# LINEAR EQUATIONS

## Numerical methods in chemical engineering

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Where innovation starts

# OVERVIEW

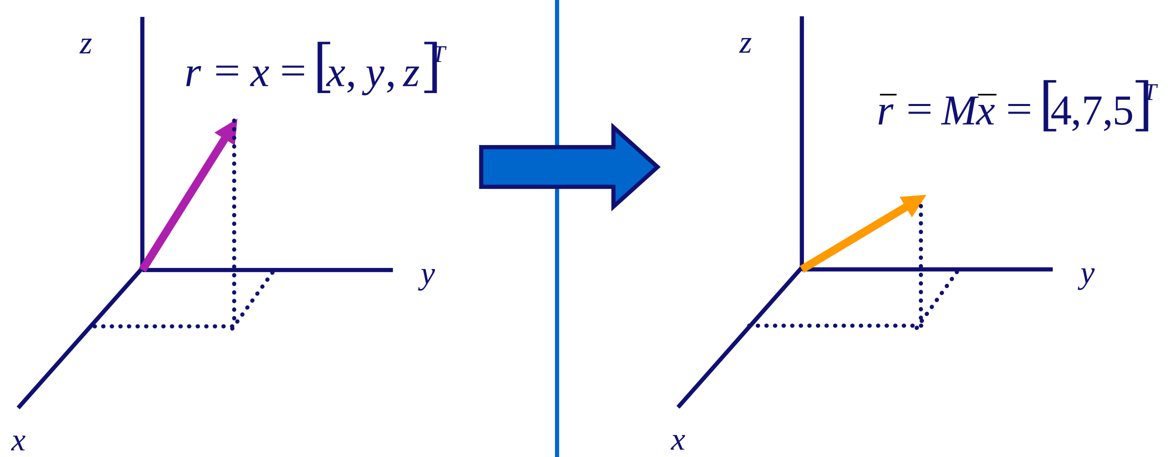
- **Different ways of looking at a system of linear equations (Matrices)**
- **The inverse, determinant and rank of a matrix**
- **The existence of a solution to a set of linear equations**

# MATLAB

- **Vector and matrix operations are an intrinsic part of matlab**
- **High level: don't worry about memorymanagement/allocation**
- **Close to 'proper' languages**
- **Command line interface user friendly**
- **It is an interpreted language (in reference to a compiler): makes it sometimes slow**

# DIFFERENT VIEWS OF LINEAR SYSTEMS

| Separate equations | Matrix mapping | Linear combination |
|---|---|---|
| $x + y + z = 4$<br>$2x + y + 3z = 7$<br>$3x + y + 6z = 5$ | $\begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 3 \\ 3 & 1 & 6 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 4 \\ 7 \\ 5 \end{bmatrix}$ | $x \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} + y \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} + z \begin{bmatrix} 1 \\ 3 \\ 6 \end{bmatrix} = \begin{bmatrix} 4 \\ 7 \\ 5 \end{bmatrix}$ |
| (2-1) | (2-2) | (2-3) |

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# INVERSE OF A MATRIX

- Inverse is defined such that:

$$M\,M^{-1} = I \quad and \quad M^{-1}M = I$$

- Use the inverse to solve a set of linear equations:

$$M\bar{x} = \bar{b}$$

$$M^{-1}M\bar{x} = M^{-1}\bar{b}$$

$$I\bar{x} = M^{-1}\bar{b}$$

$$\bar{x} = M^{-1}\bar{b}$$

# HOW TO CALCULATE AN INVERSE?

- Inverse of an *N*x*N* matrix, can be calculated using the co-factors of each element of the matrix:

$$M^{-1} = \frac{1}{\det(M)} \begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix}^T$$

Det(M) = the **determinant** of M and

$C_{ij}$ is the **co-factor** of the ij^th element in M.

# AN EXAMPLE

- **The example:**

$$M = \begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 3 \\ 3 & 1 & 6 \end{bmatrix}$$

- **Let's calculate $C_{11}$**

# CO-FACTORS

- **A co-factor is defined to be the determinant of the stuff left over when you cover up the row and column of the element in question:**

$$\begin{bmatrix} \boxed{1} & * & * \\ * & \boxed{1} & \boxed{3} \\ * & \boxed{1} & \boxed{6} \end{bmatrix}$$

# THE NEXT STEP

- **Also multiply by +/-1, depending of the position of the element, for the 3x3 matrix, the following table holds:**

$$\begin{bmatrix} \boxed{+} & - & + \\ - & + & - \\ + & - & + \end{bmatrix}$$

# CALCULATING THE INVERSE

- **So, the co-factor $C_{11}$ can be calculated as:**

$$C_{11} = +\det\begin{bmatrix} 1 & 3 \\ 1 & 6 \end{bmatrix} = 6\times1-3\times1=3$$

$$M = \begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 3 \\ 3 & 1 & 6 \end{bmatrix} \quad \begin{bmatrix} \boxed{+} & - & + \\ - & + & - \\ + & - & + \end{bmatrix} \quad \begin{bmatrix} \boxed{1} & * & * \\ * & 1 & 3 \\ * & 1 & 6 \end{bmatrix}$$

# BACK TO THE EXAMPLE

- **You'll find:**

$$\begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 3 \\ 3 & 1 & 6 \end{bmatrix}^{-1} = \frac{1}{\det(M)} \begin{bmatrix} 3 & -3 & -1 \\ -5 & 3 & 2 \\ 2 & -1 & -1 \end{bmatrix}^T$$

Determinant is very important.

Determinant = 0 →The inverse does not exist!! (The matrix is singular)

# CALCULATING THE DETERMINANT

- **Compute the determinant by multiplication of each element on a row (or column) by its cofactor and adding the results:**

$$\det\left(\begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 3 \\ 3 & 1 & 6 \end{bmatrix}\right) = +\det\begin{bmatrix} 1 & 3 \\ 1 & 6 \end{bmatrix} - \det\begin{bmatrix} 2 & 3 \\ 3 & 6 \end{bmatrix} + \det\begin{bmatrix} 2 & 1 \\ 3 & 1 \end{bmatrix} = -1$$

$$\det\left(\begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 3 \\ 3 & 1 & 6 \end{bmatrix}\right) = +\det\begin{bmatrix} 2 & 1 \\ 3 & 1 \end{bmatrix} - 3\det\begin{bmatrix} 1 & 1 \\ 3 & 1 \end{bmatrix} + 6\det\begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix} = -1$$

# SOLVING A LINEAR SYSTEM

- **Our example:**

$$x + y + z = 4$$
$$2x + y + 3z = 7$$
$$3x + y + 6z = 5$$

- **The solution is:**

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \frac{1}{-1}\begin{bmatrix} 3 & -5 & 2 \\ -3 & 3 & -1 \\ -1 & 2 & -1 \end{bmatrix}\begin{bmatrix} 4 \\ 7 \\ 5 \end{bmatrix} = \frac{1}{-1}\begin{bmatrix} -13 \\ 4 \\ 5 \end{bmatrix} = \begin{bmatrix} 13 \\ -4 \\ -5 \end{bmatrix}$$

**The inverse exists, because det(M)=-1**

# How to do this in Matlab

- Create matrix: A = [1 1 1; 2 1 3; 3 1 6];
- Create solution vector: b = [4 7 5]’
- Inverse: Ainv = inv(A)
- Solution: x = Ainv * b
- Another way: x = A\b

- These are black boxes! We are going over some methods later!

- Exercise: use tic toc to compute the time for different size matrix inversions, and plot the results… What kind of growth do you see?

# How to do this in Excel

- Create matrix A in 3x3 cells (1 1 1; 2 1 3; 3 1 6);
- Create solution vector b in 3 vertical cells (4 7 5)
- Inverse:
  - Select an empty 3x3 area
  - Type (cell numbers are examples): =MINVERSE(B2:D4)
  - Close with CTRL+Shift+Enter
- Solution:
  - Select 3 vertical cells
  - Type (cell numbers are examples): =MMULT(H2:J4,B6:B8)
  - Close with CTRL+Shift+Enter
- Try another inverse

# LARGE SYSTEMS

- Computation of determinants and inverses of large matrices in this way is too difficult (slow), so we need other methods to calculate the inverse of a large matrix (large systems).
- Determinant: det(A)

# USEFUL PROPERTIES

- **Triangular matrices:**

(2-14)

$$\det(M_{trian}) = \prod_{i=1}^{n} a_{ii}$$

$$M = \begin{bmatrix} 5 & 3 & 2 \\ 0 & 9 & 1 \\ 0 & 0 & 1 \end{bmatrix} \Rightarrow \det(M) = 5 \times 9 \times 1 = 45$$

- **Matrix multiplication:**

$$\det(AM) = \det(A) * \det(M)$$

$$A = \begin{bmatrix} a & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \Rightarrow \det(AM) = \det(A) * \det(M) = a * \det(M)$$

# USEFUL PROPERTIES

- **Matrix multiplication:**

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} ; \det(A) = 1$$

$$\det(AM) = \det(A) * \det(M) = \det(M)$$

Using rules like this, you can compute the determinant of a matrix using row operations!

# MATRIX RANK

- **Rank of a matrix: the number of linearly independent columns (columns that can not be expressed as a linear combination of the other columns) of a matrix**

$$M = \begin{bmatrix} 5 & 3 & 2 \\ 0 & 9 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

3 independent columns:

rank(M)=3

Column 2 and 4 are not independent

$$M = \begin{bmatrix} 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Col 2 = 2 * col 1

Col 4 = col 3 – col 1

So:

2 independent columns:

Rank(M)=2

# SOLUTIONS OF LINEAR SYSTEMS

- **The solution of a system of linear equations may or may not exist, and it may or may not be unique. Existence of solutions can be determined by comparing the rank of the Matrix *M* with the rank of the augmented matrix $M_a$.**

**Linear system**

$$M = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{bmatrix}, \quad b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \Rightarrow M_a = \begin{bmatrix} a_{11} & a_{21} & a_{31} & b_1 \\ a_{12} & a_{22} & a_{32} & b_2 \\ a_{13} & a_{23} & a_{33} & b_3 \end{bmatrix}$$

$$M\bar{x} = \bar{b}$$

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# SOLUTIONS OF LINEAR SYSTEMS

- **Rank($M$)=$n$**
- **Rank($M$) < $n$ and rank($M$)=rank($M_a$)**
- **Rank($M$) < $n$ and rank($M$)<rank($M_a$)**

- **Unique solution**
- **Infinite number of solutions**
- **No solution**

# TWO EXAMPLES

$$M = \begin{bmatrix} 1 & 1 & 2 \\ 0 & 3 & 1 \\ 0 & 0 & 2 \end{bmatrix}, \bar{b} = \begin{bmatrix} 17 \\ 11 \\ 4 \end{bmatrix} \Rightarrow M_a = \begin{bmatrix} 1 & 1 & 2 & 17 \\ 0 & 3 & 1 & 11 \\ 0 & 0 & 2 & 4 \end{bmatrix}$$

Rank(M) = 3 = n → unique solution

**Rank, solution??**

$$M = \begin{bmatrix} 1 & 1 & 2 \\ 0 & 3 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \bar{b} = \begin{bmatrix} 17 \\ 11 \\ 0 \end{bmatrix} \Rightarrow M_a = \begin{bmatrix} 1 & 1 & 2 & 17 \\ 0 & 3 & 1 & 11 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Rank(M)=rank($M_a$)=2 < n → infinite number of solutions

# SUMMARY

- Linear equations can be written as matrices
- Using the inverse, the solution can be determined
  - Inverse via cofactors
  - Inverse and solution in Matlab
  - Inverse and solution in Excel
- A solution depends on the rank of a matrix