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NUMERICAL METHODS & OPTIMISATION

Part I: 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 Naïve-Gauss and Gause Jordan methods
  - Apply linear algebraic equations to solve engineering problems

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

Overview Linear Algebraic Equations

- This chapter deals with simultaneous linear algebraic equations:

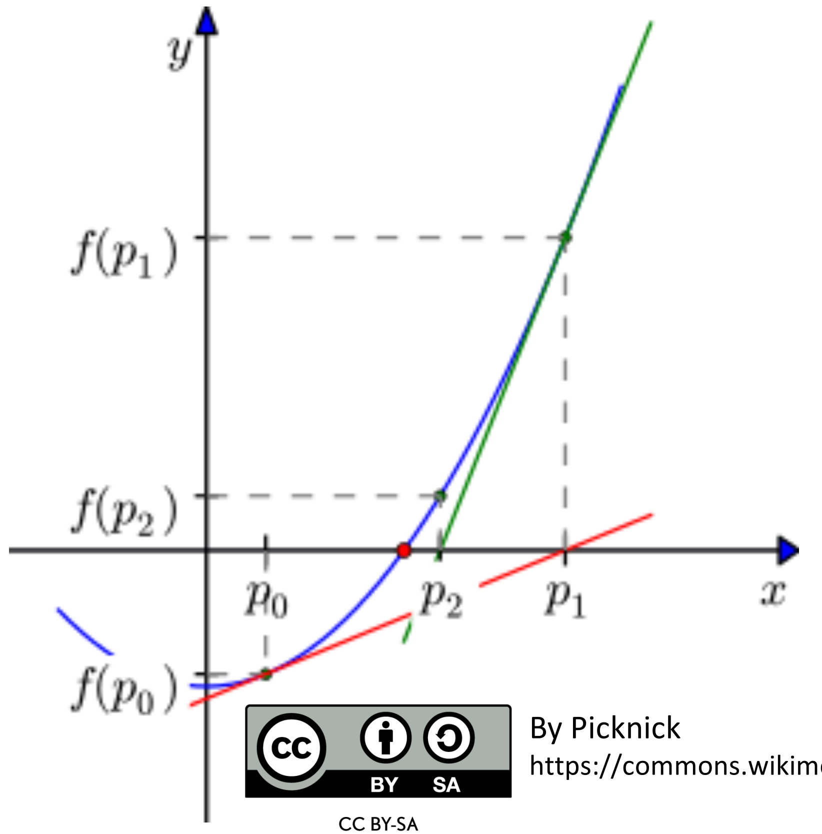
$$a_{11}x_1 + a_{12}x_2 + \ldots\ldots a_{1n}x_n = b_1$$
$$a_{21}x_1 + a_{22}x_2 + \ldots\ldots a_{2n}x_n = b_2$$
$$a_{n1}x_1 + a_{n2}x_2 + \ldots\ldots a_{nn}x_n = b_n$$

where a's are constant coefficient and b's are constants

- Gauss elimination – involves combining equations to eliminate unknowns
- Why Gauss elimination?
  - Algorithm used in popular software packages
  - Most important algorithm
  - Basis of linear equation solution

Overview Linear Algebraic Equations (cont'd)

- Two simultaneous equations can be solved through:
  - Graphical method
  - Determinants & Cramer's Rule
  - Elimination of unknowns



- Graphical method

$$a_{11}x_1 + a_{12}x_2 = b_1$$

$$a_{21}x_1 + a_{22}x_2 = b_2$$

$$x_2 = -\left(\frac{a_{11}}{a_{12}}\right)x_1 + \frac{b_1}{a_{12}}$$

$$x_2 = -\left(\frac{a_{21}}{a_{22}}\right)x_1 + \frac{b_2}{a_{22}}$$

Overview Linear Algebraic Equations (cont'd)

- Determinants & Cramer's Rule
  - Alternative to graphical method
  - Used to solve unknowns from small number of simultaneous equations
  - Expresses the solution of linear equations in terms of ratios of determinants

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

$$A_1 = a_{22}a_{33} - a_{23}a_{32}$$

$$A_2 = a_{21}a_{33} - a_{23}a_{31}$$

$$A_3 = a_{21}a_{32} - a_{22}a_{31}$$

$$D=\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} \qquad D=\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} \qquad D=\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}$$

$$x_1 = \frac{\begin{vmatrix} b_1 & a_{12} & a_{13} \\ b_2 & a_{22} & a_{23} \\ b_3 & a_{32} & a_{33} \end{vmatrix}}{D}$$

$$D = a_{11}\begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{12}\begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + a_{13}\begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}$$

Overview Linear Algebraic Equations (cont'd)

- Elimination of unknowns
  - Involves two basic steps: a) combining equations b) Substitution
  - Used to solve two simultaneous equations
  - Basis for Naïve-Gauss Elimination method

Overview Linear Algebraic Equations (cont'd)

Linear Algebraic Equation Solvers

- **Gauss Elimination**
  - **Naive Gauss**
  - **Gauss-Jord**
- **LU Decomposition & Matrix Inversion**
- **Gauss-Seidel**

Naïve-Gauss Elimination

- An extension of elimination of unknowns method – to solve higher number of equations – *n* sets

- Solved in two stages:
  - Forward elimination
  - Back substitution

Naïve-Gauss Elimination: Algorithm

- Naïve-Gauss Elimination usually suitable to be solved by computers – ability to avoid zero division
- Manual calculations unable to avoid zero division – Naïve
- Consider the following two equations:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1 \quad (1)$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2 \quad (2)$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3 \quad (3)$$

Phase 1: Forward elimination

1. Multiplication of (1) by $\frac{a_{21}}{a_{11}}$ gives:

$$a_{21}x_1 + \frac{a_{21}}{a_{11}}a_{12}x_2 + \frac{a_{21}}{a_{11}}a_{13}x_3 = \frac{a_{21}}{a_{11}}b_1 \quad (12)$$

Naïve-Gauss Elimination: Algorithm (cont'd)

2. Subtraction of (1a) from (2) gives:

$$\left(a_{22}-\frac{a_{21}}{a_{11}}a_{12}\right)x_2+\ldots.+\left(a_{2n}-\frac{a_{21}}{a_{11}}a_{13}\right)x_3=b_2-\frac{a_{21}}{a_{11}}b_1$$

$$a'_{22}x_2+\ldots.+a'_{23}x_3=b'_2$$

Which can be simplified to

3. Multiplication of (1) by $\frac{a_{31}}{a_{11}}$ and subtraction of the resulting equation from (3) yield:

$$a_{11}x_1+a_{12}x_2+a_{13}x_3=b_1 \qquad (1)$$

$$a'_{22}x_2+a'_{23}x_3\ldots..a'_{2n}x_n=b'_2 \qquad (2a)$$

$$\vdots \qquad \vdots$$

$$a'_{n2}x_2+a'_{n3}x_3\ldots..a'_{nn}x_n=b'_n \qquad (3a)$$

Naïve-Gauss Elimination: Algorithm (cont'd)

4. Elimination of second unknown from (3a) by multiplying (2a) to $\frac{a'_{32}}{a'_{22}}$ and subtraction of the resulting equation from (3a) yield:

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

$$a'_{22}x_2 + a'_{23}x_3 \ldots\ldots a'_{2n}x_n = b'_2 \quad (2a)$$

$$\vdots \qquad\qquad \vdots$$

$$a'_{n3}x_3 \ldots\ldots a'_{nn}x_n = b''_n \quad (3b)$$

5. The elimination process can be repeated until the equations are transformed into a triangular system:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

$$a'_{22}x_2 + a'_{23}x_3 = b'_2$$

$$a''_{33}x_3 = b''_3$$

Naïve-Gauss Elimination: Algorithm (cont'd)

Phase 2: Back substitution

6. x_3 can be solved by using the previous equations:

$$x_3 = \frac{b_3^{''}}{a_{33}^{''}}$$

7. The process of substitution is repeated for x_1 and x_2.

Reference: Example 9.2

Gauss-Jordan Elimination

- During the forward elimination of Naïve-Gauss elimination, there are instances where division (a.k.a pivot coefficient) will get zero
- Example:

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

- Removing x1 from Equation 2 & 3 using 0 as pivot coefficient leads to the division of 4 by 0
- Gauss-Jordan eliminates this possibility by converting the coefficients of equations into identity matrix

Gauss-Jordan Elimination (cont'd)

- It is a variation of Naïve-Gauss elimination.

- The major differences are:
  1. An unknown is eliminated from all other equations.
  2. Elimination step results in an identity matrix.

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

$$\downarrow$$

$$
\begin{bmatrix}
1 & 0 & 0 & b_1'' \\
0 & 1 & 0 & b_2'' \\
0 & 0 & 1 & b_3''
\end{bmatrix}
$$

Identity matrix

Gauss-Jordan Elimination: Algorithm

- Consider Example 9.12 as reference to explain Gauss-Jordan elimination

$$
\begin{aligned}
3x_1 - 0.1x_2 - 0.2x_3 &= 7.85 \\
0.1x_1 + 7x_2 - 0.3x_3 &= -19.3 \\
0.3x_1 - 0.2x_2 + 10x_3 &= 71.4
\end{aligned}
$$

1. Express the coefficients and the equivalences as an augmented matrix

$$
\begin{array}{l}
1^{st}\text{ row} \\
2^{nd}\text{ row} \\
3^{rd}\text{ row}
\end{array}
\quad
\begin{bmatrix}
3 & -0.1 & -0.2 & 7.85 \\
0.1 & 7 & -0.3 & -19.3 \\
0.3 & -0.2 & 10 & 71.4
\end{bmatrix}
$$

Gauss-Jordan Elimination: Algorithm (cont'd)

2. Normalize 1st row by the pivot coefficient of 1st row:

$$\begin{bmatrix} 1 & -0.0333333 & -0.066667 & 2.61667 \\ 0.1 & 7 & -0.3 & -19.3 \\ 0.3 & -0.2 & 10 & 71.4 \end{bmatrix}$$

3. Eliminate x_1 from 2nd row and 3rd row.
   a) Multiply the 1st row by 0.1 and subtract it from the 2nd row
   b) Multiply the 1st row by 0.3 and subtract it from the 3rd row

$$\begin{bmatrix} 1 & -0.0333333 & -0.066667 & 2.61667 \\ 0 & 7.00333 & -0.293333 & -19.5617 \\ 0 & -0.190000 & 10.0200 & 70.6150 \end{bmatrix}$$

Gauss-Jordan Elimination: Algorithm (cont'd)

4. Normalize the 2nd row by the pivot coefficient of 2nd row:

$$\begin{bmatrix} 1 & -0.0333333 & -0.066667 & 2.61667 \\ 0 & 1 & -0.0418848 & -2.79320 \\ 0 & -0.190000 & 10.0200 & 70.6150 \end{bmatrix}$$

5. Eliminate x_2 from 1st row and 3rd row.
   a) Multiply the 2nd row by -0.0333333 and subtract it from the 1st row
   b) Multiply the 2nd row by -0.19 and subtract it from the 3rd row

$$\begin{bmatrix} 1 & 0 & -0.0680629 & 2.52356 \\ 0 & 1 & -0.0418848 & -2.79320 \\ 0 & 0 & 10.01200 & 70.0843 \end{bmatrix}$$

Gauss-Jordan Elimination: Algorithm (cont'd)

6. Normalize 3rd row by the pivot coefficient of 3rd row:

$$\begin{bmatrix} 1 & 0 & -0.0680629 & 2.52356 \\ 0 & 1 & -0.0418848 & -2.79320 \\ 0 & 0 & 1 & 7.0000 \end{bmatrix}$$

7. Eliminate x_3 from 1st row and 2nd row.
   a) Multiply the 3rd row by -0.0680629 and subtract it from the 1st row
   b) Multiply the 3rd row by -0.0418848 and subtract it from the 2nd row

$$\begin{bmatrix} 1 & 0 & 0 & 3.0000 \\ 0 & 1 & 0 & -2.5000 \\ 0 & 0 & 1 & 7.0000 \end{bmatrix}$$

Conclusion

- The Naïve – Gauss and Gauss – Jordan 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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