



中国科学院大学

University of Chinese Academy of Sciences

Mining Massive Datasets

Dimensionality Reduction

SVD&CUR

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Dimensionality Reduction

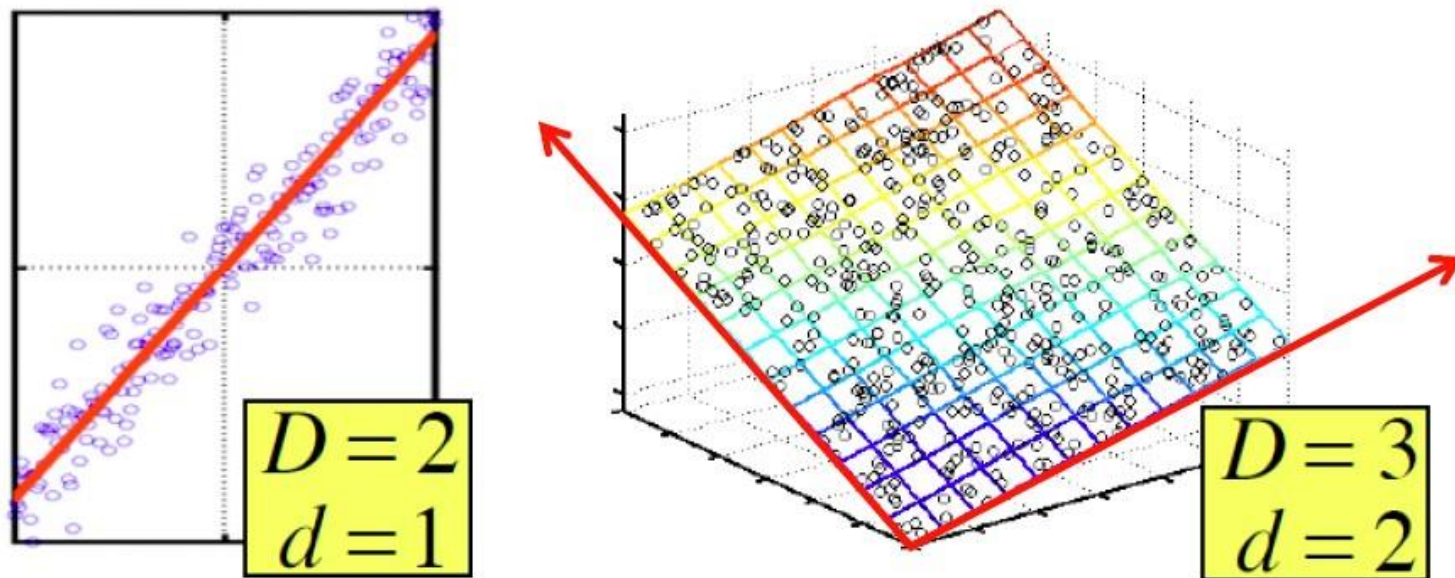
- **Compress / reduce dimensionality:**
 - 10^6 rows; 10^3 columns; no updates
 - Random access to any cell(s); **small error: OK**

customer	day	We 7/10/96	Th 7/11/96	Fr 7/12/96	Sa 7/13/96	Su 7/14/96
ABC Inc.		1	1	1	0	0
DEF Ltd.		2	2	2	0	0
GHI Inc.		1	1	1	0	0
KLM Co.		5	5	5	0	0
Smith		0	0	0	2	2
Johnson		0	0	0	3	3
Thompson		0	0	0	1	1

The above matrix is really “2-dimensional.” All rows can be reconstructed by scaling $[1 \ 1 \ 1 \ 0 \ 0]$ or $[0 \ 0 \ 0 \ 1 \ 1]$



Dimensionality Reduction



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

Why Reduce Dimensions?

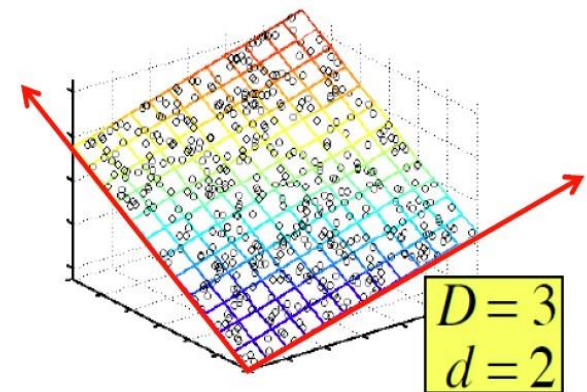
- Some features may be irrelevant
- We want to visualize high dimensional data
- “Intrinsic” dimensionality may be smaller than the number of features
- In particular, choose projection that minimizes the squared error in reconstructing original data



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

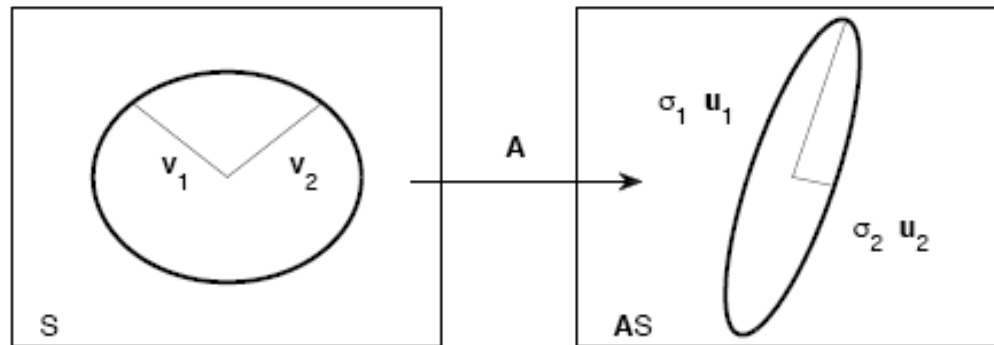
$$A_{[m \times n]} = U_{[m \times r]} \Sigma_{[r \times r]} (V_{[n \times r]})^T$$

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



SVD-decomposition

- The SVD, much as illustrated in the following figure, is essentially a transformation that stretches/compresses and rotates a given set of vectors



the transformation from the unit sphere to the hyperellipse

$$\mathbf{A}\mathbf{v}_j = \sigma_j \mathbf{u}_j,$$
$$\mathbf{A}^T \mathbf{u}_i = \sigma_j \mathbf{v}_j.$$



SVD–Eigenvalue & Eigenvector

Given a $n \times n$ matrix $A^T A$, for any σ and v , if

$$A^T A v_j = \sigma_j v_j$$

Then σ is called eigenvalue, and w is called eigenvector.

- To gain insight into the SVD, treat the rows of an $m \times n$ matrix A as n points in a n -dimensional space and consider the problem of finding the best r -dimensional subspace with respect to the set of points. Here best means minimize the sum of the squares of the perpendicular distances of the points to the subspace.



SVD-decomposition

- The objective of the rotation transformation is to find the maximal variance. We Projection of data along v is Av . Variance:

$$\sigma^2 = (Av)^T (Av) = v^T A^T Av$$

where $A^T A$ is the covariance matrix of the data

Objective: maximize variance subject to constraint $v^T v = 1$.

Maximize $f = v^T A^T Av - \lambda(v^T v - 1)$

λ is the Lagrange multiplier, Differentiating with respect to v yields Eigenvalue equation:

$$A^T Av = \lambda v$$



SVD-decomposition

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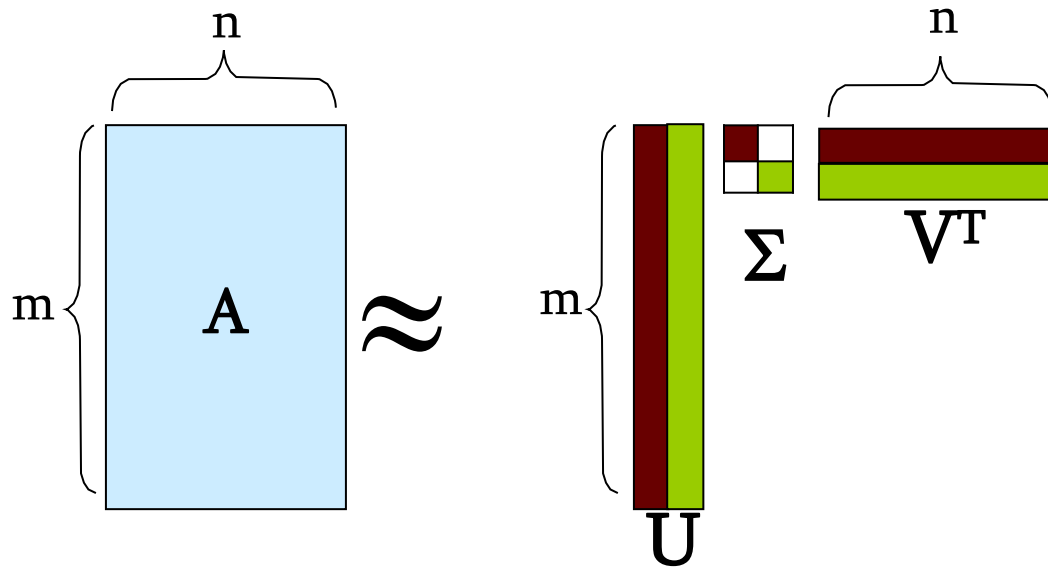
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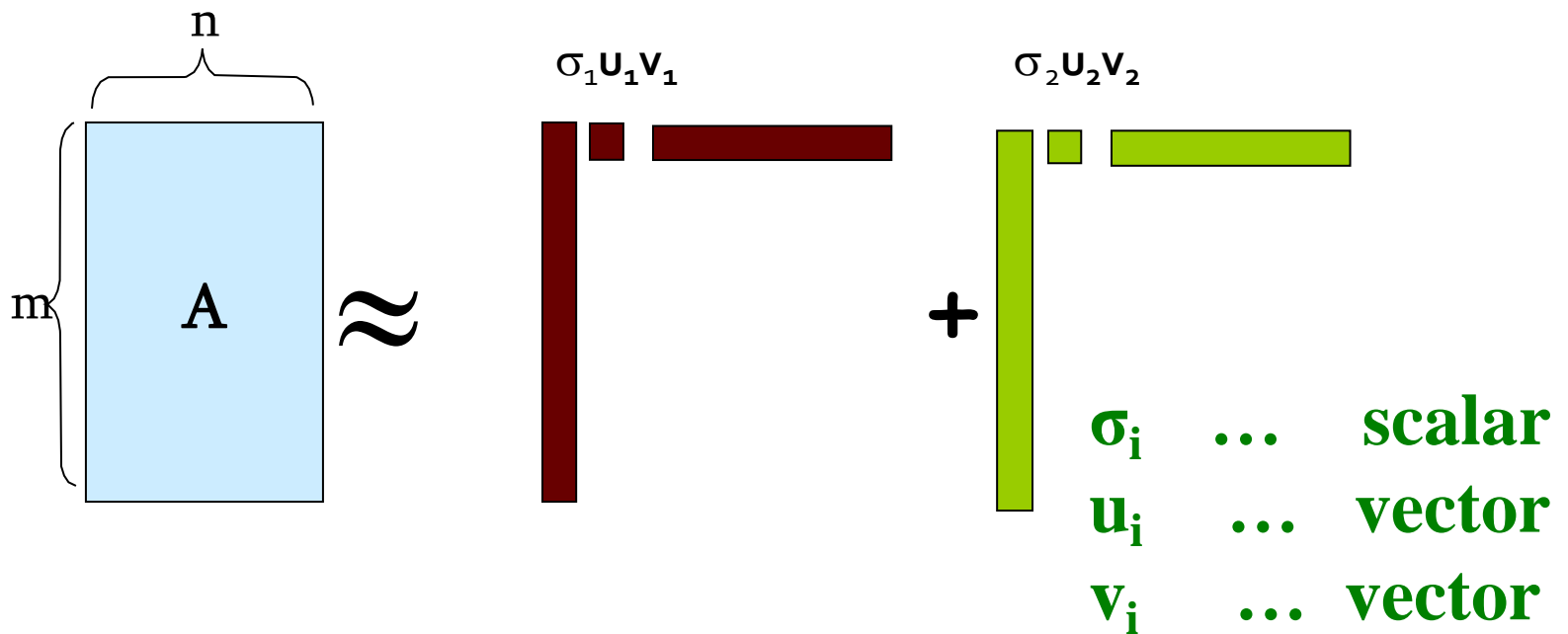
SVD

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



SVD

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



SVD

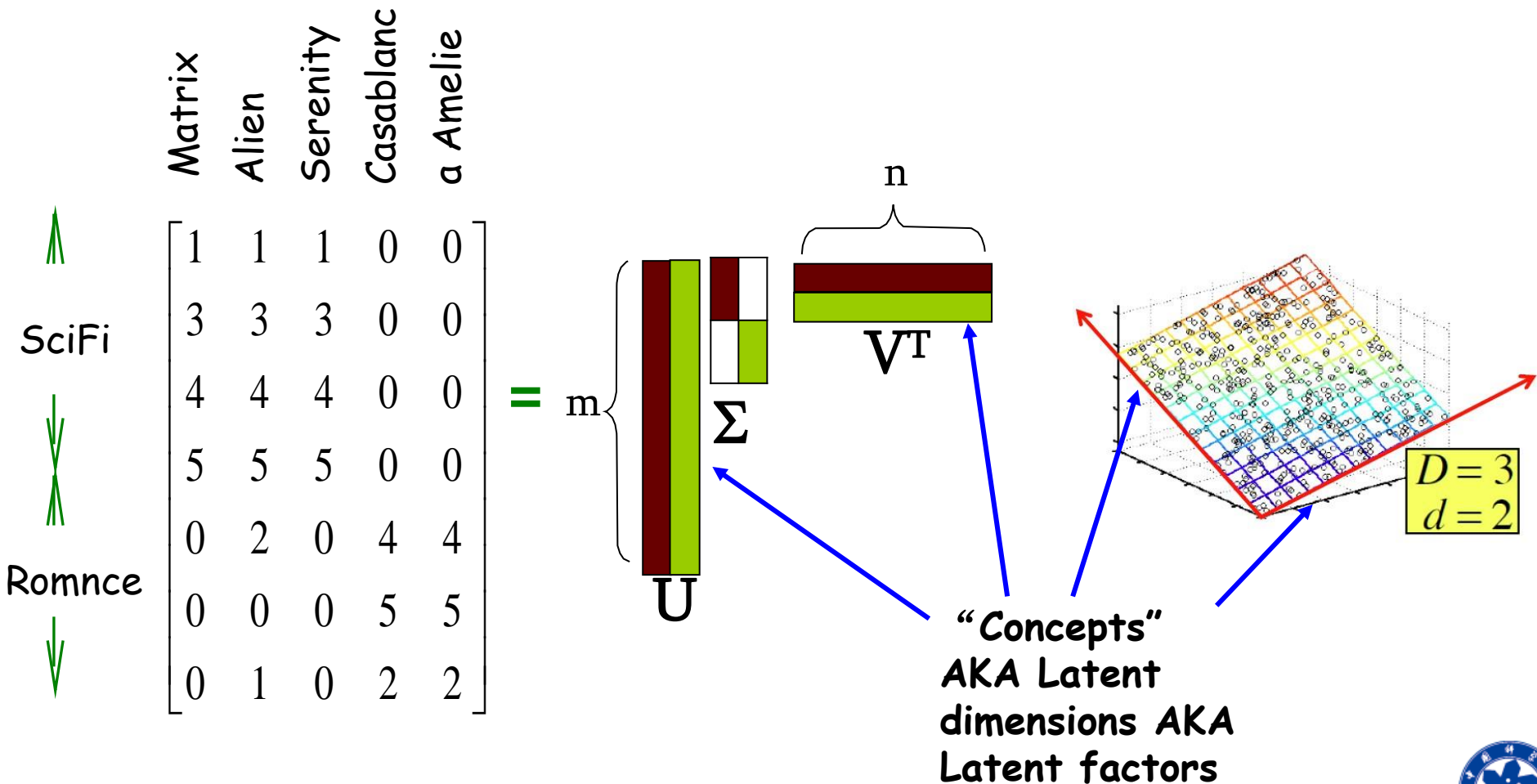
It is **always** possible to decompose a real matrix A into $A = U \Sigma V^T$, where

- 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 ($\sigma_1 \geq \sigma_2 \geq \dots \geq 0$)



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

SciFi \uparrow
 \downarrow
 Romnce \uparrow
 \downarrow

	Matrix	Alien	Serenity	Casablanc	a 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

$$=$$

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

$$\times$$

12.4	0	0
0	9.5	0
0	0	1.3

$$\times$$

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



SVD-Example:Users-to-Movies

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

Matrix

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

SciFi-concept

Romance-concept

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

SciFi

Romance



SVD-Example:Users-to-Movies

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

Matrix

	Alien	Serenity	Casablanca	Amelie
SciFi	1	1	0	0
	3	3	0	0
	4	4	0	0
	5	5	0	0
Romnce	0	2	4	4
	0	0	5	5
	0	1	2	2

SciFi-concept Romance-concept

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



SVD-Example:Users-to-Movies

■ $A = U\Sigma V^T$ - example:

Matrix

	Alien	Serenity	Casablanca	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

SciFi-concept

SciFi

Romance

SciFi-concept

"strength" of the SciFi-concept

12.4

9.5

1.3

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

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



SVD-Example:Users-to-Movies

- $A = U\Sigma V^T$ - example: V is "movie-to-concept" similarity matrix

Matrix

	Alien	Serenity	Casablanca	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

SciFi-concept

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

SciFi

Romance

\times

12.4	0	0
0	9.5	0
0	0	1.3

 \times

SciFi-concept

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



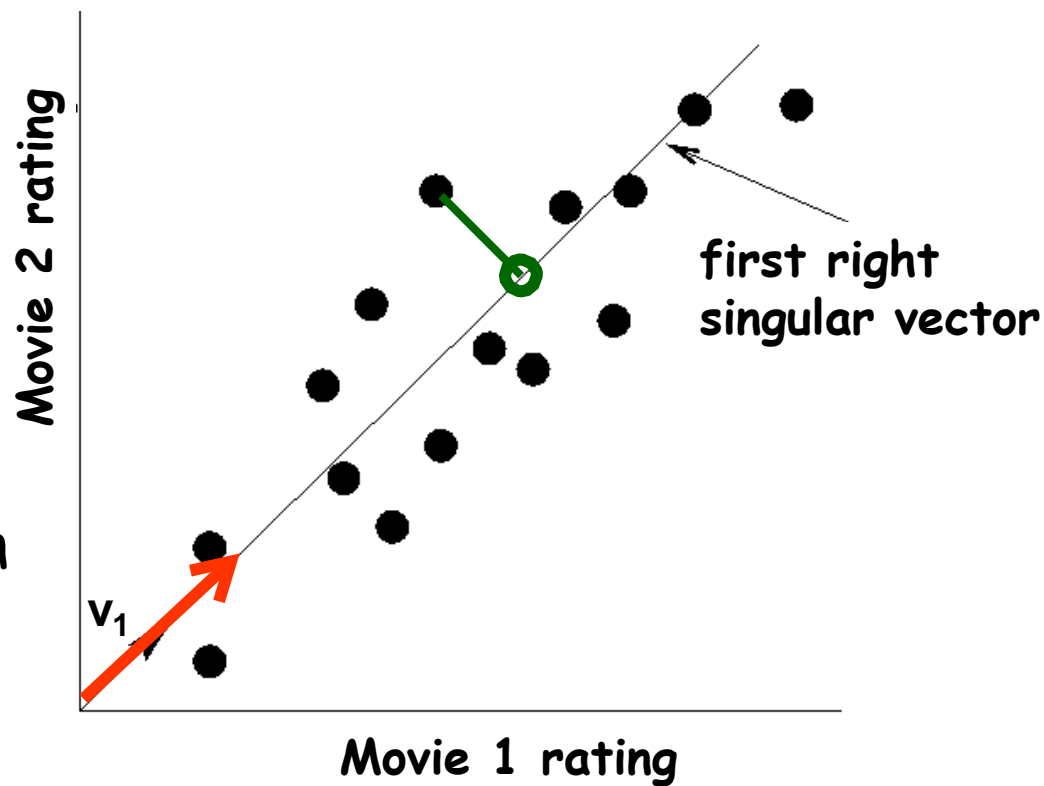
'movies', 'users' and 'concepts':

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



SVD-Interpretation #2

- SVD gives 'best' axis to project on:
- 'best' = min sum of squares of projection errors
- In other words, minimum reconstruction error



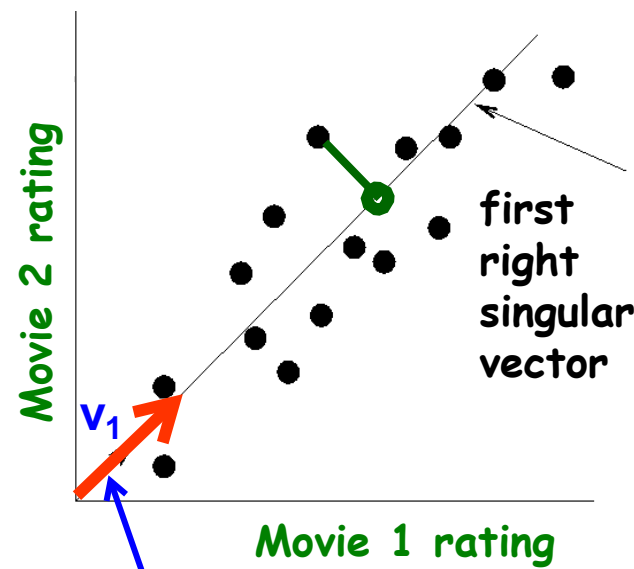
SVD-Interpretation #2

- $A = U\Sigma V^T$ - **example:**
 - V : "movie-to-concept" matrix
 - U : "user-to-concept" matrix

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

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

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



SVD-Interpretation #2

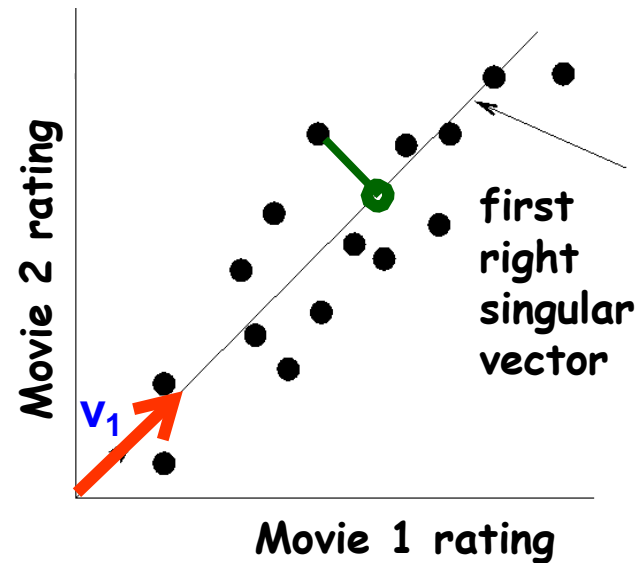
■ $A = U\Sigma V^T$ - example:

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

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variance ('spread')
on the v_1 axis



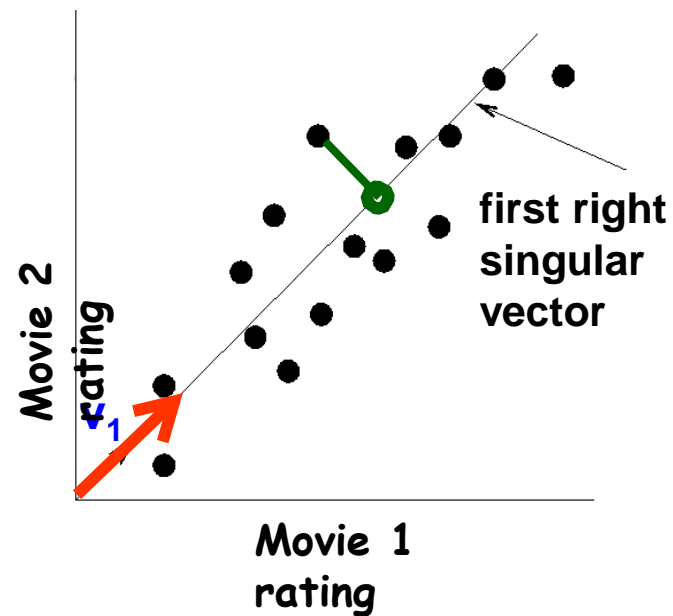
SVD-Interpretation #2

■ $A = U\Sigma V^T$ - example:

■ $U\Sigma$: Gives the coordinates of the points in the projection axis

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

Projection of users
on the "Sci-Fi"
axis $((U\Sigma)^T)$



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



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-Interpretation #2

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

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



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



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:

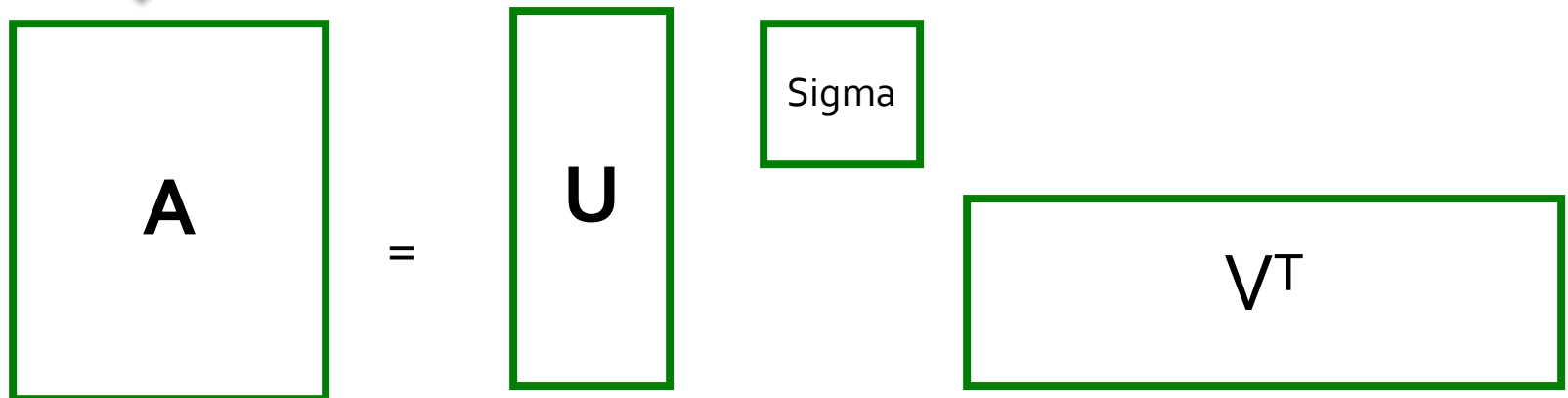
$$\|M\|_F = \sqrt{\sum_{ij} M_{ij}^2}$$

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

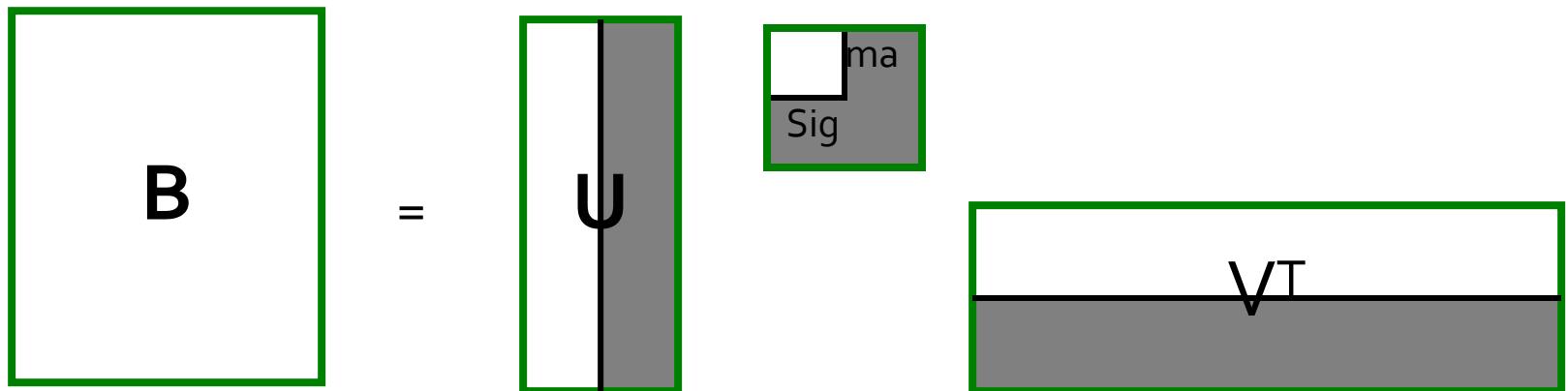
is “small”



SVD-Best Low Rank Approx.



B is best approximation of A



SVD-Best Low Rank Approx.

- Theorem: Let $A = U \Sigma V^T$ ($\sigma_1 \geq \sigma_2 \geq \dots$, $\text{rank}(A)=r$)
then $B = U S V^T$

- S = diagonal $n \times n$ matrix where $s_i = \sigma_i$ ($i=1 \dots k$) else $s_i=0$
is a best rank- k approximation to A :

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

$$\begin{pmatrix} x_{11} & x_{12} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & \\ \vdots & \vdots & \ddots & \\ x_{m1} & & & x_{mn} \end{pmatrix}_{m \times n} = \begin{pmatrix} u_{11} & \dots & & \\ \vdots & \ddots & & \\ u_{m1} & & & \end{pmatrix}_{m \times r} \begin{pmatrix} \sigma_1 & 0 & \dots \\ 0 & \ddots & \\ \vdots & & \end{pmatrix}_{r \times r} \begin{pmatrix} v_{11} & \dots & v_{1n} \\ \vdots & \ddots & \\ v_{r1} & \dots & \end{pmatrix}_{r \times n}$$

- **We will need 2 facts:**

- $\|M\|_F^2 = \sum_i (q_{ii})^2$ where $M = P Q R$ is SVD of M
- $U \Sigma V^T - U S V^T = U (\Sigma - S) V^T$



SVD-Best Low Rank Approx.

- **We will need 2 facts:**

- $\|M\|_F^2 = \sum_k (q_{kk})^2$ where $M = P Q R$ is SVD of M

$$\|M\|^2 = \sum_i \sum_j (m_{ij})^2 = \sum_i \sum_j \left(\sum_k \sum_\ell p_{ik} q_{k\ell} r_{\ell j} \right)^2$$

$$\|M\|^2 = \sum_i \sum_j \sum_k \sum_\ell \sum_n \sum_m p_{ik} q_{k\ell} r_{\ell j} p_{in} q_{nm} r_{mj}$$

$$\sum_i p_{ik} p_{in} \text{ is 1 if } k = n \text{ and 0 otherwise}$$

- $U \Sigma V^T - U S V^T = U (\Sigma - S) V^T$

We apply:

-- P column

orthonormal

-- R row orthonormal

-- Q is diagonal



SVD-Best Low Rank Approx.

- $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T$, $\mathbf{B} = \mathbf{U} \mathbf{S} \mathbf{V}^T$ ($\sigma_1 \geq \sigma_2 \geq \dots \geq 0$, $\text{rank}(\mathbf{A})=r$)
 - \mathbf{S} = diagonal $n \times n$ matrix where $s_i = \sigma_i$ ($i=1 \dots k$) else $s_i=0$
- then \mathbf{B} is solution to $\min_{\mathbf{B}} \|\mathbf{A} - \mathbf{B}\|_F$, $\text{rank}(\mathbf{B})=k$

■ Why?

$$\min_{\mathbf{B}, \text{rank}(\mathbf{B})=k} \|\mathbf{A} - \mathbf{B}\|_F = \min \|\mathbf{\Sigma} - \mathbf{S}\|_F = \min_s \sum_{i=1}^r (\sigma_i^2 - s_i^2)$$

We used: $\mathbf{U} \mathbf{\Sigma} \mathbf{V}^T - \mathbf{U} \mathbf{S} \mathbf{V}^T = \mathbf{U} (\mathbf{\Sigma} - \mathbf{S}) \mathbf{V}^T$

- We want to choose s_i to minimize $\sum (\sigma_i - s_i)^2$
 - We set $s_i = \sigma_i$ ($i=1 \dots k$) and other $s_i=0$

$$= \min_{s_i} \sum_{i=1} (\sigma_i - s_i)^2 + \sum_{i=k+1} \sigma_i^2 = \sum_{i=k+1} \sigma_i^2$$



SVD-Interpretation #2

Equivalent:

'spectral decomposition' of the matrix:

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



SVD-Interpretation #2

Equivalent:

'spectral decomposition' of the matrix:

$$\begin{array}{c} \text{← m →} \\ \begin{array}{c} \text{↑} \\ \text{↓} \\ n \end{array} \left[\begin{array}{ccccc} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{array} \right] \end{array} = \begin{array}{c} \text{← k terms →} \\ \sigma_1 \begin{array}{c} \text{u}_1 \\ \text{v}_1^T \end{array} + \sigma_2 \begin{array}{c} \text{u}_2 \\ \text{v}_2^T \end{array} + \dots \\ \begin{array}{cc} n \times 1 & 1 \times m \end{array} \end{array}$$

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



SVD-Interpretation #2

Q: How many σ_s to keep? A:
Rule-of-a thumb:

keep 80-90% of 'energy' ($=\sum \sigma_i^2$)

$$\begin{array}{c} \updownarrow \\ n \end{array} \begin{array}{c} \leftarrow m \rightarrow \\ \begin{vmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{vmatrix} \end{array} = \sigma_1 \mathbf{U}_1 \mathbf{V}_1^T + \sigma_2 \mathbf{U}_2 \mathbf{V}_2^T + \dots$$

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



- **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 ...



SVD-Conclusions so far

- **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



Relation to Eigen-decompositon

- **SVD gives us:**

- $A = U \Sigma V^T$

- **Eigen-decomposition:**

- $A = X \Lambda X^T$

- A is symmetric

- U, V, X are orthonormal ($U^T U = I$),

- Λ, Σ are diagonal

- **What is:**

- $AA^T = U \Sigma V^T (U \Sigma V^T)^T = U \Sigma V^T (V \Sigma^T \Sigma U^T) = U^T \Sigma \Sigma^T U^T$

- $A^T A = V \Sigma^T U^T (U \Sigma V^T) = V \Sigma \Sigma^T V^T$



Relation to Eigen-decompositon

- **SVD gives us:**

- $A = U \Sigma V^T$

- **Eigen-decomposition:**

- $A = X \Lambda X^T$

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- **What is:**

- $AA^T = U \Sigma V^T (U \Sigma V^T)^T = U \Sigma V^T (V \Sigma^T U^T) = U \Sigma \Sigma^T U^T$

- $A^T A = V \Sigma^T U^T (U \Sigma V^T) = V \Sigma \Sigma^T V^T$

Shows how to
compute SVD using
eigenvalue
decomposition!



$$\begin{array}{ccc} X & \Lambda & X^T \\ \downarrow & \downarrow & \downarrow \end{array}$$

So, $\lambda_i = \sigma_i^2$



Case study: How to query?

		Matrix	Alien	Serenity	Casablanca	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	

↑ SciFi
↓
↑ Romnce
↓

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

- Q: Find users that like 'Matrix'
- A: Map query into a 'concept space' - how?

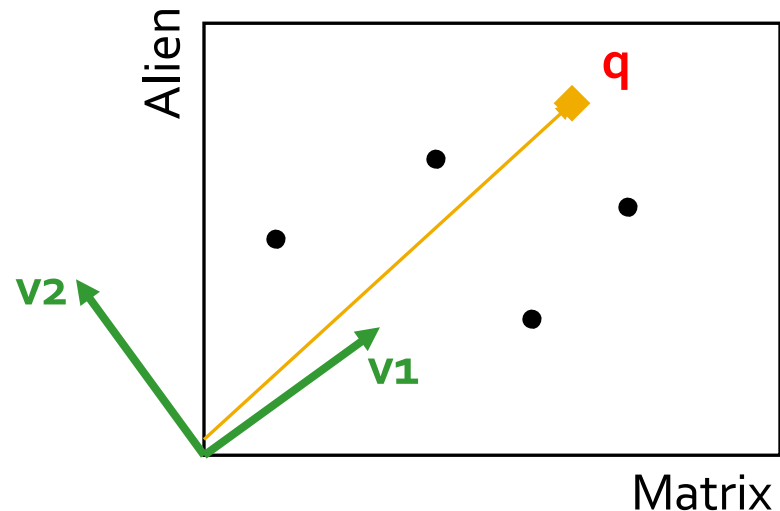


Case study: How to query?

- Q: Find users that like 'Matrix'
- A: Map query into a 'concept space' – how?

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

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

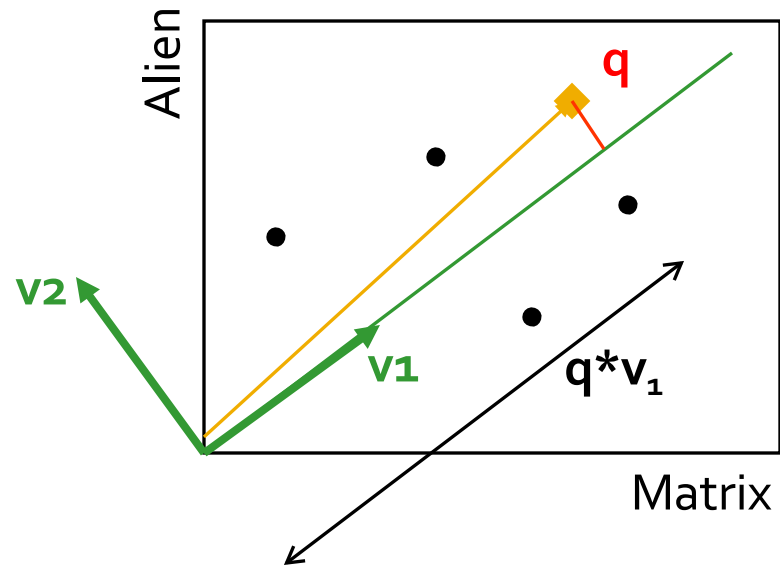


Case study: How to query?

- Q: Find users that like 'Matrix'
- A: Map query into a 'concept space' – how?

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

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



Case study: How to query?

Compactly, we have: $q_{\text{concept}} = q V$

E.g.:

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

movie-to-concept similarities (V)



Case study: How to query?

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

$$\mathbf{d}_{\text{concept}} = \mathbf{d} \mathbf{V}$$

E.g.:

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

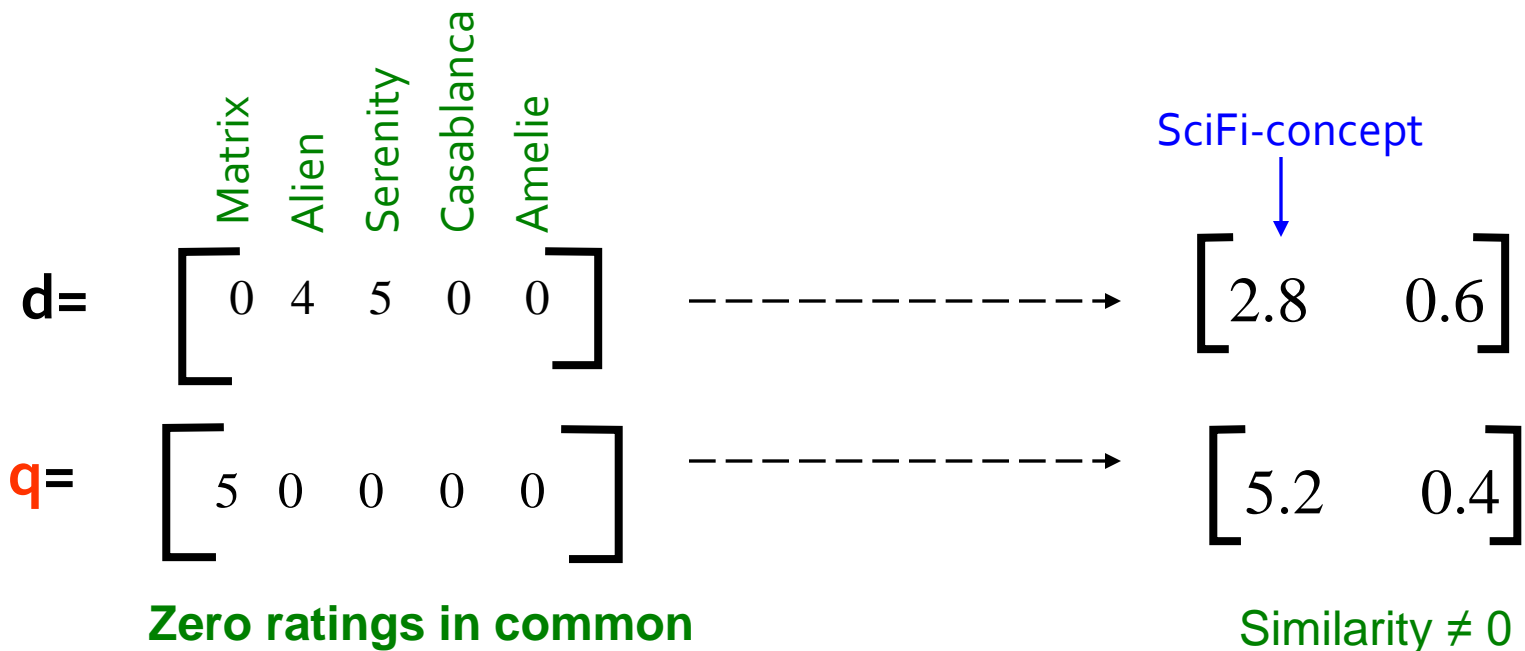
movie-to-concept
similarities (V)

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!**



Optimal low-rank approximation

in terms of Frobenius norm

- Interpretability problem:

- A singular vector specifies a linear combination of all input columns or rows

- Lack of sparsity:

- Singular vectors are **dense**!

The diagram illustrates the SVD decomposition of a matrix A into three components: U , Σ , and V^T . Matrix A is represented by a rectangle containing 6 black dots, indicating it is sparse. It is followed by an equals sign. Matrix U is represented by a tall, narrow rectangle that is almost entirely filled with black dots, indicating it is dense. To the right of U is a small square labeled Σ , which contains a few black dots. To the right of Σ is a wide, short rectangle labeled V^T , which is also almost entirely filled with black dots, indicating it is dense.

CUR Decomposition



CUR Decomposition

Frobenius norm:

$$\|X\|_F = \sqrt{\sum_{ij} X_{ij}^2}$$

- Goal: Express A as a product of matrices C, U, R Make $\|A - C \cdot U \cdot R\|_F$ small

$$\left(\begin{array}{|c|} \hline \text{Red} \\ \hline \end{array} \quad \begin{array}{|c|} \hline \text{Blue} \\ \hline \end{array} \right) A \approx \left(\begin{array}{|c|c|c|c|} \hline \text{Red} & \text{Red} & \text{Red} & \text{Blue} \\ \hline \end{array} \right) \cdot \left(\begin{array}{|c|} \hline U \\ \hline \end{array} \right) \cdot \left(\begin{array}{|c|} \hline R \\ \hline \end{array} \right)$$

A
 C
 U
 R

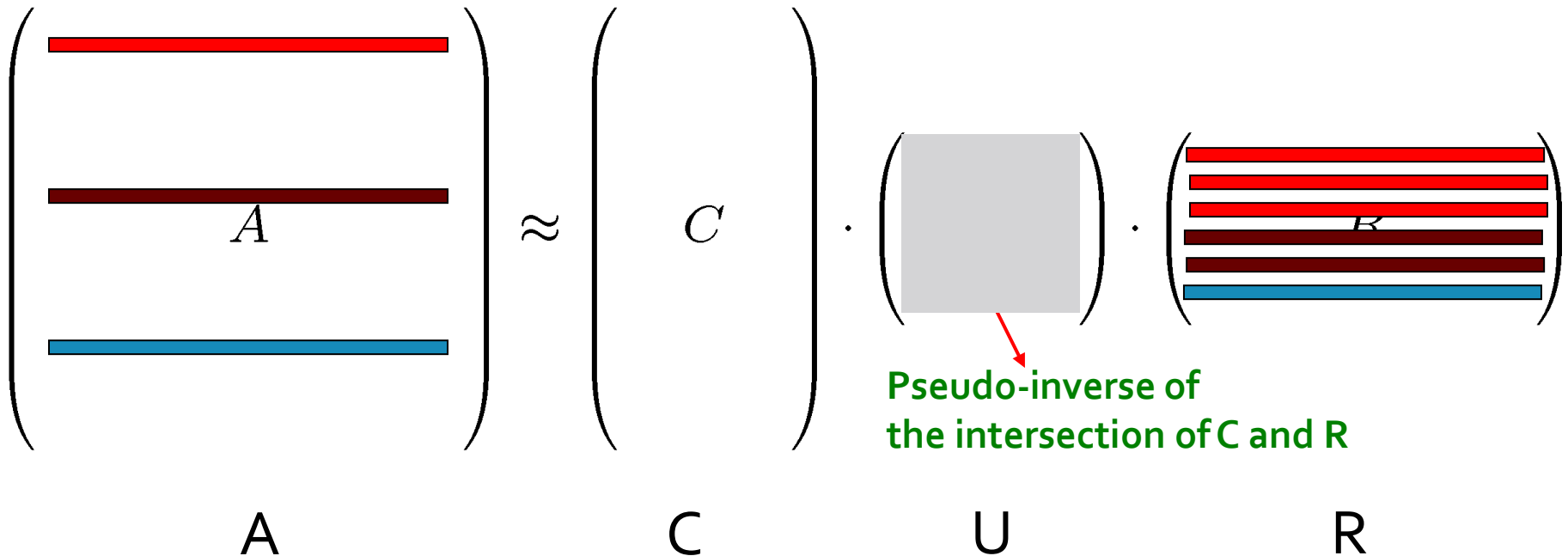


CUR Decomposition

Frobenius norm:

$$\|X\|_F = \sqrt{\sum_{ij} X_{ij}^2}$$

- Goal: Express A as a product of matrices C, U, R Make $\|A - C \cdot U \cdot R\|_F$ small
- "Constraints" on C and R :



CUR: Provably good approx.to SVD

- **Let:**

A_k be the “best” rank k approximation to A (that is, A_k is SVD of A)

Theorem [Drineas et al.]

CUR in $O(m \cdot n)$ time achieves

- $\|A - CUR\|_F \leq \|A - A_k\|_F + \varepsilon \|A\|_F$

with probability at least $1 - \delta$ by picking

- $O(k \log(1/\delta) / \varepsilon^2)$ columns, and

- $O(k^2 \log^3(1/\delta) / \varepsilon^6)$ rows

In practice:

Pick $4k$

cols/rows



■ Sampling columns (similarly for rows):

Input: matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, sample size c

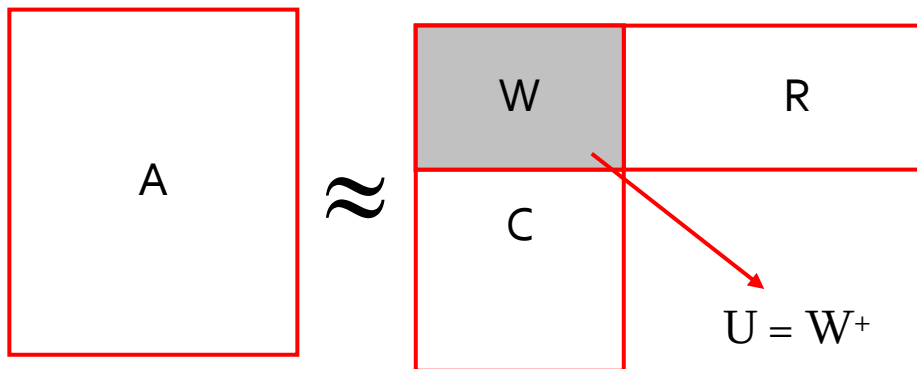
Output: $\mathbf{C}_d \in \mathbb{R}^{m \times c}$

1. for $x = 1 : n$ [column distribution]
2. $P(x) = \sum_i \mathbf{A}(i, x)^2 / \sum_{i,j} \mathbf{A}(i, j)^2$
3. for $i = 1 : c$ [sample columns]
4. Pick $j \in 1 : n$ based on distribution $P(x)$
5. Compute $\mathbf{C}_d(:, i) = \mathbf{A}(:, j) / \sqrt{cP(j)}$



Computing U

- Let **W** be the “intersection” of sampled columns **C** and rows **R**
 - Let SVD of **W** = **X Z Y^T**
- **Then: $U = W^+ = Y Z^+ X^T$**
 - **Z^+ : reciprocals of non-zero singular values: $Z^+_{ii} = 1/Z_{ii}$**
 - **W^+ is the “pseudoinverse”**



Why pseudoinverse works?

$W = X Z Y$ then $W^{-1} = X^{-1} Z^{-1} Y^{-1}$

Due to orthonormality $X^{-1} = X^T$ and $Y^{-1} = Y^T$

Since **Z** is diagonal $Z^{-1} = 1/Z_{ii}$

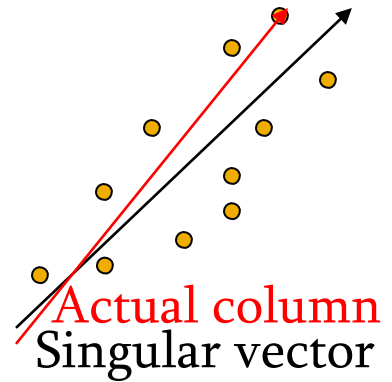
Thus, if **W** is nonsingular, pseudoinverse is the true inverse



CUR: Pros&Cons

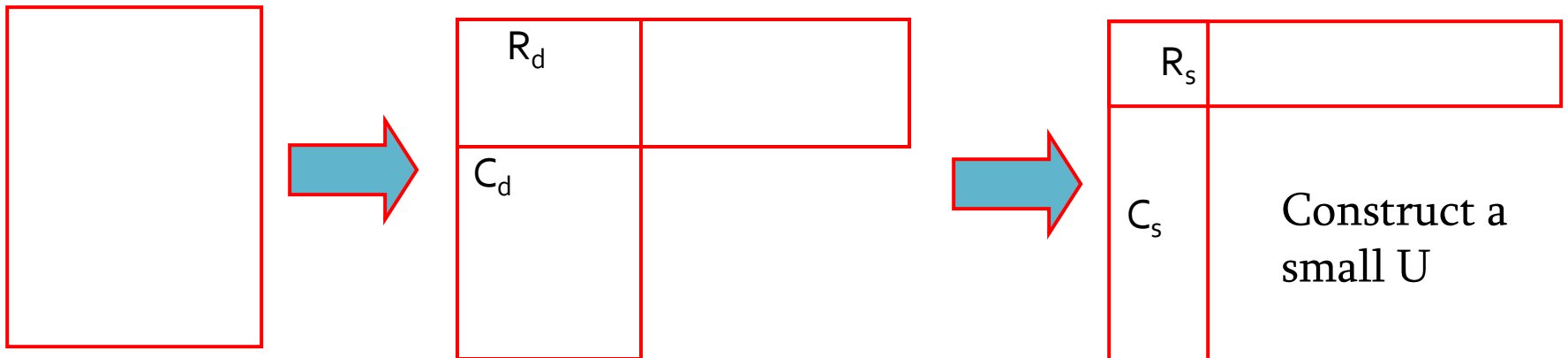
+ Easy interpretation

- Since the basis vectors are actual columns and rows
- + **Sparse basis**
- Since the basis vectors are actual columns and rows
- **Duplicate columns and rows**
 - Columns of large norms will be sampled many times



Solution

- If we want to get rid of the duplicates:
 - Throw them away
 - Scale (multiply) the columns/rows by the square root of the number of duplicates



SVD VS. CUR

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

Annotations for SVD:

- A : Huge but sparse
- U : Big and dense
- Σ : sparse and small
- V^T : Big and dense

CUR: $A = C U R$

Annotations for CUR:

- A : Huge but sparse
- C : Big but sparse
- U : dense but small
- R : Big but sparse

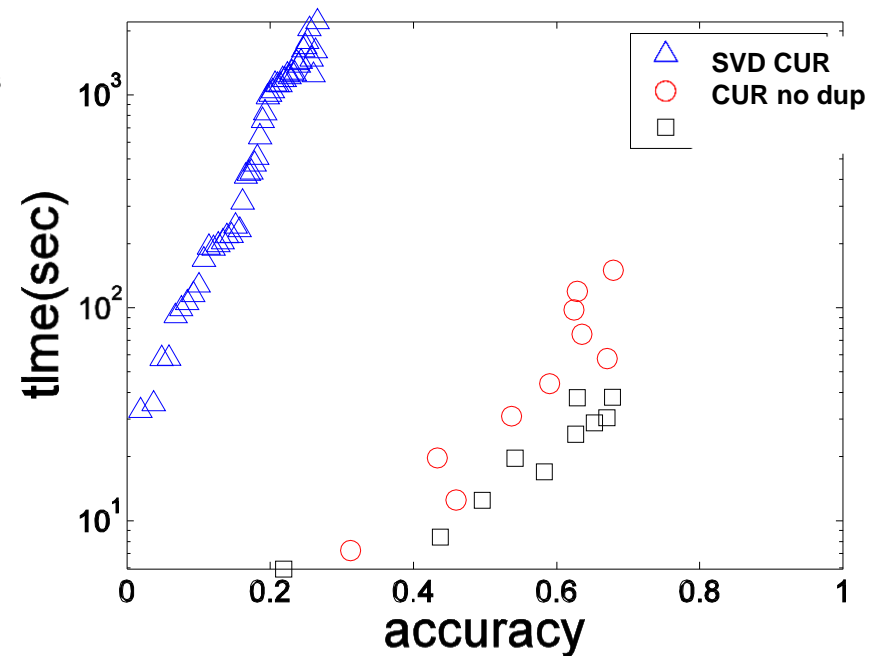
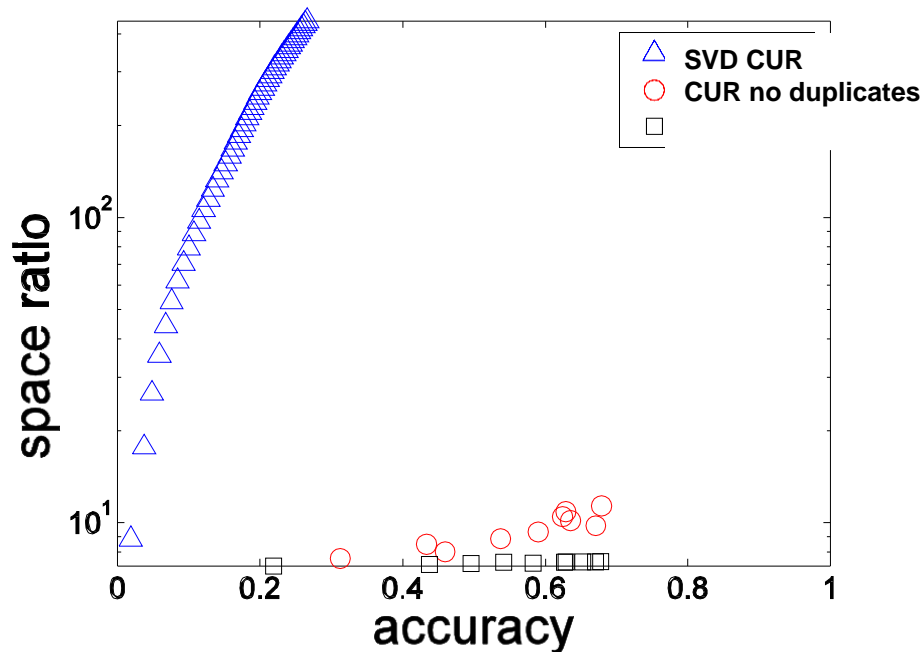


Simple Experiment

- **DBLP bibliographic data**
 - Author-to-conference big sparse matrix
 - A_{ij} : Number of papers published by author i at conference j
 - 428K authors (rows), 3659 conferences (columns)
 - Very sparse
- **Want to reduce dimensionality**
 - How much time does it take?
 - What is the reconstruction error?
 - How much space do we need?



Results : DBLP-big sparse matrix



- **Accuracy:**
 - 1 - relative sum squared errors
- **Space ratio:**
 - $\# \text{output matrix entries} / \# \text{input matrix entries}$
- **CPU time**



What about linearity assumption?

- **SVD is limited to linear projections:**

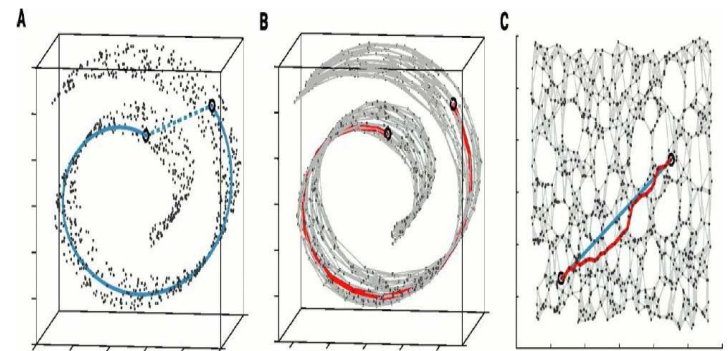
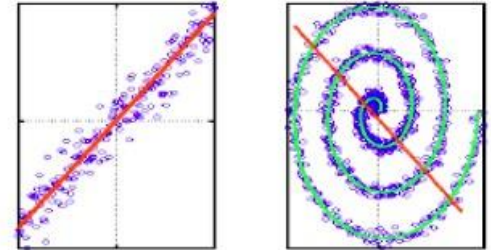
- Lower-dimensional linear projection that preserves Euclidean distances

- Non-linear methods: **Isomap**

- Data lies on a nonlinear low-dim curve aka manifold
 - Use the distance as measured along the manifold

- **How?**

- Build adjacency graph
- Geodesic distance is graph distance
- SVD/PCA the graph pairwise distance matrix



Further Reading: CUR

- Drineas et al., *Fast Monte Carlo Algorithms for Matrices III: Computing a Compressed Approximate Matrix Decomposition*, SIAM Journal on Computing, 2006.
- J. Sun, Y. Xie, H. Zhang, C. Faloutsos: *Less is More: Compact Matrix Decomposition for Large Sparse Graphs*, SDM 2007
- *Intra- and interpopulation genotype reconstruction from tagging SNPs*, P. Paschou, M. W. Mahoney, A. Javed, J. R. Kidd, A. J. Pakstis, S. Gu, K. K. Kidd, and P. Drineas, Genome Research, 17(1), 96-107 (2007)
- *Tensor-CUR Decompositions For Tensor-Based Data*, M. W. Mahoney, M. Maggioni, and P. Drineas, Proc. 12-th Annual SIGKDD, 327-336 (2006)



Tell me and I forget.
Show me and I remember.
Involve me and I understand.

Thank you! Q&A

