Computational Techniques
Module 3: Linear Equations

Dr. Niket Kaisare
Department of Chemical Engineering
Indian Institute of Technology - Madras

Prerequisite

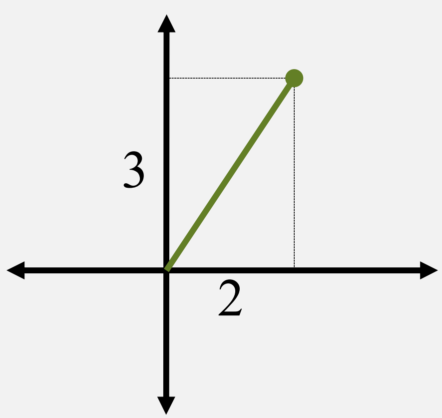
- We will assume some familiarity with the concept of linear algebra, vectors and matrices
- Please review your +2 and First Year Undergraduate syllabi for familiarity

A Quick Recap

- Scalar: A single real number $a = 1.23$
- Vector: An ordered set of scalars
  # of scalars is "*dimension*"
  Has "*length*" and "*direction*"

$$\mathbf{x} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$$

Geometric Interpretation: A point in n-dimensional space



$$\mathbf{x} \in \Re^2$$

~~Size~~ → Norm

A Quick Recap

- Matrix: A rectangular array of numbers

$$A = \begin{bmatrix} 1 & 0.5 \\ 2 & 3 \\ 0 & 2 \end{bmatrix}$$ Dimension: 3x2

- Linear operations:
  Addition, subtraction, scalar multiplication
- Matrix multiplication rules
- Eigenvalues and Eigenvectors

A Linear Equation

Coefficients

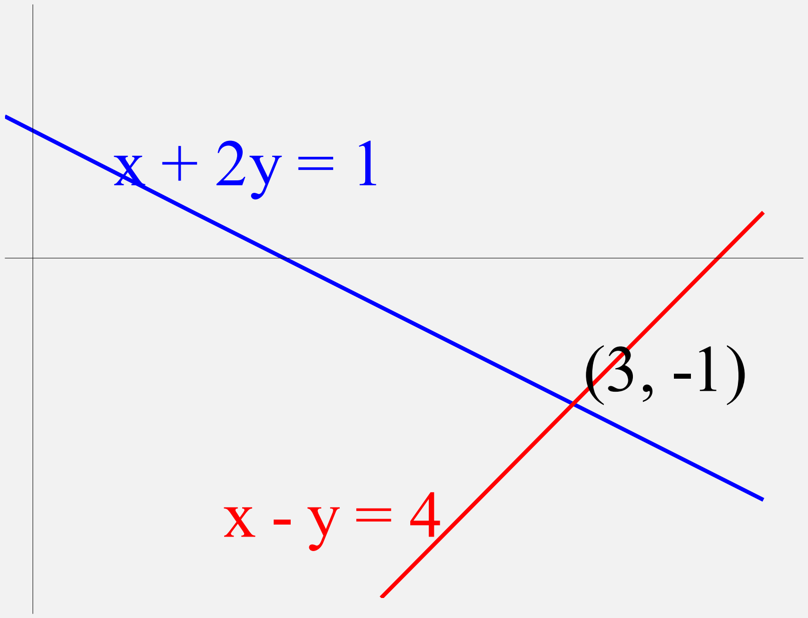
$$3x + 4y + 7z + 2w = 17$$

Variables

A Simple Example

- Consider the following example

$$x + 2y = 1$$
$$x - y \quad = 4$$



Solution is the point of intersection of the two lines

Matrix Form of Linear Equations

$$x + 2y = 1$$
$$x - y \quad = 4$$

$$\underbrace{\begin{bmatrix} 1 & 2 \\ 1 & -1 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x \\ y \end{bmatrix}}_{\mathbf{x}} = \underbrace{\begin{bmatrix} 1 \\ 4 \end{bmatrix}}_{\mathbf{b}}$$

The Determinant Method

- Cramer's Rule
  - D = determinant of matrix $\mathbf{A}$
  - D_i = determinant of $\mathbf{A}_i$, where
  - $\mathbf{A}_i$ is obtained by replacing the i^th^ column of $\mathbf{A}$ with $\mathbf{b}$

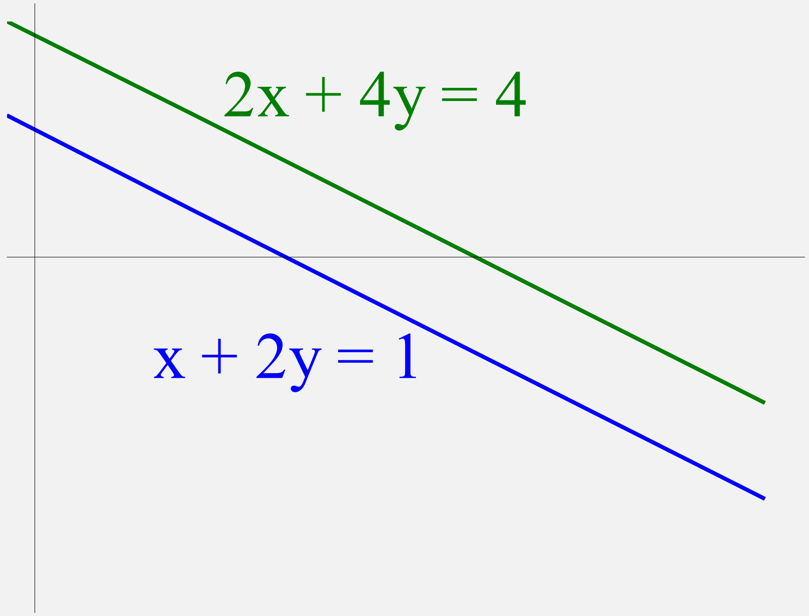
$$D = \begin{vmatrix} 1 & 2 \\ 1 & -1 \end{vmatrix} = -3 \qquad D_1 = \begin{vmatrix} 1 & 2 \\ 4 & -1 \end{vmatrix} = -9 \qquad D_2 = \begin{vmatrix} 1 & 1 \\ 1 & 4 \end{vmatrix} = 3$$

- A unique solution exists if $D \neq 0$

$$x_1 = \frac{D_1}{D} = 3; \qquad x_2 = \frac{D_2}{D} = -1$$

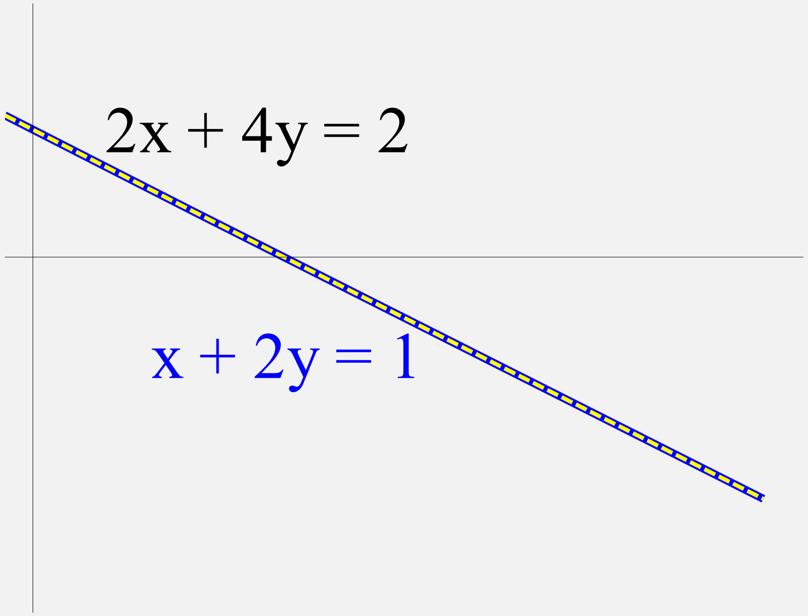
Parallel Lines: No Solution

$$x \quad + 2y = 1$$
$$2x + 4y = 4$$



Co-Incident Lines: Infinite Solutions

$$x + 2y = 1$$
$$2x + 4y = 2$$



Condition Number

$$\begin{aligned} x \quad + 2y \quad &= 1 \\ 2x + 3.999y &= 2.001 \end{aligned} \Rightarrow x = 3;\ y = -1$$

$$\begin{aligned} x \quad + 2y \quad &= 1 \\ 2x + 3.999y &= 2 \end{aligned} \Rightarrow x = 1;\ y = 0$$

$$A = \begin{bmatrix} 1 & 2 \\ 2 & 3.999 \end{bmatrix} \xrightarrow{\text{Eigenvalues}} \lambda_1 = -2 \times 10^{-4};\ \lambda_2 = 4.99;$$

Examples of Linear ChE Systems

- Reactor Network
- Heat Exchange Network
- Separation Processes
- Plug Flow Reactor

Extension to Larger Dimensions

Questions to think about

- How to represent n equations in n unknowns?
- Does the system have unique solution?
- Does the system have no solution?

General n×n System

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n &= b_1 \\
a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n &= b_2 \\
&\vdots \\
a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n &= b_n
\end{aligned}
$$

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

Outline of Linear Algebra Methods

- Cramer's Rule (and why it is not used)
- Direct Methods
  - Gauss Elimination
    - Analysis
    - Computational Effort
    - Pivoting
  - Gauss Jordan
  - Matrix Inversion
  - LU Decomposition

Outline of Linear Algebra Methods

- Sparse Matrices: Thomas Algorithm
- Iterative Methods
  - Gauss-Siedel
  - Jacobi Iteration
  - Relaxation Methods
- Eigenvalues and Eigenvectors