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NUMERICAL METHODS & OPTIMISATION

Part II: Linear Algebraic Equations

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Chapter Description

- Aims
  - Apply numerical methods in solving engineering problem and optimisation

- Expected Outcomes
  - Solve simultaneous equations by using LU Decomposition and Matrix Inversion methods
  - Apply linear algebraic equations to solve engineering problems

- References
  - Steven C. Chapra and Raymond P. Canale (2009), Numerical Methods for Engineers, McGraw-Hill, 6th Edition

LU Decomposition

- Given the system of linear algebraic equation in matrix form:

$$[A]\{X\}=\{B\}$$

- In LU decomposition, [A] is decomposed into upper triangle form known as [U] and lower triangle form known as [L]

$$[U]=\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & a''_{33} \end{bmatrix} \qquad [L]=\begin{bmatrix} 1 & 0 & 0 \\ f_{21} & 1 & 0 \\ f_{31} & f_{32} & 1 \end{bmatrix}$$

Decomposition of [A] into [U] and [L]

- Given [A] in the form of:

$$[A]=\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

- This matrix can be decomposed into [L] & [U] by using the principles of Naïve-Gauss Elimination.
  - [U] is a direct product of forward elimination:

$$[U]=\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & a''_{33} \end{bmatrix}$$

  - The factors used to eliminate a_{21}, a_{31} and a_{32} are stored in [L] in the form of:

$$[L]=\begin{bmatrix} 1 & 0 & 0 \\ f_{21} & 1 & 0 \\ f_{31} & f_{32} & 1 \end{bmatrix}$$

LU Decomposition: Example 10.1 & 10.2

$$3x_1 - 0.1x_2 - 0.2x_3 = 7.85$$

$$0.1x_1 + 7x_2 - 0.3x_3 = -19.3$$

$$0.3x_1 - 0.2x_2 + 10x_3 = 71.4$$

$$\begin{bmatrix} 3 & -0.1 & -0.2 \\ 0.1 & 7 & -0.3 \\ 0.3 & -0.2 & 10 \end{bmatrix}$$

1. Use Naïve-Gauss Elimination to obtain [U]:

$$\begin{bmatrix} 3 & -0.1 & -0.2 \\ 0 & 7.00333 & -0.293333 \\ 0 & 0 & 10.0120 \end{bmatrix} = [U]$$

$$[L] = \begin{bmatrix} 1 & 0 & 0 \\ f_{21} & 1 & 0 \\ f_{31} & f_{32} & 1 \end{bmatrix}$$

$$f_{21} = \frac{a_{21}}{a_{11}} \quad f_{31} = \frac{a_{31}}{a_{11}} \quad f_{32} = \frac{a'_{32}}{a'_{22}}$$

LU Decomposition: Example 10.1 & 10.2 (cont'd)

2. The lower matrix [L] becomes:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0.03333 & 1 & 0 \\ 0.10000 & -0.0271300 & 1 \end{bmatrix} = [L]$$

3. [L] is used to generate an intermediate vector known as {D}

$$[L]\{D\} = \{B\} \qquad \begin{bmatrix} 1 & 0 & 0 \\ 0.03333 & 1 & 0 \\ 0.10000 & -0.0271300 & 1 \end{bmatrix} \begin{Bmatrix} d_1 \\ d_2 \\ d_3 \end{Bmatrix} = \begin{Bmatrix} 7.85 \\ -19.3 \\ 71.4 \end{Bmatrix}$$

$$d_1 = 7.85 \qquad d_2 = -19.5617 \qquad d_3 = 70.0843$$

LU Decomposition: Example 10.1 & 10.2 (cont'd)

4. {D} is then used to calculate {x} by using [U]:

$$[U]\{X\} = \{D\}$$

$$\begin{bmatrix} 3 & -0.1 & -0.2 \\ 0 & 7.00333 & -0.293333 \\ 0 & 0 & 10.0120 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 7.85 \\ -19.5617 \\ 70.0843 \end{Bmatrix}$$

$$x_1 = 3 \qquad x_2 = -2.5 \qquad x_3 = 7.0000$$

Matrix Inverse

- Matrix inverse can be calculated numerically by using LU decomposition
- **Example**: Use LU decomposition to generate a matrix inverse for [A}:

  - Decompose [A] into [L] & [U]
  - [L] is used to generate an intermediate vector, {D} using:

$$[L]\{D\} = \{B\}$$

  - The inverse of [A] can be calculated in a column by column fashion:
    - 1st column, 2nd column and 3rd column of [A] can be calculated by replacing {B} with:

$$\{B\} = \begin{Bmatrix} 1 \\ 0 \\ 0 \end{Bmatrix} \qquad \{B\} = \begin{Bmatrix} 0 \\ 1 \\ 0 \end{Bmatrix} \qquad \{B\} = \begin{Bmatrix} 0 \\ 0 \\ 1 \end{Bmatrix}$$

Matrix Inverse (cont'd)

- Example (cont'd)
  - {D} is then used to calculate {x} by using:

$$[U]\{X\} = \{D\}$$

  - The x values are the values for the first column of the matrix inverse of [A]
  - Calculation can be repeated until all columns are determined

Matrix Inverse: Example 10.3

1. Consider [A] as:

$$\begin{bmatrix} 3 & -0.1 & -0.2 \\ 0.1 & 7 & -0.3 \\ 0.3 & -0.2 & 10 \end{bmatrix}$$

2. Decompose [A] into [L] and [U]

$$\begin{bmatrix} 3 & -0.1 & -0.2 \\ 0 & 7.00333 & -0.293333 \\ 0 & 0 & 10.0120 \end{bmatrix} = [U] \qquad \begin{bmatrix} 1 & 0 & 0 \\ 0.03333 & 1 & 0 \\ 0.10000 & -0.0271300 & 1 \end{bmatrix} = [L]$$

3. [L] is used to generate an intermediate vector, {D} using:

$$[L]\{D\} = \{B\}$$

Matrix Inverse: Example 10.3 (cont'd)

4. For the first column:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0.03333 & 1 & 0 \\ 0.10000 & -0.0271300 & 1 \end{bmatrix} \begin{Bmatrix} d_1 \\ d_2 \\ d_3 \end{Bmatrix} = \begin{Bmatrix} 1 \\ 0 \\ 0 \end{Bmatrix}$$

$$d_1 = 1$$

$$d_2 = -0.03333$$

$$d_3 = -0.1009$$

5. The values of {D} are used to replace the following eqn from which values of x can be determined: $[U]\{X\} = \{D\}$

$$\begin{bmatrix} 3 & -0.1 & -0.2 \\ 0 & 7.00333 & -0.293333 \\ 0 & 0 & 10.0120 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 1 \\ -0.03333 \\ -0.1009 \end{Bmatrix}$$

$$x_1 = 0.33249$$

$$x_2 = -0.00518$$

$$x_3 = -0.01008$$

$$[A]^{-1} = \begin{bmatrix} 0.33249 & 0 & 0 \\ -0.00518 & 0 & 0 \\ -0.01008 & 0 & 0 \end{bmatrix}$$

Matrix Inverse: Example 10.3 (cont'd)

4. The calculation can be repeated for the 2nd and 3rd columns until the inversion of [A] is generated:

$$\{B\} = \begin{Bmatrix} 0 \\ 1 \\ 0 \end{Bmatrix} \qquad \{B\} = \begin{Bmatrix} 0 \\ 0 \\ 1 \end{Bmatrix} \qquad [A]^{-1} = \begin{bmatrix} 0.33249 & 0.004944 & 0.006798 \\ -0.00518 & 0.142903 & 0.004183 \\ -0.01008 & 0.00271 & 0.09988 \end{bmatrix}$$

Gauss-Seidel Elimination

- The Gauss-Seidel method is the most commonly used iterative method
- For 3 x 3 matrix, if the diagonal elements are all non zero, the first equation can be solved for x1, the second for x2 and the third for x_3 to yield:

$$[A]\{X\}=\{B\}$$

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$$

$$x_1 = \frac{b_1 - a_{12}x_2 - a_{13}x_3}{a_{11}}$$

$$x_2 = \frac{b_2 - a_{21}x_1 - a_{23}x_3}{a_{22}}$$

$$x_3 = \frac{b_3 - a_{31}x_1 - a_{32}x_2}{a_{33}}$$

Gauss-Seidel Elimination: Algorithm

- The values of x are initially guessed by assuming all of them are zero
- These zero are substituted into the following equation:

$$x_1 = \frac{b_1 - a_{12}x_2 - a_{13}x_3}{a_{11}}$$

- The substitution will result in a new value of $x_1 = b_1/a_{11}$
- The new value and $x_3=0$ are used to determine new value of x_2 by using the following equation:

$$x_2 = \frac{b_2 - a_{21}x_1 - a_{23}x_3}{a_{22}}$$

- The above steps are repeated to determine new x_3 using:

$$x_3 = \frac{b_3 - a_{31}x_1 - a_{32}x_2}{a_{33}}$$

Gauss-Seidel Elimination: Algorithm (cont'd)

- Upon the estimation of x_3, the whole process is repeated until the values of x_1, x_2, and x_3 converge to the true values.
- Convergence can be checked by using the following equation:

$$\left|\varepsilon_{a,i}\right| = \left|\frac{x_i^j - x_i^{j-1}}{x_i^j}\right| \times 100\% \qquad < \varepsilon_s$$

Gauss-Seidel Elimination: Example 11.3

- Use the Gauss-Seidel elimination to obtain the solution of the same system used in Example 11.1:

$$3x_1 - 0.1x_2 - 0.2x_3 = 7.85$$

$$0.1x_1 + 7x_2 - 0.3x_3 = -19.3$$

$$0.3x_1 - 0.2x_2 + 10x_3 = 71.4$$

- Recall that the true solution is x1 = 3, x2 = -2.5 and x3 = 7

$$x_1 = \frac{7.85 + 0.1x_2 + 0.2x_3}{3} \qquad x_2 = \frac{-19.3 - 0.1x_1 + 0.3x_3}{7} \qquad x_3 = \frac{71.4 - 0.3x_1 + 0.2x_2}{10}$$

Gauss-Seidel Elimination: Example 11.3 (cont'd)

- By assuming x_2 and x_3 are zero, calculate x_1:

$$x_1 = \frac{7.85 + 0 + 0}{3} = 2.616667$$

- Use $x_1 = 2.616667$ with $x_3 = 0$ to calculate x_2:

$$x_2 = \frac{-19.3 - 0.1(2.616667) + 0}{7} = -2.794524$$

- Substitute values for x_1 and x_2 into eqn to calculate x_3:

$$x_3 = \frac{71.4 - 0.3(2.616667) + 0.2(-2.794524)}{10} = 7.00561$$

Gauss-Seidel Elimination: Example 11.3 (cont'd)

- **Second iteration:**

$$x_1 = \frac{7.85 + 0.1(-2.794524) + 0.2(7.005610)}{3} = 2.990557$$

$$x_2 = \frac{-19.3 - 0.1(2.990557) + 0.3(7.005610)}{7} = -2.499625$$

$$x_3 = \frac{71.4 - 0.3(2.990557) + 0.2(-2.499625)}{10} = 7.000291$$

- **ε_a for x_1:**

$$\left|\varepsilon_{a,1}\right| = \left|\frac{2.990557 - 2.616667}{2.990557}\right| 100\% = 12.5\%$$

- **For x_2 and x_3, $\varepsilon_{a,2} = 11.8\%$, and $\varepsilon_{a,3} = 0.076\%$.**

Gauss-Seidel Elimination: Exercise

- The following system of equations is designed to determine concentrations (in g/m³) in a series of coupled reactors as a function of amount of mass input to each reactor (g/day). Solve the problem using Gauss Seidel method to $\varepsilon_s = 5\%$

$$15c_1 - 3c_2 - c_3 = 3800$$
$$-3c_1 + 18c_2 - 6c_3 = 1200$$
$$-4c_1 - c_2 + 12c_3 = 2350$$

- Use Gauss Seidel method to solve the following equations until the percent relative error falls below $\varepsilon_s = 5\%$

$$10x_1 + 2x_2 - 3x_3 = 27$$
$$-3x_1 - 6x_2 + 2x_3 = -61.5$$
$$x_1 + x_2 + 5x_3 = -21.5$$

Conclusion

- The LU Decomposition, Matrix Inversion & Gauss-Siedel methods can be used to solve the simultaneous equations

Main Reference

Steven C. Chapra and Raymond P. Canale (2009), Numerical Methods for Engineers, McGraw-Hill, 6th Edition

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