Practical Numerical Training UKNum

Linear Equations

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Programm:

1) Introduction
2) Gauss elimination
3) Gauss with partial pivoting
4) Determinants
5) LU decomposition
6) Inverse of matrix using LU

Linear Equations

$$[A][X]=[C]$$

- Gaussian Elimination
- Gaussian Elimination with Partial Pivoting
- LU Decomposition / QR Decomposition
- Gauss-Seidel Iteration
- Sparce Matrix Solvers (e.g. Cholesky Decomposition)
- ...

Gaussian Elimination

Major: All Engineering Majors

Author(s): Autar Kaw

http://numericalmethods.eng.usf.edu

Transforming Numerical Methods Education for STEM Undergraduates

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

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

$$\downarrow$$

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

Forward Elimination

A set of n equations and n unknowns

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

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

$$\vdots \qquad \vdots$$

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

(n-1) steps of forward elimination

Forward Elimination

Step 1

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

$$\left[\frac{a_{21}}{a_{11}}\right](a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n = b_1)$$

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

Forward Elimination

Subtract the result from Equation 2.

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

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

$$\left(a_{22} - \frac{a_{21}}{a_{11}}a_{12}\right)x_2 + \ldots + \left(a_{2n} - \frac{a_{21}}{a_{11}}a_{1n}\right)x_n = b_2 - \frac{a_{21}}{a_{11}}b_1$$

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

Forward Elimination

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

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

End of Step 1

Forward Elimination

Step 2

Repeat the same procedure for the 3rd term of Equation 3.

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\
a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n &= b'_2 \\
a''_{33}x_3 + \ldots + a''_{3n}x_n &= b''_3 \\
\vdots \qquad \vdots \qquad & \\
a''_{n3}x_3 + \ldots + a''_{nn}x_n &= b''_n
\end{aligned}
$$

End of Step 2

Forward Elimination

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

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

End of Step (n-1)

Matrix Form at End of Forward Elimination

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a_{22}^{'} & a_{23}^{'} & \cdots & a_{2n}^{'} \\ 0 & 0 & a_{33}^{''} & \cdots & a_{3n}^{''} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & 0 & a_{nn}^{(n-1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2^{'} \\ b_3^{''} \\ \vdots \\ b_n^{(n\text{-}1)} \end{bmatrix}$$

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

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\
a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n &= b'_2 \\
a''_{33}x_3 + \ldots + a''_{n}x_n &= b''_3 \\
&\vdots \\
a_{nn}^{(n-1)}x_n &= b_n^{(n-1)}
\end{aligned}
$$

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

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

Then:

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

Or:

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

Naïve Gauss Elimination Pitfalls

http://numericalmethods.eng.usf.edu

Pitfall#1. Division by zero

Example 1:

$$10x_2 - 7x_3 = 3$$
$$6x_1 + 2x_2 + 3x_3 = 11$$
$$5x_1 - x_2 + 5x_3 = 9$$

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

Is division by zero an issue here?

Example 2:

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

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

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

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

Is division by zero an issue here? YES

Example 2:

$$12x_1 + 10x_2 - 7x_3 = 15$$
$$6x_1 + 5x_2 + 3x_3 = 14$$
$$24x_1 - x_2 + 5x_3 = 28$$

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

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

Pitfall#2. Large Round-off Errors

Example:

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

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

- Does decrease 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 kth 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.

Matrix Form at Beginning of 2nd 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 (2nd 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 (2nd 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 2nd 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

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

Back Substitution Starting Eqns

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\
a_{22}^{'}x_2 + a_{23}^{'}x_3 + \ldots + a_{2n}^{'}x_n &= b_2^{'} \\
a_{33}^{"}x_3 + \ldots + a_n^{"}x_n &= b_3^{"} \\
&\vdots \\
a_{nn}^{(n-1)}x_n &= b_n^{(n-1)}
\end{aligned}
$$

Back Substitution

…all the same!

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

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

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

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, $\frac{64}{144} = 0.4444$

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix} \times 0.4444 = \begin{bmatrix} 63.99 & 5.333 & 0.4444 & \vdots & 124.1 \end{bmatrix}$$

Subtract the result from Equation 2

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

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.)

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

Divide Equation 1 by 144 and multiply it by 25, $\dfrac{25}{144} = 0.1736$

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix} \times 0.1736 = \begin{bmatrix} 25.00 & 2.083 & 0.1736 & \vdots & 48.47 \end{bmatrix}$$

Subtract the result from Equation 3

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

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, $\frac{2.667}{2.917} = 0.9143.$

$$\begin{bmatrix} 0 & 2.917 & 0.8264 & \vdots & 58.33 \end{bmatrix} \times 0.9143 = \begin{bmatrix} 0 & 2.667 & 0.7556 & \vdots & 53.33 \end{bmatrix}$$

Subtract the result from Equation 3

$$\begin{array}{r} \begin{bmatrix} 0 & 2.667 & 0.5556 & \vdots & 53.10 \end{bmatrix} \\ -\begin{bmatrix} 0 & 2.667 & 0.7556 & \vdots & 53.33 \end{bmatrix} \\ \hline \begin{bmatrix} 0 & 0 & -0.2 & \vdots & -0.23 \end{bmatrix} \end{array}$$

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

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

Solving for a_3

$$-0.2a_3 = -0.23$$

$$a_3 = \frac{-0.23}{-0.2}$$

$$= 1.15$$

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

$$2.917a_2 + 0.8264a_3 = 58.33$$

$$a_2 = \frac{58.33 - 0.8264a_3}{2.917}$$

$$= \frac{58.33 - 0.8264 \times 1.15}{2.917}$$

$$= 19.67$$

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

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

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

Theorem of Determinants

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

Theorem of Determinants

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

$$\det(\mathrm{A}) = a_{11} \times a_{22} \times \ldots \times a_{ii} \times \ldots \times a_{nn}$$

$$= \prod_{i=1}^{n} a_{ii}$$

Forward Elimination of a Square Matrix

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

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

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

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…

Finding the Determinant

After forward elimination

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

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

Determinants and Pivoting ?

What to do if division by zero may occur?

You can do pivoting, but be careful! The determinant may change sign!

<u>Theorem 3</u>

$[A]_{nxn}$ is a n x n matrix. If $[B]_{nxn}$ is a matrix created by switching collumns or rows in $[A]_{nxn}$,then det(A)=-det(B).

LU Decomposition

Major: All Engineering Majors

Authors: Autar Kaw

http://numericalmethods.eng.usf.edu

Transforming Numerical Methods Education for STEM Undergraduates

LU Decomposition

LU Decomposition is another method to solve a set of simultaneous linear equations

Which is better, Gauss Elimination or LU Decomposition?

To answer this, a closer look at LU decomposition is needed.

LU Decomposition

Method

For most non-singular matrix [A] that one could conduct Naïve Gauss Elimination forward elimination steps, one can always write it as

$$[A] = [L][U]$$

where

$[L]$ = lower triangular matrix

$[U]$ = upper triangular matrix

How does LU Decomposition work?

If solving a set of linear equations	$[A][X] = [C]$
If $[A] = [L][U]$ then	$[L][U][X] = [C]$
Multiply by	$[L]^{-1}$
Which gives	$[L]^{-1}[L][U][X] = [L]^{-1}[C]$
Remember $[L]^{-1}[L] = [I]$ which leads to	$[I][U][X] = [L]^{-1}[C]$
Now, if $[I][U] = [U]$ then	$[U][X] = [L]^{-1}[C]$
Now, let	$[L]^{-1}[C]=[Z]$
Which ends with	$[L][Z] = [C] \quad (1)$
and	$[U][X] = [Z] \quad (2)$

LU Decomposition

How can this be used?

Given $[A][X] = [C]$

1. Decompose $[A]$ into $[L]$ and $[U]$
2. Solve $[L][Z] = [C]$ for $[Z]$
3. Solve $[U][X] = [Z]$ for $[X]$

When is LU Decomposition better than Gaussian Elimination?

To solve $[A][X] = [B]$

Table. Time taken by methods

Gaussian Elimination	LU Decomposition
$T\left(\frac{8n^3}{3} + 12n^2 + \frac{4n}{3}\right)$	$T\left(\frac{8n^3}{3} + 12n^2 + \frac{4n}{3}\right)$

where T = clock cycle time and n = size of the matrix

So both methods are equally efficient.

To find inverse of [A]

Time taken by Gaussian Elimination

$$= n\left(CT|_{FE} + CT|_{BS}\right)$$

$$= T\left(\frac{8n^4}{3} + 12n^3 + \frac{4n^2}{3}\right)$$

Time taken by LU Decomposition

$$= CT|_{LU} + n \times CT|_{FS} + n \times CT|_{BS}$$

$$= T\left(\frac{32n^3}{3} + 12n^2 + \frac{20n}{3}\right)$$

Table 1 Comparing computational times of finding inverse of a matrix using LU decomposition and Gaussian elimination.

n	10	100	1000	10000
$CT\|_{\text{inverse GE}} / CT\|_{\text{inverse LU}}$	3.28	25.83	250.8	2501

Method: [A] Decompose to [L] and [U]

$$[A] = [L][U] = \begin{bmatrix} 1 & 0 & 0 \\ \ell_{21} & 1 & 0 \\ \ell_{31} & \ell_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

[*U*] is the same as the coefficient matrix at the end of the forward elimination step.

[*L*] is obtained using the *multipliers* that were used in the forward elimination process

Finding the [*U*] matrix

Using the Forward Elimination Procedure of Gauss Elimination

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

Step 1:

$$\frac{64}{25} = 2.56; \quad Row2 - Row1(2.56) = \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 144 & 12 & 1 \end{bmatrix}$$

$$\frac{144}{25} = 5.76; \quad Row3 - Row1(5.76) = \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & -16.8 & -4.76 \end{bmatrix}$$

Finding the [U] Matrix

Matrix after Step 1:

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

Step 2:

$$\frac{-16.8}{-4.8} = 3.5; \quad Row3 - Row2(3.5) = \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix}$$

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

Finding the [*L*] matrix

$$\begin{bmatrix} 1 & 0 & 0 \\ \ell_{21} & 1 & 0 \\ \ell_{31} & \ell_{32} & 1 \end{bmatrix}$$

Using the multipliers used during the Forward Elimination Procedure

From the first step of forward elimination

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

$$\ell_{21} = \frac{a_{21}}{a_{11}} = \frac{64}{25} = 2.56$$

$$\ell_{31} = \frac{a_{31}}{a_{11}} = \frac{144}{25} = 5.76$$

Finding the [L] Matrix

From the second step of forward elimination

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & -16.8 & -4.76 \end{bmatrix} \quad \ell_{32} = \frac{a_{32}}{a_{22}} = \frac{-16.8}{-4.8} = 3.5$$

$$[L] = \begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix}$$

Does [L][U] = [A]?

$$[L][U] = \begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix} \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} = \quad ?$$

Using LU Decomposition to solve SLEs

Solve the following set of linear equations using LU Decomposition

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

Using the procedure for finding the [*L*] and [*U*] matrices

$$[A] = [L][U] = \begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix} \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix}$$

Example

Set $[L][Z]=[C]$

$$\begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix}\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

Solve for $[Z]$

$$z_1 = 106.8$$

$$2.56z_1 + z_2 = 177.2$$

$$5.76z_1 + 3.5z_2 + z_3 = 279.2$$

Example

Complete the forward substitution to solve for $[Z]$

$$
\begin{aligned}
z_1 &= 106.8 \\
z_2 &= 177.2 - 2.56 z_1 \\
&= 177.2 - 2.56(106.8) \\
&= -96.2 \\
z_3 &= 279.2 - 5.76 z_1 - 3.5 z_2 \\
&= 279.2 - 5.76(106.8) - 3.5(-96.21) \\
&= 0.735
\end{aligned}
$$

$$
[Z] = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.21 \\ 0.735 \end{bmatrix}
$$

Example

Set $[U][X] = [Z]$

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

Solve for $[X]$

The 3 equations become

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

$$-4.8a_2 - 1.56a_3 = -96.21$$

$$0.7a_3 = 0.735$$

http://

Example

From the 3rd equation

$$0.7a_3 = 0.735$$

$$a_3 = \frac{0.735}{0.7}$$

$$a_3 = 1.050$$

Substituting in a_3 and using the second equation

$$-4.8a_2 - 1.56a_3 = -96.21$$

$$a_2 = \frac{-96.21 + 1.56a_3}{-4.8}$$

$$a_2 = \frac{-96.21 + 1.56(1.050)}{-4.8}$$

$$a_2 = 19.70$$

Example

Substituting in a_3 and a_2 using the first equation

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

$$\begin{aligned} a_1 &= \frac{106.8 - 5a_2 - a_3}{25} \\ &= \frac{106.8 - 5(19.70) - 1.050}{25} \\ &= 0.2900 \end{aligned}$$

Hence the Solution Vector is:

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0.2900 \\ 19.70 \\ 1.050 \end{bmatrix}$$

Finding the inverse of a square matrix

The inverse [B] of a square matrix [*A*] is defined as

$$[A][B] = [I] = [B][A]$$

Finding the inverse of a square matrix

How can LU Decomposition be used to find the inverse?

Assume the first column of $[B]$ to be $[b_{11} \ \ b_{12} \ \ \ldots \ b_{n1}]^T$

Using this and the definition of matrix multiplication

First column of $[B]$

$$[A]\begin{bmatrix} b_{11} \\ b_{21} \\ \vdots \\ b_{n1} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Second column of $[B]$

$$[A]\begin{bmatrix} b_{12} \\ b_{22} \\ \vdots \\ b_{n2} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}$$

The remaining columns in $[B]$ can be found in the same manner

Example: Inverse of a Matrix

Find the inverse of a square matrix [*A*]

$$[A]=\begin{bmatrix}25 & 5 & 1\\ 64 & 8 & 1\\ 144 & 12 & 1\end{bmatrix}$$

Using the decomposition procedure, the [*L*] and [*U*] matrices are found to be

$$[A]=[L][U]=\begin{bmatrix}1 & 0 & 0\\ 2.56 & 1 & 0\\ 5.76 & 3.5 & 1\end{bmatrix}\begin{bmatrix}25 & 5 & 1\\ 0 & -4.8 & -1.56\\ 0 & 0 & 0.7\end{bmatrix}$$

Example: Inverse of a Matrix

Solving for the each column of [*B*] requires two steps

1) Solve [*L*] [*Z*] = [*C*] for [*Z*]

2) Solve [*U*] [*X*] = [*Z*] for [*X*]

Step 1:

$$[L][Z]=[C]\rightarrow\begin{bmatrix}1 & 0 & 0\\ 2.56 & 1 & 0\\ 5.76 & 3.5 & 1\end{bmatrix}\begin{bmatrix}z_1\\ z_2\\ z_3\end{bmatrix}=\begin{bmatrix}1\\ 0\\ 0\end{bmatrix}$$

This generates the equations:

$$\begin{aligned} z_1 &= 1 \\ 2.56z_1 + z_2 &= 0 \\ 5.76z_1 + 3.5z_2 + z_3 &= 0 \end{aligned}$$

Example: Inverse of a Matrix

Solving for [*Z*]

$$
\begin{aligned}
z_1 &= 1 \\
z_2 &= 0 - 2.56 z_1 \\
&= 0 - 2.56(1) \\
&= -2.56 \\
z_3 &= 0 - 5.76 z_1 - 3.5 z_2 \\
&= 0 - 5.76(1) - 3.5(-2.56) \\
&= 3.2
\end{aligned}
$$

$$[Z] = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -2.56 \\ 3.2 \end{bmatrix}$$

Example: Inverse of a Matrix

Solving [U][X] = [Z] for [X]

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \end{bmatrix} = \begin{bmatrix} 1 \\ -2.56 \\ 3.2 \end{bmatrix}$$

$$25b_{11} + 5b_{21} + b_{31} = 1$$

$$-4.8b_{21} - 1.56b_{31} = -2.56$$

$$0.7b_{31} = 3.2$$

Example: Inverse of a Matrix

Using Backward Substitution

$$b_{31} = \frac{3.2}{0.7} = 4.571$$

$$b_{21} = \frac{-2.56 + 1.560 b_{31}}{-4.8}$$

$$= \frac{-2.56 + 1.560(4.571)}{-4.8} = -0.9524$$

$$b_{11} = \frac{1 - 5b_{21} - b_{31}}{25}$$

$$= \frac{1 - 5(-0.9524) - 4.571}{25} = 0.04762$$

So the first column of the inverse of [*A*] is:

$$\begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \end{bmatrix} = \begin{bmatrix} 0.04762 \\ -0.9524 \\ 4.571 \end{bmatrix}$$

Example: Inverse of a Matrix

Repeating for the second and third columns of the inverse

Second Column

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix}\begin{bmatrix} b_{12} \\ b_{22} \\ b_{32} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} b_{12} \\ b_{22} \\ b_{32} \end{bmatrix} = \begin{bmatrix} -0.08333 \\ 1.417 \\ -5.000 \end{bmatrix}$$

Third Column

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix}\begin{bmatrix} b_{13} \\ b_{23} \\ b_{33} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} b_{13} \\ b_{23} \\ b_{33} \end{bmatrix} = \begin{bmatrix} 0.03571 \\ -0.4643 \\ 1.429 \end{bmatrix}$$

Example: Inverse of a Matrix

The inverse of [*A*] is

$$[A]^{-1} = \begin{bmatrix} 0.04762 & -0.08333 & 0.03571 \\ -0.9524 & 1.417 & -0.4643 \\ 4.571 & -5.000 & 1.429 \end{bmatrix}$$

To check your work do the following operation

$$[A][A]^{-1} = [I] = [A]^{-1}[A]$$

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

http://numericalmethods.eng.usf.edu/topics/gauss_seidel.html

Exercise:

Free Training

- Start writing routines using the
  1. Naive Gaussian Elimination Method and
  2. Naive Gaussian Elimination with Partial Pivoting.
  3. Think how to implement the LU decomposition of a matrix A

  to solve the following set of linear equations:

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b},$$

where

$$\mathbf{A} = \begin{pmatrix} 13 & 4 & 7 & 9 \\ 10 & 6 & 5 & 12 \\ 1 & 8 & 2 & 16 \\ 3 & 14 & 15 & 11 \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 111 \\ 118 \\ 114 \\ 163 \end{pmatrix}.$$

Assignment for the Afternoon / Homework, 20 Points

- **Exercise 1, 10 points**: Print the upper triangular matrix and the new **b**-vector after the *forward* Gaussian elimination and show the solution of **x**. Also, use the method to calculate the determinant of matrix **A**.

- **Exercise 2, 10 points**: Write a routine which does the LU decomposition on a square matrix. Use the above matrix **A** to test your program.
  - Print out the L and U parts of the matrix **A**.
  - Solve the above equation.
  - **Optional:** Compute the inverse of the matrix **A**.