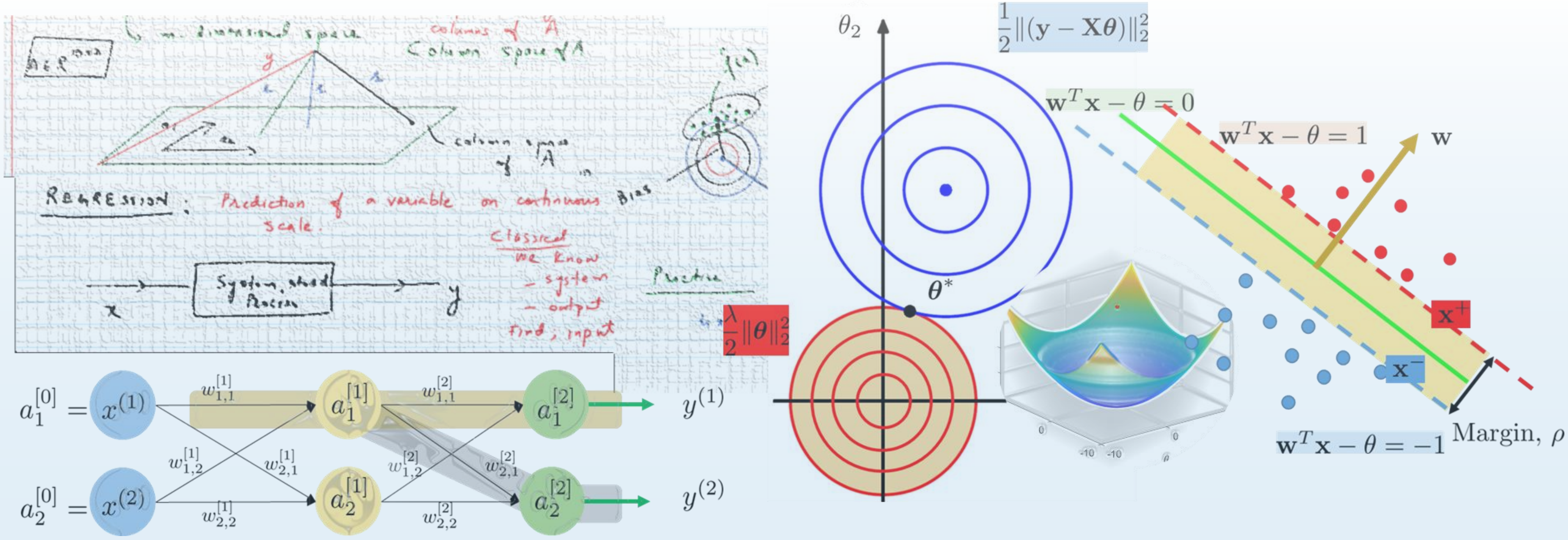

AI-501 Mathematics for AI

Singular Value Decomposition and Spaces

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LUMS

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Outline

- Eigenvalue Decomposition
  - Eigenvectors, Eigenvalue overview
  - Formulation
  - Interpretation

Eigenvalue Decomposition (EVD)

Eigenvectors and Eigenvalues:

For square matrices, *eigenvectors* and *eigenvalues* are vectors and numbers represent the *eigen-decomposition* of a matrix; analyzes the structure of this matrix.

For a matrix $A \in \mathbf{R}^{n \times n}$

a vector $q \in \mathbf{R}^n$, $q \neq 0$, is called an eigenvector of A if

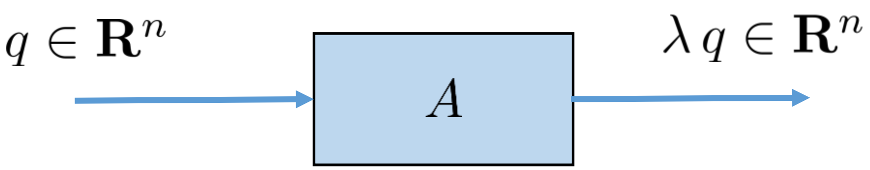
$$A\,q = \lambda\,q$$

Eigenvalue Equation

- λ is referred to as an eigenvalue of A associated with the eigenvector q

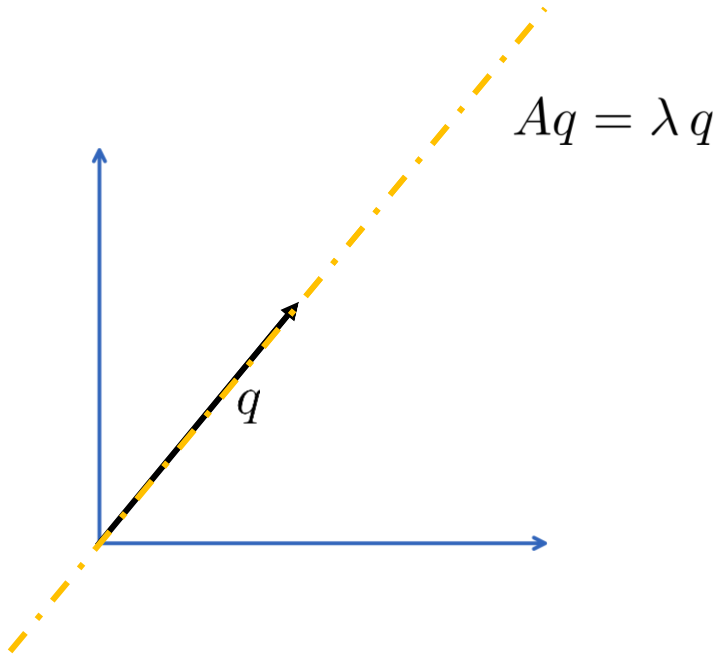
Eigenvalue Decomposition (EVD)

Linear transformation interpretation:



Only scaling

Graphically



Eigenvalue Decomposition (EVD)

Eigenvectors and Eigenvalues:

How to compute eigenvalues?

$$Aq = \lambda q \qquad \Rightarrow \qquad Aq - \lambda q = 0$$

$p(\lambda) = \det(Aq - \lambda q) = 0$ Characteristic polynomial; degree *n*

n eigenvalues — Eigenspectrum: set of eigenvalues

n eigenvectors — Eigenspace: span of eigenevectors

Eigenvalue Decomposition (EVD)

Eigenvectors and Eigenvalues:

$$A\,q = \lambda\,q$$

n eigenvalues $\lambda_1,\ \lambda_2, \ldots, \lambda_n$

n eigenvectors $q_1,\ q_2, \ldots, q_n \in \mathbf{R}^n$

$$A\,q_1 = \lambda_1\,q_1, \quad A\,q_2 = \lambda_2\,q_2, \ \ldots$$

$$A\,Q = Q\,\Lambda$$

$$A = Q\,\Lambda\,Q^{-1}$$

Eigen-decomposition

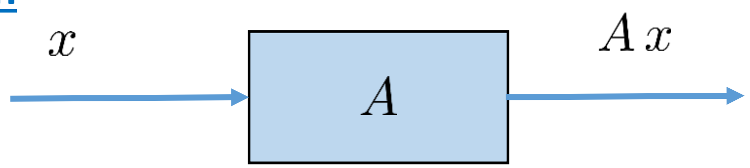
$$\Lambda = \begin{bmatrix} \lambda_1 & 0 & \ldots & 0 \\ 0 & \lambda_2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \lambda_n \end{bmatrix}$$

$$Q = \begin{bmatrix} (q_1)_1 & (q_2)_1 & \ldots & (q_n)_1 \\ (q_1)_2 & (q_2)_2 & \ldots & (q_n)_2 \\ \vdots & \vdots & \ddots & \vdots \\ (q_1)_n & (q_2)_n & \ldots & (q_n)_n \end{bmatrix}$$

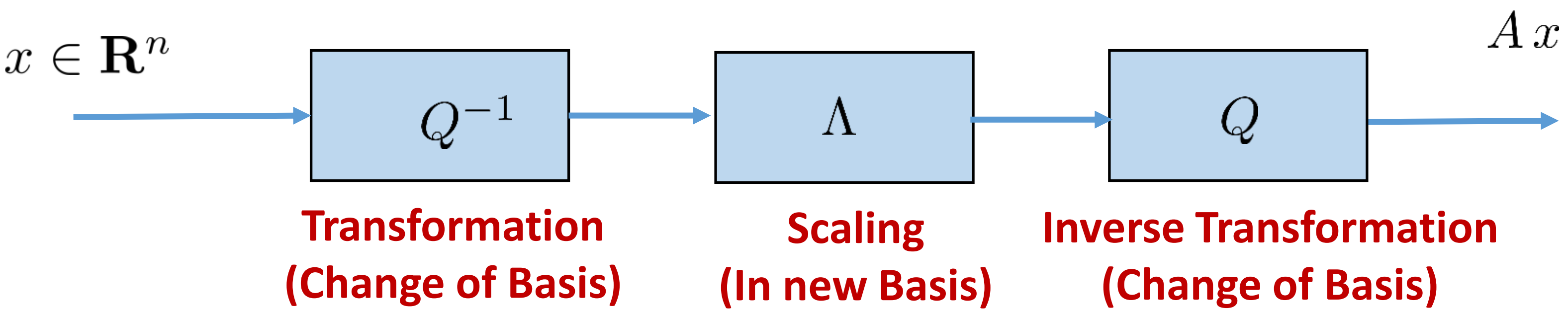
Eigenvalue Decomposition

What does eigenvector and eigenvalues reveal about A?

Linear Transformation



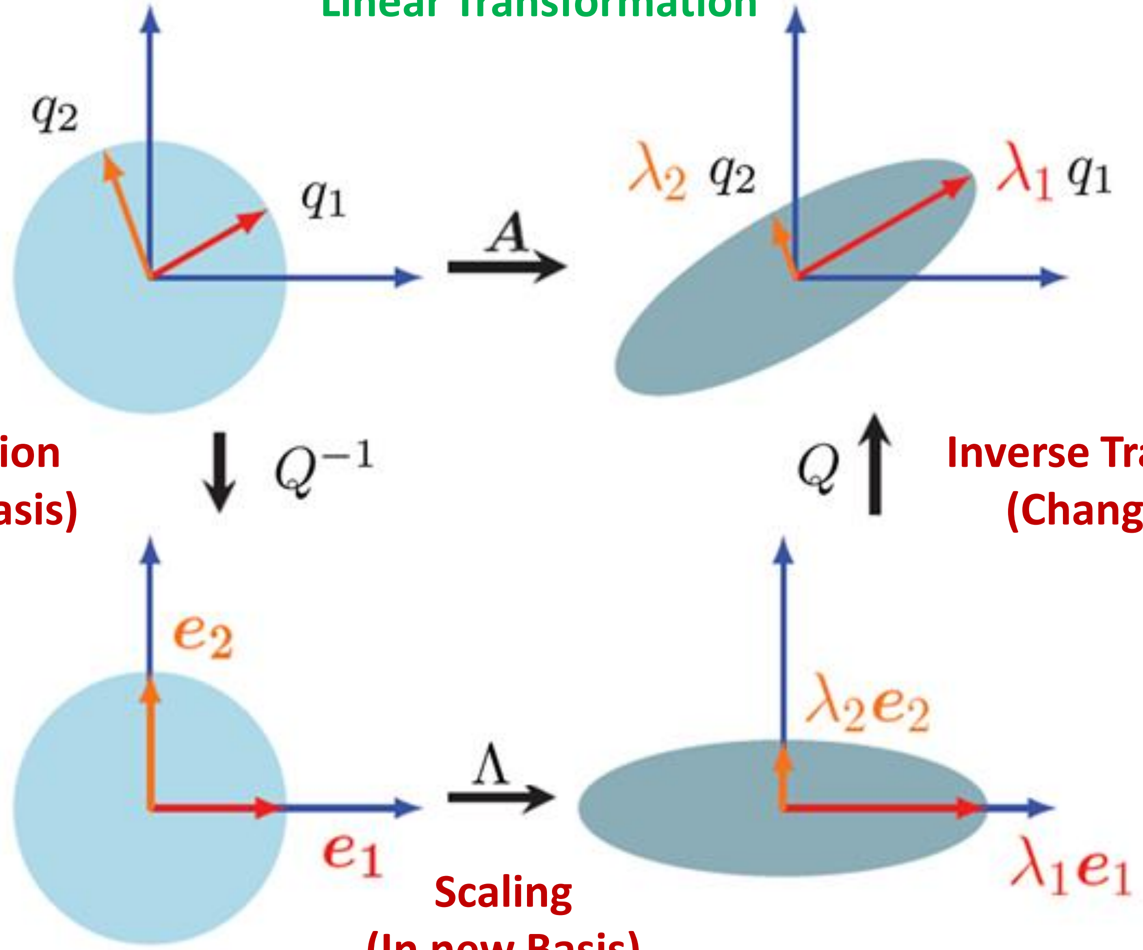
Linear Transformation Interpretation in terms of Eigen-decomposition of the Matrix



Eigenvalue Decomposition

Linear Transformation Interpretation in terms of Eigen-decomposition of the Matrix - Visualization

Linear Transformation



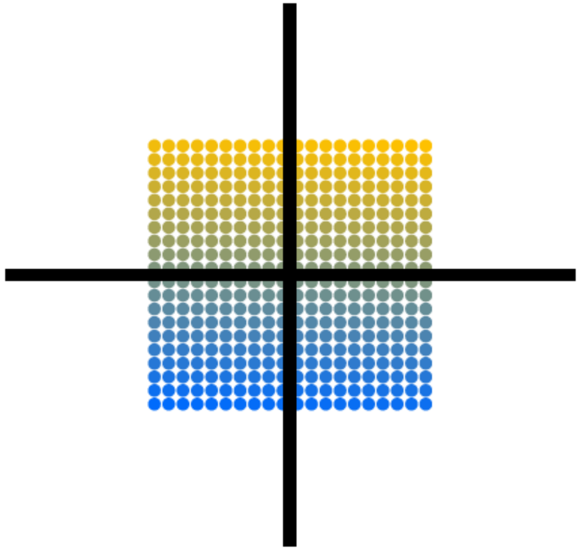
Transformation
(Change of Basis)

Inverse Transformation
(Change of Basis)

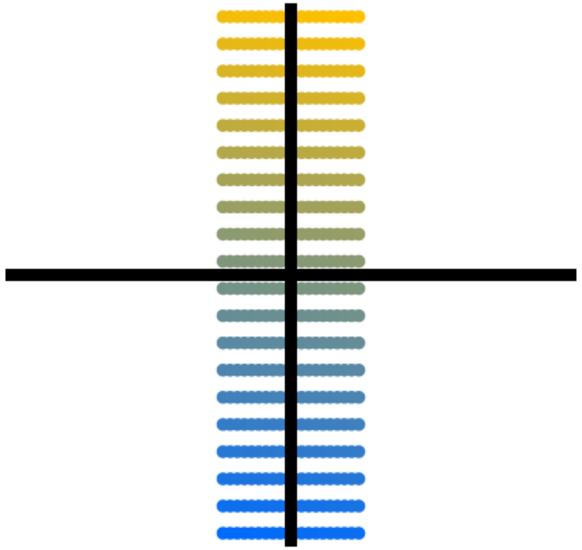
Scaling
(In new Basis)

Eigenvalue Decomposition

Eigen-decomposition of the Matrix - Example

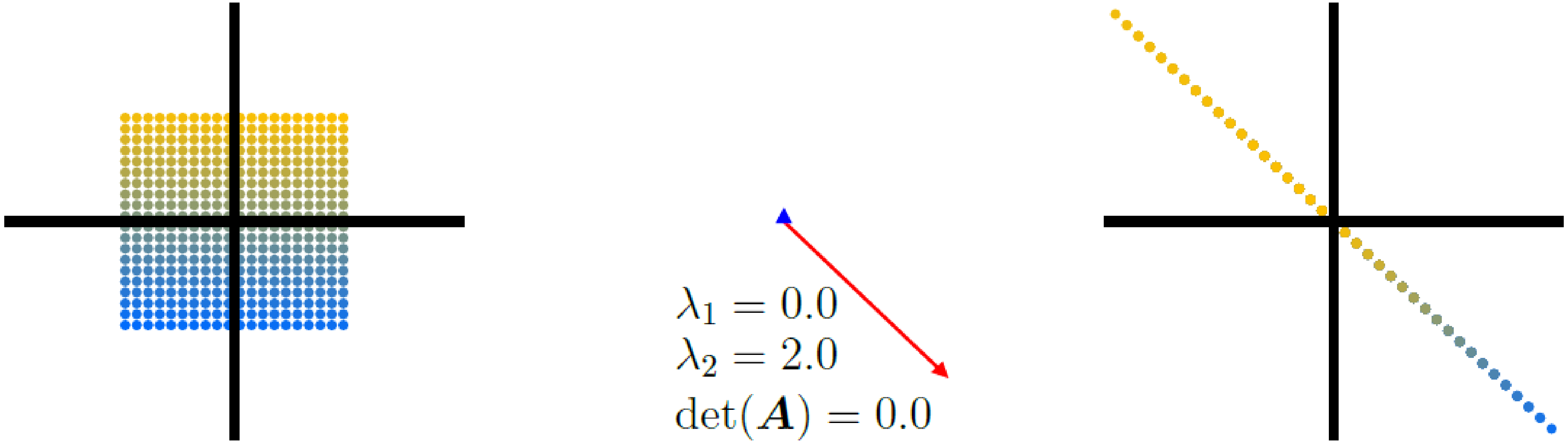


$$\lambda_1 = 2.0$$
$$\lambda_2 = 0.5$$
$$\det(\boldsymbol{A}) = 1.0$$



Eigenvalue Decomposition

Eigen-decomposition of the Matrix - Example



Eigenvalue Decomposition

Determinant in terms of Eigenvalues

- Determinant of a matrix $A \in \mathbf{R}^{n\times n}$ is given by the product of eigenvalues, that is,

$$\det(A) = \det(Q\Lambda Q^{-1}) = \det(Q)\det(\Lambda)\det(Q^{-1})$$

$$\det(A) = \det(Q\Lambda Q^{-1}) = \det(Q)\left(\prod_{i=1}^{n}\lambda_i\right)\frac{1}{\det(Q)}$$

$$\det(A) = \prod_{i=1}^{n}\lambda_i$$

- If one of the eigenvalues is zero, determinant of the matrix is zero.

  - I encourage you to connect this with the interpretation of determinant and (eigenvectors, eigenvalues).

Eigenvalue Decomposition (EVD)

EVD of Inverse Matrix:

- Matrix inverse A^{-1} has same eigenvectors but eigenvalues are given by inverse of the eigenvalues of the original matrix A.
- This can be shown in multiple ways. Let's use eigenvalue equation to show this.

For a matrix $A \in \mathbf{R}^{n \times n}$

$$A\,q = \lambda\,q$$

Eigenvalue Equation

- Assuming A is invertible, that is, all eigenvalues are non-zero.

$$A^{-1}A\,q = \lambda\,A^{-1}q \qquad \frac{1}{\lambda}q = A^{-1}q$$

This implies q is an eigenvector of A^{-1} with associated eigenvalue $\frac{1}{\lambda}$.

Eigenvalue Decomposition

Power of a matrix

$$AA = A^2 = Q\Lambda Q^{-1}\ Q\Lambda Q^{-1} = Q\Lambda^2 Q^{-1}$$

$$A^n = Q\Lambda^n Q^{-1}$$

- I encourage you to connect this with the interpretation of linear transformation using EVD of a matrix.

Eigenvalue Decomposition

Zero eigenvalues; Columns of A are not linearly independent

- If one of the eigenvalues is zero and q is an associated eigenvector.

$$A\,q = \lambda\,q \;=\; 0$$

- It simply follows from the definition of linear independence that the columns are not linearly independent since Aq represents the linear combination of columns of A.

Eigenvalue Decomposition

Eigenvalues of a Symmetric Matrix

- (Spectral Theorem) For a symmetric matrix $A \in \mathbf{R}^{n\times n}$, there exists an orthonormal basis of the corresponding vectors space cossisting of eigenvectors of A and each eigenvalue is real.

$$A = Q \Lambda Q^{-1}$$

$$A^T = (Q^{-1})^T \Lambda Q^T$$

Since $A = A^T$, we have $(Q^{-1} = Q^T$

⇩

Orthonormal matrix

- Summary: For a symmetric matrix, eigenvectors are orthonromal and eigenvalues are real.

Outline

- Positive/negative definite and semi-definite matrices
- Singular Value Decomposition (SVD)
  - Formulation
  - Interpretation
  - Application examples
- Column space and Null Space

Positive/Negative Definite/Semi-Definite Matrices

Definition:

For a matrix $A \in \mathbf{R}^{n \times n}$, if

$x^T A x \geq 0$	$\forall \ x \in \mathbf{R}^n$	A is positive semi-definite (PSD)
$x^T A x > 0$	$\forall \ x \in \mathbf{R}^n$	A is positive definite (PD)
$x^T A x \leq 0$	$\forall \ x \in \mathbf{R}^n$	A is negative semi-definite (NSD)
$x^T A x < 0$	$\forall \ x \in \mathbf{R}^n$	A is negative definite (ND)

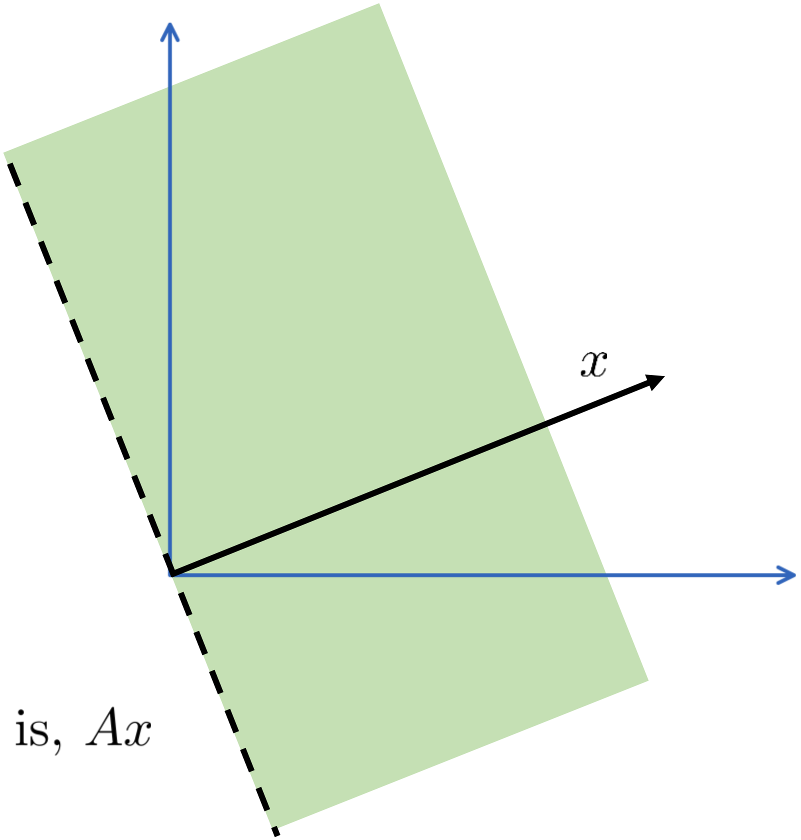
Positive Definite and Semi-Definite Matrices

Interpretation:

A is positive semi-definite (PSD)

$$x^T A x \geq 0$$

- Let $y = Ax$
  - y is a linear transformation defined by the matrix A.
- $x^T y \geq 0$ implies angle between x and y is less than or equal to $\frac{\pi}{2}$.
- $x^T y \geq 0$ implies angle between x and linearly transformed x, that is, Ax is less than or equal to $\frac{\pi}{2}$.



Graphically, a vector x when transformed by a matrix A, that is, Ax can be anywhere in the green region including the dashed boundary where $x^T Ax = 0$

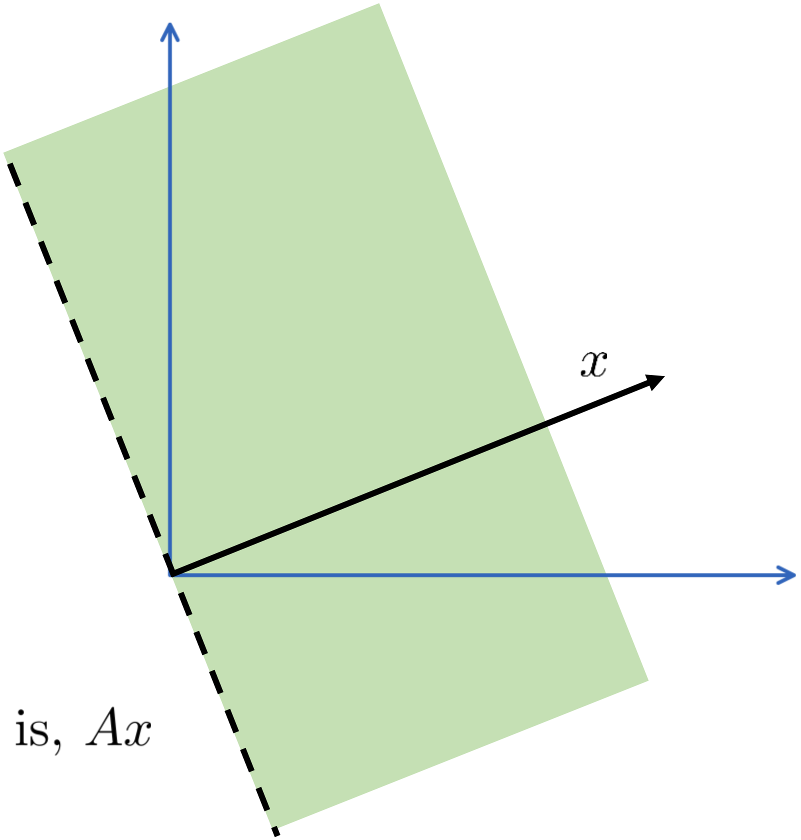
Positive Definite and Semi-Definite Matrices

Interpretation:

A is positive definite (PD)

$$x^T A x > 0$$

- Let $y = Ax$
  - y is a linear transformation defined by the matrix A.
- $x^T y > 0$ implies angle between x and y is less than $\frac{\pi}{2}$.
- $x^T y \geq 0$ implies angle between x and linearly transformed x, that is, Ax is less than $\frac{\pi}{2}$.



Graphically, a vector x when transformed by a matrix A, that is, Ax can be anywhere in the green region excluding the dashed boundary where $x^T A x = 0$

Positive Definite and Semi-Definite Matrices

Eigenvalues of symmetric PSD/PD matrix:

For a symmetric and PD matrix A, eigenvalues are positive.

How?

- We already know that the eigenvalues of a symmetric matrix are real.
- For a PD symmetric, we require $x^T Ax > 0$
- If we take $x = q$, where q is an eigenvector with an associated eigenvalue λ

$$q^T Aq > 0 \Rightarrow \lambda\, q^T q > 0 \Rightarrow \lambda\, \|q\|_2^2 > 0 \Rightarrow \lambda > 0$$

Similarly, we can show the following:

For a symmetric and PSD matrix A, eigenvalues are non-negative.

For a symmetric and NSD matrix A, eigenvalues are non-positive.

For a symmetric and ND matrix A, eigenvalues are negative.

Outline

- Positive/negative definite and semi-definite matrices
- Singular Value Decomposition (SVD)

Outline

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    - Formulation
    - Interpretation
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- Column space and Null Space

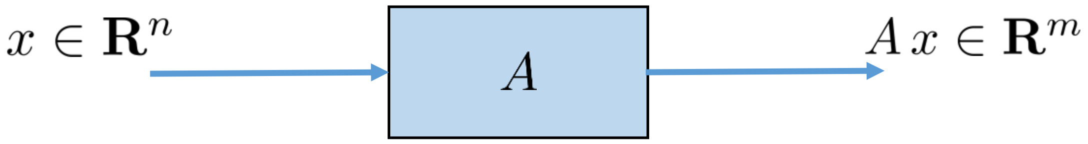
Singular Value Decomposition

Overview:

- The singular value decomposition (SVD) of a matrix is a central matrix decomposition method in linear algebra.

- It has been referred to as the "**fundamental theorem of linear algebra**" (Strang, 1993) because it can be applied to all matrices, not only to square matrices, and it always exists.

- For $A \in \mathbf{R}^{m\times n}$, we have



- SVD explains the underlying geometry of this linear transformation.

Singular Value Decomposition

Formulation:

- For any matrix $A \in \mathbf{R}^{m\times n}$, we have a singular value decomposition (SVD) given by

$$A = U\,\Sigma\,V^T$$

- Matrix $U \in \mathbf{R}^{m\times m}$ is an orthonormal matrix.
- Matrix $V \in \mathbf{R}^{n\times n}$ is an orthonormal matrix.
- Matrix $\Sigma \in \mathbf{R}^{m\times n}$ is a (special) diagonal matrix.

$m < n$

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & 0 & \dots & 0 \\ 0 & 0 & \dots & \sigma_m & 0 & \dots & 0 \end{bmatrix}$$

$m = n$

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \end{bmatrix}$$

$m > n$

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix}$$

Singular Value Decomposition

Formulation:

$$A = U \Sigma V^T$$

- Columns of U are referred to as left singular vectors of matrix A.
- Columns of V are referred to as right singular vectors of matrix A.
- $\sigma_1, \sigma_2, \ldots, \sigma_{\min(m,n)}$ are singular values of matrix A, which are (usually) indexed such that

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{\min(m,n)} \geq 0$$

Singular Value Decomposition

How to Compute SVD?

- For a matrix $A \in \mathbf{R}^{m\times n}$, we define a matrix $G = AA^T$.
- Using $A = U\,\Sigma\,V^T$, we can write G as

$$G = U\,\Sigma\,V^T\,V\,\Sigma^T\,U^T = U\,\Sigma\,\Sigma^T\,U^T$$

- What is special about matrix G?
  - G is symmetric by definition.
  - G is positive semi-definite. How? You are fully equipped to show this.
- We note that $\Sigma\Sigma^T$ is a diagonal matrix of size $m \times m$.
- Eigenvalue decomposition of G gives columns of U as eigenvectors and diagonal entries of $\Sigma\Sigma^T$ as eigenvalues.
- In other words, left singular vectors of A are eigenvectors of AA^T and $\sigma^2 = \lambda$ (eigenvalue of AA^T). Furthermore, $\lambda \geq 0$ since $G = AA^T$ is PSD.

Eigenvalue decomposition of AA^T gives m left singular vectors of A and first m singular values.

Singular Value Decomposition

How to Compute SVD?

- Now we define a matrix $G = A^T A$.
- Using $A = U \Sigma V^T$, we can write G as

$$G = V \Sigma^T U^T U \Sigma V^T = V \Sigma^T \Sigma V^T$$

- What is special about matrix G?
  - G is symmetric by definition.
  - G is positive semi-definite. *How? You are fully equipped to show this.*
- We note that $\Sigma^T \Sigma$ is a diagonal matrix of size $n \times n$.
- Eigenvalue decomposition of G gives columns of V as eigenvectors and diagonal entries of $\Sigma^T \Sigma$ as eigenvalues.
- In other words, right singular vectors of A are eigenvectors of $A^T A$ and $\sigma^2 = \lambda$ (eigenvalue of $A^T A$). Furthermore, $\lambda \geq 0$ since G is PSD.

Eigenvalue decomposition of $A^T A$ gives n right singular vectors of A and first n singular values.

Now you can explain the non-negativity of the singular values.

Singular Value Decomposition

SVD Summary

- Singular value decomposition (SVD) of a matrix $A \in \mathbf{R}^{m \times n}$ is given by

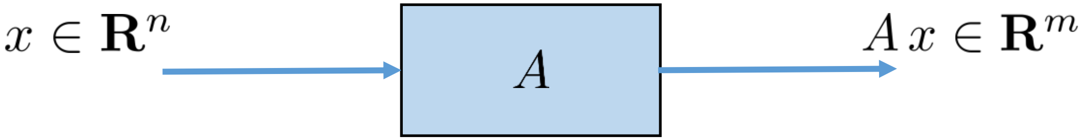
$$A = U\,\Sigma\,V^T$$

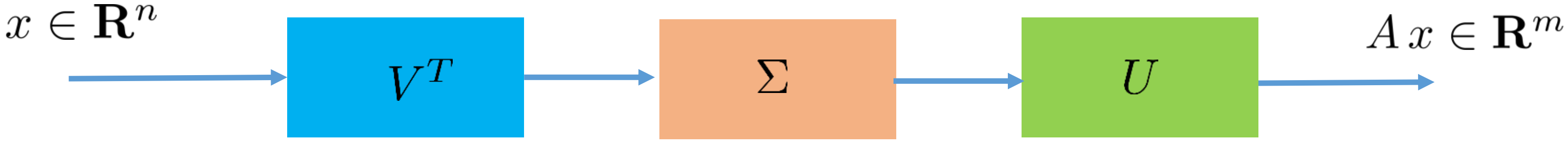
- EVD of AA^T gives U and first m singular values.
- EVD of A^TA gives V and first n singular values.
- U and V are always orthogonal.
- SVD always exists.
- Singular values are non-negative, that is,

$$\sigma_1 \geq \sigma_2 \geq \ \ldots \ \geq \sigma_{\min(m,n)} \geq 0$$

Singular Value Decomposition

Geometric Interpretation





Transformation (Change of Basis)

Scaling (In new Basis)

Transformation (Change of Basis)

Change of basis in $\mathbf{R}^n$

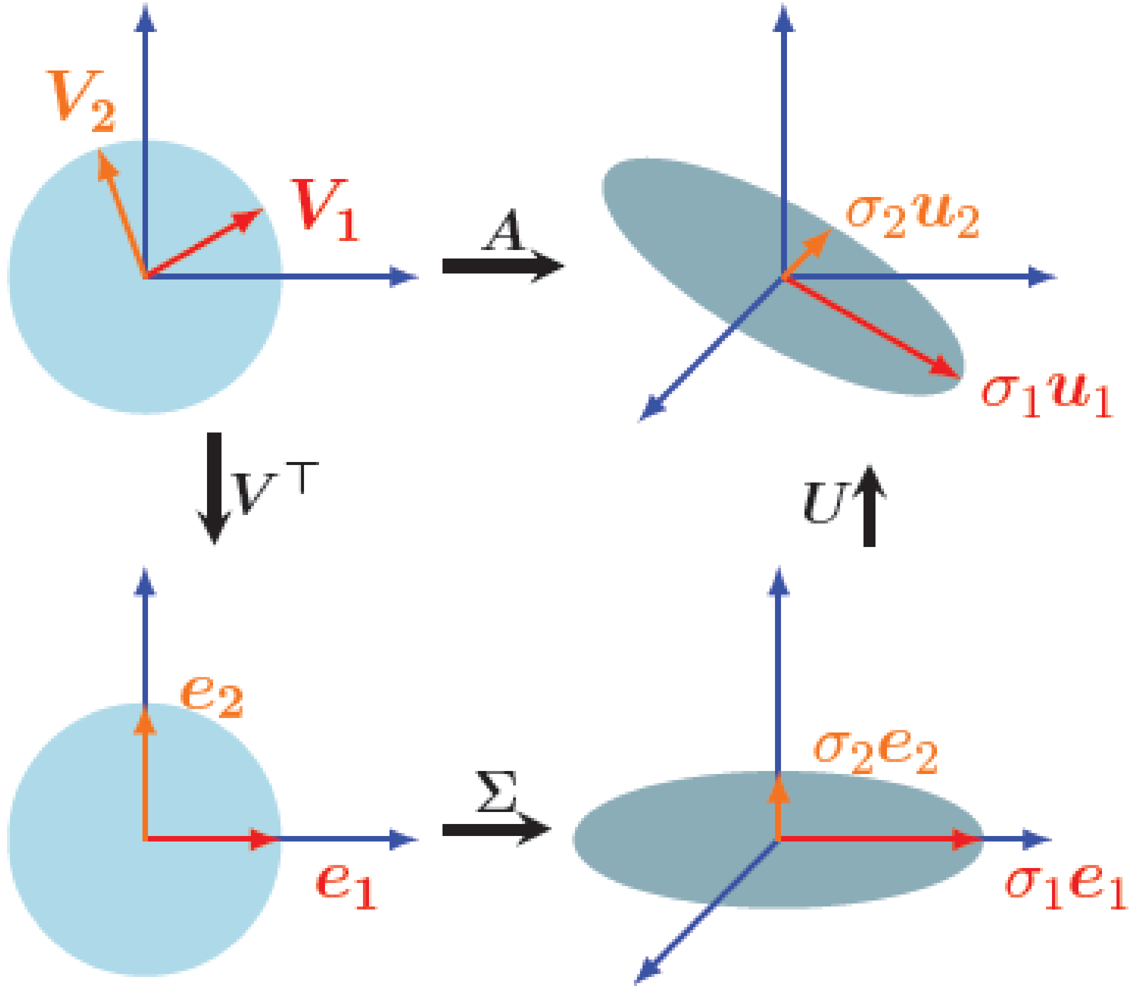
Change of basis in $\mathbf{R}^m$

Scaling along the new basis by singular values.

- $m < n$ - Drop the last $n - m$ basis (impact of columns of zeros in Σ)
- $m > n$ - Append $m - n$ basis (impact of rows of zeros in Σ)

Singular Value Decomposition

Geometric Interpretation

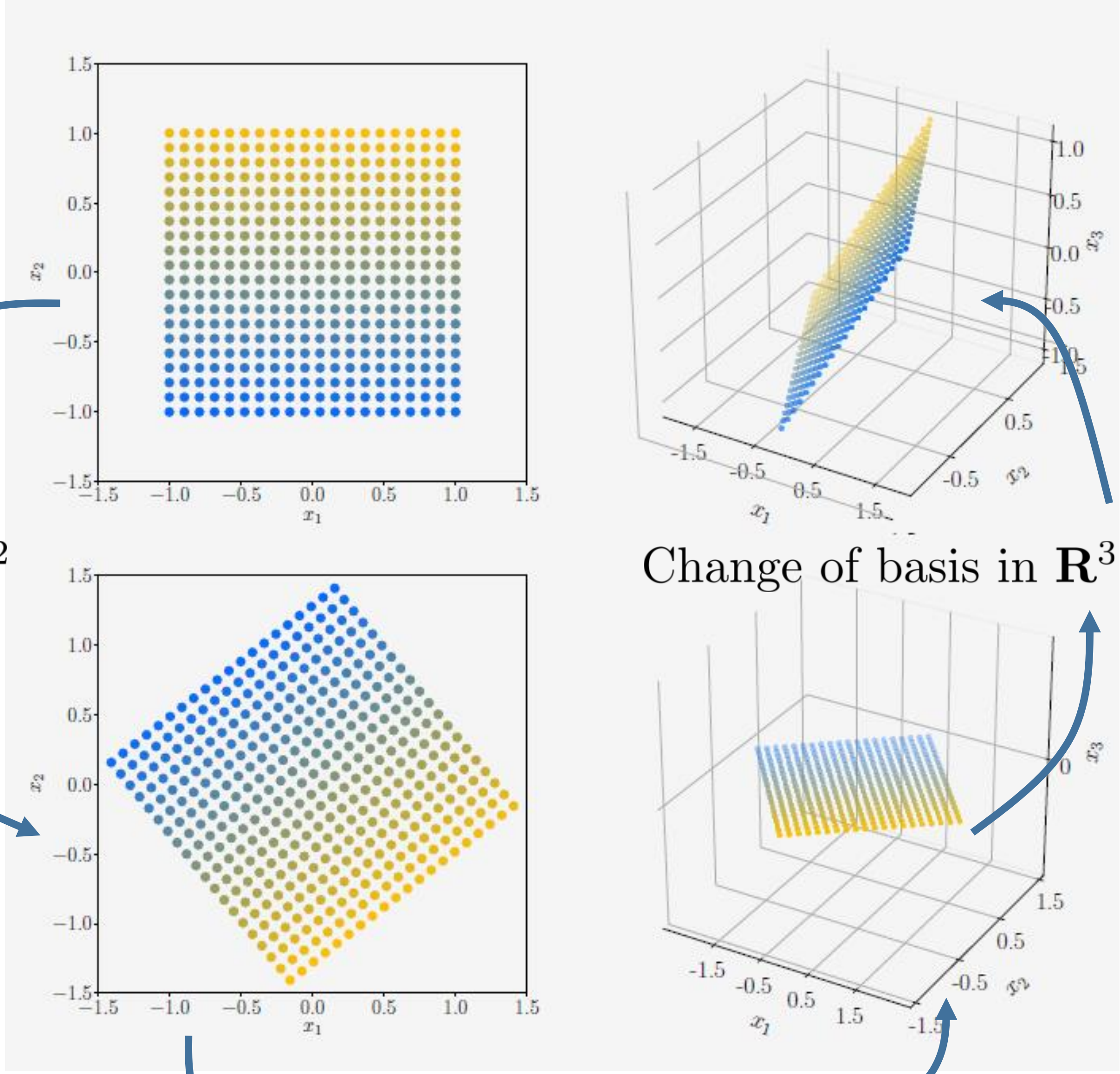


Singular Value Decomposition

Geometric Interpretation - Example

$$A = \begin{bmatrix} 1 & -0.8 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} = U\Sigma V^\top$$

$$= \begin{bmatrix} -0.79 & 0 & -0.62 \\ 0.38 & -0.78 & -0.49 \\ -0.48 & -0.62 & 0.62 \end{bmatrix} \begin{bmatrix} 1.62 & 0 \\ 0 & 1.0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} -0.78 & 0.62 \\ -0.62 & -0.78 \end{bmatrix}$$



Change of basis in $\mathbf{R}^2$

Change of basis in $\mathbf{R}^3$

- Append 1 more basis (impact of a row of zeros in Σ)

Singular Value Decomposition

Rank of a Matrix:

- The rank of a matrix is equal to the number of non-zero singular values.

How?

- Since $A^T A$ and A have the same rank and we know that the rank of any square matrix equals the number of nonzero eigenvalues.

Application Example – Rank Estimation:

We use SVD for the estimation of rank while analyzing data. **How?**

- Suppose that we have n data points $a_1, a_2, \ldots, a_n$, all of which live in $\mathbf{R}^m$, where n is much larger than m. Let A be the $m \times n$ matrix with columns $a_1, a_2, \ldots, a_n$.

- Assume that the the data points satisfy some linear relations, such that $a_1, a_2, \ldots, a_n$ all lie in an r dimensional subspace of $\mathbf{R}^m$. Then we would expect the matrix A to have rank r.

- If the data points are obtained from measurements with errors, then the matrix A will probably have full rank m. But only r of the singular values of A will be large, and the other singular values will be close to zero.

- Using SVD, we can can estimate an "approximate rank" of A by counting the number of singular values which are much larger than the others.

Singular Value Decomposition

Application: Matrix Approximation

- A matrix $A \in \mathbf{R}^{m \times n}$ can be decomposed using SVD as

$$A = U\,\Sigma\,V^T = \sum_{i=1}^{\min(m,n)} u_i \sigma_i v_i^T$$

- If rank of a matrix is $r \leq \min(m, n)$, we can truncate the summationion at r

$$A = \sum_{i=1}^{r} u_i \sigma_i v_i^T$$

- Using SVD formulation, we can define k rank approximation of the matrix A by including first k singular vectors and associated singular values in the representation, that is,

$$A \approx \sum_{i=1}^{k} u_i \sigma_i v_i^T$$

(k-rank approximation)

Outline

- Positive/negative definite and semi-definite matrices
- Singular Value Decomposition (SVD)
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- Column space and Null Space

Column Space and Null Space

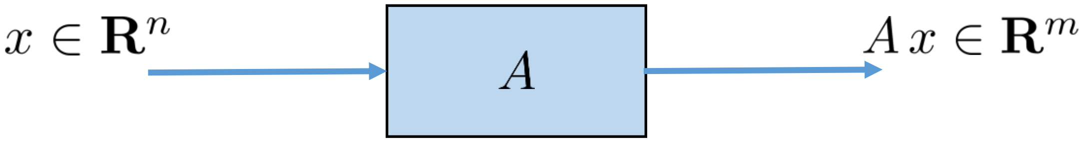
Column Space:

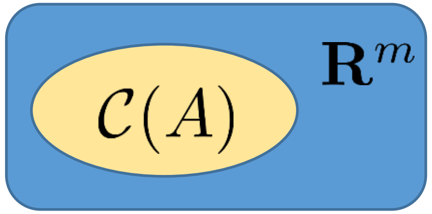
- For a matrix $A \in \mathbf{R}^{m \times n}$, the column space, denoted by $\mathcal{C}(A)$, is the span of the columns of A.
- If $a_1, a_2, \ldots, a_n \in \mathbf{R}^m$ are the columns of A, column space is given by

$$\mathcal{C}(A) = \text{span}(a_1, a_2, \ldots, a_n)$$

$$\mathcal{C}(A) = \{Ax | x \in \mathbf{R}^n\}$$ *(all possible linear combinations of columns of A)*

- In other words, column space is a linear transformation of every point in $\mathbf{R}^n$, that is,





- Consequently, $\mathcal{C}(A)$ is the subspace of $\mathbf{R}^m$.
- What is the dimension of column space $\mathcal{C}(A)$? Number of linearly independent columns of A=rank(A).

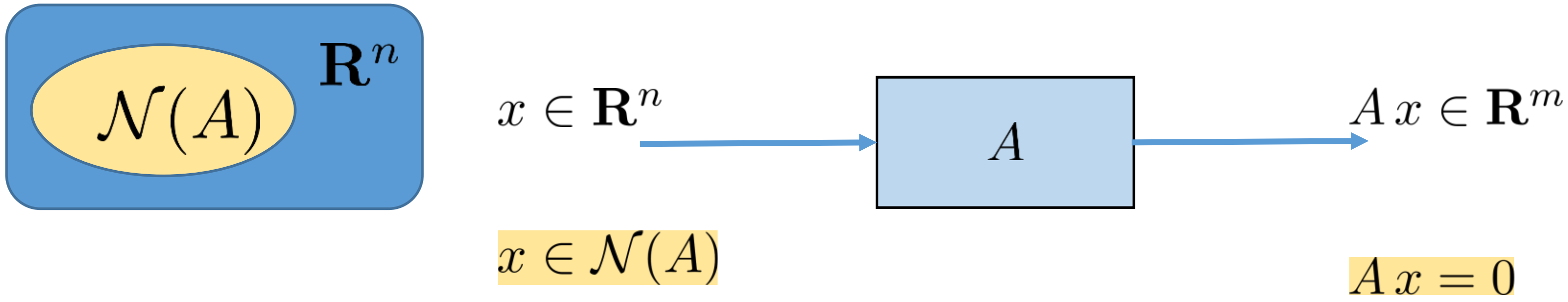
Column Space and Null Space

Null Space:

- For a matrix $A \in \mathbf{R}^{m \times n}$, the null space, denoted by $\mathcal{N}(A)$, is the subspace of $\mathbf{R}^n$ such that

$$\mathcal{N}(A) = \{x \in \mathbf{R}^n \mid Ax = 0\}$$ *(all points that are mapped to zero by matrix A*

- In other words, null space is an inverse linear transformation of $0 \in \mathbf{R}^m$.



- Nullity of the matrix, that is, the dimension of the null-space $\mathcal{N}(A)$ is given by the following rank-nullity theorem (also known as rank+nullity theorem).

$$\text{rank}(A) + \text{nullity}(A) = \text{ number of columns of } A$$

$$\dim(\mathcal{C}(A)) + \dim(\mathcal{N}(A)) = \text{ number of columns of } A$$

Column Space and Null Space

Example:

$$A = \begin{bmatrix} 1 & 1 & 2 \\ 2 & 1 & 3 \\ 3 & 1 & 4 \\ 4 & 1 & 5 \end{bmatrix}$$

- $m = 4$, $n = 3$
- $\mathcal{C}(A)$ is a subspace of $\mathbf{R}^4$.
- $\mathcal{N}(A)$ is a subspace of $\mathbf{R}^3$.

- Note that a third column is a sum of first two columns and therefore number of linearly independent columns is equal to 2.
- Consequently, $\mathcal{C}(A)$ is a 2-dimensional subspace of $\mathbf{R}^4$.