k,k}$

    Do j = k+1 to n

      $a_{i,j} = a_{i,j} - \text{factor} * a_{k,j}$

    End Do

    $b_i = b_i - \text{factor} * b_k$

  End Do

End Do

Pseudo-Code: Back Substitution

```
x_n = b_n / a_{n,n}
Do i = n-1 downto 1
   sum = b_i
   Do j = i+1 to n
         sum = sum – a_{i,j} * x_j
   End Do
   x_i = sum / a_{i,i}
End Do
```

Problems with Gaussian Elimination

- The Gaussian Elimination may fail for very simple cases.

  (The pivoting element is zero).

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

- **Very small pivoting element may result in serious computation errors**

$$\begin{bmatrix} 10^{-3} & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \qquad \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1.0010 \\ 0.999 \end{bmatrix}$$

How Do Know If a Solution is Good or Not

Given AX=B

X is a solution if AX-B=0

Compute the residual vector R= AX-B

Due to rounding error, R may not be zero

$$\text{The solution is acceptable if } \max_i |r_i| \leq \varepsilon$$

How Good is the Solution?

$$\begin{bmatrix} 1 & -1 & 2 & 1 \\ 3 & 2 & 1 & 4 \\ 5 & -8 & 6 & 3 \\ 4 & 2 & 5 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ -1 \end{bmatrix}$$

$$solution \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -1.8673 \\ -0.3469 \\ 0.3980 \\ 1.7245 \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}_{Exact} = \begin{bmatrix} -1.917 \\ -0.349 \\ 0.393 \\ 1.726 \end{bmatrix} \quad solution \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -1.8673 \\ -0.3469 \\ 0.3980 \\ 1.7245 \end{bmatrix} \quad \text{Residues } R = \begin{bmatrix} 0.005 \\ 0.002 \\ 0.003 \\ 0.001 \end{bmatrix}$$

Gauss Elimination Method Example 1

Solve the following system using Gauss Elimination.

$$
\begin{aligned}
6x_1 - 2x_2 + 2x_3 + 4x_4 &= 16 \\
12x_1 - 8x_2 + 6x_3 + 10x_4 &= 26 \\
3x_1 - 13x_2 + 9x_3 + 3x_4 &= -19 \\
-6x_1 + 4x_2 + x_3 - 18x_4 &= -34
\end{aligned}
$$

Step 0: Form the augmented matrix

$$
\left[\begin{array}{cccc|c}
6 & -2 & 2 & 4 & 16 \\
12 & -8 & 6 & 10 & 26 \\
3 & -13 & 9 & 3 & -19 \\
-6 & 4 & 1 & -18 & -34
\end{array}\right]
\begin{array}{l}
\\
R2-2R1 \\
R3-0.5R1 \\
R4-(-R1)
\end{array}
$$

Gauss Elimination Method
Example 1 (cont'd)

Step 1: Forward elimination

1. Eliminate x_1

$\boxed{6}$	−2	2	4	|	16	(Does not change. Pivot is 6)
0	−4	2	2	|	−6	
0	−12	8	1	|	−27	R3−6R2
0	2	3	−14	|	−18	R4−(−0.5R2)

2. Eliminate x_2

6	−2	2	4	|	16	**(Does not change.)**
0	$\boxed{-4}$	2	2	|	−6	**(Does not change. Pivot is-4)**
0	0	2	−5	|	−9	
0	0	4	−13	|	−21	R4−2R3

3. Eliminate x_3

6	−2	2	4	|	16	**(Does not change.)**
0	−4	2	2	|	−6	**(Does not change.)**
0	0	$\boxed{2}$	−5	|	−9	**(Does not change. Pivot is 2)**
0	0	0	−3	|	−3	

Naive Gauss Elimination Method

Example 1 (cont'd)

Step 2: Back substitution

Find x_4 $\quad x_4 = (-3)/(-3) = 1$

Find x_3 $\quad x_3 = (-9+5*1)/2 = -2$

Find x_2 $\quad x_2 = (-6-2*(-2)-2*1)/(-4) = 1$

Find x_1 $\quad x_1 = (16+2*1-2*(-2)-4*1)/6 = 3$

Gauss Elimination Method Example 2

(Using 6 Significant Figures)

$$
\begin{aligned}
3.0\, x_1 - 0.1\, x_2 - 0.2\, x_3 &= 7.85 \\
0.1\, x_1 + 7.0\, x_2 - 0.3\, x_3 &= -19.3 \qquad R2-(0.1/3)R1 \\
0.3\, x_1 - 0.2\, x_2 + 10.0\, x_3 &= 71.4 \qquad R3-(0.3/3)R1
\end{aligned}
$$

Step 1: Forward elimination

$$
\begin{aligned}
3.00000\, x_1 - 0.100000\, x_2 - 0.200000\, x_3 &= 7.85000 \\
7.00333\, x_2 - 0.293333\, x_3 &= -19.5617 \\
-\,0.190000\, x_2 + 10.0200\, x_3 &= 70.6150
\end{aligned}
$$

$$
\begin{aligned}
3.00000\, x_1 - 0.100000\, x_2 - 0.20000\, x_3 &= 7.85000 \\
7.00333\, x_2 - 0.293333\, x_3 &= -19.5617 \\
10.0120\, x_3 &= 70.0843
\end{aligned}
$$

Gauss Elimination Method Example 2 (cont'd)

Step 2: **Back substitution**

$x_3 = 7.00003$

$x_2 = -2.50000$

$x_1 = 3.00000$

Exact solution:

$x_3 = 7.0$

$x_2 = -2.5$

$x_1 = 3.0$

Residue of solution:

$x_3 = 0.00003$

$x_2 = 1e-7$

$x_1 = 1e-7$

Pitfalls of Gauss Elimination Methods

1. **Division by zero**

$$\begin{aligned} 0 \qquad\; 2x_2 + 3x_3 &= 8 \\ 4x_1 + 6x_2 + 7x_3 &= -3 \\ 2x_1 + x_2 + 6x_3 &= 5 \end{aligned}$$

$a_{11} = 0$
(the pivot element)

It is possible that during both elimination and back-substitution phases a division by zero can occur.

2. **Round-off errors**

In the previous example where up to 6 digits were kept during the calculations and still end up with close to the real solution.

$x_3 = 7.00003$, instead of $x_3 = 7.0$

Pitfalls of Gauss Elimination (cont'd)

$$\begin{bmatrix} 400 & -201 \\ -800 & 401 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 200 \\ -200 \end{bmatrix} \quad x_1 = -100 \text{ and } x_2 = -200$$

3. Ill-conditioned systems

$$\begin{bmatrix} 401 & -201 \\ -800 & 401 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 200 \\ -200 \end{bmatrix} \quad x_1 = 40000 \text{ and } x_2 = 79800$$

$$x_1 + 2x_2 = 10$$
$$1.1x_1 + 2x_2 = 10.4$$

$\rightarrow x_1 = 4.0$ & $x_2 = 3.0$

$$x_1 + 2x_2 = 10$$
$$1.05x_1 + 2x_2 = 10.4$$

$\rightarrow x_1 = 8.0$ & $x_2 = 1.0$

Ill conditioned systems are those where small changes in coefficients result in large change in solution. Alternatively, it happens when two or more equations are nearly identical, resulting a wide ranges of answers to approximately satisfy the equations. Since round off errors can induce small changes in the coefficients, these changes can lead to large solution errors.

Pitfalls of Gauss Elimination (cont'd)

4. **Singular systems.**

- When two equations are identical, would loose one degree of freedom and be dealing with case of *n-1* equations for *n* unknowns.

To check for singularity:

- After getting the forward elimination process and getting the triangle system, then the determinant for such a system is the product of all the diagonal elements. If a zero diagonal element is created, the determinant is Zero then have a singular system.
- The determinant of a singular system is zero.

Techniques for Improving Solutions

1. **Use of more significant figures** to solve for the **round-off error.**
2. **Pivoting**. If a pivot element is zero, elimination step leads to division by zero. The same problem may arise, when the pivot element is close to zero. This Problem can be avoided by:
   - **Partial pivoting**. Switching the rows so that the largest element is the pivot element.
   - **Complete pivoting**. Searching for the largest element in all rows and columns then switching.
3. **Scaling**
   - Solve problem of ill-conditioned system.
   - Minimize round-off error

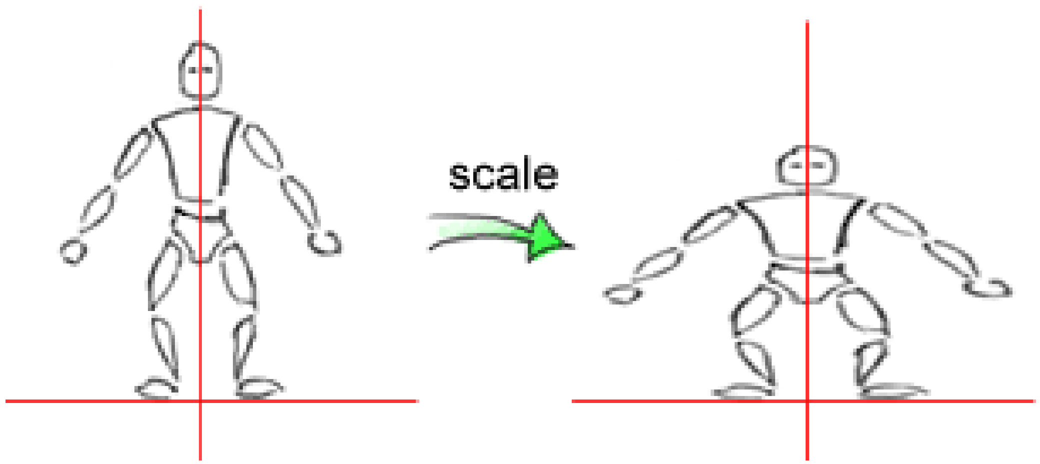
$$A = \begin{bmatrix} 1 & -1 \\ 1000 & 1000 \end{bmatrix}$$

$$A^{-1} = \begin{bmatrix} 0.5 & 0.0005 \\ -0.5 & 0.0005 \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \quad A^{-1} = \begin{bmatrix} 0.5 & 0.5 \\ -0.5 & 0.5 \end{bmatrix}$$

Partial Pivoting

Before each row is normalized, find the largest available coefficient in the column below the pivot element. The rows can then be switched so that the largest element is the pivot element so that the largest coefficient is used as a pivot.



Use of more significant figures to solve for the round-off error : Example

Use Gauss Elimination to solve these 2 equations: (keeping only 4 sig. figures)

$$0.0003\ x_1 + 3.0000\ x_2 = 2.0001$$
$$1.0000\ x_1 + 1.0000\ x_2 = 1.000$$

$$0.0003\ x_1 + 3.0000\ x_2 = 2.0001$$
$$-\ 9999.0\ x_2 = -6666.0$$

Solve: $x_2 = 0.6667$ & $x_1 = 0.0$

$$1.0000\ x_1 + 1.0000\ x_2 = 1.000$$
$$0.0003\ x_1 + 3.0000\ x_2 = 2.0001$$

$$1.0000\ x_1 + 1.0000\ x_2 = 1.000$$
$$-\ 9999.0\ x_2 = -6666.0$$

Solve: $x_2 = 0.6667$ & $x_1 = 0.3333$

The exact solution is $x_2 = 2/3$ & $x_1 = 1/3$

Use of more significant figures to solve for the round-off error :Example (cont'd).

$$0.0003\, x_1 + 3.0000\, x_2 = 2.0001$$
$$1.0000\, x_1 + 1.0000\, x_2 = 1.000$$

$$x_2 = \frac{2}{3}$$

$$x_1 = \frac{2.0001 - 3(2/3)}{0.0003}$$

Significant Figures	x_2	x_1
3	0.667	-3.33
4	0.6667	0.000
5	0.66667	0.3000
6	0.666667	0.33000
7	0.6666667	0.333000

Pivoting: Example

Now, solving the pervious example using the partial pivoting technique:

$$1.0000\ x_1 + 1.0000\ x_2 = 1.000$$
$$0.0003\ x_1 + 3.0000\ x_2 = 2.0001$$

The pivot is 1.0

$$1.0000\ x_1 + 1.0000\ x_2 = 1.000$$
$$2.9997\ x_2 = 1.9998$$

$$x_2 = 0.6667 \ \& \ x_1 = 0.3333$$

Checking the effect of the # of significant digits:

# of dig	x_2	x_1	Ea% in x1
4	0.6667	0.3333	0.01
5	0.66667	0.33333	0.001

Scaling: Example

- Solve the following equations using (naïve) gauss elimination:

  (keeping only 3 sig. figures)

  $$2\,x_1 + 100{,}000\,x_2 = 100{,}000$$

  $$x_1 + x_2 = 2.0$$

Forward elimination (naïve):

$$2\,x_1 + 100.000\,x_2 = 100.000$$

$$-500000x_2 = -500000$$

Solve $x_2 = 1$ & $x_1 = 0$

- **Forward elimination (**gauss elimination)**:**

  $$\mathbf{2\,x_1 + 100.000\,x_2 = 100.000}$$

  $$\mathbf{-\,99998\,x_2 = -99996}$$

  Solve $x_2 = 0.9998$ & $x_1 = 1.0002$

- The exact solution is $x_1 = 1.00002$ & $x_2 = 0.99998$

Scaling: Example (cont'd)

B) Using the scaling algorithm to solve:

$$2\,x_1 + 100{,}000\,x_2 = 100{,}000$$
$$x_1 + x_2 = 2.0$$

Scaling the first equation by dividing by 100,000:

$$0.00002\,x_1 + x_2 = 1.0$$
$$x_1 + x_2 = 2.0$$

Rows are pivoted:

$$x_1 + x_2 = 2.0$$
$$0.00002\,x_1 + x_2 = 1.0$$

Forward elimination yield:

$$x_1 + x_2 = 2.0$$
$$x_2 = 1.00$$

Solve: $x_2 = 1.00$ & $x_1 = 1.00$

The exact solution is $x_1 = 1.00002$ & $x_2 = 0.99998$

Scaling: Example (cont'd)

C) The scaled coefficient indicate that pivoting is necessary.

Even use pivot but retain the original coefficient to give:

$$x_1 + x_2 = 2.0$$

$$2\,x_1 + 100{,}000\,x_2 = 100{,}000$$

Forward elimination yields:

$$x_1 + x_2 = 2.0$$

$$100{,}000\,x_2 = 100{,}000$$

Solve: $x_2 = 1.00$ & $x_1 = 1.00$

Thus, scaling was useful in determining whether pivoting was necessary, but the equation themselves did not require scaling to arrive at a correct result.

Determinate Evaluation

The determinate can be simply evaluated at the end of the forward elimination step, when the program employs partial pivoting:

$$D = a_{11} a'_{22} a''_{33} \ldots a_{nn}^{(n-1)} (-1)^{p}$$

where:

p represents the number of times that rows are pivoted

Example: Gauss Elimination

$$
\begin{array}{lllll}
 & +2x_2 & & +x_4 & =0 \\
2x_1 & +2x_2 & +3x_3 & +2x_4 & =-2 \\
4x_1 & -3x_2 & & +x_4 & =-7 \\
6x_1 & +x_2 & -6x_3 & -5x_4 & =6
\end{array}
$$

a) Forward Elimination

$$
\left[\begin{array}{cccc|c}
0 & 2 & 0 & 1 & 0 \\
2 & 2 & 3 & 2 & -2 \\
4 & -3 & 0 & 1 & -7 \\
6 & 1 & -6 & -5 & 6
\end{array}\right]
\quad R1 \rightleftarrows R4 \quad
\left[\begin{array}{cccc|c}
6 & 1 & -6 & -5 & 6 \\
2 & 2 & 3 & 2 & -2 \\
4 & -3 & 0 & 1 & -7 \\
0 & 2 & 0 & 1 & 0
\end{array}\right]
$$

Example: Gauss Elimination (cont'd)

$$\left[\begin{array}{cccc|c} 6 & 1 & -6 & -5 & 6 \\ 2 & 2 & 3 & 2 & -2 \\ 4 & -3 & 0 & 1 & -7 \\ 0 & 2 & 0 & 1 & 0 \end{array}\right] \begin{array}{l} \\ R2-0.33333\cdot R1 \\ R3-0.66667\cdot R1 \\ \\ \end{array}$$

$$\left[\begin{array}{cccc|c} 6 & 1 & -6 & -5 & 6 \\ 0 & 1.6667 & 5 & 3.6667 & -4 \\ 0 & -3.6667 & 4 & 4.3333 & -11 \\ 0 & 2 & 0 & 1 & 0 \end{array}\right] R2 \rightleftarrows R3$$

$$\left[\begin{array}{cccc|c} 6 & 1 & -6 & -5 & 6 \\ 0 & -3.6667 & 4 & 4.3333 & -11 \\ 0 & 1.6667 & 5 & 3.6667 & -4 \\ 0 & 2 & 0 & 1 & 0 \end{array}\right]$$

Example: Gauss Elimination (cont'd)

$$\left[\begin{array}{cccc|c} 6 & 1 & -6 & -5 & 6 \\ 0 & -3.6667 & 4 & 4.3333 & -11 \\ 0 & 1.6667 & 5 & 3.6667 & -4 \\ 0 & 2 & 0 & 1 & 0 \end{array}\right] \begin{array}{l} \\ \\ R3+0.45455\cdot R2 \\ R4+0.54545\cdot R2 \end{array}$$

$$\left[\begin{array}{cccc|c} 6 & 1 & -6 & -5 & 6 \\ 0 & -3.6667 & 4 & 4.3333 & -11 \\ 0 & 0 & 6.8182 & 5.6364 & -9.0001 \\ 0 & 0 & 2.1818 & 3.3636 & -5.9999 \end{array}\right] \begin{array}{l} \\ \\ \\ R4-0.32000\cdot R3 \end{array}$$

$$\left[\begin{array}{cccc|c} 6 & 1 & -6 & -5 & 6 \\ 0 & -3.6667 & 4 & 4.3333 & -11 \\ 0 & 0 & 6.8182 & 5.6364 & -9.0001 \\ 0 & 0 & 0 & 1.5600 & -3.1199 \end{array}\right]$$

Example: Gauss Elimination (cont'd)

$$\left[\begin{array}{cccc|c} 6 & 1 & -6 & -5 & 6 \\ 0 & -3.6667 & 4 & 4.3333 & -11 \\ 0 & 0 & 6.8182 & 5.6364 & -9.0001 \\ 0 & 0 & 0 & 1.5600 & -3.1199 \end{array}\right]$$

b) Back Substitution

$$x_4 = \frac{-3.1199}{1.5600} = -1.9999$$

$$x_3 = \frac{-9.0001 - 5.6364(-1.9999)}{6.8182} = 0.33325$$

$$x_2 = \frac{-11 - 4.3333(-1.9999) - 4(0.33325)}{-3.6667} = 1.0000$$

$$x_1 = \frac{6 + 5(-1.9999) + 6(0.33325) - 1(1.0000)}{6} = -0.50000$$

Naïve Gauss Elimination (cont'd)

$$\left[\begin{array}{cccc|c} 6 & 1 & -6 & -5 & 6 \\ 0 & -3.6667 & 4 & 4.3333 & -11 \\ 0 & 0 & 6.8182 & 5.6364 & -9.0001 \\ 0 & 0 & 0 & 1.5600 & -3.1199 \end{array}\right]$$

$$\left[\begin{array}{cccc|c} 1 & 1 & -6 & -5 & 6 \\ 0 & 1 & 4 & 4.3333 & -11 \\ 0 & 0 & 1 & 5.6364 & -9.0001 \\ 0 & 0 & 0 & 1 & -2.05 \end{array}\right]$$

b) Back Substitution

$$x_4 = \frac{-3.1199}{1.5600} = -1.9999$$

$$x_3 = \frac{-9.0001 - 5.6364(-1.9999)}{6.8182} = 0.33325$$

$$x_2 = \frac{-11 - 4.3333(-1.9999) - 4(0.33325)}{-3.6667} = 1.0000$$

$$x_1 = \frac{6 + 5(-1.9999) + 6(0.33325) - 1(1.0000)}{6} = -0.50000$$