Summer Class: Machine Learning and Data Science

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Matrix as a Vector Transformer

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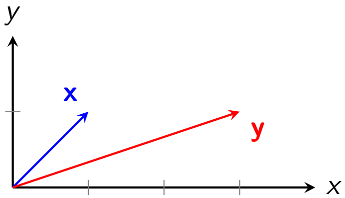

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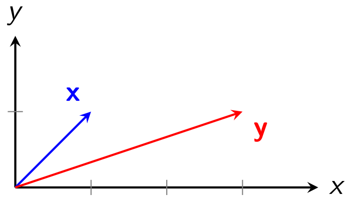

What does this mean geometrically?

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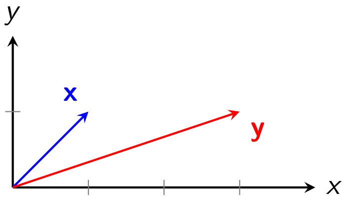
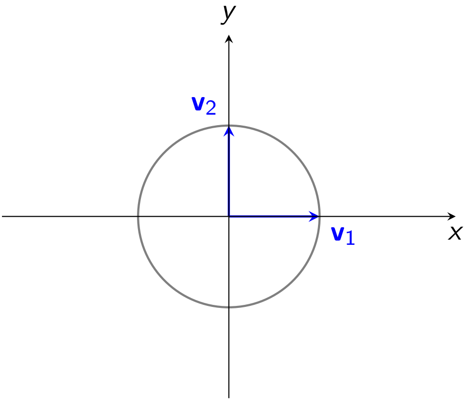


What does this mean geometrically?

- Changes length (scaling).
- Changes direction (rotation/skewing).
- May collapse dimensions.

Transforming a Set of Vectors

Input space: Unit Circle



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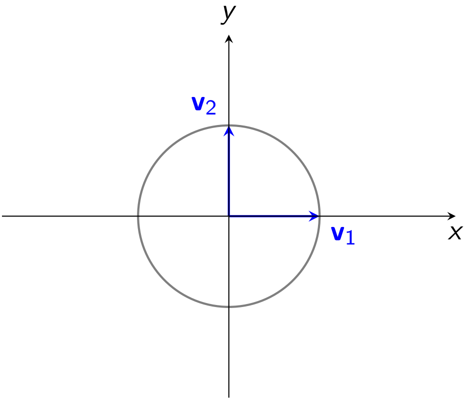
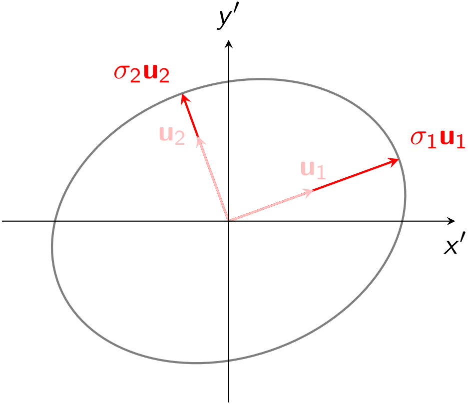


After A, Output space: Ellipse



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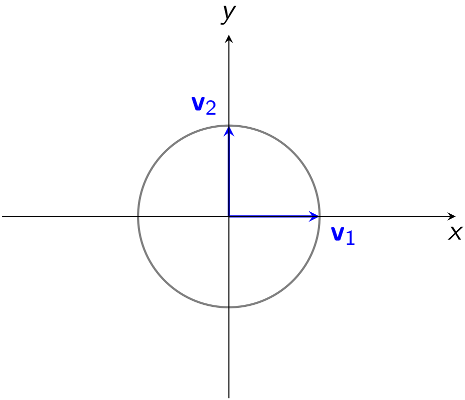

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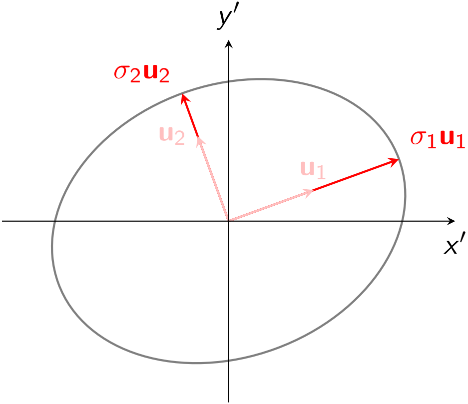

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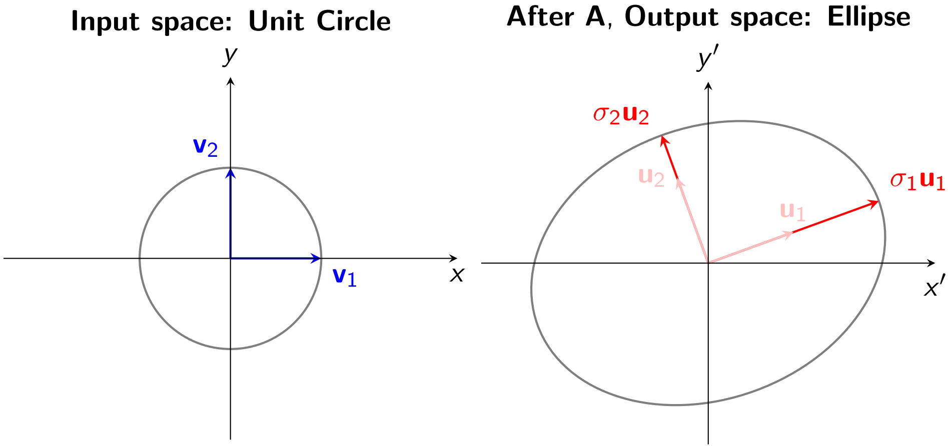

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$$Av_i = \sigma_i u_i \Rightarrow AV = U\Sigma \Rightarrow A = U\Sigma V^*.$$

What is Singular Value Decomposition?

- The Singular Value Decomposition (SVD) is a fundamental matrix factorization in linear algebra. It asserts that any real or complex matrix $A \in \mathbb{C}^{m \times n}$ can be decomposed into the product of three specific matrices.

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- $U \in \mathbb{C}^{m \times m}$: An orthogonal (or unitary for complex) matrix whose columns are the left singular vectors.
- $\Sigma \in \mathbb{C}^{m \times n}$: A diagonal matrix (with non-negative real numbers in decreasing order on the diagonal) containing the singular values σ.
- $V \in \mathbb{C}^{n \times n}$: An orthogonal (or unitary for complex) matrix whose columns are the right singular vectors.

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  - If $m > n$, $\Sigma = \begin{bmatrix} \hat{\Sigma} \in \mathbb{C}^{n\times n} \\ 0 \end{bmatrix}$. If $m < n$, $\Sigma = \left[\hat{\Sigma} \in \mathbb{C}^{m\times m}, 0\right]$. If $m = n$, $\Sigma = \hat{\Sigma} \in \mathbb{C}^{m\times n}$.

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   - Σ is a diagonal matrix. It scales the rotated vectors along these new axes.
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3. Rotation by U:
   - U is an orthogonal matrix. It rotates the scaled vectors into their final positions in the codomain (output space $\mathbb{R}^m$).
   - It aligns the scaled vectors with the basis vectors of the range (u_i).

Visualizing the Transformation

Let's start with an ellipse and apply the transformation matrix:

$$A = \begin{pmatrix} 0.4330 & -0.7500 \\ 1.2500 & -0.4330 \end{pmatrix}$$

.

- **Rotation (V^T):** Rotation by 30°.

$$V^T = \begin{pmatrix} 0.866 & -0.5 \\ 0.5 & 0.866 \end{pmatrix} \approx R(30^\circ)$$

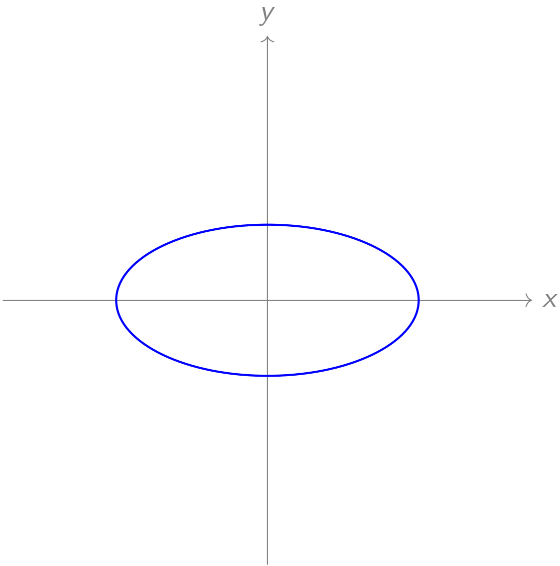
- **Scaling (Σ):**

$$\Sigma = \begin{pmatrix} 1.5 & 0 \\ 0 & 0.5 \end{pmatrix}$$

- **Rotation (U):** Rotation by 60°.

$$U = \begin{pmatrix} 0.5 & -0.866 \\ 0.866 & 0.5 \end{pmatrix} \approx R(60^\circ)$$

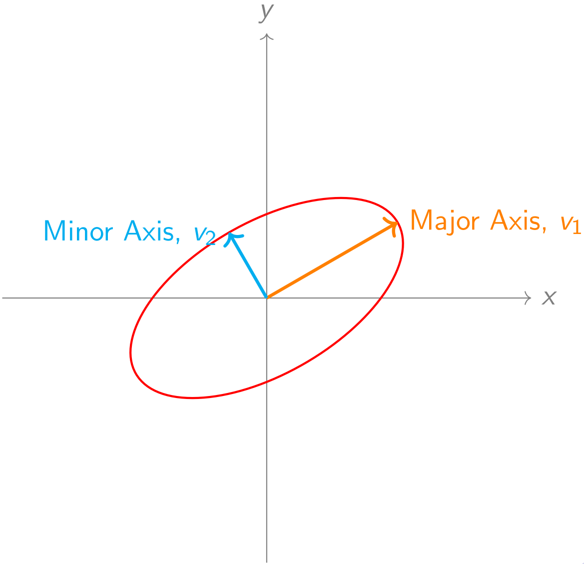
Visualizing the Transformation



Start: Ellipse

$x_0 \in \mathbb{R}^2$

Visualizing the Transformation

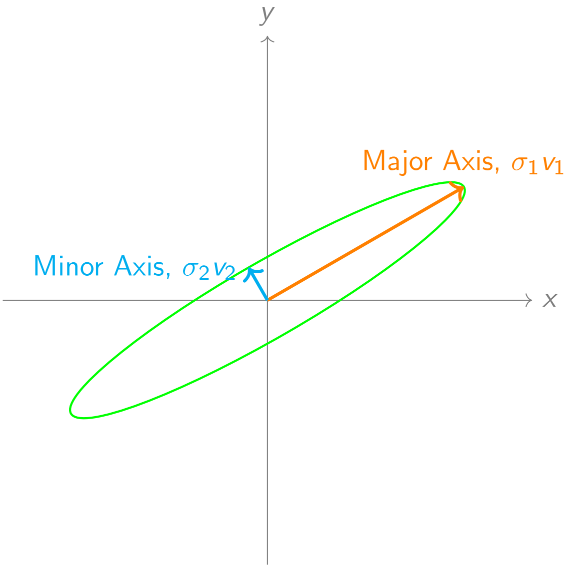


Step 1: Apply $V^\top$

$$x_1 = V^\top x_0$$

$V^\top$ rotates the entire coordinate system so that the directions we want to stretch and shrink are perfectly aligned with the main x and y axes (major and minor axes are rotated to lie along the 30° and 120° lines).

Visualizing the Transformation

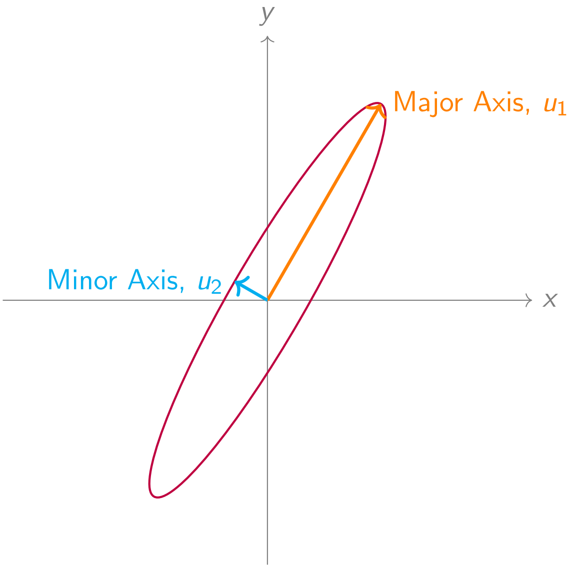


Step 2: Apply Σ

$$x_2 = \Sigma x_1 = \Sigma V^\top x_0$$

It scales everything by 1.5 along the new 30° direction and by 0.5 along the new 120° direction.

Visualizing the Transformation



Step 3: Apply U

$$x_{\text{new}} = Ux_2 = U\Sigma V^\top x_0$$

The columns of the U define the directions of the final ellipse's axes.

Final rotation gives:

$$\boxed{x_{\text{new}} = Ax_0}$$

Full vs Economy (Reduced) SVD

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    - **Case 1: Tall-and-Skinny Matrix** $(m > n)$

$$A_{m\times n} = \underbrace{\begin{bmatrix} | & & | \\ u_1 & \cdots & u_n \\ | & & | \end{bmatrix}}_{U\in\mathbb{C}^{m\times n}} \underbrace{\begin{bmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_n \end{bmatrix}}_{\Sigma\in\mathbb{C}^{n\times n}} \underbrace{\begin{bmatrix} - & v_1^\top & - \\ & \vdots & \\ - & v_n^\top & - \end{bmatrix}}_{V^\top\in\mathbb{C}^{n\times n}}$$

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  - **Case 2: Short-and-Fat Matrix** ($m < n$)

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  - Row-space correlation matrix:

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- Eigenvalues: Σ^2

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- Standard SVD algorithms can be computationally expensive for very large matrices.
- For "Big Data" scenarios where m and n are in the tens of thousands, millions, or more, computing the full SVD becomes impractical in terms of time and memory.
- However, many large real-world matrices are approximately low-rank, or we are only interested in a low-rank approximation (e.g., top k singular values/vectors).

Basic Idea of rSVD

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   - How:
     1. Generate a random matrix $\Omega \in \mathbb{R}^{n \times l}$.
     2. Form the "sketch" or "sample" matrix $Y = A\Omega \in \mathbb{R}^{m \times l}$. Multiplying A by random vectors effectively samples its range.
     3. Compute an orthonormal basis for the columns of Y, typically via QR decomposition: $Y = QR$. The matrix $Q \in \mathbb{R}^{m \times l}$ is our approximate basis.

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   The insight here is that random projections can preserve the essential geometric structure of the original matrix A, particularly its dominant components, allowing us to work with a much smaller sketch Y.

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     3. The final SVD approximation for A is then $A \approx (Q\tilde{U})\Sigma V^T$. Let $U_{rSVD} = Q\tilde{U}$ and then $A \approx U_{rSVD}\Sigma V^T$.

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1. **Generate random test matrix:** $\Omega \in \mathbb{R}^{n\times(k+p)} \quad (l = k + p)$
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MATLAB Demonstration.

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where:

- $r = \text{rank}(A)$.
- σ_i is the i-th singular value.
- u_i is the i-th left singular vector (column of U).
- v_i is the i-th right singular vector (column of V).
- Each item $\sigma_i u_i v_i^T$ is an $m \times n$ matrix of rank 1.

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This means any matrix A can be expressed as a weighted sum of r rank-one matrices. The weights are the singular values σ_i. Since $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r \geq 0$, the first few terms in this sum capture the most "significant" parts of the matrix A.

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- A_k is constructed using the k largest singular values and their corresponding singular vectors.
- This process effectively filters out information associated with smaller singular values, which often corresponds to noise or less significant details.

Optimal Truncation – Eckart-Young-Mirsky Theorem

The Eckart-Young-Mirsky theorem formalizes the optimality of the SVD-based low-rank approximation.

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- Frobenius norm

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- p-norms

$$\|A\|_p = \sup_{x\neq 0}\frac{\|Ax\|_p}{\|x\|_p} = \sup_{x:\|x\|_p=1}\|Ax\|_p, \|A\|_2 = \sigma_1$$

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Theorem (Eckart-Young-Mirsky)

For either $\|\cdot\|_2$ or $\|\cdot\|_F$,

$$\|A - A_k\| \leq \|A - B\| \text{for all rank-k matrices } B.$$

Moreover,

$$\|A - A_k\| = \begin{cases} \sigma_{k+1}, \|\cdot\|_2 \text{ norm} \\ \left(\sum_{i=k+1}^{r} \sigma_i^2\right)^{\frac{1}{2}}, \|\cdot\|_F \text{ norm.} \end{cases}$$

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- MATLAB Demonstration (SVD and rSVD).

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Can we predict the values of the '?' cells?

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

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- **Why is Low Rank?**
  - The columns (and rows) are not independent; they are combinations of a few "basis" vectors.
  - Think of movie ratings: they are driven by a few latent factors like genre, actors, etc.
- **How does SVD help?**
  - SVD finds the best low-rank approximation of any matrix.
  - It decomposes a matrix A into:

$$A = USV^T$$

  - By keeping only the top k singular values in S and setting others to zero (S_k), we get the best rank-k approximation: $A_k = US_kV^T$.

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4. **Repeat:** Go back to Step 2 and repeat. The guesses for the missing values will converge.

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- **Matrix:** Rows are users, columns are movies, and entries are ratings (1-5 stars).
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	1	2	3	4	5	6
a	5		1	1		2
b		2		4		4
c	4	5		1	1	2
d			3	5	2	
e	2		1		4	4

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Standard Solution: $\beta = (X^T X)^{-1} X^T y$ ($X^T X$ is invertible).

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- If columns are nearly linearly dependent (high multicollinearity), $X^T X$ is ill-conditioned, leading to the numerical instability.

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- The regression coefficients are found by:

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This solution minimizes the least-squares error $\|y - X\beta\|_2^2$.

Linear Regression with SVD

MATLAB Demonstration.

$$\begin{bmatrix} | & | & \cdots & | \\ 1 & x_1 & \cdots & x_n \\ | & | & \cdots & | \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

Summary of What You've Learned Today

- Properties of SVD, U, Σ, V.
- Computation of SVD: Conventional method and randomized SVD.
- Geometric Interpretation of SVD
- Applications
  - Matrix Approximation: Image Compression.
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See you on Wednesday (7/2) for Lecture 3 on
Singular Value Decomposition (PCA, POD, LSA).

Principal Component Analysis (PCA)

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- PCs are ordered such that PC1 explains the most variance, PC2 the second most (and is orthogonal to PC1), and so on.

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4. Projection onto lower-dimensional subspace: $P = U^T A_c \in \mathbb{R}^{r \times n}$.

Principal Component Analysis (PCA)

MATLAB Demonstration.

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$$X = U\Sigma V^\top \quad \Rightarrow \quad \text{Eigenfaces} = U_{:,1:k}$$

Eigenfaces

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We can reconstruct the original face using only the top k eigenfaces:

$$x_{\text{recon}} = U_k U_k^\top x$$

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Idea: Project each face image onto a low-dimensional subspace spanned by eigenfaces.

- Each image becomes a vector of coefficients $\alpha \in \mathbb{R}^k$.
- Use classifiers (e.g., k-means, k-NN, SVM) on α instead of original image.
- Efficient and robust to noise, simple.

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- The decomposition takes the form:

$$X(x,t) \approx \sum_{k=1}^{r} a_k(t)\phi_k(x)$$

Proper Orthogonal Decomposition (POD)

Proper Orthogonal Decomposition

- Goal: To decompose a complex, high-dimensional dataset into a set of dominant, energy-ranked spatial patterns called POD modes and their corresponding temporal evolution.
- POD finds the most efficient (optimal) orthogonal basis to represent the data. This means that a truncated set of POD modes captures more energy (variance) of the system than any other basis of the same size.
- The decomposition takes the form:

$$X(x,t) \approx \sum_{k=1}^{r} a_k(t)\phi_k(x)$$

  - $\phi_k(x)$: The k-th POD mode (spatial pattern).
  - $a_k(t)$: The time coefficient for the k-th mode.

Proper Orthogonal Decomposition (POD)

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3. Perform SVD: $A = U\Sigma V^T$.
4. Interpret the POD Components:
   - U (Left Singular Vectors): The columns of U are the POD modes (spatial patterns). Each column is an orthonormal basis vector representing a dominant structure.
   - Σ (Singular Values): The squared singular values (σ_i^2) represent the "energy" of each mode. A rapid decay indicates the dynamics are dominated by a few modes.
   - V (Right Singular Vectors): The columns of V represent the temporal coefficients or evolution of each corresponding spatial mode.

POD on Spring-Mass Networks

MATLAB Demonstration

POD on Spring-Mass Networks

MATLAB Demonstration

- **Data Collection:**
- A 1D chain of masses connected by random springs.
- Dynamics are governed by Newton's second law:

$$M\ddot{u}(t) + Ku(t) = F(t).$$

POD on Spring-Mass Networks

MATLAB Demonstration

- **Data Collection:**
- A 1D chain of masses connected by random springs.
- Dynamics are governed by Newton's second law:

$$M\ddot{u}(t) + Ku(t) = F(t).$$

- Fix a node.
- Apply a short impulse at another node to excite the system.

POD on Spring-Mass Networks

MATLAB Demonstration

- **POD:**
- Collect displacement snapshots: $A = [u(t_1), u(t_2), \ldots]$.
- Apply Singular Value Decomposition:

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MATLAB Demonstration

- **POD:**
- Collect displacement snapshots: $A = [u(t_1), u(t_2), \dots]$.
- Apply Singular Value Decomposition:

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

- Extract:
  - Spatial modes: $\Phi = U(:, 1:r)$.
  - Time coefficients: $a(t) = \Sigma_r V_r^T$.

Latent Semantic Analysis (LSA)

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- Instead of matching keywords, it understands text based on underlying **concepts** and **topics**.

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- LSA is a technique to analyze relationships between documents and the terms they contain.
- Its goal is to uncover the **latent semantic structure** of text.
- Instead of matching keywords, it understands text based on underlying **concepts** and **topics**.
- This helps overcome the limitations of simple keyword matching.

Latent Semantic Analysis (LSA)

Keywords Aren't Meanings: Traditional search methods struggle with two common language issues:

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1. Synonymy

Different words can have the same meaning.

- A search for "**auto**" won't find a document that only uses the word "**car**".

Latent Semantic Analysis (LSA)

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1. Synonymy

Different words can have the same meaning.

- A search for "**auto**" won't find a document that only uses the word "**car**".

2. Polysemy

The same word can have multiple meanings.

- A search for "**jaguar**" could return documents about the animal instead of the car brand.

Latent Semantic Analysis (LSA)

The Core Idea: The Term-Document Matrix

LSA starts by creating a matrix where:

- Each **row** corresponds to a unique **term** (word).
- Each **column** corresponds to a **document**.
- Each **cell** contains a count of how many times a term appears in a document.

Term	**Doc 1**	**Doc 2**	**Doc 3**	**Doc 4**
nasa	1	1	0	0
mars	1	0	0	0
space	1	1	0	0
data	0	0	1	1
python	0	0	1	0

Latent Semantic Analysis (LSA)

LSA uses SVD to decompose the term-document matrix (A) and then reduces its dimensions to find k concepts.

$$A \approx U_k \cdot S_k \cdot V_k^T$$

- U_k Term-Concept Matrix: Shows how each term relates to a concept.
- S_k Concept Strength Matrix: Shows the importance of each concept.
- V_k Document-Concept Matrix: Shows how each document relates to a concept.

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This reduction forces the model to generalize, merging synonyms and clarifying ambiguous terms.

Latent Semantic Analysis (LSA)

After applying SVD, we have a low-dimensional "concept space"

- Find conceptually similar documents, even if they don't share keywords.
- Find semantically related terms.
- Compare a search query against documents in the new space.

Latent Semantic Analysis (LSA)

MATLAB Demonstration.

Latent Semantic Analysis (LSA)

MATLAB Demonstration.

Example

1. NASA sends a rover to explore the surface of Mars
2. The James Webb space telescope captures images of distant stars
3. Machine learning in Python makes data analysis simple
4. Data scientists develop new algorithms for data mining

Latent Semantic Analysis (LSA)

MATLAB Demonstration.

Example

1. NASA sends a rover to explore the surface of Mars
2. The James Webb space telescope captures images of distant stars
3. Machine learning in Python makes data analysis simple
4. Data scientists develop new algorithms for data mining

Two concepts: space exploration, data science

Summary of What You've Learned Today

- Principal Component Analysis (PCA): High Dimensional Data.
- Proper Orthogonal Decomposition (POD): Time Series.
- Latent Semantic Analysis (LSA): Natural Language Processing.

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See you on Monday (7/7) for Lecture 4 on
Fourier Analysis.