

Dimensionality Reduction 1

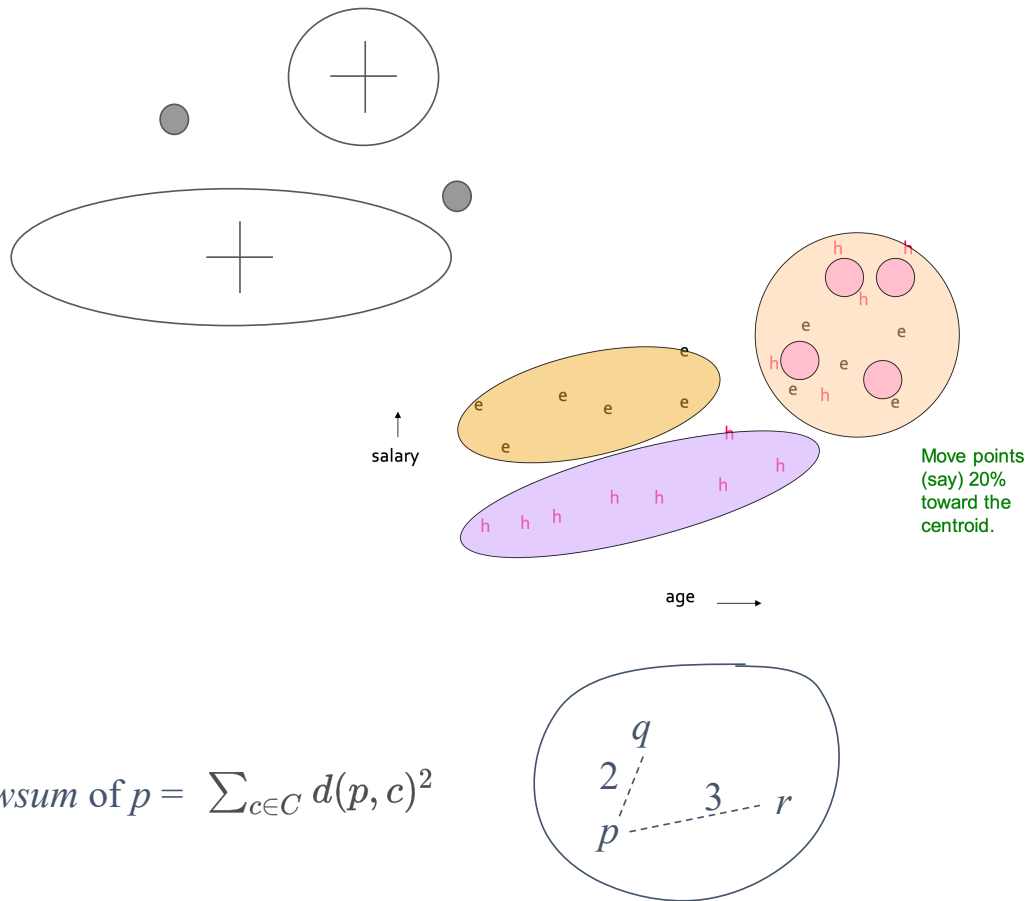
EE412: Foundation of Big Data Analytics

Announcements

- Homeworks
 - HW1 (due: 10/05)
 - HW2 (will be posted at 10/10; due: 11/02)
 - Clustering
 - Dimensionality reduction
 - Recommender systems
 - Midterm (10/19)

Recap

- BFR Algorithm
 - Cluster representation
 - Three classes of sets
- CURE Algorithm
 - Representative points
- GRGPF Algorithm
 - Rowsum
 - Estimation of a rowsum



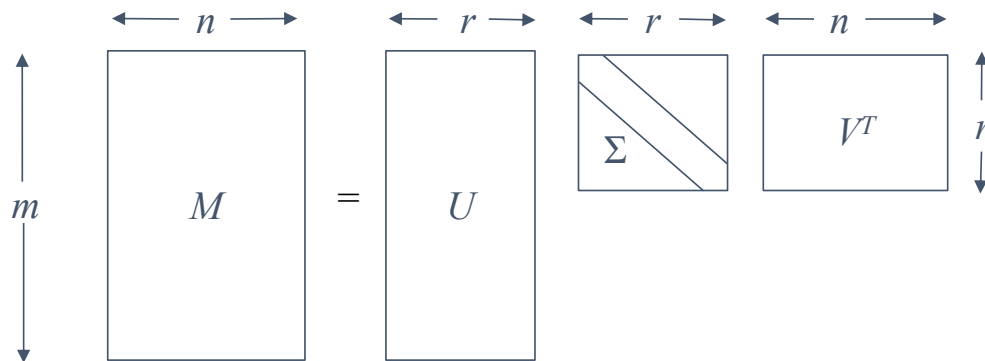
$$\text{rowsum of } p = \sum_{c \in C} d(p, c)^2$$

Outline

1. **Dimensionality Reduction**
2. Principal Component Analysis
3. Singular Value Decomposition (SVD)
4. Dimensionality Reduction with SVD

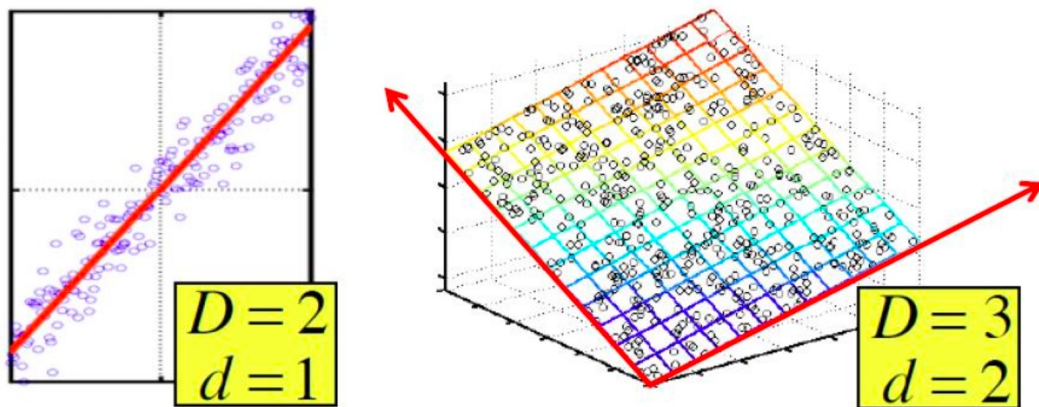
Dimensionality Reduction

- Many sources of data can be viewed as a large matrix
 - E.g., an $m \times n$ matrix for m points with n features
- **Dimensionality reduction**
 - Approximate a matrix by the product of smaller matrices
 - **Example of SVD:** Expect $(m + n + 1)r \ll mn$



Latent Factors

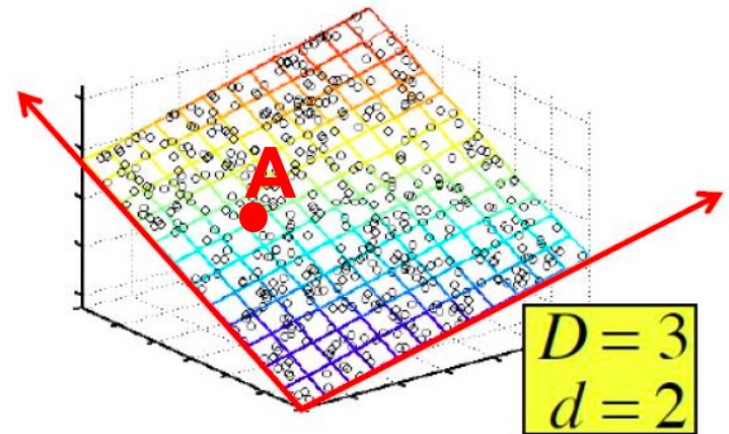
- **Q:** Do we lose information after dimensionality reduction?
- **A:** Maybe not. There can be hidden, or **latent factors** that
 - Explain why the values are as they appear in the data matrix



Source: Stanford CS246 (2022)

Rank is “Dimensionality”

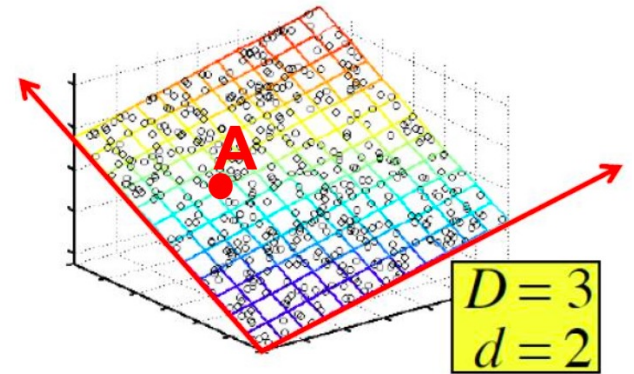
- **Q:** What is the **rank** of a matrix M ?
- **A:** Number of linearly independent rows (or columns) of M
 - **Independence:** There is no nonzero linear sum of these rows that is $\mathbf{0}$
- Consider 3 points in a 3D space:
 - $\begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$ (1 row per point)
- Rank is two, since \Rightarrow dependent on A & B
 - $A - B - C = \mathbf{0}$ (in terms of rows)
 - $5c_1 - 3c_2 + c_3 = \mathbf{0}$ (in terms of columns)



Source: Stanford CS246 (2022)

Rank is “Dimensionality”

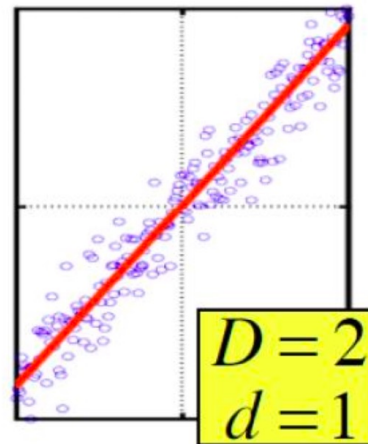
- We can **rewrite the coordinates** efficiently
 - $\begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$
- Old basis vectors: $[1 \ 0 \ 0], [0 \ 1 \ 0], [0 \ 0 \ 1]$
 - $A = 1u_1 + 2u_2 + 1u_3$
- **New basis vectors:** $[1 \ 2 \ 1], [-2 \ -3 \ 1]$
 - $A = 1u_1 + 0u_2$
 - M has new coordinates: $A: [1 \ 0], B: [0 \ 1], C: [1 \ -1]$
 - We reduced the number of dimensions!



Source: Stanford CS246 (2022)

Dimensionality Reduction

- **Goal:** Discover **the axes** of data
 - Represent each point with 1 coordinate
 - Follow the red line (a.k.a. the manifold)
- By doing this, we incur a **bit of error**
 - Since the points do not exactly lie on the line
 - There will be no error if the rank is one



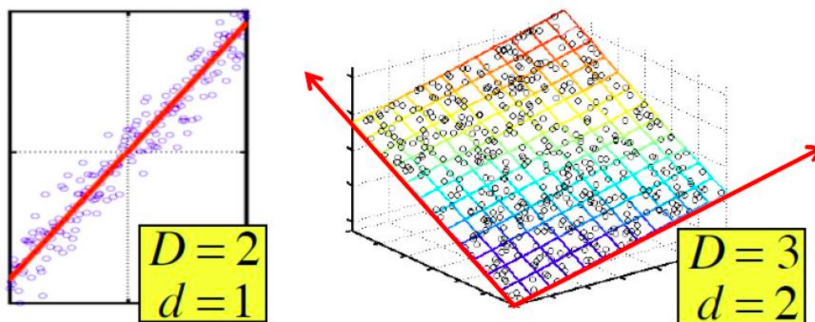
Source: Stanford CS246 (2022)

Outline

1. Dimensionality Reduction
2. **Principal Component Analysis**
3. Singular Value Decomposition (SVD)
4. Dimensionality Reduction with SVD

Principal Component Analysis

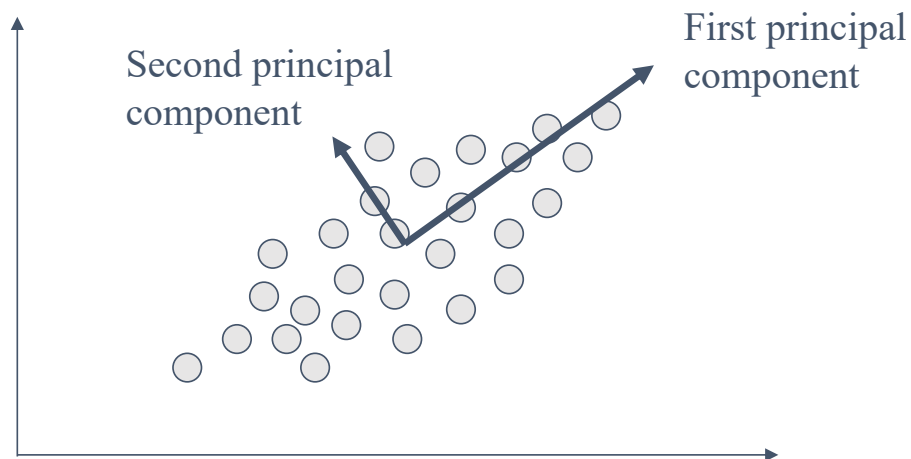
- The axes of these dimensions can be chosen by:
 - **First dimension:** Direction in which the points exhibit the greatest variance
 - **Second dimension:** Direction in which points show the 2nd greatest variance
 - Orthogonal to the first
 - And so on..., until you have enough dimensions that variance is really low



Source: Stanford CS246 (2022)

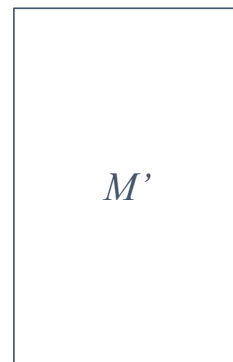
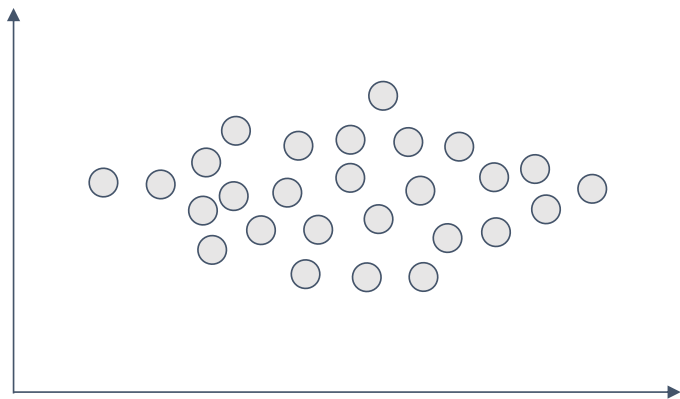
Principal Component Analysis

- **Principal component analysis (PCA)** is an algorithm for that
 - The new dimensions are called **principal components**

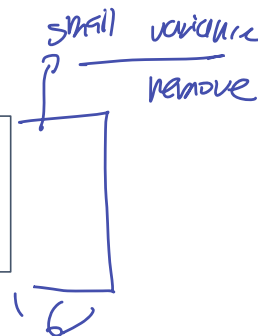
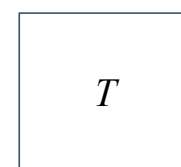


Output of PCA

- The goal of PCA is to create an $n \times n$ **transformation matrix** T
 - $M' = MT$ puts an $m \times n$ data matrix M on new axes
 - The i -th column of T creates the i -th principal component
 - We want it to be a **unit vector** (i.e., $\|t_i\|_2 = 1$)
 - Dimensionality reduction is done if we use the first r columns



=



Optimization Problem

- **Q:** How can we efficiently find the principal components?
- In order to maximize variance, the first column t_1 should satisfy.

$$t_1 = \operatorname{argmax}_{\|t=1\|} \sum_{i=1}^m \underbrace{(M'_i - \bar{\mathbf{m}}')^2}_{//}$$

- M'_i : The i -th row of the new data matrix M'
- $\bar{\mathbf{m}}'$: The elementwise mean of all rows in M'

Optimization Problem

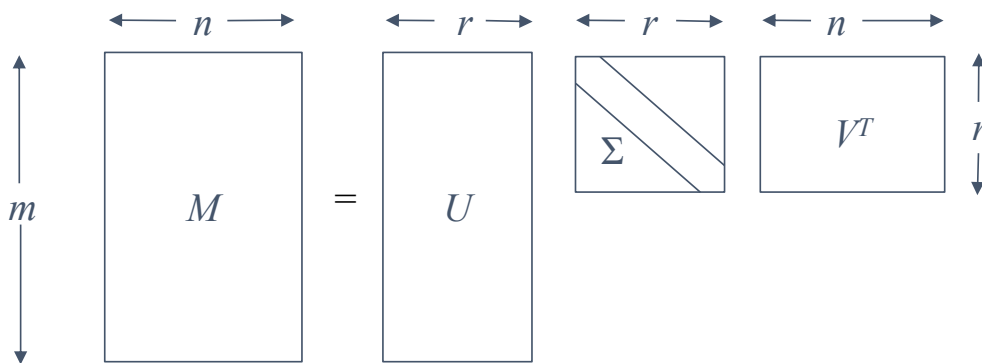
- **Q:** How can we efficiently find the principal components?
- **A:** **Singular value decomposition (SVD)** is a standard way to do that
 - The problem is related to the **eigenvectors** of $M^T M$
 - PCA has its own way, which is effective if r is very low

Outline

1. Dimensionality Reduction
2. Principal Component Analysis
3. **Singular Value Decomposition (SVD)**
4. Dimensionality Reduction with SVD

Singular Value Decomposition

- Decomposition of any matrix into a product of three matrices
- Choose any number r of **intermediate concepts** (latent factors)
 - In a way that minimizes the reconstruction error
 - The error is zero when $r \geq \text{rank}(M)$



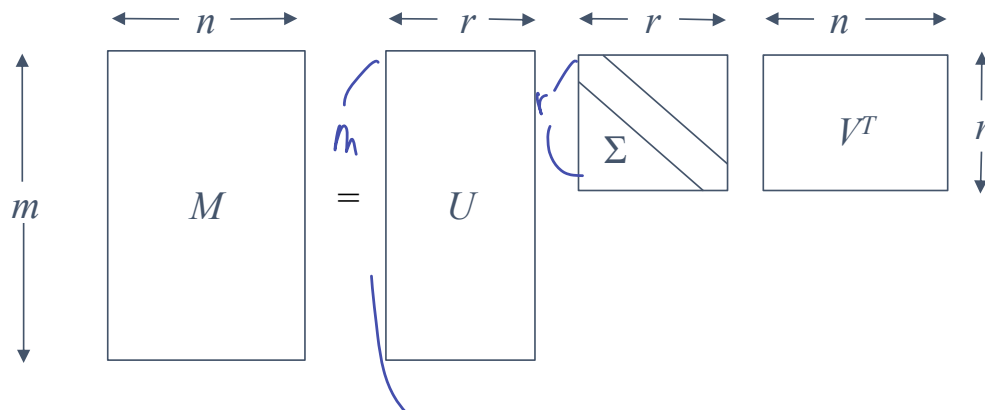
Definition of SVD

$$\begin{cases} u = m \times 1 \\ v = n \times 1 \end{cases}$$

$$u^T v = s$$

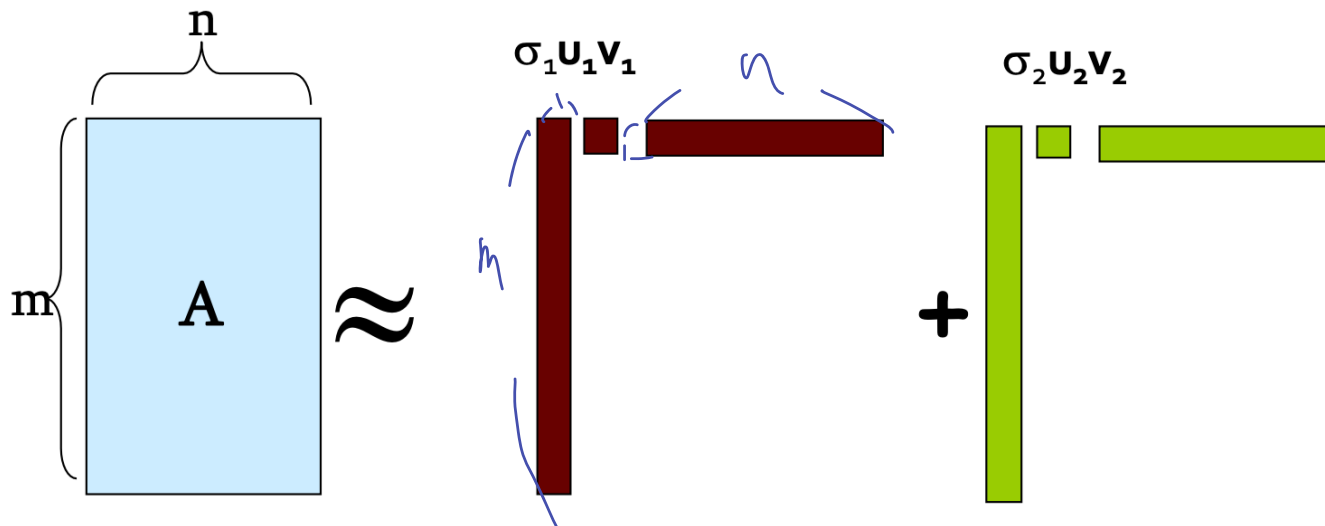
$$u v^T = \begin{bmatrix} & \\ & \end{bmatrix}_{m \times n}$$

- $M \approx U \Sigma V^T$ (equality if $r \geq \text{rank}(M)$)
 - M is an $m \times n$ **input data matrix**
 - U is an $m \times r$ matrix of **left singular vectors**
 - V is an $n \times r$ matrix of **right singular vectors**
 - Σ is an $r \times r$ diagonal matrix of **singular values** (strength of each “concept”)



Different View of SVD

- $M \approx U\Sigma V^T = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^T$ (σ_i : scalar, $\mathbf{u}_i, \mathbf{v}_i$: vectors)



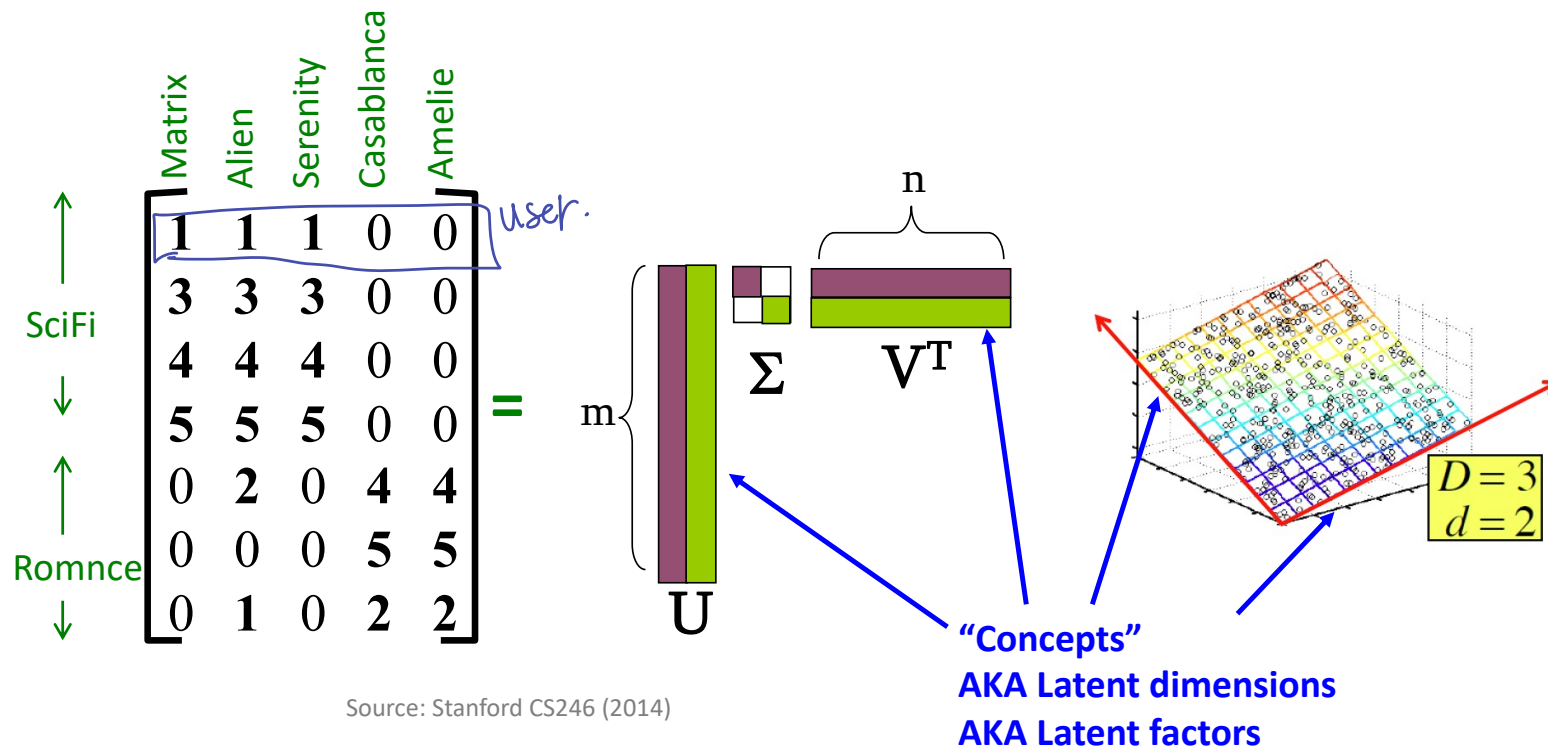
Source: Stanford CS246 (2022)

Properties of SVD

- **Always possible to decompose a real matrix** as $M = U\Sigma V^T$
- U, Σ, V : Unique
- U, V : Column orthonormal
 - Columns are orthogonal unit vectors
 - $U^T U = I; V^T V = I$ (I : Identity matrix)
- Σ : diagonal
 - Entries (singular values) are non-negative, and sorted in decreasing order
 - $\sigma_1 \geq \sigma_2 \geq \dots \geq 0$

Example: SVD

- Consider a matrix of ratings from users; **What does SVD do?**



Source: Stanford CS246 (2014)

Example: SVD

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

“strength” of the SciFi-concept

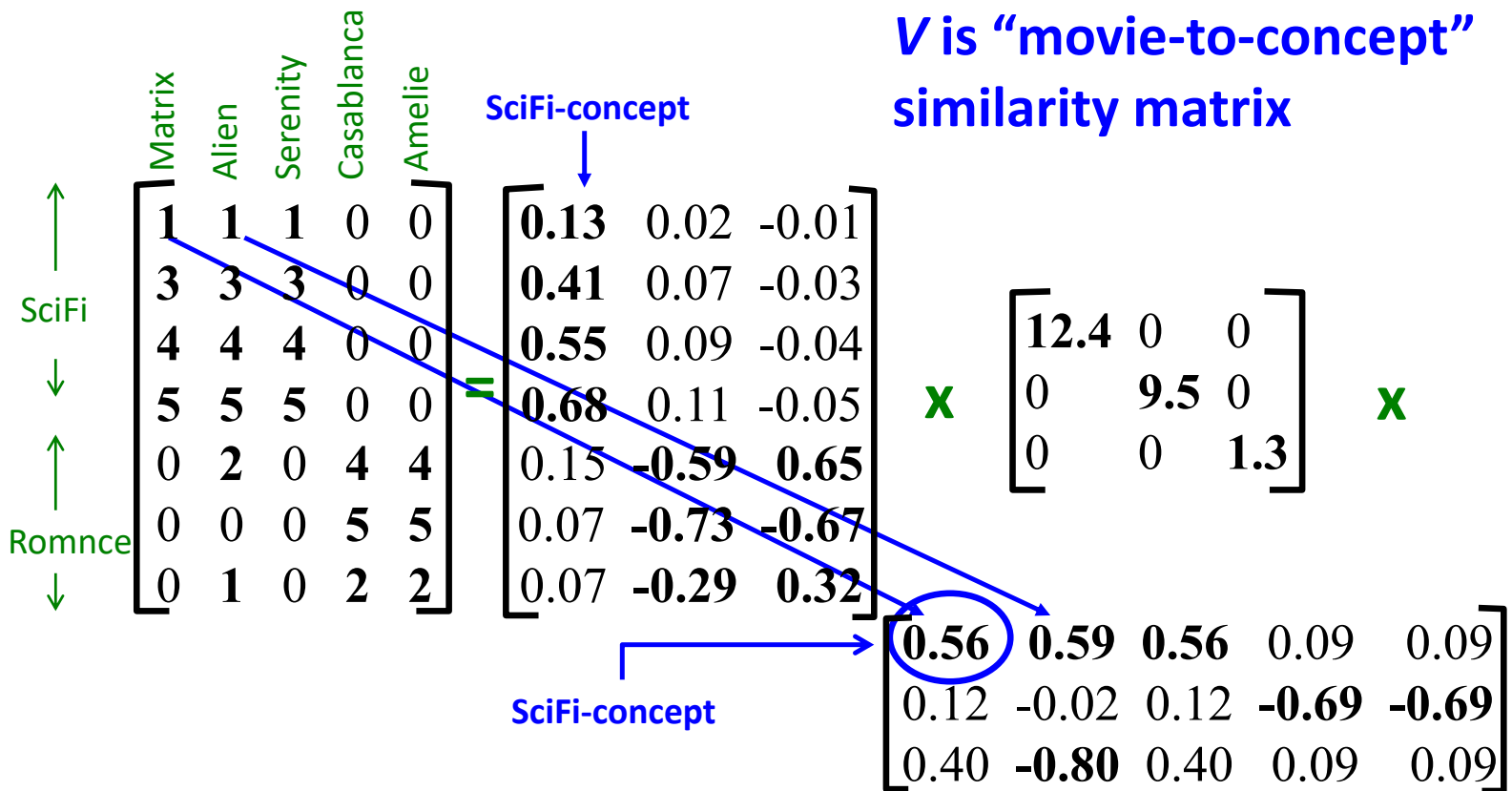
Example: SVD

U is “user-to-concept” similarity matrix

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

(Note: In the original image, the value 0.13 in the SciFi-concept row is circled in green. The value 1.3 in the diagonal matrix is circled in blue with a handwritten note "noise" pointing to it.)

Example: SVD



Example: SVD

Matrix Alien Serenity Casablanca Amelie

SciFi ↑

↓

Romnce ↑

↓

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

What concept?

concept ↓

no vie

concept

Example: SVD

Movies, users and concepts:

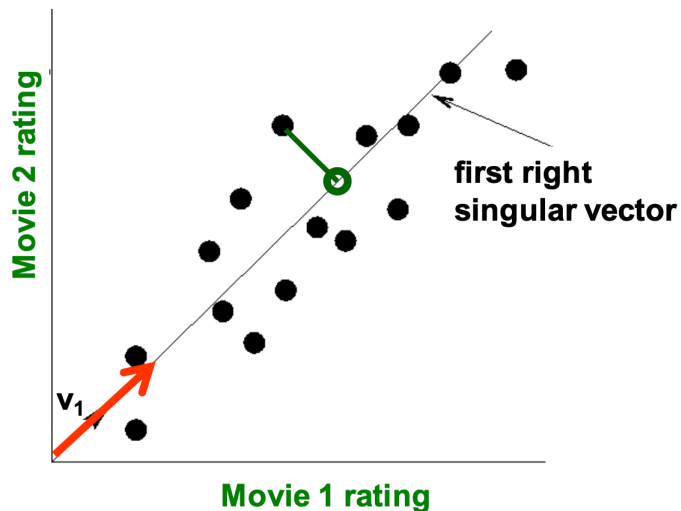
- U : User (row)-to-concept matrix
- V : Movie (column)-to-concept matrix
- Σ : Its diagonal elements: “strength” of each concept

Outline

1. Dimensionality Reduction
2. Principal Component Analysis
3. Singular Value Decomposition (SVD)
4. **Dimensionality Reduction with SVD**

SVD for Dimensionality Reduction

- Let's use fewer coordinates to describe point positions
 - Consider an example of N users for 2 movies of 1 concept
 - Point's position is its location along vector v_1



Source: Stanford CS246 (2022)

Jaemin Yoo

Example: SVD

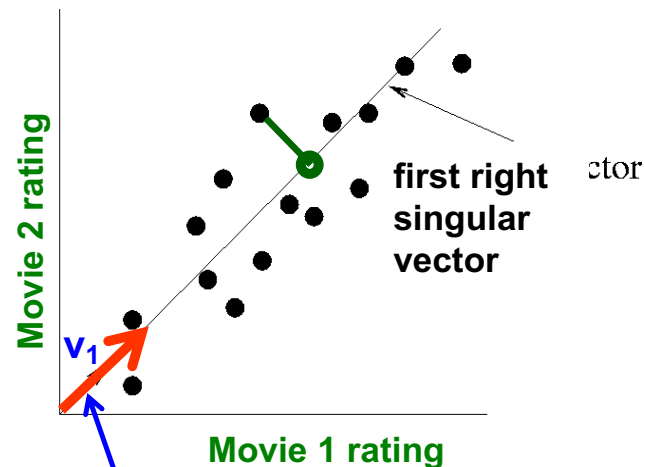
- U is about users, V is about movies
- Each column of V becomes a **new axis**

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

$$\begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 1.3 \end{bmatrix} \times$$

$$\begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\ 0.40 & -0.80 & 0.40 & 0.09 & 0.09 \end{bmatrix}$$

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



Example: SVD

- First column of V
 - Has the largest variance

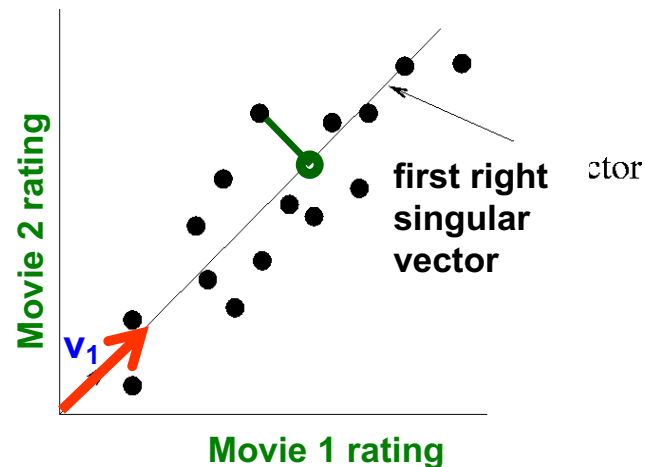
variance ('spread')
on the v_1 axis

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

$$\begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 1.3 \end{bmatrix} \times$$

$$\begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\ 0.40 & -0.80 & 0.40 & 0.09 & 0.09 \end{bmatrix}$$

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



Example: SVD

- $U\Sigma$ gives the coordinates of the points
 - In the projection axis

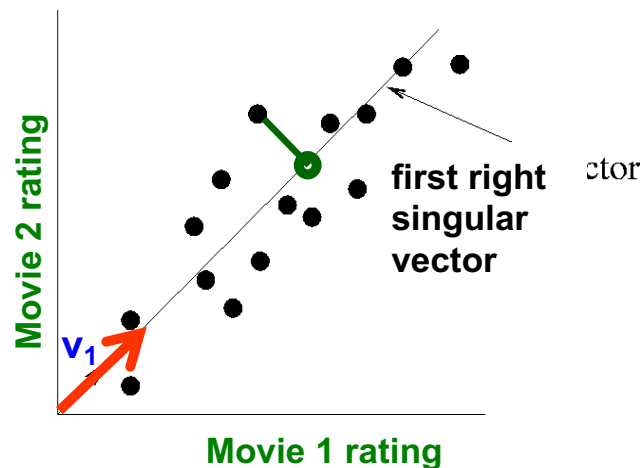
$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix}$$

Projection of users
on the “Sci-Fi” axis

$U\Sigma V^T$:

$$\begin{bmatrix} 1.61 & 0.19 & -0.01 \\ 5.08 & 0.66 & -0.03 \\ 6.82 & 0.85 & -0.05 \\ 8.43 & 1.04 & -0.06 \\ 1.86 & -5.60 & 0.84 \\ 0.86 & -6.93 & -0.87 \\ 0.86 & -2.75 & 0.41 \end{bmatrix}$$

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



SVD for Dimensionality Reduction

- **Q:** How exactly is dimensionality reduction done by SVD?
- **A:** **Set smallest singular values to zero**

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

The diagram illustrates the SVD decomposition of a 7x5 matrix into three matrices: a 7x3 matrix of left singular vectors, a 3x3 diagonal matrix of singular values, and a 3x5 matrix of right singular vectors. The singular values are 12.4, 9.5, and 1.3. The right singular vectors are shown as a 3x5 matrix. The smallest singular value (1.3) and its corresponding right singular vector row are crossed out with a red 'X', indicating the process of setting the smallest singular values to zero for dimensionality reduction.

SVD for Dimensionality Reduction

- Reconstruction error is quantified by the **Frobenius norm**:

- Definition:** $\|A\|_F = \sqrt{\sum_{ij} A_{ij}^2}$, **This case:** $\|M - B\|_F = \sqrt{\sum_{ij} (M_{ij} - B_{ij})^2}$

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix}$$

\approx

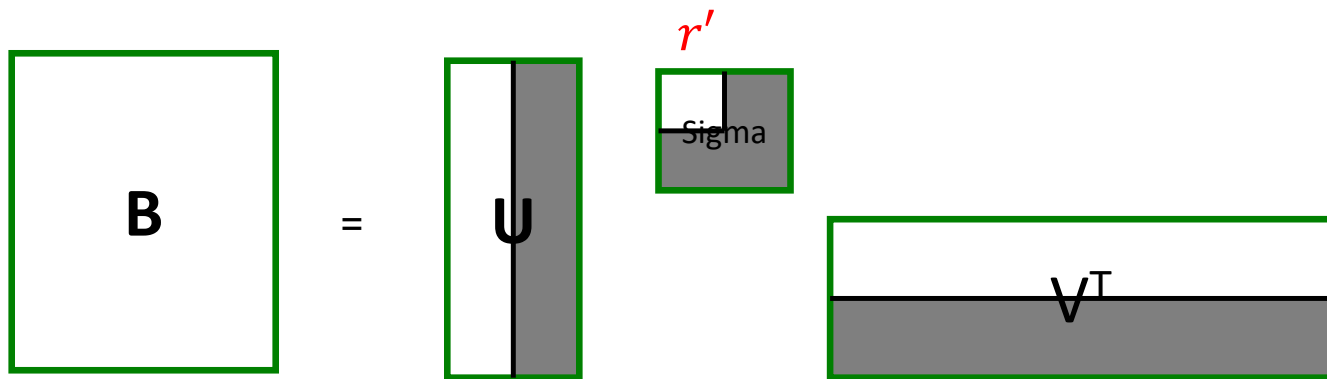
$$\begin{bmatrix} 0.92 & 0.95 & 0.92 & 0.01 & 0.01 \\ 2.91 & 3.01 & 2.91 & -0.01 & -0.01 \\ 3.90 & 4.04 & 3.90 & 0.01 & 0.01 \\ 4.82 & 5.00 & 4.82 & 0.03 & 0.03 \\ 0.70 & 0.53 & 0.70 & 4.11 & 4.11 \\ -0.69 & 1.34 & -0.69 & 4.78 & 4.78 \\ 0.32 & 0.23 & 0.32 & 2.01 & 2.01 \end{bmatrix}$$

Reconstructed
data matrix B

Best Low Rank Approximation

- Given $r' < r$, SVD gives the best axes to project on

- Minimizing the reconstruction error $\|M - B\|_F = \sqrt{\sum_{ij} (M_{ij} - B_{ij})^2}$



Source: Stanford CS246 (2022)

Determining the Low Rank

- **Q:** What is a good value for r' (# of latent factors)?
- **A:** Pick r' to have at least 90% of the total energy
 - Let the **energy** of singular values be the sum of their squares
- Back to our example:
 - Singular values are 12.4, 9.5, and 1.3 (total energy = 245.7)
 - If we drop 1.3, whose square is 1.7, the remaining is energy 244.0
 - The remaining energy is over 99% of the total energy

Summary

1. Dimensionality Reduction
 - Latent factors
 - Rank of a matrix
2. Principal Component Analysis
3. Singular Value Decomposition (SVD)
 - Singular values and singular vectors
4. Dimensionality Reduction with SVD
 - Reconstruction error
 - Best low rank approximation