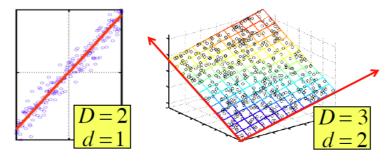
# 大数据分析

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.mmds.org

# Rank of a Matrix

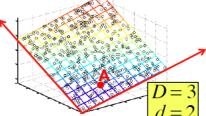
- Q: What is rank of a matrix A?
- A: Number of linearly independent columns of A
- **■** For example:
  - □ Matrix A =  $\begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$  has rank r=2
    - Why? The first two rows are linearly independent, so the rank is at least 2, but all three 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]

-

# Rank is "Dimensionality"

- Cloud of points 3D space:
  - □ Think of point positions as a matrix:  $\begin{bmatrix} 1 & 2 & 1 \end{bmatrix}$

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

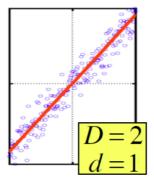


■ We can rewrite coordinates more efficiently

- 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!

# **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).

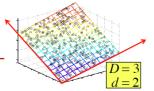
By doing this we incur a bit of **error** as the points do not exactly lie on the line

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
- Easier storage and processing of the data



# **SVD** - Definition

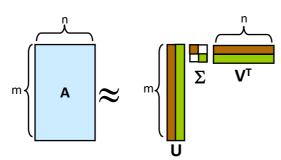
$$\mathbf{A}_{[m \times n]} = \mathbf{U}_{[m \times r]} \Sigma_{[r \times r]} (\mathbf{V}_{[n \times r]})^{\mathsf{T}}$$

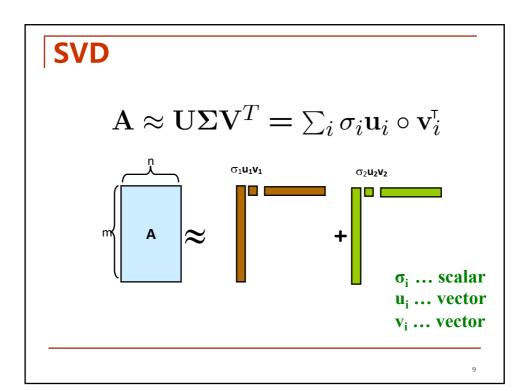
- A: Input data matrix
  - m x n matrix (e.g., m documents, n terms)
- U: Left singular vectors
  - m x r matrix (m documents, r concepts)
- **Σ**: Singular values
  - r x r diagonal matrix (strength of each 'concept')(r: rank of the matrix A)
- V: Right singular vectors
  - n x r matrix (n terms, r concepts)

7

# **SVD**

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



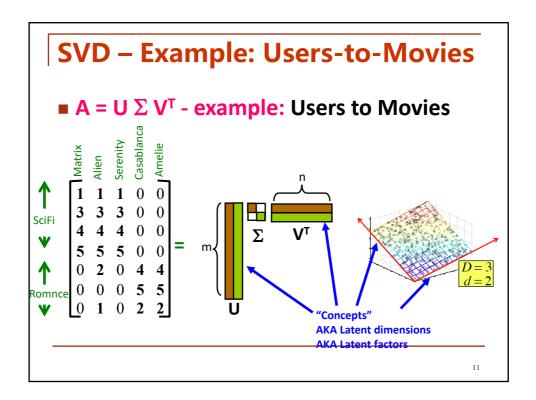


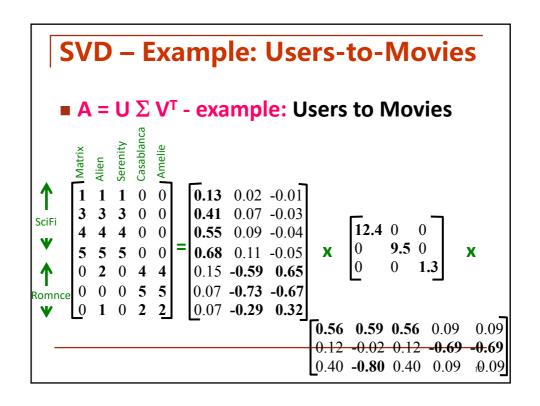
# **SVD - Properties**

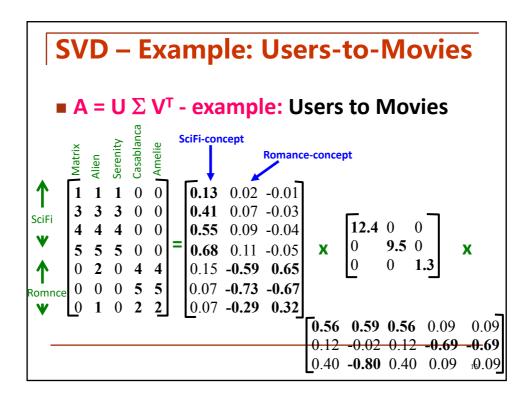
It is always possible to decompose a real matrix A into  $A = U \sum V^T$ , where

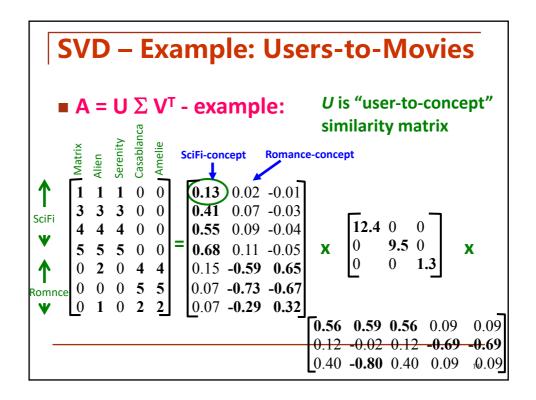
- U,  $\Sigma$ , V: unique
- *U, V*: column orthonormal
  - $U^T U = I; V^T V = I$  (I: identity matrix)
  - (Columns are orthogonal unit vectors)
- $\Sigma$ : diagonal
  - □ Entries (singular values) are positive, and sorted in decreasing order  $(\sigma_1 \ge \sigma_2 \ge ... \ge 0)$

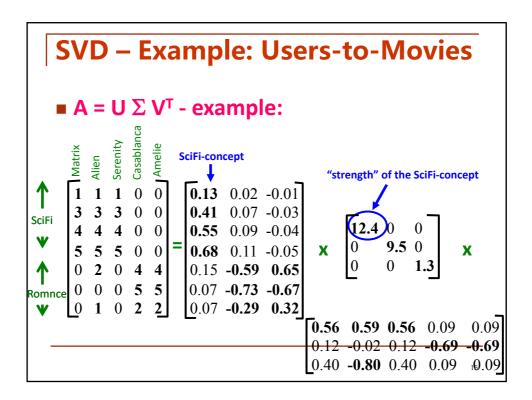
Nice proof of uniqueness: http://www.mpi-inf.mpg.de/~bast/ir-seminar-ws04/lecture2.pdf

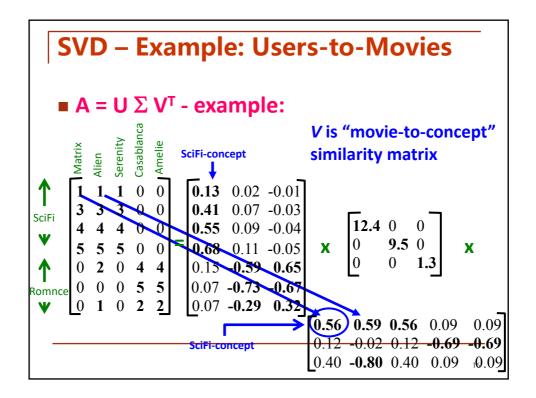












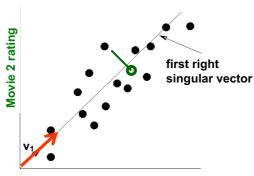
### 'movies', 'users' and 'concepts':

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

17

# Dimensionality Reduction with SVD

# **SVD – Dimensionality Reduction**

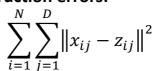


Movie 1 rating

- 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

# **SVD – Dimensionality Reduction**

Goal: Minimize the sum of reconstruction errors:

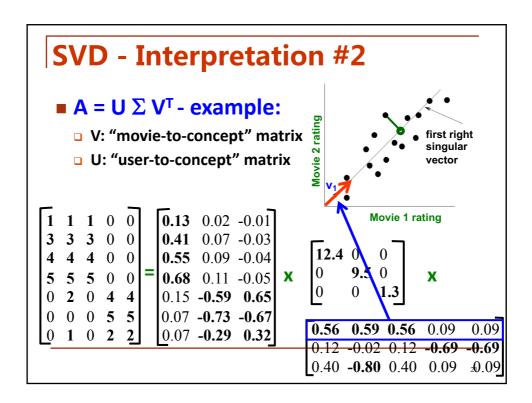


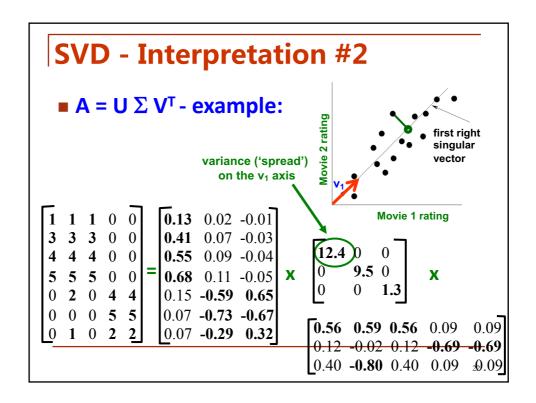
Movie 1 rating

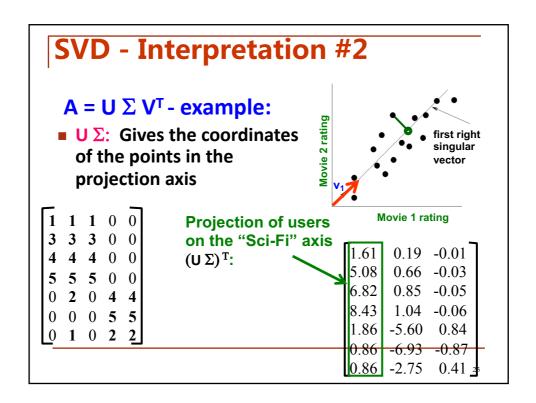
singular vector

- 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







### **More details**

Q: How exactly is dim. reduction done?

$$\begin{bmatrix} \mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & 0 \\ \mathbf{3} & \mathbf{3} & \mathbf{3} & 0 & 0 \\ \mathbf{4} & \mathbf{4} & \mathbf{4} & 0 & 0 \\ \mathbf{5} & \mathbf{5} & \mathbf{5} & 0 & 0 \\ 0 & \mathbf{2} & 0 & \mathbf{4} & \mathbf{4} \\ 0 & 0 & 0 & \mathbf{5} & \mathbf{5} \\ 0 & \mathbf{1} & 0 & \mathbf{2} & \mathbf{2} \end{bmatrix} = \begin{bmatrix} \mathbf{0}.\mathbf{13} & 0.02 & -0.01 \\ \mathbf{0}.\mathbf{41} & 0.07 & -0.03 \\ \mathbf{0}.\mathbf{55} & 0.09 & -0.04 \\ \mathbf{0}.\mathbf{68} & 0.11 & -0.05 \\ 0.15 & -0.59 & \mathbf{0}.\mathbf{65} \\ 0.07 & -0.73 & -0.67 \\ 0.07 & -0.29 & \mathbf{0}.\mathbf{32} \end{bmatrix} \times \begin{bmatrix} \mathbf{12.4} & 0 & 0 \\ 0 & \mathbf{9.5} & 0 \\ 0 & 0 & \mathbf{1.3} \end{bmatrix} \times \begin{bmatrix} \mathbf{12.4} & 0 & 0 \\ 0 & \mathbf{9.5} & 0 \\ 0 & 0 & \mathbf{1.3} \end{bmatrix} \times \begin{bmatrix} \mathbf{0.56} & \mathbf{0.59} & \mathbf{0.56} & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\ 0.40 & -0.80 & 0.40 & 0.09 & 0.09 \end{bmatrix}$$

# **SVD** – Best Low Rank Approx.

### **■** Theorem:

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

### What do we mean by "best":

 $\square$  B is a solution to min<sub>B</sub>  $||A-B||_F$  where rank(B)=k

$$\begin{pmatrix} x_{11} & x_{12} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & \\ \vdots & \vdots & \ddots & \\ x_{m1} & & & x_{mn} \end{pmatrix} = \begin{pmatrix} u \\ u_{11} & \dots \\ \vdots & \ddots \\ u_{m1} & & & \\ m \times r \end{pmatrix} \begin{pmatrix} \boldsymbol{\sigma}_{11} & \boldsymbol{0} & \dots \\ \boldsymbol{0} & \ddots & \\ \vdots & \ddots & \\ \vdots & \ddots & \\ r \times r \end{pmatrix} \begin{pmatrix} \boldsymbol{v}^{\mathsf{T}} & \boldsymbol{v}^{\mathsf{T}} \\ v_{11} & \dots & v_{1n} \\ \vdots & \ddots & \\ r \times n \end{pmatrix}$$

$$||A - B||_F = \sqrt{\sum_{ij} (A_{ij} - B_{ij})_{25}^2}$$

# **SVD** - Interpretation #2

### **More details**

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

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

### **More details**

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

```
0.13 0.02 -0.01
  1 1 0 0
              0.41 0.07 -0.03
 3 3 0 0
                                 12.4 0 0
              0.55 0.09 -0.04
 4 4 0 0
                                     9.5 0
              0.68 0.11 -0.05
 5 5 0 0
0 2 0 4 4
              0.15 -0.59 0.65
0 0 0 5 5
              0.07 -0.73 -0.67
                                0.56 0.59 0.56 0.09 0.09
              0.07 -0.29 0.32
                                0.12 -0.02 0.12 -0.69 -0.69
                                0.40 -0.80 0.40 0.09 £0.09
```

# **SVD** - Interpretation #2

### **More details**

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

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \approx \begin{bmatrix} 0.13 & 0.02 & -0.01 \\ 0.41 & 0.07 & -0.03 \\ 0.55 & 0.09 & -0.04 \\ 0.68 & 0.11 & -0.05 \\ 0.15 & -0.59 & 0.65 \\ 0.07 & -0.73 & -0.67 \\ 0.07 & -0.29 & 0.32 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 3.3 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 3.3 \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\ 0.40 & -0.80 & 0.40 & 0.09 & 0.09 \end{bmatrix}$$

### **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} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5
```

# **SVD** - Interpretation #2

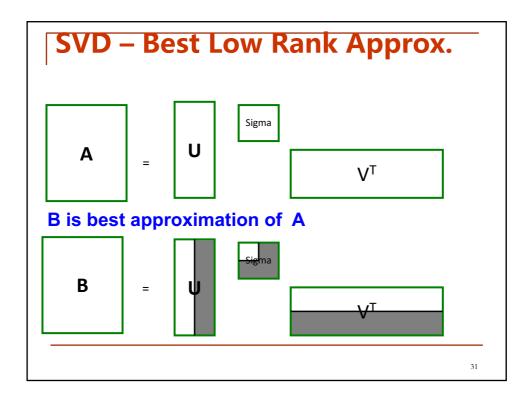
### **More details**

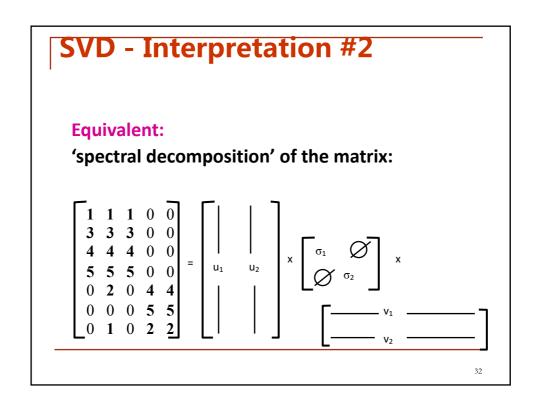
- Q: How exactly is dim. reduction done?
- A: Set smallest singular values to zero

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

### Frobenius norm:

$$\|\mathbf{M}\|_{F} = \sqrt{\sum_{ij} M_{ij}^{2}} \qquad \|\mathbf{A} - \mathbf{B}\|_{F} = \sqrt{\sum_{ij} (\mathbf{A}_{ij} - \mathbf{B}_{ij})^{2}}$$
is "small"





### **Equivalent:**

'spectral decomposition' of the matrix

Assume:  $\sigma_1 \ge \sigma_2 \ge \sigma_3 \ge ... \ge 0$ 

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

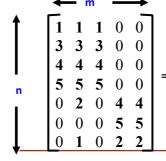
31

# **SVD** - Interpretation #2

Q: How many  $\sigma_s$  to keep?

A: Rule-of-a thumb:

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



$$\sigma_1$$
  $u_1$   $v_1^T$  +  $\sigma_2$   $u_2$   $v_2^T$  +...

Assume:  $\sigma_1 \ge \sigma_2 \ge \sigma_3 \ge ...$ 

# **SVD** - Complexity

- To compute SVD:
  - □ O(nm²) or O(n²m) (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 ...

3.

# **SVD** - Conclusions

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