

CS3319 Foundations of Data Science

# 7. Dimensionality Reduction

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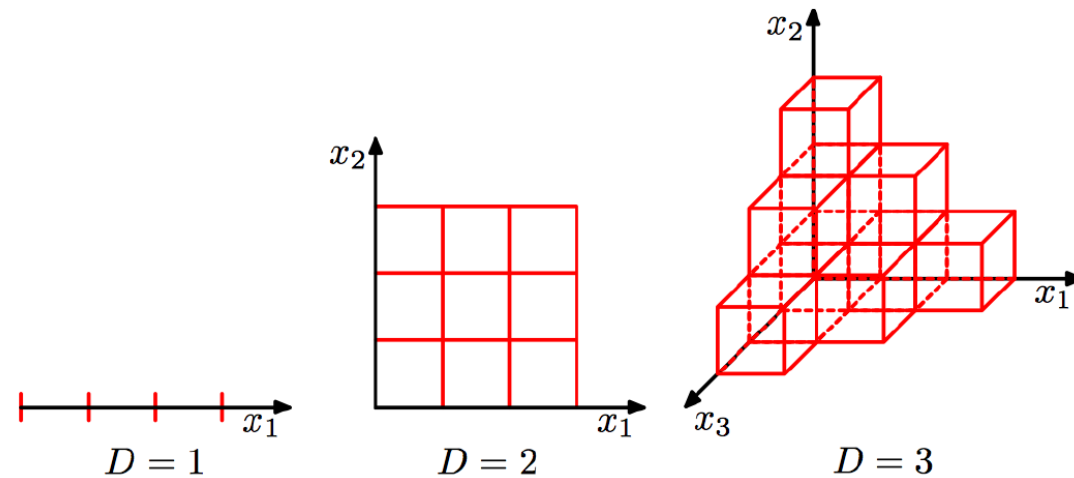
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# Curse of Dimensionality

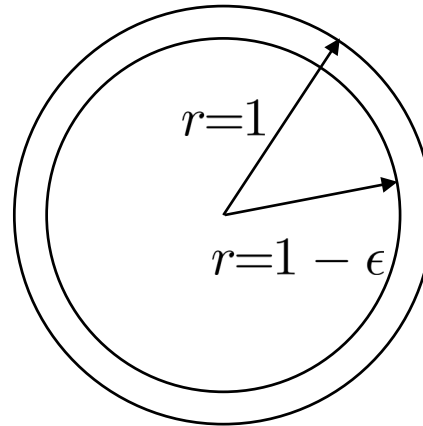
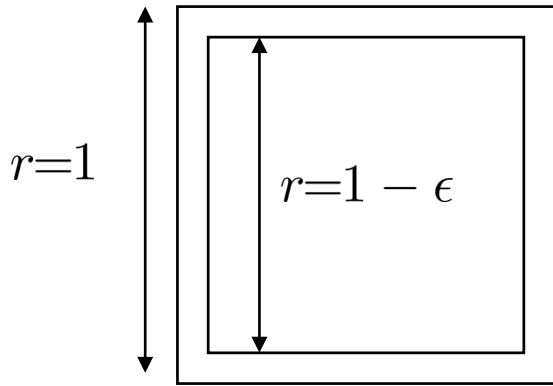
- The high dimensional spaces are **empty**
  - The sample sizes to cover the space grow **exponentially** with the dimension



# Curse of Dimensionality

- Most of its volume is **near the surface** in high dimensional spaces
  - Given a  $d$ -dim volume, shrink this volume by a small amount  $\epsilon$

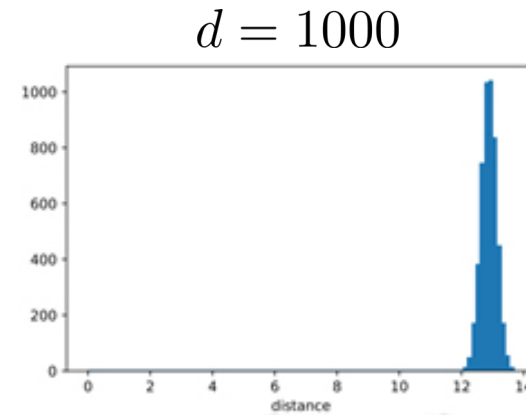
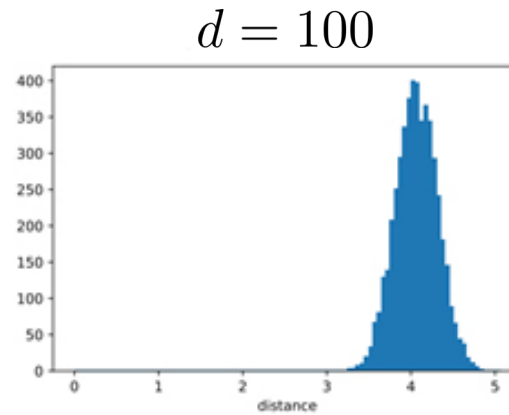
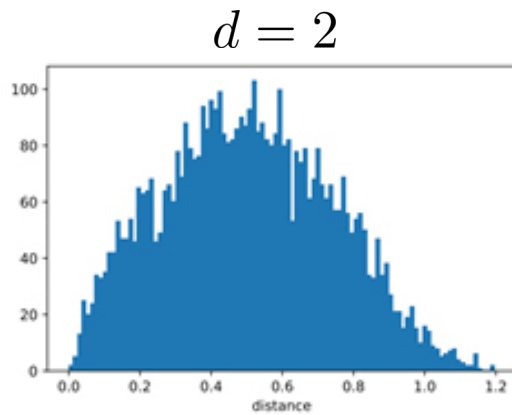
hypercube  $V_d(r) = r^d$       hypersphere  $V_d(r) = \frac{2r^d \pi^{\frac{d}{2}}}{d\Gamma(\frac{d}{2})}$



$$\lim_{d \rightarrow \infty} \frac{V_d(1 - \epsilon)}{V_d(1)} = \lim_{d \rightarrow \infty} (1 - \epsilon)^d = 0$$

# Curse of Dimensionality

- Points are **isolated** in high dimensional spaces
  - $x, y$  are two independent variables, with uniform distribution on  $[0,1]^d$ , their mean Euclidean distance satisfies  $E(\|x - y\|_{\ell_2}) = \sqrt{\frac{d}{6}}$

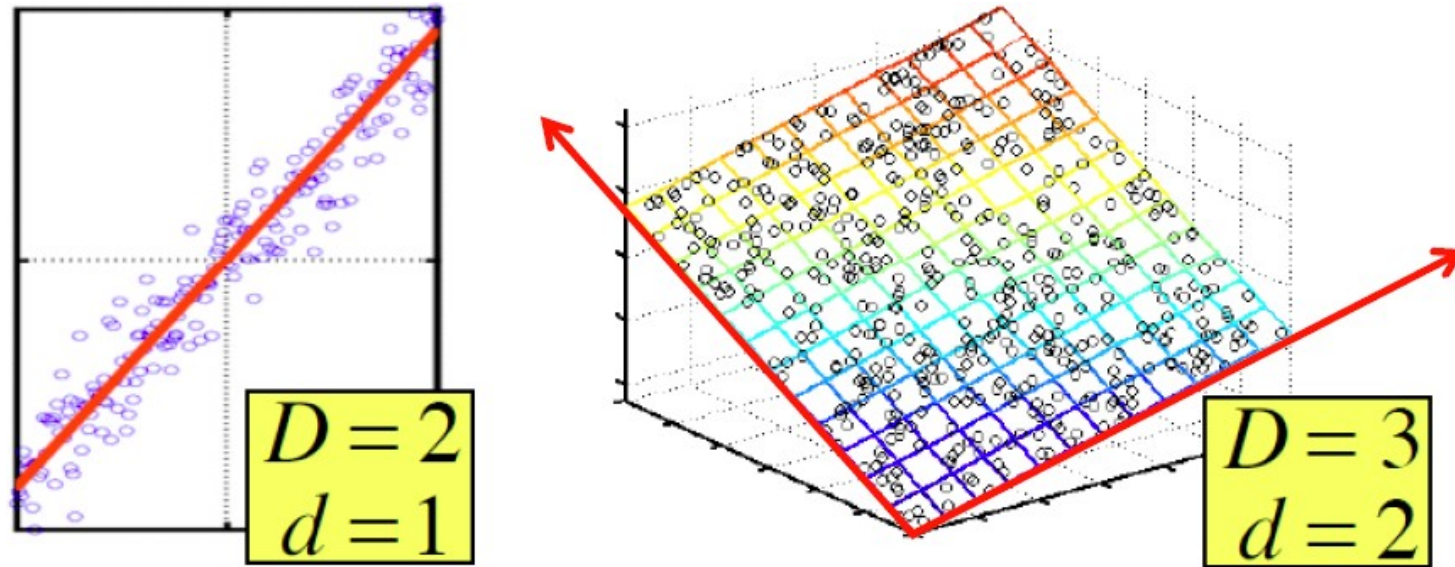


# Curse of dimensionality

- Sample space is large
- Almost all points are near the surface
- Distance metric starts losing their effectiveness

Solution: **dimensionality reduction**

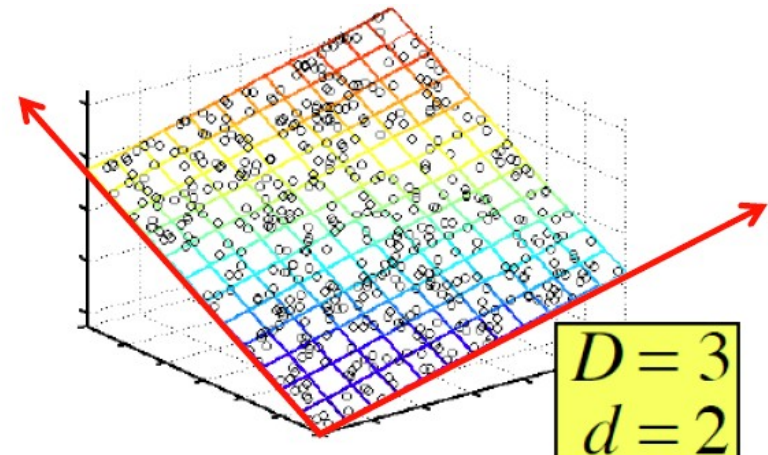
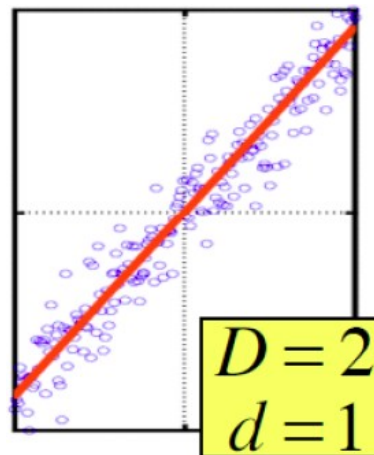
# Dimensionality Reduction



- There are hidden, or **latent factors, latent dimensions** that – to a close approximation – explain why the values are as they appear in the data matrix.
- **Goal of dimensionality reduction is to discover the axes of data!**

# Dimensionality Reduction

- The axes of these dimensions can be chosen by:
  - The first dimension is the direction in which the points exhibit the **greatest variance**.
  - The second dimension is the direction, **orthogonal** to the first, in which points show the **2<sup>nd</sup> greatest variance**.
  - And so on..., until you have enough dimensions that variance is really low.



# SVD: Singular Value Decomposition

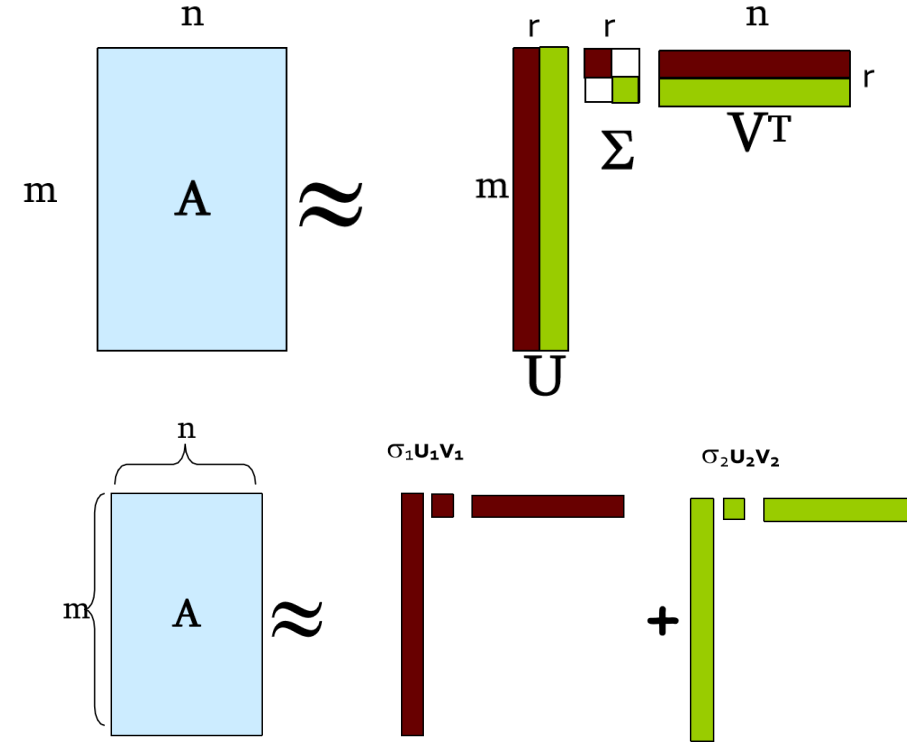


# SVD

It is **always** possible to decompose a real matrix **A** into

where 
$$\mathbf{A} \approx \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \sum_i \sigma_i \mathbf{u}_i \circ \mathbf{v}_i$$

- **U,  $\Sigma$ , V:** unique
- **A: Input data matrix**
  - $m \times n$  matrix;
- **U: Left singular vectors**
  - $m \times r$  matrix; column orthonormal  $\mathbf{U}^T \mathbf{U} = \mathbf{I}$
- **$\Sigma$ : Singular values**
  - $r \times r$  diagonal matrix,  $r$  : rank of the matrix **A**
  - Entries are non-negative, and sorted in decreasing order ( $\sigma_1 \geq \sigma_2 \geq \dots \geq 0$ )
- **V: Right singular vectors**
  - $n \times r$  matrix; column orthonormal  $\mathbf{V}^T \mathbf{V} = \mathbf{I}$



# How to Compute SVD

- First we need a method for finding the **principal eigenvalue** (the largest one) and the corresponding **eigenvector** of a symmetric matrix
  - $M$  is *symmetric* if  $m_{ij} = m_{ji}$  for all  $i$  and  $j$ .
- **Method:**
  - Start with any random eigenvector  $x_0$
  - Construct  $x_{k+1} = \frac{Mx_k}{\|Mx_k\|}$  for  $k = 0, 1, \dots$ 
    - $\| \dots \|$  denotes the Frobenius norm
  - Stop when consecutive  $x_k$  show little change

# Example: Iterative Eigenvector

$$M = \begin{pmatrix} 1 & 2 \\ 2 & 3 \end{pmatrix} \quad \mathbf{x}_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\frac{M\mathbf{x}_0}{\|M\mathbf{x}_0\|} = \begin{pmatrix} 3 \\ 5 \end{pmatrix} / \sqrt{34} = \begin{pmatrix} 0.51 \\ 0.86 \end{pmatrix} = \mathbf{x}_1$$

$$\frac{M\mathbf{x}_1}{\|M\mathbf{x}_1\|} = \begin{pmatrix} 2.23 \\ 3.60 \end{pmatrix} / \sqrt{17.93} = \begin{pmatrix} 0.53 \\ 0.85 \end{pmatrix} = \mathbf{x}_2$$

# Finding the Principal Eigenvalue

- Once you have the principal eigenvector  $\mathbf{x}$ , you find its eigenvalue  $\lambda$  by  $\lambda = \mathbf{x}^T \mathbf{M} \mathbf{x}$ .
  - We know  $\mathbf{x} \lambda = \mathbf{M} \mathbf{x}$  if  $\lambda$  is the eigenvalue; multiply both sides by  $\mathbf{x}^T$  on the left.
  - Since  $\mathbf{x}^T \mathbf{x} = \mathbf{1}$ , we have  $\lambda = \mathbf{x}^T \mathbf{M} \mathbf{x}$ .
- **Example:** If we take  $\mathbf{x}^T = [0.53, 0.85]$ , then

$$\lambda = [0.53 \ 0.85] \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 0.53 \\ 0.85 \end{bmatrix} = 4.25$$

# Finding More Eigenpairs

- Eliminate the portion of the matrix that can be generated by the first eigenpair,  $\lambda$  and  $\mathbf{x}$ :

$$\mathbf{M}^* := \mathbf{M} - \lambda \mathbf{x} \mathbf{x}^T$$

- Recursively find the principal eigenpair for  $\mathbf{M}^*$ , eliminate the effect of that pair, and so on.
- Example:

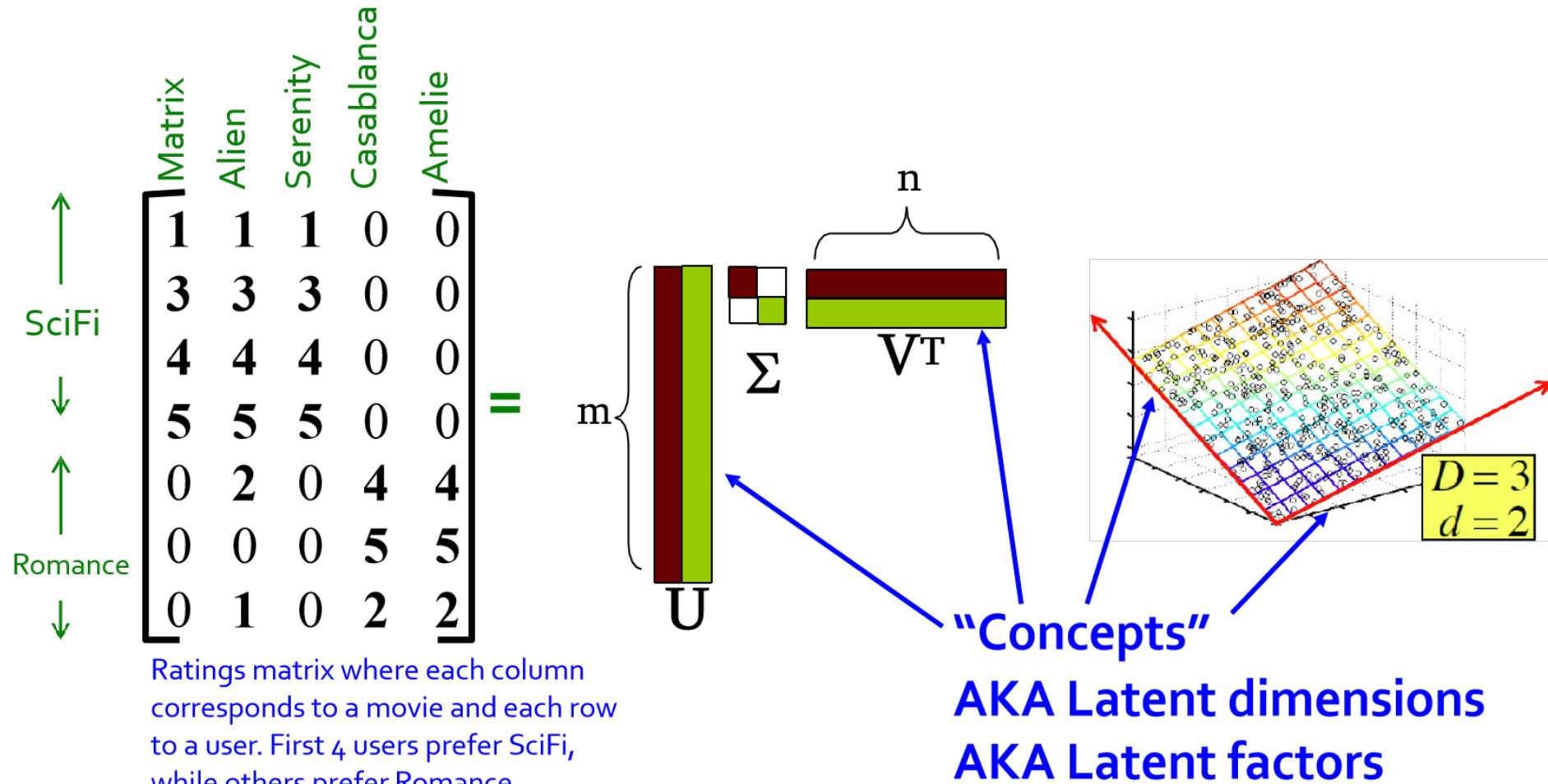
$$\mathbf{M}^* = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} - 4.25 \begin{bmatrix} 0.53 \\ 0.85 \end{bmatrix} \begin{bmatrix} 0.53 & 0.85 \end{bmatrix} = \begin{bmatrix} -0.19 & 0.09 \\ 0.09 & 0.07 \end{bmatrix}$$

# How to Compute SVD

- Start by  $A = U\Sigma V^T$
- $A^T A = V\Sigma U^T U\Sigma V^T = V\Sigma^2 V^T$ 
  - $U$  is orthonormal, so  $U^T U$  is an identity matrix.
  - Also note that  $\Sigma^2$  is a diagonal matrix whose  $i$ -th element is the square of the  $i$ -th element of  $\Sigma$ .
- $A^T A V = V\Sigma^2 V^T V = V\Sigma^2$ 
  - $V$  is also orthonormal.
  - **Note** that therefore the  $i$ -th column of  $V$  is an eigenvector of  $A^T A$ , and its eigenvalue is the  $i$ -th element of  $\Sigma^2$ .
- Symmetric argument,  $AA^T$  gives us  $U$ .

# Interpreting SVD

- What does SVD do?



# SVD-Example: Users-to-Movies

- $A = U\Sigma V^T$  -example: Users to Movies

$$\begin{array}{c}
 \begin{array}{c} \uparrow \\ \text{SciFi} \\ \downarrow \\ \uparrow \\ \text{Romance} \\ \downarrow \end{array}
 \begin{array}{c} \text{Matrix} \\ \text{Alien} \\ \text{Serenity} \\ \text{Casablanca} \\ \text{Amelie} \end{array}
 \begin{bmatrix}
 1 & 1 & 1 & 0 & 0 \\
 3 & 3 & 3 & 0 & 0 \\
 4 & 4 & 4 & 0 & 0 \\
 5 & 5 & 5 & 0 & 0 \\
 0 & 2 & 0 & 4 & 4 \\
 0 & 0 & 0 & 5 & 5 \\
 0 & 1 & 0 & 2 & 2
 \end{bmatrix}
 =
 \begin{bmatrix}
 0.13 & 0.02 & -0.01 \\
 0.41 & 0.07 & -0.03 \\
 0.55 & 0.09 & -0.04 \\
 0.68 & 0.11 & -0.05 \\
 0.15 & -0.59 & 0.65 \\
 0.07 & -0.73 & -0.67 \\
 0.07 & -0.29 & 0.32
 \end{bmatrix}
 \times
 \begin{bmatrix}
 12.4 & 0 & 0 \\
 0 & 9.5 & 0 \\
 0 & 0 & 1.3
 \end{bmatrix}
 \times
 \begin{bmatrix}
 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
 0.40 & -0.80 & 0.40 & 0.09 & 0.09
 \end{bmatrix}
 \end{array}$$



# SVD-Example: Users-to-Movies

U is "user-to-concept" factor matrix

$$\begin{array}{c}
 \begin{array}{c} \uparrow \\ \text{SciFi} \\ \downarrow \\ \uparrow \\ \text{Romance} \\ \downarrow \end{array}
 \begin{bmatrix}
 \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \\
 1 & 1 & 1 & 0 & 0 \\
 3 & 3 & 3 & 0 & 0 \\
 4 & 4 & 4 & 0 & 0 \\
 5 & 5 & 5 & 0 & 0 \\
 0 & 2 & 0 & 4 & 4 \\
 0 & 0 & 0 & 5 & 5 \\
 0 & 1 & 0 & 2 & 2
 \end{bmatrix}
 =
 \begin{array}{c}
 \text{SciFi-concept} \\
 \downarrow \\
 \text{Romance-concept} \swarrow
 \end{array}
 \begin{bmatrix}
 0.13 & 0.02 & -0.01 \\
 0.41 & 0.07 & -0.03 \\
 0.55 & 0.09 & -0.04 \\
 0.68 & 0.11 & -0.05 \\
 0.15 & -0.59 & 0.65 \\
 0.07 & -0.73 & -0.67 \\
 0.07 & -0.29 & 0.32
 \end{bmatrix}
 \times
 \begin{bmatrix}
 12.4 & 0 & 0 \\
 0 & 9.5 & 0 \\
 0 & 0 & 1.3
 \end{bmatrix}
 \times
 \begin{bmatrix}
 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
 0.40 & -0.80 & 0.40 & 0.09 & 0.09
 \end{bmatrix}
 \end{array}$$

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# SVD-Example: Users-to-Movies

Diagram illustrating the SVD decomposition of a User-Movie rating matrix.

**Rating Matrix (Users to Movies):**

	Matrix	Alien	Serenity	Casablanca	Amelie
SciFi	1	1	1	0	0
	3	3	3	0	0
	4	4	4	0	0
	5	5	5	0	0
Romance	0	2	0	4	4
	0	0	0	5	5
	0	1	0	2	2

**SVD Decomposition:**

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} = \begin{bmatrix} 0.13 & 0.02 & -0.01 \\ 0.41 & 0.07 & -0.03 \\ 0.55 & 0.09 & -0.04 \\ 0.68 & 0.11 & -0.05 \\ 0.15 & -0.59 & 0.65 \\ 0.07 & -0.73 & -0.67 \\ 0.07 & -0.29 & 0.32 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 1.3 \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\ 0.40 & -0.80 & 0.40 & 0.09 & 0.09 \end{bmatrix}$$

**Annotations:**

- SciFi-concept:** Points to the first column of the first matrix.
- "strength" of the SciFi-concept:** Points to the value 12.4 in the second matrix.
- SciFi:** Points to the first row of the rating matrix.
- Romance:** Points to the last row of the rating matrix.

# SVD-Example: Users-to-Movies

$$\begin{matrix}
 \uparrow \text{SciFi} \\
 \downarrow \\
 \uparrow \text{Romance} \\
 \downarrow
 \end{matrix}
 \begin{matrix}
 \text{Matrix} \\
 \text{Alien} \\
 \text{Serenity} \\
 \text{Casablanca} \\
 \text{Amelie}
 \end{matrix}
 \begin{bmatrix}
 1 & 1 & 1 & 0 & 0 \\
 3 & 3 & 3 & 0 & 0 \\
 4 & 4 & 4 & 0 & 0 \\
 5 & 5 & 5 & 0 & 0 \\
 0 & 2 & 0 & 4 & 4 \\
 0 & 0 & 0 & 5 & 5 \\
 0 & 1 & 0 & 2 & 2
 \end{bmatrix}
 =
 \begin{matrix}
 \text{SciFi-concept} \\
 \downarrow
 \end{matrix}
 \begin{bmatrix}
 0.13 & 0.02 & -0.01 \\
 0.41 & 0.07 & -0.03 \\
 0.55 & 0.09 & -0.04 \\
 0.68 & 0.11 & -0.05 \\
 0.15 & -0.59 & 0.65 \\
 0.07 & -0.73 & -0.67 \\
 0.07 & -0.29 & 0.32
 \end{bmatrix}
 \times
 \begin{matrix}
 \text{V is "movie-to-concept" factor matrix} \\
 \\
 \end{matrix}
 \begin{bmatrix}
 12.4 & 0 & 0 \\
 0 & 9.5 & 0 \\
 0 & 0 & 1.3
 \end{bmatrix}
 \times
 \begin{matrix}
 \\
 \\
 \end{matrix}
 \begin{bmatrix}
 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
 0.40 & -0.80 & 0.40 & 0.09 & 0.09
 \end{bmatrix}$$

The diagram illustrates the SVD decomposition of a user-movie rating matrix. The first matrix (User-Movie) is decomposed into three matrices: a user-concept matrix (labeled "SciFi-concept" with a blue arrow), a diagonal matrix of singular values, and a movie-concept matrix (labeled "V is 'movie-to-concept' factor matrix"). The resulting user-concept matrix is a 7x3 matrix, and the movie-concept matrix is a 3x5 matrix. The product of the user-concept matrix and the movie-concept matrix is shown as the final result, with the value 0.56 highlighted in a blue circle and labeled "SciFi-concept" with a blue arrow.

# SVD-Interpretation #1

- **Movies, users and concepts:**
  - $U$ : user-to-concept matrix
  - $V$ : movie-to-concept matrix
  - $\Sigma$ : its diagonal elements: 'strength' of each concept

# SVD-Interpretation #2

- **More details**

- **Q:** Further dimension reduction?

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} = \begin{bmatrix} 0.13 & 0.02 & -0.01 \\ 0.41 & 0.07 & -0.03 \\ 0.55 & 0.09 & -0.04 \\ 0.68 & 0.11 & -0.05 \\ 0.15 & -0.59 & 0.65 \\ 0.07 & -0.73 & -0.67 \\ 0.07 & -0.29 & 0.32 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 1.3 \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\ 0.40 & -0.80 & 0.40 & 0.09 & 0.09 \end{bmatrix}$$

# SVD-Interpretation #2

- **More details**

- **Q:** Further dimension reduction?
- **A:** Set **smallest singular values to zero.**

This is Rank 2 approximation to A. We could also do Rank 1 approx.  
The larger the rank the more accurate the approximation.

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \approx \begin{bmatrix} 0.13 & 0.02 & -0.01 \\ 0.41 & 0.07 & -0.03 \\ 0.55 & 0.09 & -0.04 \\ 0.68 & 0.11 & -0.05 \\ 0.15 & -0.59 & 0.65 \\ 0.07 & -0.73 & -0.67 \\ 0.07 & -0.29 & 0.32 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 1.3 \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\ 0.40 & -0.80 & 0.40 & 0.09 & 0.09 \end{bmatrix}$$

*Note: In the original image, the third column of the second matrix and the third row of the third matrix are crossed out with red lines, indicating they are the smallest singular values being set to zero for a rank-2 approximation.*

# SVD-Interpretation #2

- **More details**

- **Q:** Further dimension reduction?
- **A:** Set smallest singular values to zero.

This is Rank 2 approximation to A. We could also do Rank 1 approx.  
The larger the rank the more accurate the approximation.

Matrix A

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \approx \begin{bmatrix} 0.92 & 0.95 & 0.92 & 0.01 & 0.01 \\ 2.91 & 3.01 & 2.91 & -0.01 & -0.01 \\ 3.90 & 4.04 & 3.90 & 0.01 & 0.01 \\ 4.82 & 5.00 & 4.82 & 0.03 & 0.03 \\ 0.70 & 0.53 & 0.70 & 4.11 & 4.11 \\ -0.69 & 1.34 & -0.69 & 4.78 & 4.78 \\ 0.32 & 0.23 & 0.32 & 2.01 & 2.01 \end{bmatrix}$$

Reconstructed matrix B

Reconstruction Error is quantified by the Frobenius norm:

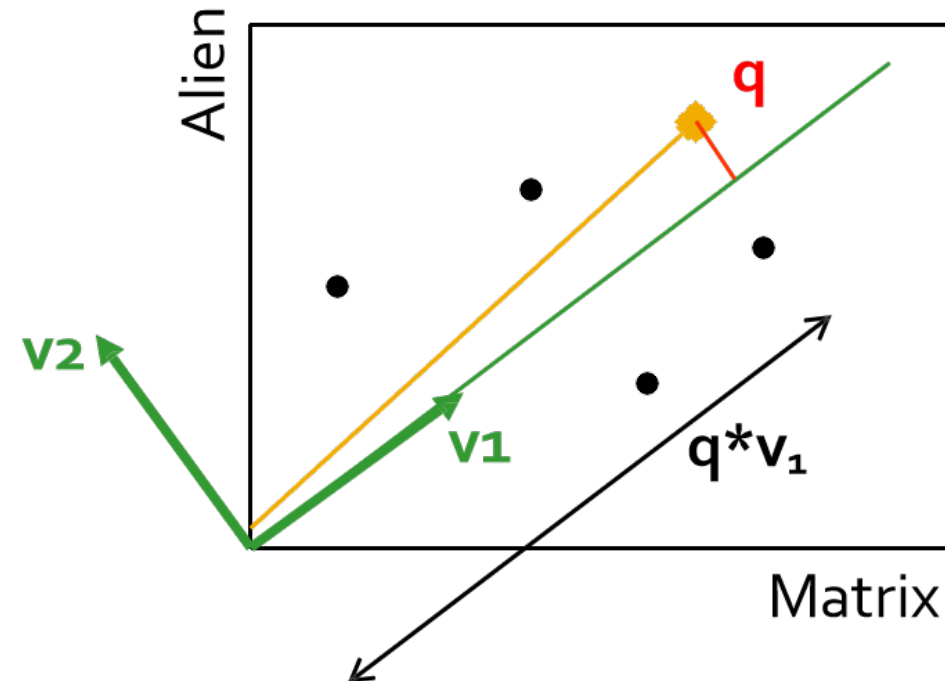
$$\|A - B\|_F = \sqrt{\sum_{ij} (A_{ij} - B_{ij})^2} = \sqrt{\text{tr}((\Sigma_A - \Sigma_B)^2)}$$

# Case Study: How to query?

- Q: A user likes `Matrix', what is her/his taste?
- A: Map query into a 'concept space' – how?

$$\mathbf{q} = \begin{bmatrix} \text{Matrix} \\ 5 \\ \text{Alien} \\ 0 \\ \text{Serenity} \\ 0 \\ \text{Casablanca} \\ 0 \\ \text{Amelie} \\ 0 \end{bmatrix}$$

**Project into concept space:**  
Inner product with each  
'concept' vector  $\mathbf{v}_i$





# Case Study: Are they similar?

- **Observation:** For user  $d$  that rated ('Alien', 'Serenity') and user  $q$  that rated ('Matrix'), are they similar or not? How to measure?

$$d = \begin{matrix} & \begin{matrix} \text{Matrix} \\ \text{Alien} \\ \text{Serenity} \\ \text{Casablanca} \\ \text{Amelie} \end{matrix} \\ \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \end{bmatrix} \end{matrix}$$

$$q = \begin{bmatrix} 5 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Zero ratings in common

# Case Study: How to query?

- Compactly, we have:

$$q_{concept} = qV$$

- E.g.:

$$q = \begin{bmatrix} \text{Matrix} \\ 5 \\ \text{Alien} \\ 0 \\ \text{Serenity} \\ 0 \\ \text{Casablanca} \\ 0 \\ \text{Amelie} \\ 0 \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.12 \\ 0.59 & -0.02 \\ 0.56 & 0.12 \\ 0.09 & -0.69 \\ 0.09 & -0.69 \end{bmatrix} = \begin{bmatrix} \text{SciFi-concept} \\ \downarrow \\ 2.8 & 0.6 \end{bmatrix}$$

movie-to-concept  
factors (V)

# Case Study: How to query?

- How would the user  $d$  that rated ('Alien', 'Serenity') be handled?

$$d_{concept} = dV$$

- E.g.:

$$d = \begin{matrix} & \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \\ \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \end{bmatrix} & \times & \begin{bmatrix} 0.56 & 0.12 \\ 0.59 & -0.02 \\ 0.56 & 0.12 \\ 0.09 & -0.69 \\ 0.09 & -0.69 \end{bmatrix} & = & \begin{bmatrix} 5.2 & 0.4 \end{bmatrix} \end{matrix}$$

movie-to-concept  
factors (V)

SciFi-concept  
↓

# Case Study: How to query?

- **Observation:** User  $d$  that rated ('Alien', 'Serenity') will be **similar** to user  $q$  that rated ('Matrix'), although  $d$  and  $q$  have **zero ratings in common**!

