10.34: Numerical Methods Applied to Chemical Engineering

Lecture 3:
Existence and uniqueness of solutions
Four fundamental subspaces

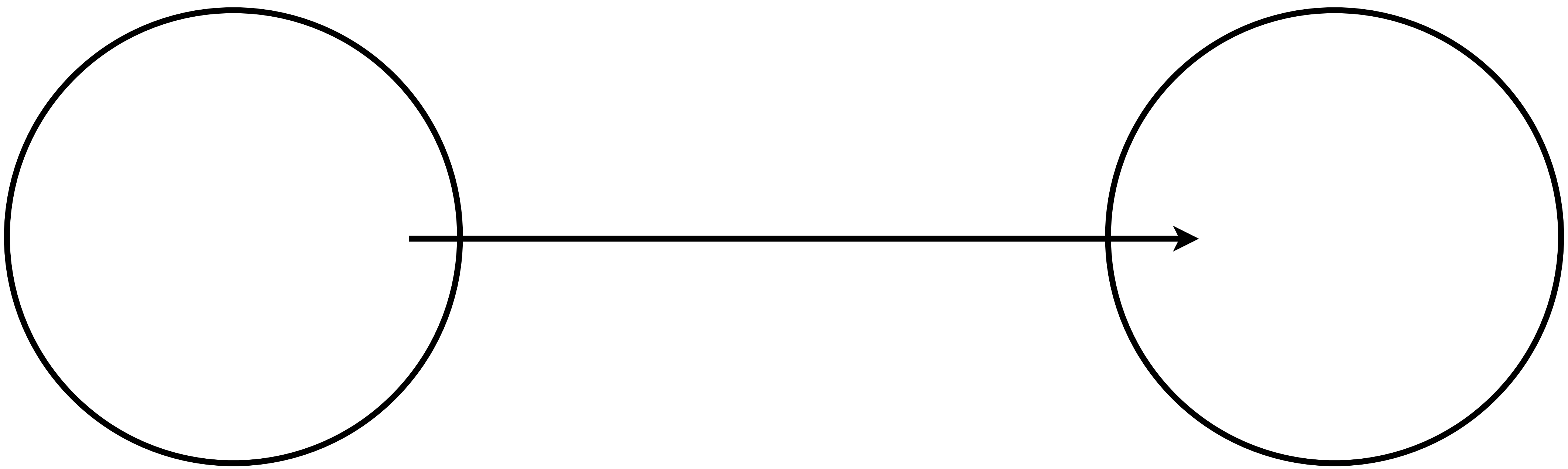
Recap

- Scalars, vectors, and matrices
  - Transformations/maps
  - Determinant
  - Induced norms
  - Condition number

Recap

- Matrices:
  - Matrices are maps between vector spaces!

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



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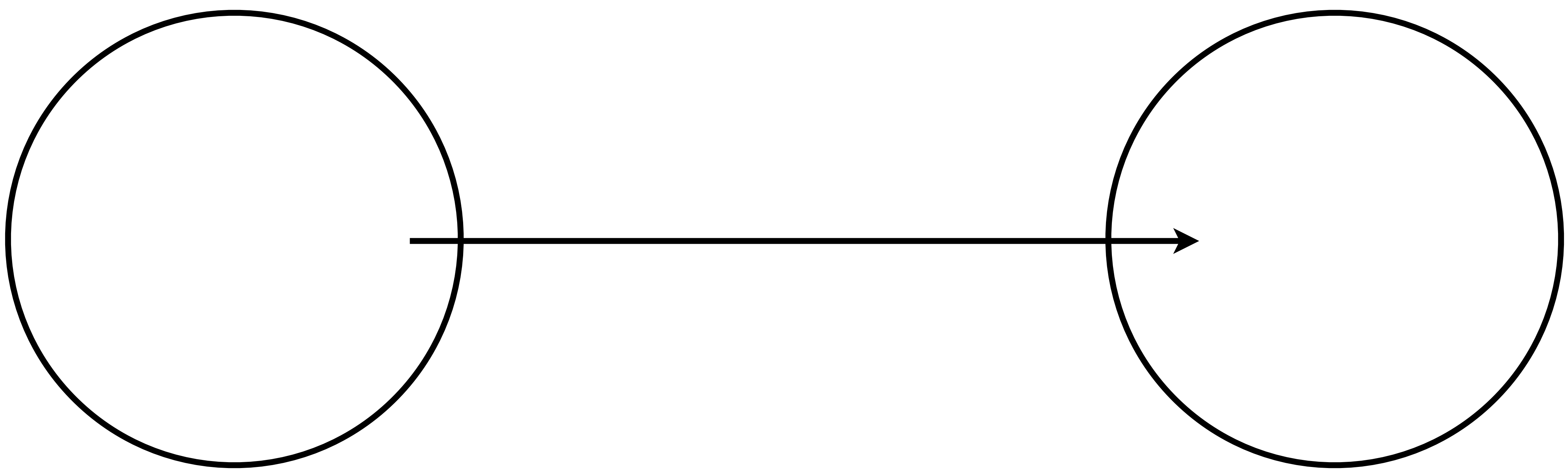

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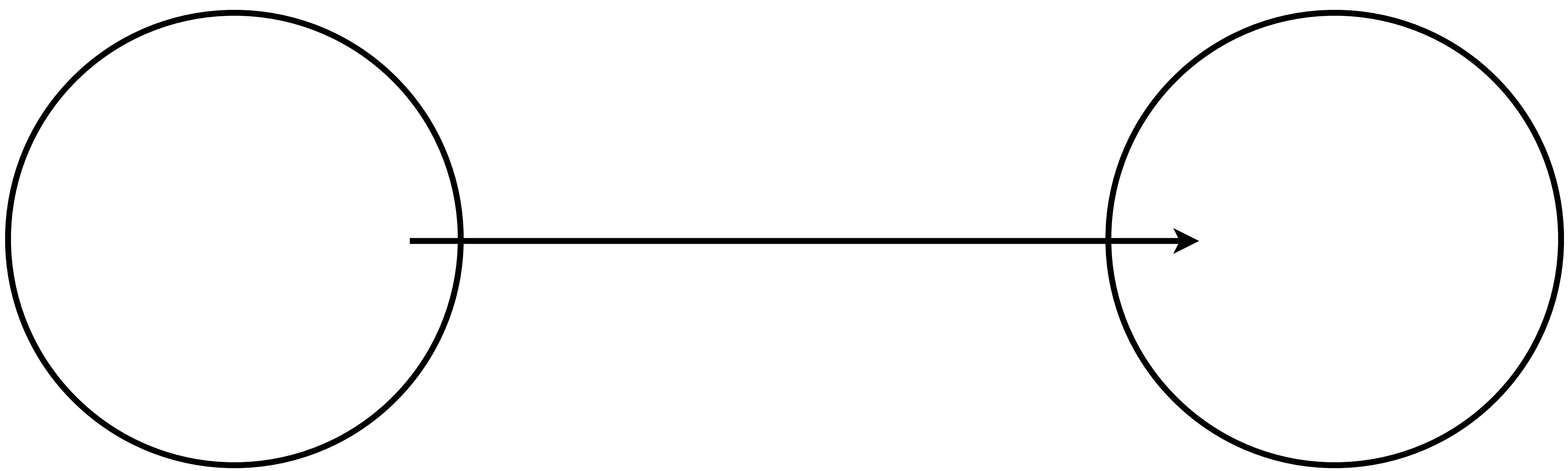

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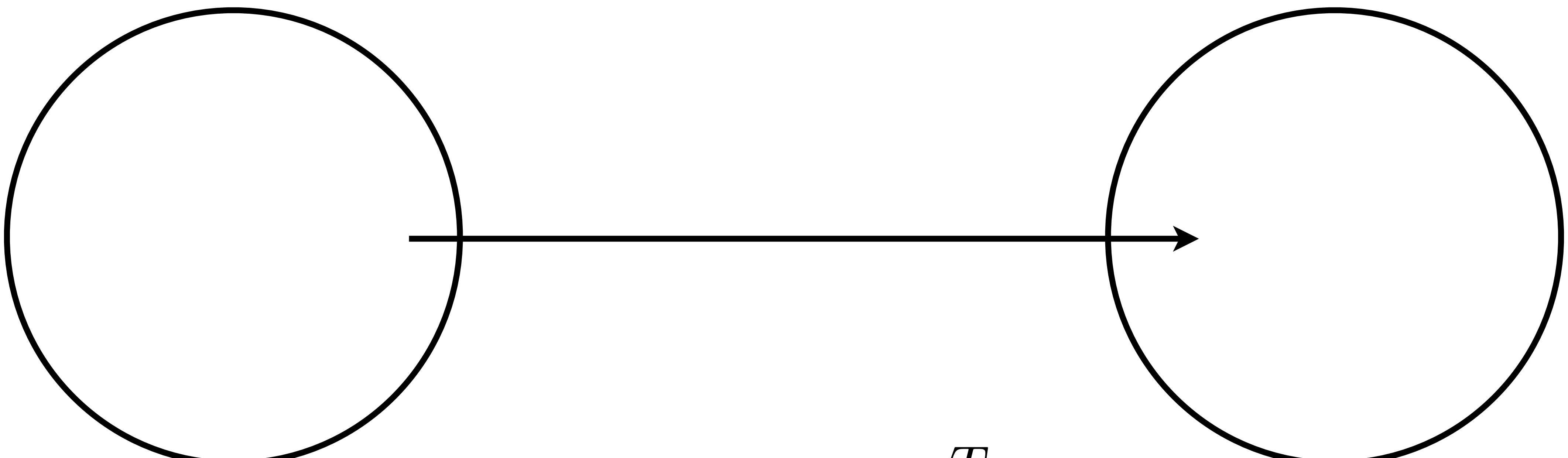
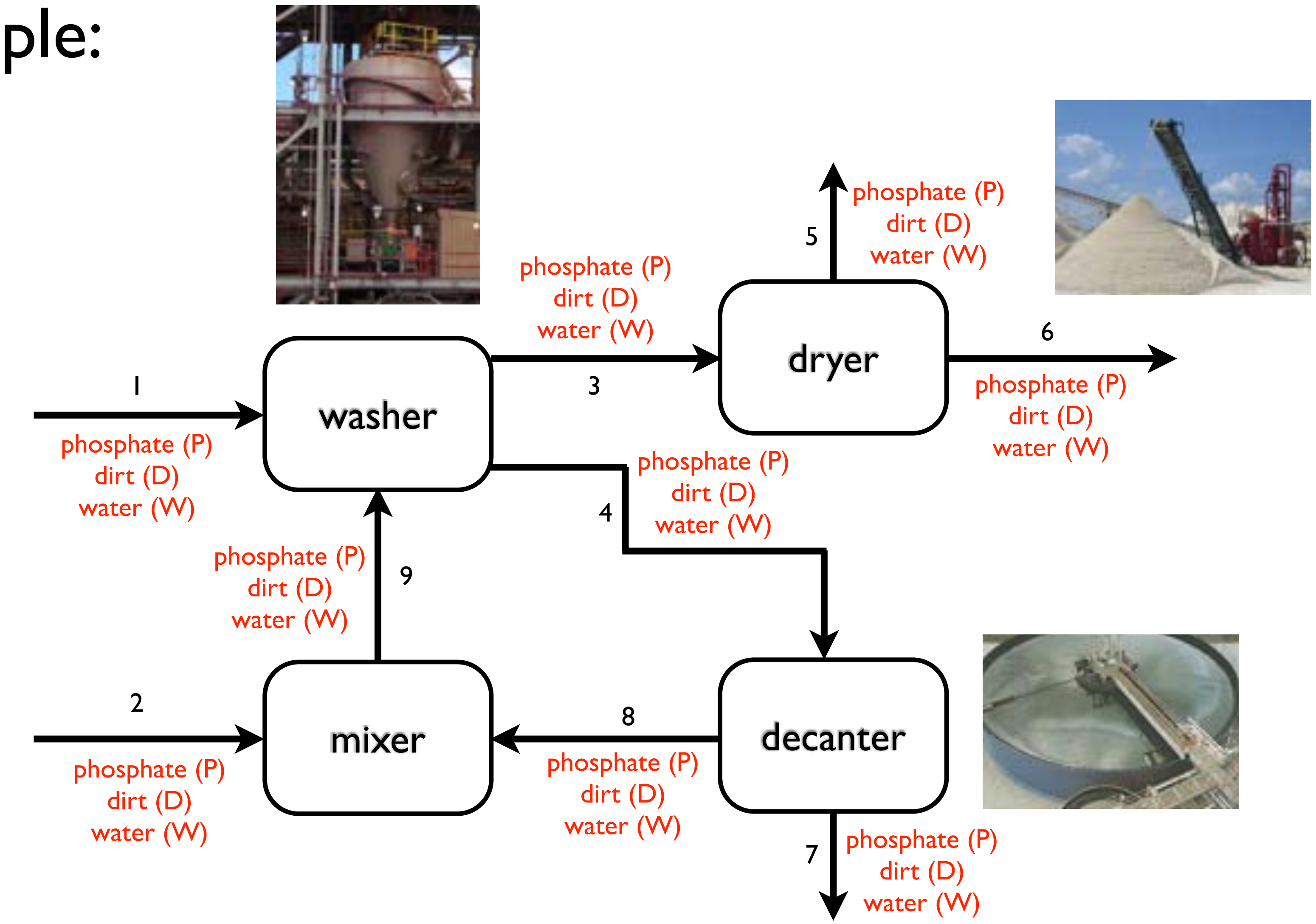


$$\mathbf{A} = \mathbf{I} - \frac{\mathbf{s}\mathbf{s}^T}{\|\mathbf{s}\|_2^2}$$

Existence and Uniqueness

- Example:



Stream 1 carries 1800 kg/hr P, 1200 kg/hr D and 0 kg/hr W
Stream 2 carries 0 kg/hr P, 0 kg/hr D and 10000 kg/hr W
Stream 3 carries 0 kg/hr D and 50% W into the washer
Stream 4 carries 0 kg/hr P
Stream 5 carries 0 kg/hr P and 0 kg/hr D
Stream 6 carries 0 kg/hr D and 0 kg/hr W
Stream 7 carries 0 kg/hr P, 95% of D into the decanter, 5% of W into the decanter
Stream 8 carries 0 kg/hr P
Stream 9 carries 0 kg/hr P

Does a solution exist? Is it unique?

Vector Spaces

- $\mathbb{R}^N$ is an example of a vector space
- A vectors space is a "special" set of vectors
- Properties of a vector space:
  - closed under addition:

$$\mathbf{x}, \mathbf{y} \in S \Rightarrow \mathbf{x} + \mathbf{y} \in S$$

  - closed under scalar multiplication:

$$\mathbf{x} \in S \Rightarrow c\mathbf{x} \in S$$

  - contains the null vector:

$$\mathbf{0} \in S$$

  - has an additive inverse:

$$\mathbf{x} \in S \Rightarrow (-\mathbf{x}) \in S : \mathbf{x} + (-\mathbf{x}) = \mathbf{0}$$

Vector Spaces

- Is this a vector space?

$$\{(1,0),(0,1)\}$$

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$$\{\mathbf{y}:\mathbf{y}=\lambda_1(1,0)+\lambda_2(0,1);\;\;\lambda_1,\lambda_2\in\mathbb{R}\}$$

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Vector Spaces

- A "subspace" is a subset of a vector space
  - It is still closed under addition and scalar multiplication
  - It still contains the null vector
  - For example, $\mathbb{R}^2$ is a subspace of $\mathbb{R}^3$
  - Is this a subspace?

$$\{\mathbf{y} : \mathbf{y} = \lambda((3,0) + (0,1));\ \ \lambda_1, \lambda_2 \in \mathbb{R}\}$$

- The linear combination of a set of vectors:

$$\mathbf{y} = \sum_{i=1}^{M} \lambda_i \mathbf{x}_i$$

- The set of all possible linear combinations of a set of vectors is a subspace:

$$\mathrm{span}\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_M\}$$

$$= \{\mathbf{y} \in \mathbb{R}^N : \mathbf{y} = \sum_{i=1}^{M} \lambda_i \mathbf{x}_i;\ \ \lambda_i \in \mathbb{R}, i = 1, \ldots, M\}$$

Linear Dependence

- If at least one non-trivial linear combination of a set of vectors is equal to the null vector, the set is said to be linearly dependent.
    - The set $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_M\}$ with $\mathbf{x}_i \in \mathbb{R}^N$ is linearly dependent if there exists at least one $\lambda_i \neq 0$ such that:

$$\sum_{i=1}^{M} \lambda_i \mathbf{x}_i = 0$$

- If M > N, then the set of vectors is always dependent

Linear Dependence

- Example: are the columns of $\mathbf{I}$ linearly dependent?

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \lambda_1 + \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \lambda_2 + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \lambda_3 = \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{pmatrix} = 0$$

- Example: are these vectors linearly dependent?

$$\begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix}, \begin{pmatrix} -1 \\ 2 \\ -1 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \\ 2 \end{pmatrix}$$

- In general, if $\mathbf{A}\mathbf{x} = 0$ has a non-trivial solution, then the vectors $(\mathbf{A}_1^c \ \mathbf{A}_2^c \ \ldots \ \mathbf{A}_M^c)$ are linearly dependent.

Linear Dependence

- Uniqueness of solutions to: $\mathbf{Ax} = \mathbf{b}$
  - If we can find one vector for which: $\mathbf{Ax} = 0$, then a unique solution cannot exist.
  - Proof:
    - Let $\mathbf{x} = \mathbf{x}^H + \mathbf{x}^P$, and $\mathbf{Ax}^H = 0$ while $\mathbf{Ax}^P = \mathbf{b}$
    - If $\mathbf{x}^H \neq 0$, $\mathbf{x} = c\mathbf{x}^H + \mathbf{x}^P$ is another solution.
    - Therefore, $\mathbf{x}$ cannot be unique.
- Uniqueness of solutions requires the columns of a matrix be linearly independent!
  - $(\mathbf{A}_1^c \ \mathbf{A}_2^c \ \ldots \ \mathbf{A}_M^c)\mathbf{x}^H = 0$ only if $\mathbf{x}^H = 0$
- If a system has more variables than equations, then a unique solution cannot exist. It is under constrained.

Linear Dependence

- The dimension of a subspace is the minimum number of linearly independent vectors required to describe the span:

$$S = \text{span}\{(1,0,0),(0,1,0),(0,0,1)\}, \;\; \dim S = 3$$

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  - Example: can $\mathbf{Ax} = \mathbf{b}$ have a unique solution?

$$\mathbf{A} = \begin{pmatrix} 1 & 4 & 0 \\ 2 & 5 & 7 \\ 3 & 6 & 8 \\ 0 & 7 & 9 \end{pmatrix}$$

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Four Fundamental Subspaces

$$\mathbf{A} \in \mathbb{R}^{N \times M}$$

- Column space (range space):

$$\mathcal{R}(\mathbf{A}) = \mathrm{span}\{\mathbf{A}_1^c, \mathbf{A}_2^c, \ldots, \mathbf{A}_M^c\}$$

- Null space:

$$\mathcal{N}(\mathbf{A}) = \{\mathbf{x} \in \mathbb{R}^M : \mathbf{A}\mathbf{x} = 0\}$$

- Row space:

$$\mathcal{R}(\mathbf{A}^T) = \mathrm{span}\{\mathbf{A}_1^r, \mathbf{A}_2^r, \ldots, \mathbf{A}_N^r\}$$

- Left null space:

$$\mathcal{N}(\mathbf{A}^T) = \{\mathbf{x} \in \mathbb{R}^N : \mathbf{A}^T\mathbf{x} = 0\}$$

Column Space

$$\mathbf{A} \in \mathbb{R}^{N\times M} \quad \mathcal{R}(\mathbf{A}) = \text{span}\{\mathbf{A}_1^c, \mathbf{A}_2^c, \ldots, \mathbf{A}_M^c\}$$

- The column space of $\mathbf{A}$ is a subspace of $\mathbb{R}^N$
- Vectors in $\mathcal{R}(\mathbf{A})$ are linear combinations of the columns of $\mathbf{A}$
- Existence of solutions:
  - Consider: $\mathbf{A}\mathbf{x} = \mathbf{b}$

$$\sum_{i=1}^{M} x_i \mathbf{A}_i^c = \mathbf{b}$$

  - If $\mathbf{x}$ exists, then $\mathbf{b}$ is a linear combination of the columns of $\mathbf{A}$. $\mathbf{b} \in \mathcal{R}(\mathbf{A})$
  - Converse: if $\mathbf{b} \notin \mathcal{R}(\mathbf{A})$, then $\mathbf{x}$ cannot exist

Existence of Solutions

$$\mathbf{A} \in \mathbb{R}^{N \times M} \quad \mathcal{R}(\mathbf{A}) = \text{span}\{\mathbf{A}_1^c, \mathbf{A}_2^c, \ldots, \mathbf{A}_M^c\}$$

- Solutions to $\mathbf{A}\mathbf{x} = \mathbf{b}$ exist only if $\mathbf{b} \in \mathcal{R}(\mathbf{A})$
- Example:
  - Does a solution exist with $\mathbf{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
  - If $\mathbf{b} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$?
  - If $\mathbf{b} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$?

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Existence of Solutions

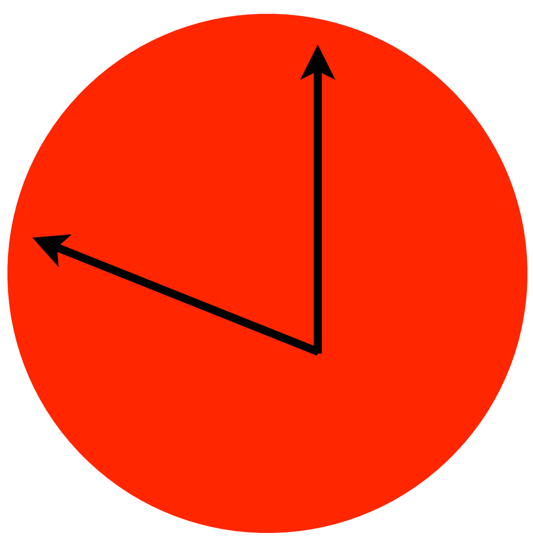
- Example:

  - Does a solution exist?

$$\begin{pmatrix} 1 & 1 \\ -2 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 0 \\ 1.1 \end{pmatrix}$$

  - What is the column space?
    -

    - Is $\mathbf{b} \in \mathcal{R}(\mathbf{A})$?



Null Space

$$\mathbf{A} \in \mathbb{R}^{N \times M}$$

- The set of all vectors that are transformed into the null vector by $\mathbf{A}$ is called the null space of $\mathbf{A}$

$$\mathcal{N}(\mathbf{A}) = \{\mathbf{x} \in \mathbb{R}^M \,:\, \mathbf{A}\mathbf{x} = 0\}$$

- The null space is a subset of $\mathbb{R}^M$
  - Not the same as $\mathcal{R}(\mathbf{A})$
- $\mathbf{0}$ is in the null space of all matrices but is trivial
- Uniqueness:
  - Consider two solutions $\mathbf{A}\mathbf{x} = \mathbf{b}, \quad \mathbf{A}\mathbf{y} = \mathbf{b}$
  - Such that $\mathbf{A}(\mathbf{x} - \mathbf{y}) = 0$
  - If $\dim \mathcal{N}(\mathbf{A}) = 0$, then $\mathbf{x} - \mathbf{y} = 0, \quad \mathbf{x} = \mathbf{y}$
    - A unique solution exists

Null Space

- Example:
  - A series of chemical reactions: $\mathrm{A} \xrightarrow{k_1} \mathrm{B} \underset{k_3}{\overset{k_2}{\longleftrightarrow}} \mathrm{C} \underset{k_5}{\overset{k_4}{\longleftrightarrow}} \mathrm{D}.$
  - Conservation equation:

$$\frac{d}{dt}\begin{pmatrix} [A] \\ [B] \\ [C] \\ [D] \end{pmatrix} = \begin{pmatrix} -k_1 & 0 & 0 & 0 \\ k_1 & -k_2 & k_3 & 0 \\ 0 & k_2 & -k_3 - k_4 & k_5 \\ 0 & 0 & k_4 & -k_5 \end{pmatrix} \begin{pmatrix} [A] \\ [B] \\ [C] \\ [D] \end{pmatrix}.$$

  - Steady state: $\begin{pmatrix} -k_1 & 0 & 0 & 0 \\ k_1 & -k_2 & k_3 & 0 \\ 0 & k_2 & -k_3 - k_4 & k_5 \\ 0 & 0 & k_4 & -k_5 \end{pmatrix} \begin{pmatrix} [A] \\ [B] \\ [C] \\ [D] \end{pmatrix} = 0$

  - Null space of the rate matrix: $\begin{pmatrix} [A] \\ [B] \\ [C] \\ [D] \end{pmatrix} = c \begin{pmatrix} 0 \\ (k_3/k_2)\,(k_5/k_4) \\ k_5/k_4 \\ 1 \end{pmatrix}$

  - What is this subspace geometrically?

Matrix Rank

$$\mathbf{A} \in \mathbb{R}^{N \times M}$$

- Rank of a matrix is the dimension of its column space

$$r = \dim \mathcal{R}(\mathbf{A})$$

- Finding the rank: transform to upper triangular form

$$\mathbf{A} \to \mathbf{U}$$

$$\boldsymbol{U} = \left(\begin{array}{cccc|ccc} U_{11} & U_{12} & \ldots & U_{1r} & U_{1(r+1)} & \ldots & U_{1M} \\ 0 & U_{22} & \ldots & U_{2r} & U_{2(r+1)} & \ldots & U_{2M} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & U_{rr} & U_{r(r+1)} & \ldots & U_{rM} \\ \hline 0 & 0 & \ldots & 0 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & 0 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & 0 & 0 & \ldots & 0 \end{array}\right)$$

- Rank nullity theorem:

$$\dim \mathcal{N}(\mathbf{A}) = M - r$$

Existence and Uniqueness

$$\mathbf{A} \in \mathbb{R}^{N \times M}$$

- Existence:
  - For any $\mathbf{b}$ in $\mathbf{Ax} = \mathbf{b}$
  - A solution exists only if $r = \dim \mathcal{R}(\mathbf{A}) = N$
- Uniqueness:
  - A solution is unique only if $\dim \mathcal{N}(\mathbf{A}) = 0$
  - Equivalently when $r = \dim \mathcal{R}(\mathbf{A}) = M$

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