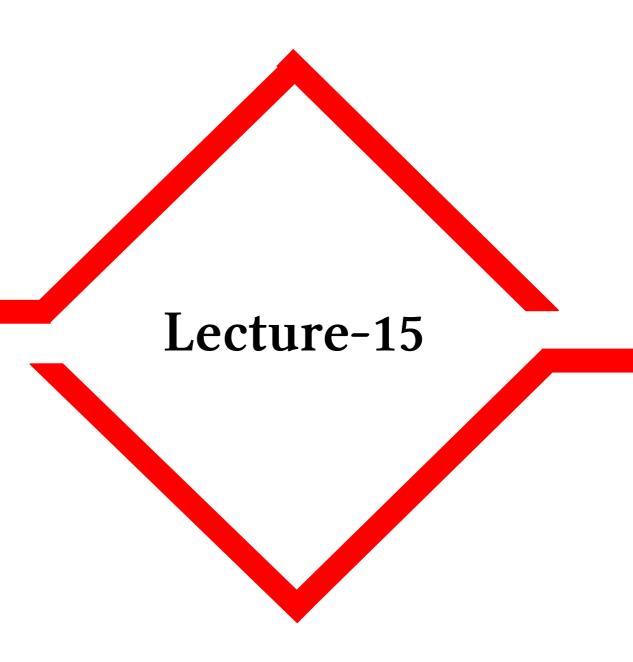
Computational Physics

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Physics Group, University of Qom



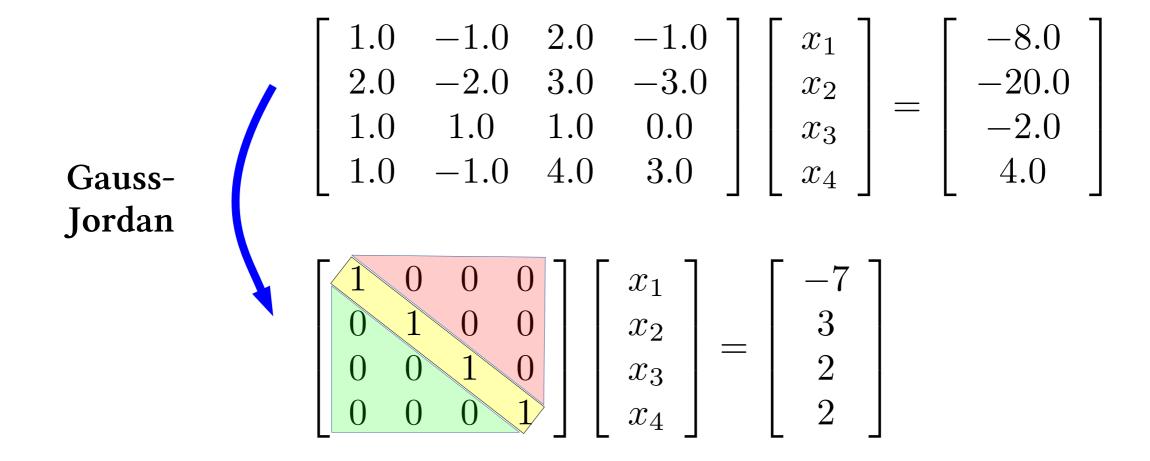
Contents

- Basis Concepts
- Numerical Differentiation
- Numerical Integration
- Numerical Finding Root
- Classical Scattering
- Solving Linear Systems

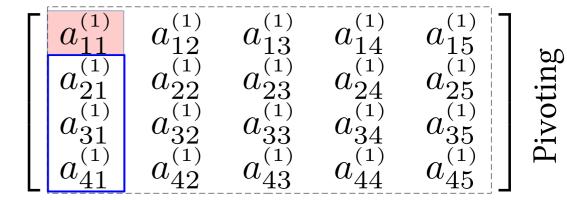
• Gauss-Jordan Method (Gauss-Jordan Elimination)

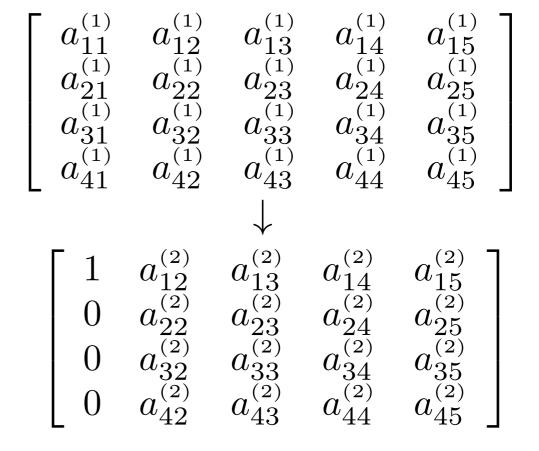
$$\begin{bmatrix} 1.0 & -1.0 & 2.0 & -1.0 \\ 2.0 & -2.0 & 3.0 & -3.0 \\ 1.0 & 1.0 & 1.0 & 0.0 \\ 1.0 & -1.0 & 4.0 & 3.0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -8.0 \\ -20.0 \\ -2.0 \\ 4.0 \end{bmatrix}$$

The basic idea of Gauss-Jordan method is to transform the original linear equation set to one that has **unit** coefficient matrix.

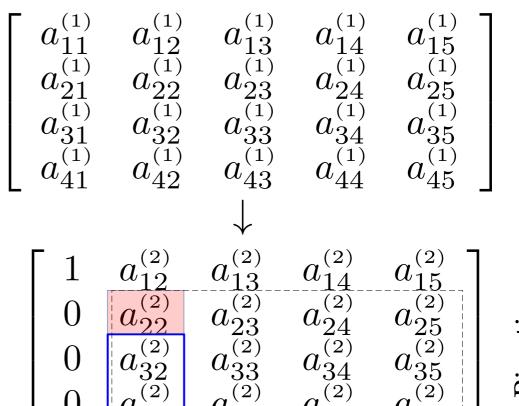


| $a_{11}^{(1)}$ | $a_{12}^{_{(1)}}$ | $a_{13}^{(1)}$ | $a_{14}^{(1)}$ | $a_{15}^{(1)}$ |
|----------------------|----------------------|----------------|---------------------------|----------------|
| $a_{21}^{\bar{(1)}}$ | $a_{22}^{\bar{(1)}}$ | $a_{23}^{(1)}$ | $a_{24}^{\overline{(1)}}$ | $a_{25}^{(1)}$ |
| $a_{31}^{(1)}$ | $a_{32}^{(1)}$ | $a_{33}^{(1)}$ | $a_{34}^{(1)}$ | $a_{35}^{(1)}$ |
| $a_{41}^{(1)}$ | $a_{42}^{(1)}$ | $a_{43}^{(1)}$ | $a_{44}^{(1)}$ | $a_{45}^{(1)}$ |

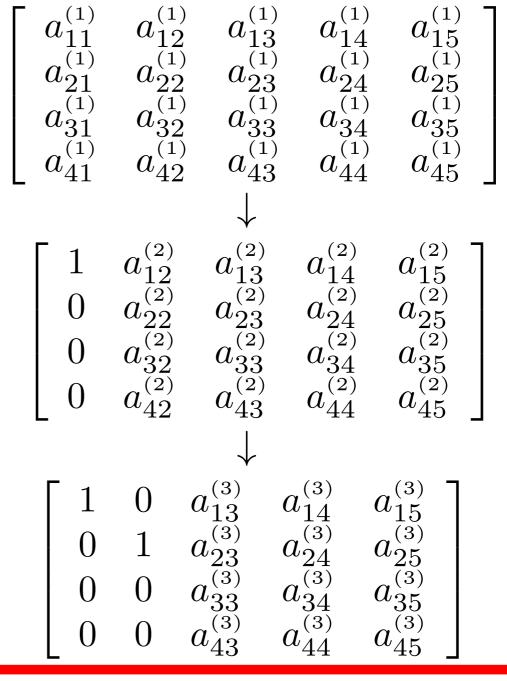


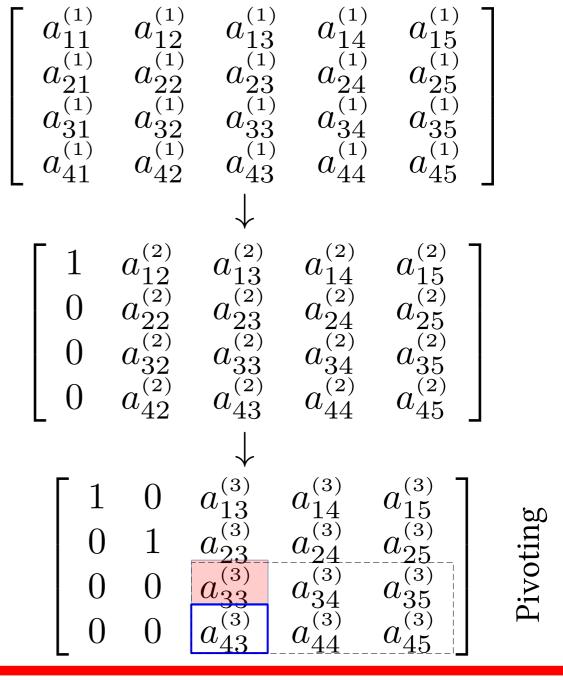


• Gauss-Jordan Method



Pivoting





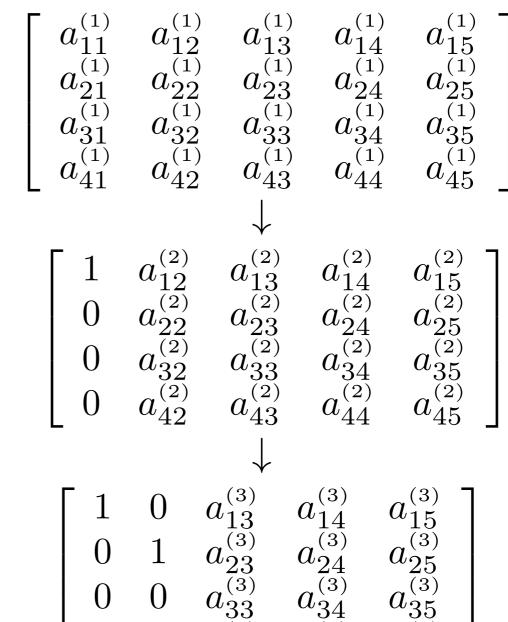
$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} & a_{14}^{(1)} & a_{15}^{(1)} \\ a_{21}^{(1)} & a_{22}^{(1)} & a_{23}^{(1)} & a_{24}^{(1)} & a_{25}^{(1)} \\ a_{31}^{(1)} & a_{32}^{(1)} & a_{33}^{(1)} & a_{34}^{(1)} & a_{35}^{(1)} \\ a_{41}^{(1)} & a_{42}^{(1)} & a_{43}^{(1)} & a_{44}^{(1)} & a_{45}^{(1)} \end{bmatrix} \\ \downarrow \\ \begin{bmatrix} 1 & a_{12}^{(2)} & a_{13}^{(2)} & a_{14}^{(2)} & a_{45}^{(2)} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & a_{24}^{(2)} & a_{25}^{(2)} \\ 0 & a_{32}^{(2)} & a_{33}^{(2)} & a_{34}^{(2)} & a_{45}^{(2)} \end{bmatrix} \\ \downarrow \\ \begin{bmatrix} 1 & 0 & a_{13}^{(3)} & a_{14}^{(3)} & a_{15}^{(3)} \\ 0 & a_{42}^{(2)} & a_{43}^{(2)} & a_{24}^{(2)} & a_{25}^{(2)} \\ 0 & 0 & a_{33}^{(3)} & a_{34}^{(3)} & a_{35}^{(3)} \\ 0 & 0 & a_{33}^{(3)} & a_{34}^{(3)} & a_{35}^{(3)} \\ 0 & 0 & a_{43}^{(3)} & a_{44}^{(3)} & a_{45}^{(3)} \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & a_{14}^{(4)} & a_{15}^{(4)} \\ 0 & 1 & 0 & a_{24}^{(4)} & a_{25}^{(4)} \\ 0 & 0 & 1 & a_{34}^{(4)} & a_{35}^{(4)} \\ 0 & 0 & 0 & a_{45}^{(4)} & a_{45}^{(4)} \end{bmatrix}$$

$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} & a_{14}^{(1)} & a_{15}^{(1)} \\ a_{21}^{(1)} & a_{22}^{(1)} & a_{23}^{(1)} & a_{24}^{(1)} & a_{25}^{(1)} \\ a_{31}^{(1)} & a_{32}^{(1)} & a_{33}^{(1)} & a_{34}^{(1)} & a_{35}^{(1)} \\ a_{41}^{(1)} & a_{42}^{(1)} & a_{43}^{(1)} & a_{44}^{(1)} & a_{45}^{(1)} \end{bmatrix} \\ \downarrow \\ \begin{bmatrix} 1 & a_{12}^{(2)} & a_{13}^{(2)} & a_{14}^{(2)} & a_{15}^{(2)} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & a_{24}^{(2)} & a_{25}^{(2)} \\ 0 & a_{32}^{(2)} & a_{33}^{(2)} & a_{34}^{(2)} & a_{45}^{(2)} \end{bmatrix} \\ \downarrow \\ \begin{bmatrix} 1 & 0 & a_{13}^{(3)} & a_{14}^{(3)} & a_{15}^{(3)} \\ 0 & a_{42}^{(2)} & a_{43}^{(2)} & a_{24}^{(2)} & a_{25}^{(2)} \\ 0 & a_{33}^{(3)} & a_{34}^{(3)} & a_{44}^{(3)} \end{bmatrix} \\ \downarrow \\ \begin{bmatrix} 1 & 0 & a_{13}^{(3)} & a_{14}^{(3)} & a_{15}^{(3)} \\ 0 & 1 & a_{23}^{(3)} & a_{24}^{(3)} & a_{25}^{(3)} \\ 0 & 0 & a_{33}^{(3)} & a_{34}^{(3)} & a_{35}^{(3)} \\ 0 & 0 & a_{43}^{(3)} & a_{44}^{(3)} & a_{45}^{(3)} \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 & a_{15}^{(5)} \\ 0 & 1 & 0 & 0 & a_{25}^{(5)} \\ 0 & 0 & 1 & 0 & a_{35}^{(5)} \\ 0 & 0 & 0 & 1 & a_{45}^{(5)} \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & a_{14}^{(4)} & a_{15}^{(4)} \\ 0 & 1 & 0 & a_{24}^{(4)} & a_{25}^{(4)} \\ 0 & 0 & 1 & a_{34}^{(4)} & a_{35}^{(4)} \\ 0 & 0 & 0 & a_{45}^{(4)} & a_{45}^{(4)} \end{bmatrix}$$



$$\begin{bmatrix} 1 & 0 & a_{13}^{(3)} & a_{14}^{(3)} & a_{15}^{(3)} \\ 0 & 1 & a_{23}^{(3)} & a_{24}^{(3)} & a_{25}^{(3)} \\ 0 & 0 & a_{33}^{(3)} & a_{34}^{(3)} & a_{35}^{(3)} \\ 0 & 0 & a_{43}^{(3)} & a_{44}^{(3)} & a_{45}^{(3)} \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 & a_{15}^{(5)} \\ 0 & 1 & 0 & 0 & a_{25}^{(5)} \\ 0 & 0 & 1 & 0 & a_{35}^{(5)} \\ 0 & 0 & 0 & 1 & a_{45}^{(5)} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & -7 \\ 0 & 1 & 0 & 0 & 3 \\ 0 & 0 & 1 & 0 & 2 \\ 0 & 0 & 0 & 1 & 2 \end{bmatrix}$$

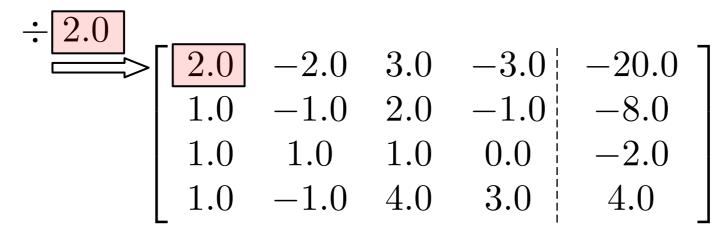
$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -7 \\ 3 \\ 2 \\ 2 \end{bmatrix}$$

Gauss-Jordan
$$\begin{bmatrix} 1.0 & -1.0 & 2.0 & -1.0 \\ 2.0 & -2.0 & 3.0 & -3.0 \\ 1.0 & 1.0 & 1.0 & 0.0 \\ 1.0 & -1.0 & 4.0 & 3.0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -8.0 \\ -20.0 \\ -2.0 \\ 4.0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -7 \\ 3 \\ 2 \\ 2 \end{bmatrix}$$

Gauss-Jordan Method

Pivot Step



$$\begin{bmatrix} 1.0 & -1.0 & 1.5 & -1.5 & -10.0 \\ 1.0 & -1.0 & 2.0 & -1.0 & -8.0 \\ 1.0 & 1.0 & 1.0 & 0.0 & -2.0 \\ 1.0 & -1.0 & 4.0 & 3.0 & 4.0 \end{bmatrix}$$

$$R_1 = \begin{bmatrix} 1.0 & -1.0 & 1.5 & -1.5 & -10.0 \\ 0 & 0 & 0.5 & 0.5 & 2.0 \\ 0 & 0 & 0.5 & 1.5 & 8.0 \\ 0 & 0 & 0 & 2.5 & 4.5 & 14.0 \end{bmatrix}$$

Gauss-Jordan Method

Pivot Step

$$\begin{bmatrix} 1.0 & -1.0 & 1.5 & -1.5 & -10.0 \\ \hline 0 & 2.0 & -0.5 & 1.5 & 8.0 \\ \hline 0 & 0 & 0.5 & 0.5 & 2.0 \\ \hline 0 & 0 & 2.5 & 4.5 & 14.0 \end{bmatrix} \leftarrow \begin{bmatrix} 1.0 & -1.0 & 1.5 & -1.5 & -10.0 \\ 0 & 0 & 0.5 & 0.5 & 2.0 \\ \hline 0 & 0 & 2.5 & 4.5 & 14.0 \end{bmatrix} \leftarrow \begin{bmatrix} 1.0 & -1.0 & 1.5 & -1.5 & -10.0 \\ 0 & 0 & 0.5 & 0.5 & 2.0 \\ \hline 0 & 2.0 & -0.5 & 1.5 & 8.0 \\ \hline 0 & 0 & 2.5 & 4.5 & 14.0 \end{bmatrix} \leftarrow \begin{bmatrix} 1.0 & -1.0 & 1.5 & -1.5 & -10.0 \\ 0 & 0 & 0.5 & 0.5 & 2.0 \\ \hline 0 & 2.0 & -0.5 & 1.5 & 8.0 \\ \hline 0 & 0 & 2.5 & 4.5 & 14.0 \end{bmatrix}$$

$$R_1 - (-1) \times R_2 \begin{bmatrix} 1.0 & 0.0 & 1.25 & -0.75 & -6.0 \\ 0 & 1.0 & -0.25 & 0.75 & 4.0 \\ R_3 - 0 \times R_2 & 0 & 0.5 & 0.5 & 2.0 \\ R_4 - 0 \times R_2 & 0 & 0 & 2.5 & 4.5 & 14.0 \end{bmatrix}$$

2.5

4.5

Gauss-Jordan Method

Pivot Step

$$\begin{bmatrix} 1.0 & 0.0 & 1.25 & -0.75 & | -6.0 \\ 0 & 1.0 & -0.25 & 0.75 & | 4.0 \\ \hline 0 & 0 & 2.5 & | 4.5 & | 14.0 \\ \hline 0 & 0 & 0.5 & | 0.5 & | 2.0 \end{bmatrix} \begin{bmatrix} 1.0 & 0.0 & 1.25 & -0.75 & | -6.0 \\ 0 & 1.0 & -0.25 & | 0.75 & | 4.0 \\ \hline 0 & 0 & 0.5 & | 0.75 & | -6.0 \\ \hline 0 & 1.0 & -0.25 & | 0.75 & | 4.0 \\ \hline 0 & 0 & 0.5 & | 0.5 & | 2.0 \end{bmatrix}$$

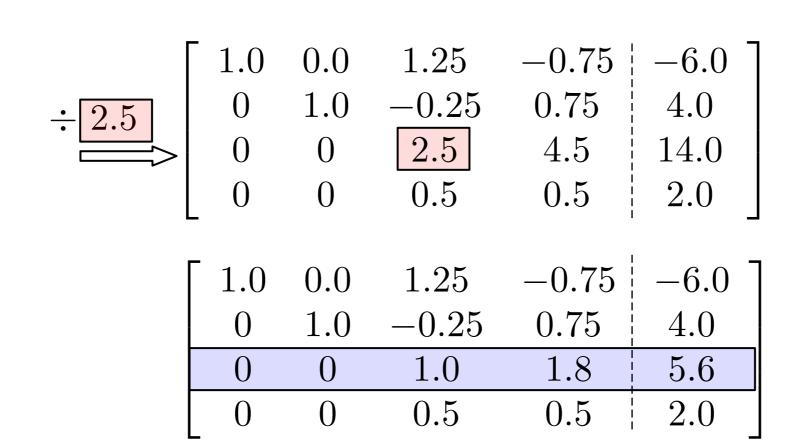
0

0

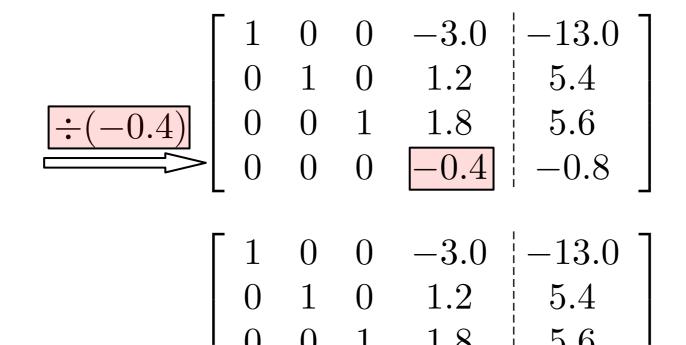
14.0

14.0

4.5



$$R_1 - 1.25 \times R_3$$
 $R_2 - (-0.25) \times R_3$
 R_3
 $R_4 - 0.5 \times R_3$
 R_3
 $R_4 - 0.5 \times R_3$
 R_3
 $R_4 - 0.5 \times R_3$
 R_5
 R_6
 R_7
 R_8
 R_8
 R_9
 R_9



$$R_1 - (-3.0) \times R_4$$
 $R_2 - 1.2 \times R_4$
 $R_3 - 1.8 \times R_4$
 R_4
 R_5
 R_6
 R_6

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

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -7 \\ 3 \\ 2 \\ 2 \end{bmatrix}$$

$$x_1 = -7, \quad x_2 = 3, \quad x_1 = 2, \quad x_4 = 2$$