Computational Physics

Lecture-16

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Contents

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

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$AA^{-1} = A^{-1}A = I$$

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{12} & a_{12} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}, \qquad I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$A^{-1} = \begin{bmatrix} \alpha_{11} & \alpha_{12} & a_{12} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} & \alpha_{24} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} & \alpha_{34} \\ \alpha_{41} & \alpha_{42} & \alpha_{43} & \alpha_{44} \end{bmatrix}, \qquad A^{-1} = ?$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$AA^{-1} = A^{-1}A = I$$

Gauss-Jordan

$$\left[\begin{array}{cccc|cccc} a_{11} & a_{12} & a_{12} & a_{12} & 1 & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} & 0 & 1 & 0 & 0 \\ a_{31} & a_{32} & a_{33} & a_{34} & 0 & 0 & 1 & 0 \\ a_{41} & a_{42} & a_{43} & a_{44} & 0 & 0 & 0 & 1 \end{array}\right]$$

$$\left[\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & \alpha_{11} & \alpha_{12} & a_{12} & \alpha_{12} \\ 0 & 1 & 0 & 0 & \alpha_{21} & \alpha_{22} & \alpha_{23} & \alpha_{24} \\ 0 & 0 & 1 & 0 & \alpha_{31} & \alpha_{32} & \alpha_{33} & \alpha_{34} \\ 0 & 0 & 0 & 1 & \alpha_{41} & \alpha_{42} & \alpha_{43} & \alpha_{44} \end{array}\right]$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$AA^{-1} = A^{-1}A = I$$

Gauss-Jordan

$$\left[\begin{array}{cccc|cccc} a_{11} & a_{12} & a_{12} & a_{12} & 1 & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} & 0 & 1 & 0 & 0 \\ a_{31} & a_{32} & a_{33} & a_{34} & 0 & 0 & 1 & 0 \\ a_{41} & a_{42} & a_{43} & a_{44} & 0 & 0 & 0 & 1 \end{array}\right]$$

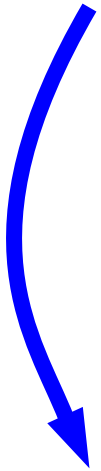
$$\left[\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & \alpha_{11} & \alpha_{12} & a_{12} & \alpha_{12} \\ 0 & 1 & 0 & 0 & \alpha_{21} & \alpha_{22} & \alpha_{23} & \alpha_{24} \\ 0 & 0 & 1 & 0 & \alpha_{31} & \alpha_{32} & \alpha_{33} & \alpha_{34} \\ 0 & 0 & 0 & 1 & \alpha_{41} & \alpha_{42} & \alpha_{43} & \alpha_{44} \end{array}\right]$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$\left[\begin{array}{cccc|cccc} 1.0 & -1.0 & 2.0 & -1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 2.0 & -2.0 & 3.0 & -3.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 \\ 1.0 & -1.0 & 4.0 & 3.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{array}\right]$$

Gauss-Jordan



$$\left[\begin{array}{cccc|cccc} 1.0 & 0.0 & 0.0 & 0.0 & -0.75 & 3.5 & 0.5 & 1.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 3.0 & -1.5 & 0.5 & -0.5 \\ 0.0 & 0.0 & 1.0 & 0.0 & 4.5 & -2.0 & 0.0 & -0.5 \\ 0.0 & 0.0 & 00 & 1.0 & -2.5 & 1.0 & 0.0 & 0.5 \end{array}\right]$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$A^{-1} = \begin{bmatrix} -0.75 & 3.5 & 0.5 & 1.0 \\ 3.0 & -1.5 & 0.5 & -0.5 \\ 4.5 & -2.0 & 0.0 & -0.5 \\ -2.5 & 1.0 & 0.0 & 0.5 \end{bmatrix}$$

$$AX = B$$

$$\xrightarrow{A^{-1}} A^{-1}AX = A^{-1}B \qquad \xrightarrow{A^{-1}A = I} IX = A^{-1}B$$

$$\xrightarrow{IX = X} X = A^{-1}B$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$A^{-1} = \begin{bmatrix} -0.75 & 3.5 & 0.5 & 1.0 \\ 3.0 & -1.5 & 0.5 & -0.5 \\ 4.5 & -2.0 & 0.0 & -0.5 \\ -2.5 & 1.0 & 0.0 & 0.5 \end{bmatrix}$$

$$X = A^{-1}B$$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -0.75 & 3.5 & 0.5 & 1.0 \\ 3.0 & -1.5 & 0.5 & -0.5 \\ 4.5 & -2.0 & 0.0 & -0.5 \\ -2.5 & 1.0 & 0.0 & 0.5 \end{bmatrix} \begin{bmatrix} -8.0 \\ -20.0 \\ -2.0 \\ 4.0 \end{bmatrix} = \begin{bmatrix} -7.0 \\ 3.0 \\ 2.0 \\ 2.0 \end{bmatrix}$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

Pivot Step

$$\left[\begin{array}{cccc|cccc}
1.0 & -1.0 & 2.0 & -1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\
2.0 & -2.0 & 3.0 & -3.0 & 0.0 & 1.0 & 0.0 & 0.0 \\
1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 \\
1.0 & -1.0 & 4.0 & 3.0 & 0.0 & 0.0 & 0.0 & 1.0
\end{array}\right]$$

$$\left[\begin{array}{cccc|cccc}
2.0 & -2.0 & 3.0 & -3.0 & 0.0 & 1.0 & 0.0 & 0.0 \\
1.0 & -1.0 & 2.0 & -1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\
1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 \\
1.0 & -1.0 & 4.0 & 3.0 & 0.0 & 0.0 & 0.0 & 1.0
\end{array}\right]$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$\div 2.0 \Longrightarrow \left[\begin{array}{cccc|cccc} \boxed{2.0} & -2.0 & 3.0 & -3.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ 1.0 & -1.0 & 2.0 & -1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 \\ 1.0 & -1.0 & 4.0 & 3.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{array}\right]$$

$$\left[\begin{array}{cccc|cccc} \boxed{1.0} & -1.0 & 1.5 & -1.5 & 0.0 & 0.5 & 0.0 & 0.0 \\ 1.0 & -1.0 & 2.0 & -1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 \\ 1.0 & -1.0 & 4.0 & 3.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{array}\right]$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$
\begin{array}{c}
R_1 \\ R_2 \\ R_3 \\ R_4
\end{array}
\left[\begin{array}{cccc:cccc}
1.0 & -1.0 & 1.5 & -1.5 & 0.0 & 0.5 & 0.0 & 0.0 \\
1.0 & -1.0 & 2.0 & -1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\
1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 \\
1.0 & -1.0 & 4.0 & 3.0 & 0.0 & 0.0 & 0.0 & 1.0
\end{array}\right]
$$

$$
\begin{array}{c}
R_1 \\ R_2 - 1.0 \times R_1 \\ R_3 - 1.0 \times R_1 \\ R_4 - 1.0 \times R_1
\end{array}
\left[\begin{array}{cccc:cccc}
1.0 & -1.0 & 1.5 & -1.5 & 0.0 & 0.5 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.5 & 0.5 & 1.0 & -0.5 & 0.0 & 0.0 \\
0.0 & 2.0 & -0.5 & 1.5 & 0.0 & -0.5 & 1.0 & 0.0 \\
0.0 & 0.0 & 2.5 & 4.5 & 0.0 & -0.5 & 0.0 & 1.0
\end{array}\right]
$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

Pivot Step

$$\left[\begin{array}{cccc|cccc} 1.0 & -1.0 & 1.5 & -1.5 & 0.0 & 0.5 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.5 & 0.5 & 1.0 & -0.5 & 0.0 & 0.0 \\ 0.0 & 2.0 & -0.5 & 1.5 & 0.0 & -0.5 & 1.0 & 0.0 \\ 0.0 & 0.0 & 2.5 & 4.5 & 0.0 & -0.5 & 0.0 & 1.0 \end{array}\right]$$

$$\left[\begin{array}{cccc|cccc} 1.0 & -1.0 & 1.5 & -1.5 & 0.0 & 0.5 & 0.0 & 0.0 \\ 0.0 & 2.0 & -0.5 & 1.5 & 0.0 & -0.5 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.5 & 0.5 & 1.0 & -0.5 & 0.0 & 0.0 \\ 0.0 & 0.0 & 2.5 & 4.5 & 0.0 & -0.5 & 0.0 & 1.0 \end{array}\right]$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$\div \boxed{2.0} \Longrightarrow \left[\begin{array}{cccc|cccc} 1.0 & -1.0 & 1.5 & -1.5 & 0.0 & 0.5 & 0.0 & 0.0 \\ 0.0 & \boxed{2.0} & -0.5 & 1.5 & 0.0 & -0.5 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.5 & 0.5 & 1.0 & -0.5 & 0.0 & 0.0 \\ 0.0 & 0.0 & 2.5 & 4.5 & 0.0 & -0.5 & 0.0 & 1.0 \end{array}\right]$$

$$\left[\begin{array}{cccc|cccc} 1.0 & -1.0 & 1.5 & -1.5 & 0.0 & 0.5 & 0.0 & 0.0 \\ \boxed{0.0} & \boxed{1.0} & \boxed{-0.25} & \boxed{0.75} & \boxed{0.0} & \boxed{-0.25} & \boxed{0.5} & \boxed{0.0} \\ 0.0 & 0.0 & 0.5 & 0.5 & 1.0 & -0.5 & 0.0 & 0.0 \\ 0.0 & 0.0 & 2.5 & 4.5 & 0.0 & -0.5 & 0.0 & 1.0 \end{array}\right]$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$
\begin{array}{c}
R_1 \\ R_2 \\ R_3 \\ R_4
\end{array}
\left[\begin{array}{cccc:cccc}
1.0 & -1.0 & 1.5 & -1.5 & 0.0 & 0.5 & 0.0 & 0.0 \\
0.0 & 1.0 & -0.25 & 0.75 & 0.0 & -0.25 & 0.5 & 0.0 \\
0.0 & 0.0 & 0.5 & 0.5 & 1.0 & -0.5 & 0.0 & 0.0 \\
0.0 & 0.0 & 2.5 & 4.5 & 0.0 & -0.5 & 0.0 & 1.0
\end{array}\right]
$$

$$
\begin{array}{r}
R_1 - (-1.0) \times R_2 \\ R_2 \\ R_3 - 0.0 \times R_2 \\ R_4 - 0.0 \times R_2
\end{array}
\left[\begin{array}{cccc:cccc}
1.0 & 0.0 & 1.25 & -0.75 & 0.0 & 0.25 & 0.5 & 0.0 \\
0.0 & 1.0 & -0.25 & 0.75 & 0.0 & -0.25 & 0.5 & 0.0 \\
0.0 & 0.0 & 0.5 & 0.5 & 1.0 & -0.5 & 0.0 & 0.0 \\
0.0 & 0.0 & 2.5 & 4.5 & 0.0 & -0.5 & 0.0 & 1.0
\end{array}\right]
$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

Pivot Step

$$\begin{bmatrix} 1.0 & 0.0 & 1.25 & -0.75 & 0.0 & 0.25 & 0.5 & 0.0 \\ 0.0 & 1.0 & -0.25 & 0.75 & 0.0 & -0.25 & 0.5 & 0.0 \\ 0.0 & 0.0 & 0.5 & 0.5 & 1.0 & -0.5 & 0.0 & 0.0 \\ 0.0 & 0.0 & 2.5 & 4.5 & 0.0 & -0.5 & 0.0 & 1.0 \end{bmatrix}$$

$$\begin{bmatrix} 1.0 & 0.0 & 1.25 & -0.75 & 0.0 & 0.25 & 0.5 & 0.0 \\ 0.0 & 1.0 & -0.25 & 0.75 & 0.0 & -0.25 & 0.5 & 0.0 \\ 0.0 & 0.0 & 2.5 & 4.5 & 0.0 & -0.5 & 0.0 & 1.0 \\ 0.0 & 0.0 & 0.5 & 0.5 & 1.0 & -0.5 & 0.0 & 0.0 \end{bmatrix}$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$\div \boxed{2.5} \Longrightarrow \left[\begin{array}{cccc|cccc} 1.0 & 0.0 & 1.25 & -0.75 & 0.0 & 0.25 & 0.5 & 0.0 \\ 0.0 & 1.0 & -0.25 & 0.75 & 0.0 & -0.25 & 0.5 & 0.0 \\ 0.0 & 0.0 & \boxed{2.5} & 4.5 & 0.0 & -0.5 & 0.0 & 1.0 \\ 0.0 & 0.0 & 0.5 & 0.5 & 1.0 & -0.5 & 0.0 & 0.0 \end{array}\right]$$

$$\left[\begin{array}{cccc|cccc} 1.0 & 0.0 & 1.25 & -0.75 & 0.0 & 0.25 & 0.5 & 0.0 \\ 0.0 & 1.0 & -0.25 & 0.75 & 0.0 & -0.25 & 0.5 & 0.0 \\ \boxed{0.0} & \boxed{0.0} & \boxed{1.0} & \boxed{1.8} & \boxed{0.0} & \boxed{-0.2} & \boxed{0.0} & \boxed{0.4} \\ 0.0 & 0.0 & 0.5 & 0.5 & 1.0 & -0.5 & 0.0 & 0.0 \end{array}\right]$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$
\begin{array}{c}
R_1 \\ R_2 \\ R_3 \\ R_4
\end{array}
\left[\begin{array}{cccc:cccc}
1.0 & 0.0 & 1.25 & -0.75 & 0.0 & 0.25 & 0.5 & 0.0 \\
0.0 & 1.0 & -0.25 & 0.75 & 0.0 & -0.25 & 0.5 & 0.0 \\
0.0 & 0.0 & 1.0 & 1.8 & 0.0 & -0.2 & 0.0 & 0.4 \\
0.0 & 0.0 & 0.5 & 0.5 & 1.0 & -0.5 & 0.0 & 0.0
\end{array}\right]
$$

$$
\begin{array}{r}
R_1 - 1.25 \times R_3 \\
R_2 - (-0.25) \times R_3 \\
R_3 \\
R_4 - 0.5 \times R_3
\end{array}
\left[\begin{array}{cccc:cccc}
1.0 & 0.0 & 0.0 & -3.0 & 0.0 & 0.5 & 0.5 & -0.5 \\
0.0 & 1.0 & 0.0 & 1.2 & 0.0 & -0.3 & 0.5 & 0.1 \\
0.0 & 0.0 & 1.0 & 1.8 & 0.0 & -0.2 & 0.0 & 0.4 \\
0.0 & 0.0 & 0.0 & -0.4 & 1.0 & -0.4 & 0.0 & -0.2
\end{array}\right]
$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$\div \boxed{(-0.4)} \Longrightarrow \left[\begin{array}{cccc|cccc} 1.0 & 0.0 & 0.0 & -3.0 & 0.0 & 0.5 & 0.5 & -0.5 \\ 0.0 & 1.0 & 0.0 & 1.2 & 0.0 & -0.3 & 0.5 & 0.1 \\ 0.0 & 0.0 & 1.0 & 1.8 & 0.0 & -0.2 & 0.0 & 0.4 \\ 0.0 & 0.0 & 0.0 & \boxed{-0.4} & 1.0 & -0.4 & 0.0 & -0.2 \end{array}\right]$$

$$\left[\begin{array}{cccc|cccc} 1.0 & 0.0 & 0.0 & -3.0 & 0.0 & 0.5 & 0.5 & -0.5 \\ 0.0 & 1.0 & 0.0 & 1.2 & 0.0 & -0.3 & 0.5 & 0.1 \\ 0.0 & 0.0 & 1.0 & 1.8 & 0.0 & -0.2 & 0.0 & 0.4 \\ \boxed{0.0} & \boxed{0.0} & \boxed{0.0} & \boxed{1.0} & \boxed{-2.5} & \boxed{1.0} & \boxed{0.0} & \boxed{0.5} \end{array}\right]$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$
\begin{array}{c}
\\
R_1 \\ R_2 \\ R_3 \\ R_4
\end{array}
\left[\begin{array}{cccc:cccc}
1.0 & 0.0 & 0.0 & -3.0 & 0.0 & 0.5 & 0.5 & -0.5 \\
0.0 & 1.0 & 0.0 & 1.2 & 0.0 & -0.3 & 0.5 & 0.1 \\
0.0 & 0.0 & 1.0 & 1.8 & 0.0 & -0.2 & 0.0 & 0.4 \\
0.0 & 0.0 & 0.0 & 1.0 & -2.5 & 1.0 & 0.0 & 0.5
\end{array}\right]
$$

$$
\begin{array}{r}
R_1 - (-3.0) \times R_4 \\
R_2 - 1.2 \times R_4 \\
R_3 - 1.8 \times R_4 \\
R_4
\end{array}
\left[\begin{array}{cccc:cccc}
1.0 & 0.0 & 0.0 & 0.0 & -7.5 & 3.5 & 0.5 & 1.0 \\
0.0 & 1.0 & 0.0 & 0.0 & 3.0 & -1.5 & 0.5 & -0.5 \\
0.0 & 0.0 & 1.0 & 0.0 & 4.5 & -2.0 & 0.0 & -0.5 \\
0.0 & 0.0 & 0.0 & 1.0 & -2.5 & 1.0 & 0.0 & 0.5
\end{array}\right]
$$

Solving Linear Systems

- **Inverse Gauss-Jordan Method**

$$\left[\begin{array}{cccc|cccc} 1.0 & 0.0 & 0.0 & 0.0 & -7.5 & 3.5 & 0.5 & 1.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 3.0 & -1.5 & 0.5 & -0.5 \\ 0.0 & 0.0 & 1.0 & 0.0 & 4.5 & -2.0 & 0.0 & -0.5 \\ 0.0 & 0.0 & 0.0 & 1.0 & -2.5 & 1.0 & 0.0 & 0.5 \end{array}\right]$$

$$A^{-1} = \left[\begin{array}{cccc} -7.5 & 3.5 & 0.5 & 1.0 \\ 3.0 & -1.5 & 0.5 & -0.5 \\ 4.5 & -2.0 & 0.0 & -0.5 \\ -2.5 & 1.0 & 0.0 & 0.5 \end{array}\right]$$