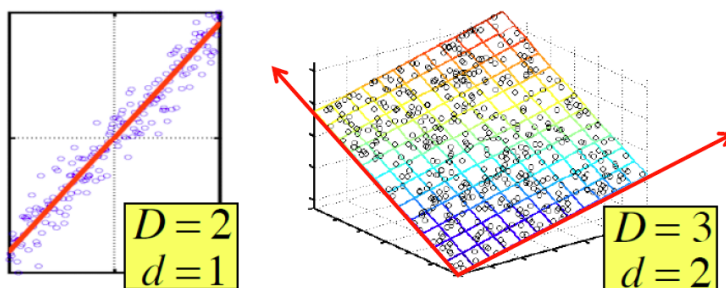


大数据分析

Large-scale computing

刘盛华

Dimensionality Reduction



- **Assumption:** Data lies on or near a low d -dimensional subspace
- **Axes of this subspace are effective representation of the data**

J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets,
<http://www.mmids.org>

2

Rank of a Matrix

■ **Q:** What is **rank** of a matrix A?

■ **A:** Number of linearly independent columns of A

■ For example:

■ Matrix A = $\begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$ has rank $r=2$

■ Why? The first two rows are linearly independent, so the rank is at least 2, but all three rows are linearly dependent (the first is equal to the sum of the second and third) so the rank must be less than 3.

■ Why do we care about low rank?

■ We can write A as two "basis" vectors: $[1 \ 2 \ 1] \ [-2 \ -3 \ 1]$

■ And new coordinates of : $[1 \ 0] \ [0 \ 1] \ [1 \ -1]$

3

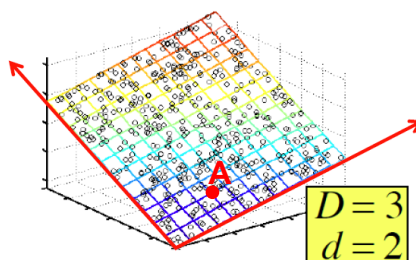
Rank is "Dimensionality"

■ Cloud of points 3D space:

■ Think of point positions

as a matrix:

1 row per point: $\begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix} \begin{matrix} A \\ B \\ C \end{matrix}$



■ We can rewrite coordinates more efficiently!

■ Old basis vectors: $[1 \ 0 \ 0] \ [0 \ 1 \ 0] \ [0 \ 0 \ 1]$

■ New basis vectors: $[1 \ 2 \ 1] \ [-2 \ -3 \ 1]$

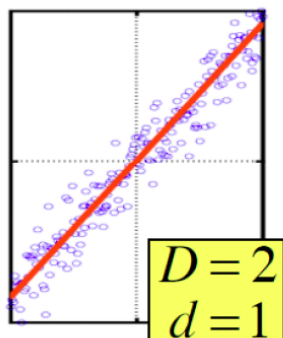
■ Then A has new coordinates: $[1 \ 0]$. B: $[0 \ 1]$, C: $[1 \ -1]$

■ Notice: We reduced the number of coordinates!

4

Dimensionality Reduction

- Goal of dimensionality reduction is to discover the axis of data!



Rather than representing every point with 2 coordinates we represent each point with 1 coordinate (corresponding to the position of the point on the red line).

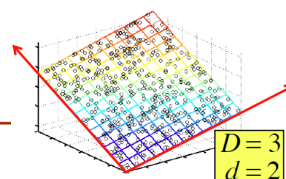
By doing this we incur a bit of **error** as the points do not exactly lie on the line

5

Why Reduce Dimensions?

Why reduce dimensions?

- Discover hidden correlations/topics
 - Words that occur commonly together
- Remove redundant and noisy features
 - Not all words are useful
- Interpretation and visualization 解释与可视化
- Easier storage and processing of the data



SVD - Definition

$r = \text{秩}$

$$\mathbf{A}_{[m \times n]} = \mathbf{U}_{[m \times r]} \mathbf{\Sigma}_{[r \times r]} (\mathbf{V}_{[n \times r]})^T$$

■ **A: Input data matrix**

- $m \times n$ matrix (e.g., m documents, n terms)

■ **U: Left singular vectors**

正交左奇异向量

- $m \times r$ matrix (m documents, r concepts)

■ **Σ : Singular values**

奇异值矩阵 对角矩阵

- $r \times r$ diagonal matrix (strength of each 'concept')
(r : rank of the matrix A)

■ **V: Right singular vectors**

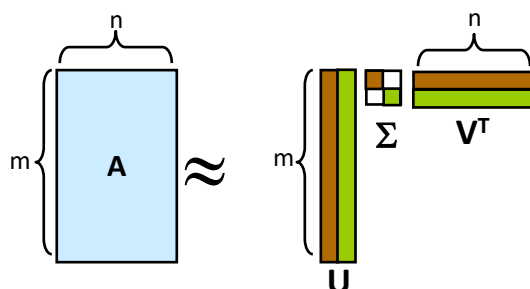
- $n \times r$ matrix (n terms, r concepts)



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SVD

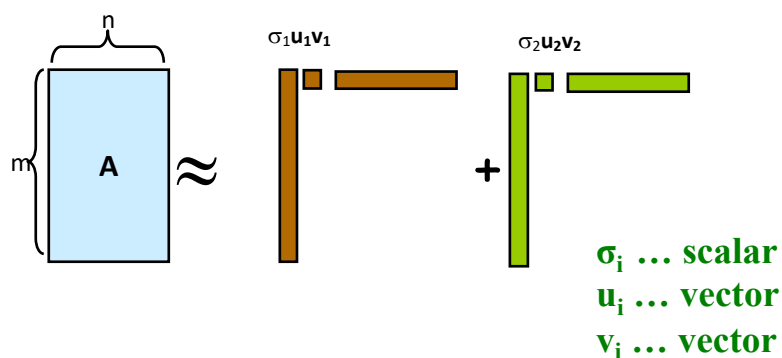
$$\mathbf{A} \approx \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T = \sum_i \sigma_i \mathbf{u}_i \circ \mathbf{v}_i^T$$



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SVD

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



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SVD - Properties

It is always possible to decompose a real matrix A into $A = U \Sigma V^T$, where

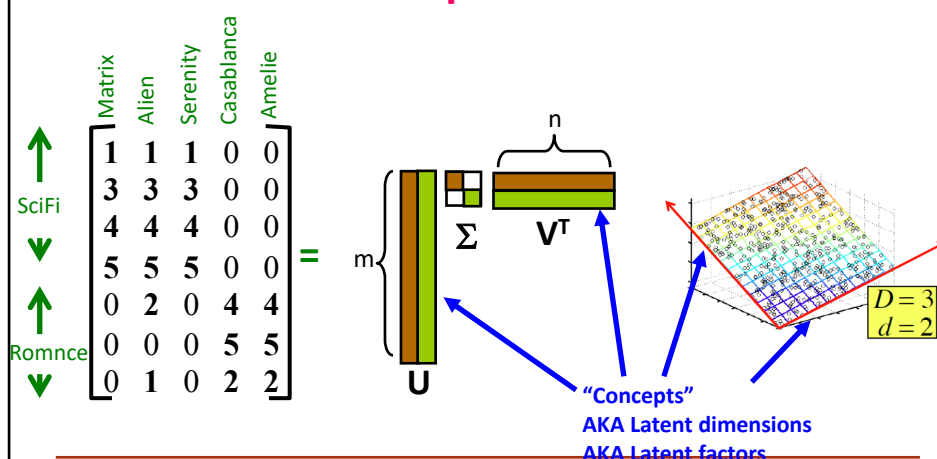
- U, Σ, V : **unique**
- U, V : **column orthonormal**
 - $U^T U = I; V^T V = I$ (I : identity matrix)
 - (Columns are orthogonal unit vectors)
- Σ : **diagonal**
 - Entries (**singular values**) are **positive**, and sorted in decreasing order ($\sigma_1 \geq \sigma_2 \geq \dots \geq 0$)

Nice proof of uniqueness: <http://www.mpi-inf.mpg.de/~bast/ir-seminar-ws04/lecture2.pdf>

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SVD – Example: Users-to-Movies

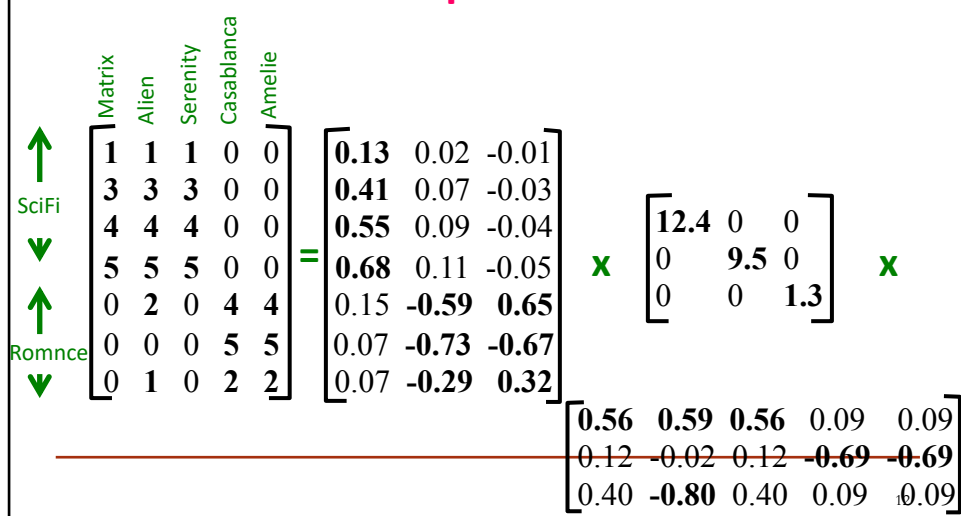
■ $A = U \Sigma V^T$ - example: Users to Movies



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SVD – Example: Users-to-Movies

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



SVD – Example: Users-to-Movies

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

Matrix Alien Serenity Casablanca Amelie

SciFi ↑ ↓ ↑ ↓

Romnce ↑ ↓

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

SciFi-concept Romance-concept

SVD – Example: Users-to-Movies

■ $A = U \Sigma V^T$ - example: U is “user-to-concept” similarity matrix

Matrix Alien Serenity Casablanca Amelie

SciFi ↑ ↓ ↑ ↓

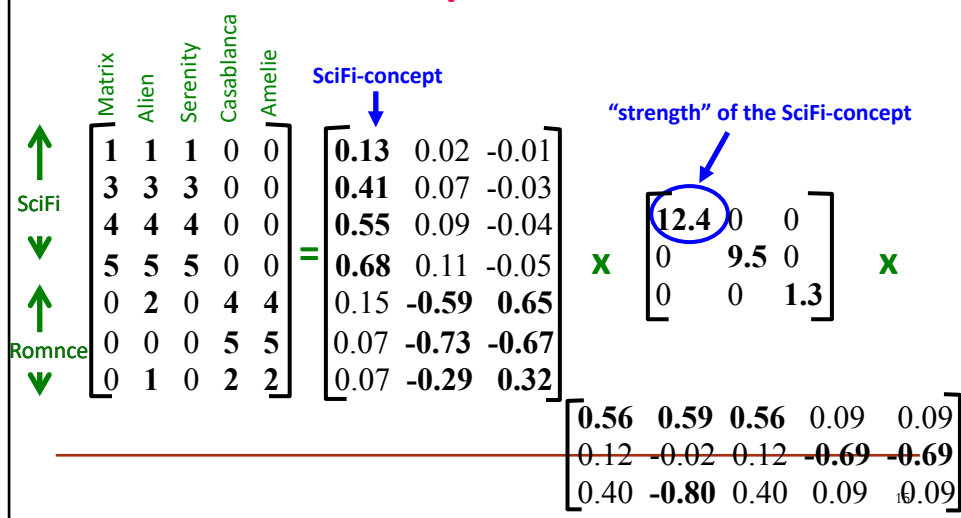
Romnce ↑ ↓

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

SciFi-concept Romance-concept

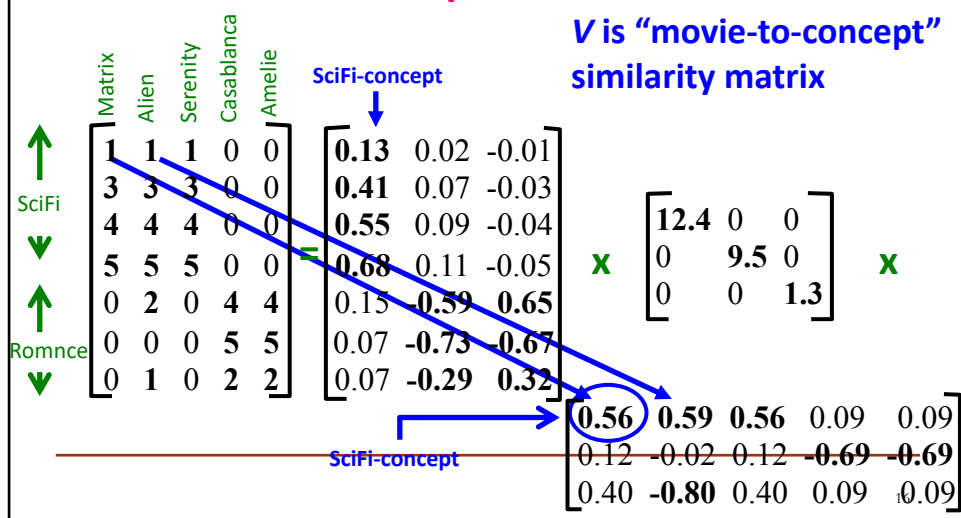
SVD – Example: Users-to-Movies

■ $A = U \Sigma V^T$ - example:



SVD – Example: Users-to-Movies

■ $A = U \Sigma V^T$ - example:



SVD - Interpretation #1

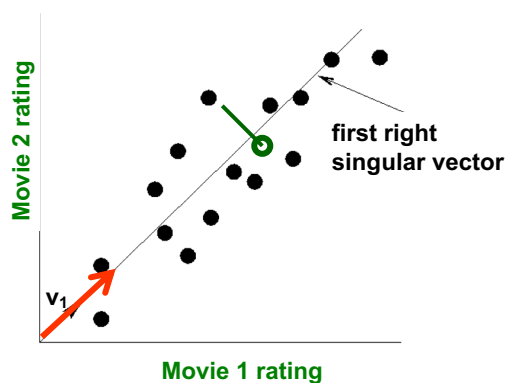
'movies', 'users' and 'concepts':

- U : user-to-concept similarity matrix
- V : movie-to-concept similarity matrix
- Σ : its diagonal elements:
 'strength' of each concept

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Dimensionality Reduction with SVD

SVD – Dimensionality Reduction



- Instead of using two coordinates (x, y) to describe point locations, let's use only one coordinate (z)
- Point's position is its location along vector v_1
- How to choose v_1 ? **Minimize reconstruction error**

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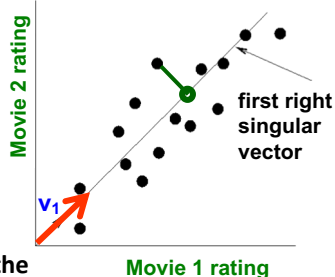
SVD – Dimensionality Reduction

- **Goal:** Minimize the sum of reconstruction errors:

$$\sum_{i=1}^N \sum_{j=1}^D \|x_{ij} - z_{ij}\|^2$$

- where x_{ij} are the "old" and z_{ij} are the "new" coordinates

- SVD gives 'best' axis to project on:
 - 'best' = minimizing the reconstruction errors
- In other words, **minimum reconstruction error**

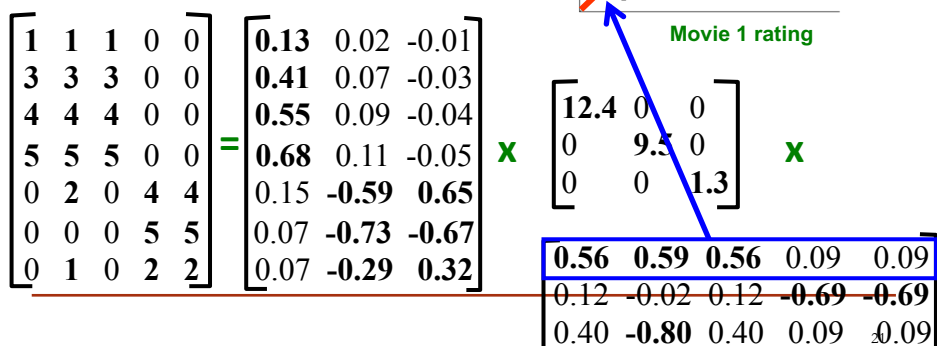


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SVD - Interpretation #2

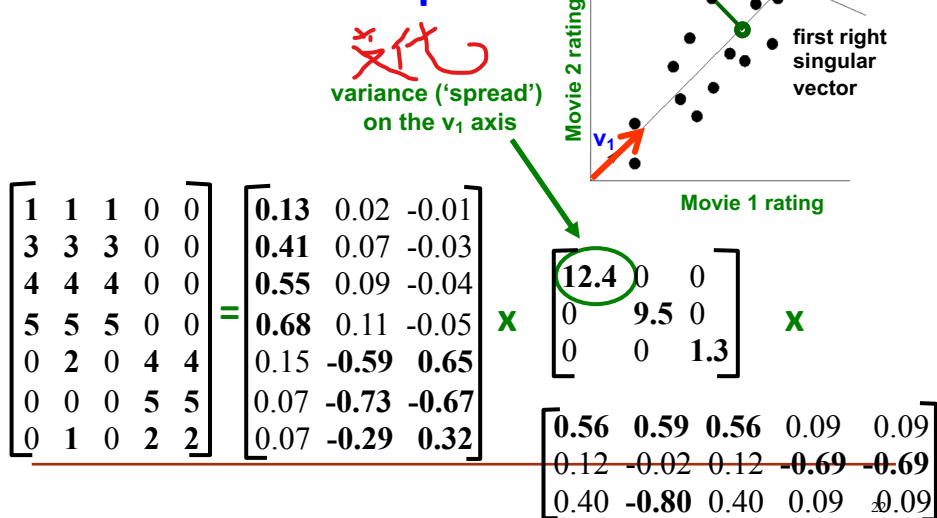
■ $A = U \Sigma V^T$ - example:

- V: "movie-to-concept" matrix
- U: "user-to-concept" matrix



SVD - Interpretation #2

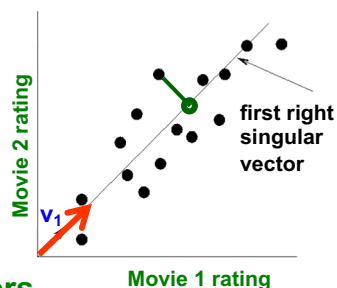
■ $A = U \Sigma V^T$ - example:



SVD - Interpretation #2

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

- $U \Sigma$: 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
($U \Sigma$)^T:

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

SVD - Interpretation #2

More details

- Q: How exactly is dim. reduction done?

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

SVD – Best Low Rank Approx.

■ Theorem:

Let $A = U \Sigma V^T$ and $B = U S V^T$ where
 S = diagonal $r \times r$ matrix with $s_i = \sigma_i$ ($i=1 \dots k$) else $s_i = 0$
 then B is a best rank(B)= k approx. to A

What do we mean by “best”:

□ B is a solution to $\min_B \|A - B\|_F$ where $\text{rank}(B) = k$

$$\begin{pmatrix} x_{11} & x_{12} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & \\ \vdots & \vdots & \ddots & \\ x_{m1} & & & x_{mn} \end{pmatrix}_{m \times n} = \begin{pmatrix} u_{11} & \dots & u_{1r} \\ \vdots & \ddots & \vdots \\ u_{m1} & & u_{mr} \end{pmatrix}_{m \times r} \begin{pmatrix} \sigma_{11} & 0 & \dots \\ 0 & \sigma_{rr} & \\ \vdots & & \ddots \end{pmatrix}_{r \times r} \begin{pmatrix} v_{11} & \dots & v_{1n} \\ \vdots & \ddots & \\ v_{r1} & & v_{rn} \end{pmatrix}_{r \times n}$$

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

SVD - Interpretation #2

More details

- Q: How exactly is dim. reduction done?
- A: Set smallest singular values to zero

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

SVD - Interpretation #2

More details

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

SVD - Interpretation #2

More details

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

SVD - Interpretation #2

More details

- **Q:** How exactly is dim. reduction done?
- **A:** Set smallest singular values to zero

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \approx \begin{bmatrix} 0.13 & 0.02 \\ 0.41 & 0.07 \\ 0.55 & 0.09 \\ 0.68 & 0.11 \\ 0.15 & -0.59 \\ 0.07 & -0.73 \\ 0.07 & -0.29 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \end{bmatrix}$$

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SVD - Interpretation #2

More details

- **Q:** How exactly is dim. reduction done?
- **A:** Set smallest singular values to zero

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

Frobenius norm:

$$\|M\|_F = \sqrt{\sum_{ij} M_{ij}^2}$$

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

is "small"

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SVD – Best Low Rank Approx.

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

B is best approximation of **A**

$$B = U \Sigma' V^T$$

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SVD - Interpretation #2

Equivalent:

'spectral decomposition' of the matrix:

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} = \begin{bmatrix} | & | \\ u_1 & u_2 \\ | & | \end{bmatrix} \times \begin{bmatrix} \sigma_1 & \emptyset \\ \emptyset & \sigma_2 \end{bmatrix} \times \begin{bmatrix} \text{---} & v_1 & \text{---} \\ \text{---} & v_2 & \text{---} \end{bmatrix}$$

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SVD - Interpretation #2

Equivalent:

'spectral decomposition' of the matrix

$$\begin{array}{c} \uparrow \\ n \\ \downarrow \end{array} \begin{array}{c} \xleftarrow{m} \xrightarrow{} \end{array} \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} = \begin{array}{c} \xleftarrow{k \text{ terms}} \xrightarrow{\phantom{k \text{ terms}}} \end{array} \sigma_1 \begin{array}{c} \nearrow \\ n \times 1 \end{array} u_1 \begin{array}{c} \nwarrow \\ 1 \times m \end{array} v_1^T + \sigma_2 u_2 v_2^T + \dots$$

Assume: $\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \dots \geq 0$

Why is setting small σ_i to 0 the right thing to do?
 Vectors u_i and v_i are unit length, so σ_i scales them.
 So, zeroing small σ_i introduces less error.

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SVD - Interpretation #2

Q: How many σ s to keep?

A: Rule-of-a thumb:

keep 80-90% of 'energy' = $\sum_i \sigma_i^2$

$$\begin{array}{c} \uparrow \\ n \\ \downarrow \end{array} \begin{array}{c} \xleftarrow{m} \xrightarrow{} \end{array} \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \dots$$

Assume: $\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \dots$

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SVD - Complexity

- **To compute SVD:**
 - $O(nm^2)$ or $O(n^2m)$ (whichever is less)
- **But:**
 - Less work, if we just want singular values
 - or if we want first k singular vectors
 - or if the matrix is sparse
- **Implemented in** linear algebra packages like
 - LINPACK, Matlab, SPlus, Mathematica ...

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SVD - Conclusions

- **SVD:** $A = U \Sigma V^T$: **unique**
 - U : user-to-concept similarities
 - V : movie-to-concept similarities
 - Σ : strength of each concept
- **Dimensionality reduction:**
 - keep the few largest singular values (80-90% of 'energy')
 - SVD: picks up linear correlations

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