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Dimensionality Reduction: SVD & CUR

CS246: Mining Massive Datasets

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Reducing Matrix Dimension

- Often, our data can be represented by an m -by- n matrix
- And this matrix can be closely approximated by the product of three matrices that share a small common dimension r

$$\begin{matrix} n \\ \text{---} \\ m \end{matrix} \boxed{A} \approx \begin{matrix} r \\ \text{---} \\ m \end{matrix} \boxed{U} \times \begin{matrix} r \\ \text{---} \\ \Sigma \end{matrix} \times \begin{matrix} n \\ \text{---} \\ r \end{matrix} \boxed{V^T}$$

Dimensionality Reduction

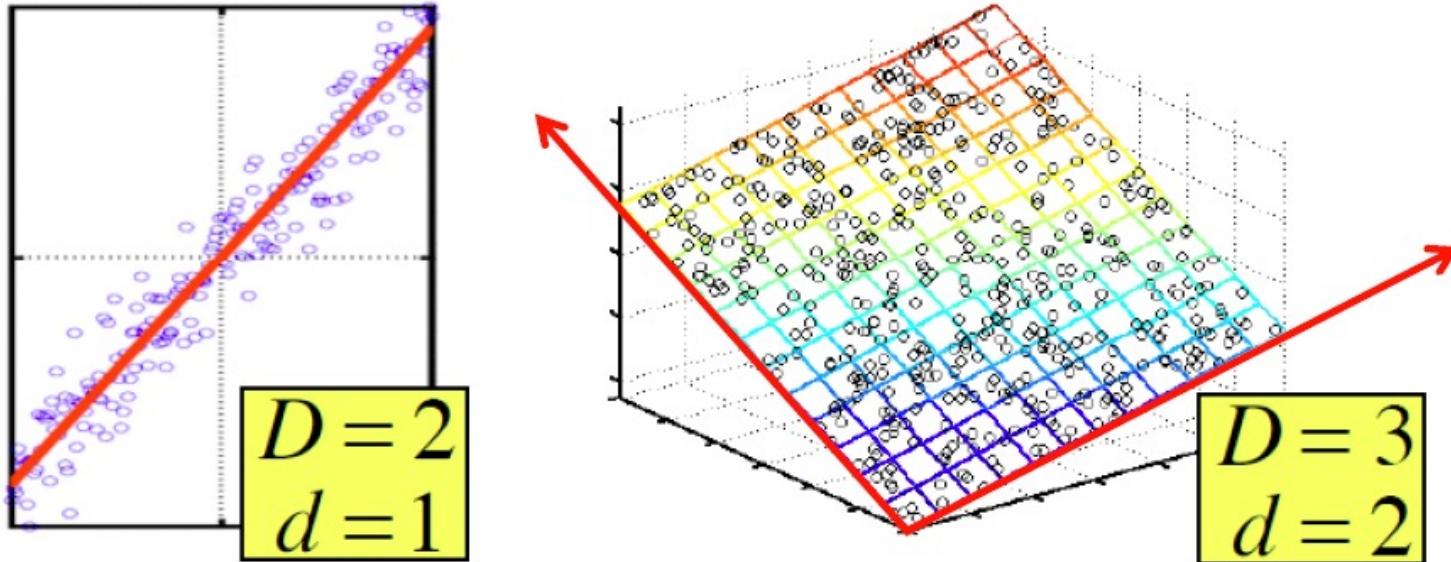
■ Compress / reduce dimensionality:

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

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

Note: 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

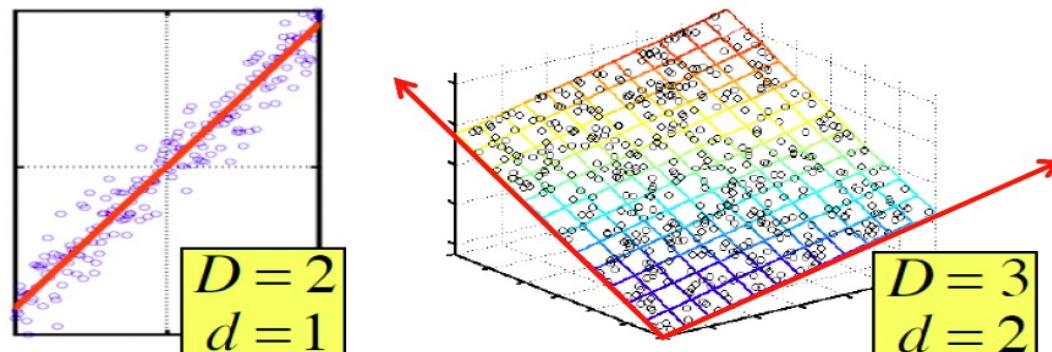


There are hidden, or **latent factors, latent dimensions** that – to a close approximation – explain why the values are as they appear in the data matrix

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 2nd greatest variance
- And so on..., until you have enough dimensions that variance is really low

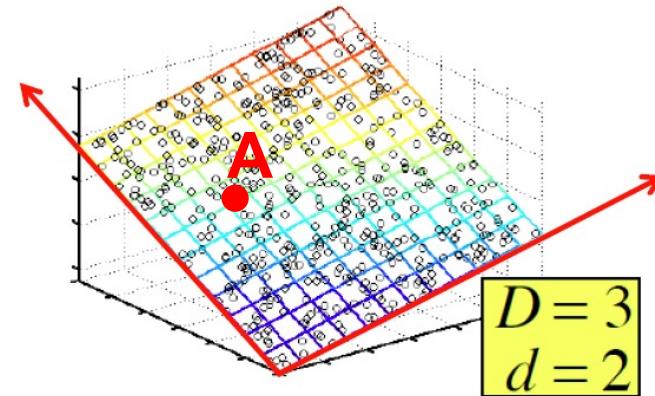


Rank is “Dimensionality”

- Q: What is **rank** of a matrix A?
- A: Number of **linearly independent** rows of A
- **Cloud of points in 3D space:**

- Think of point coordinates

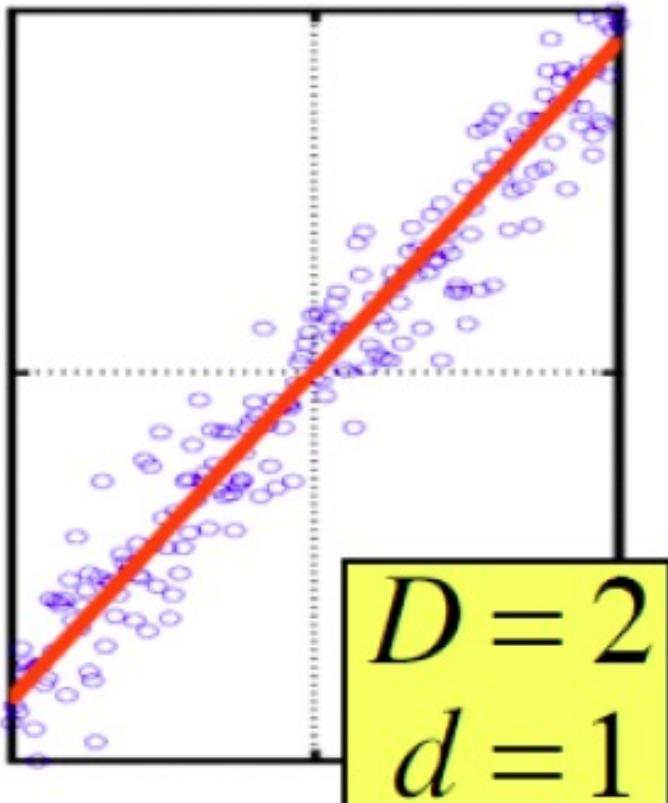
as a matrix: $\begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$ **A**
1 row per point: $\begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$ **B**
C



- 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 dimensions/coordinates!

Dimensionality Reduction

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



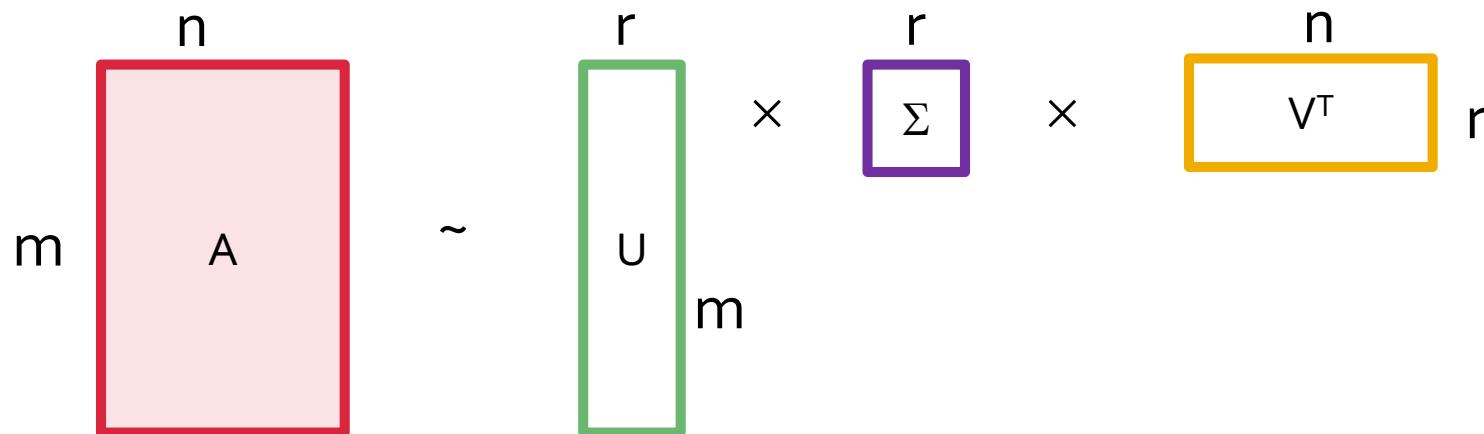
Rather than representing every point with 2 coordinates we represent each point with 1 coordinate (corresponding to the position of the point on the red line).

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

SVD: Singular Value Decomposition

Reducing Matrix Dimension

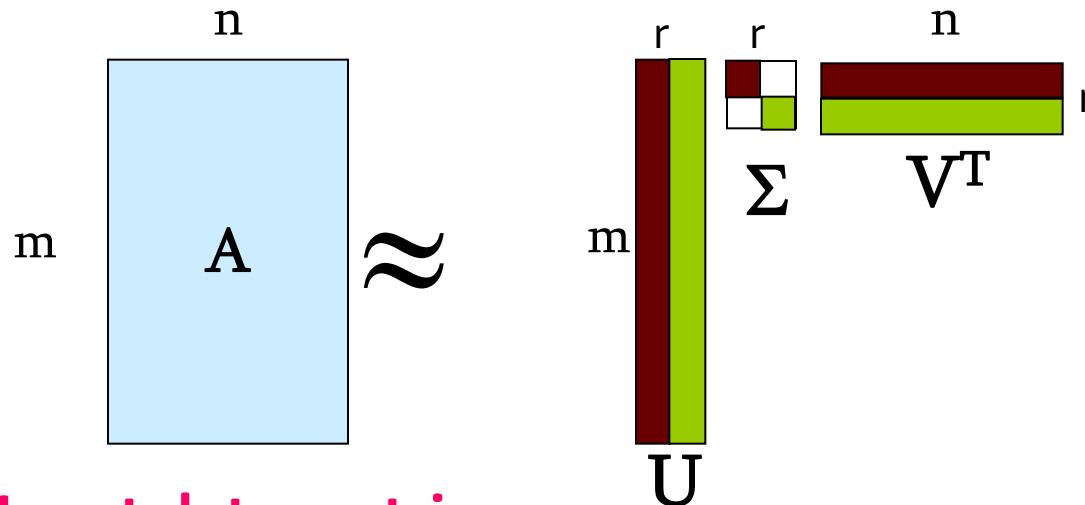
- Gives a decomposition of any matrix into a product of three matrices:



- There are strong constraints on the form of each of these matrices
 - Results in a unique decomposition
- From this decomposition, you can choose any number r of intermediate concepts (latent factors) in a way that minimizes the reconstruction error

SVD – Definition

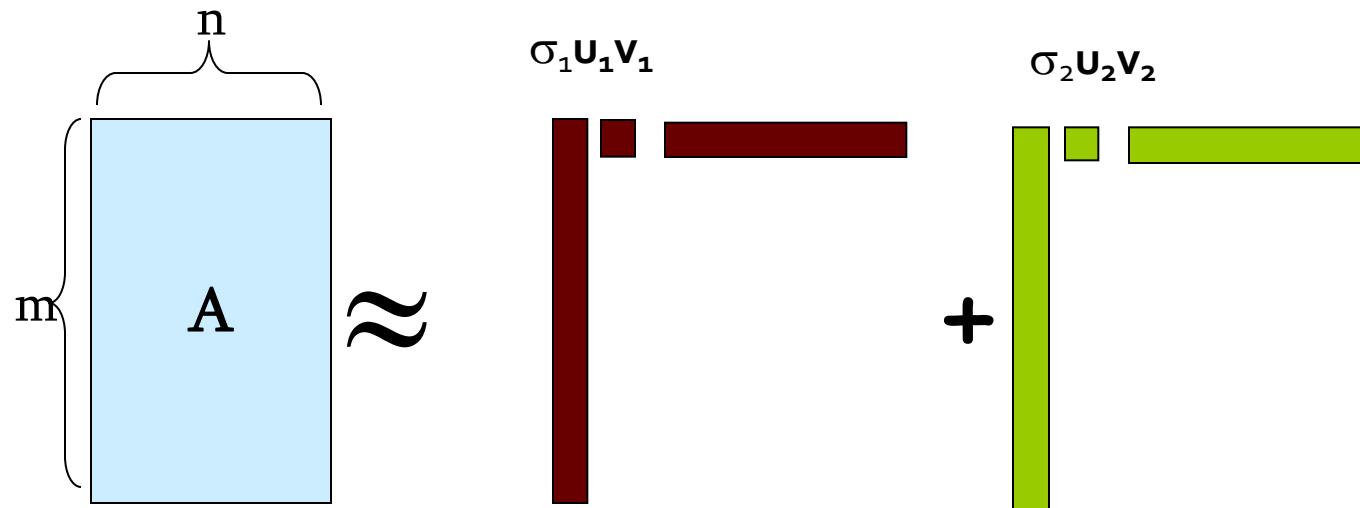
$$\mathbf{A} \approx \mathbf{U}\Sigma\mathbf{V}^T = \sum_i \sigma_i \mathbf{u}_i \circ \mathbf{v}_i^T$$



- **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

$$A \approx U\Sigma V^T = \sum_i \sigma_i u_i \circ v_i^\top$$



If we set $\sigma_2 = 0$, then the green columns may as well not exist.

σ_i ... scalar

u_i ... vector

v_i ... vector

SVD – Properties

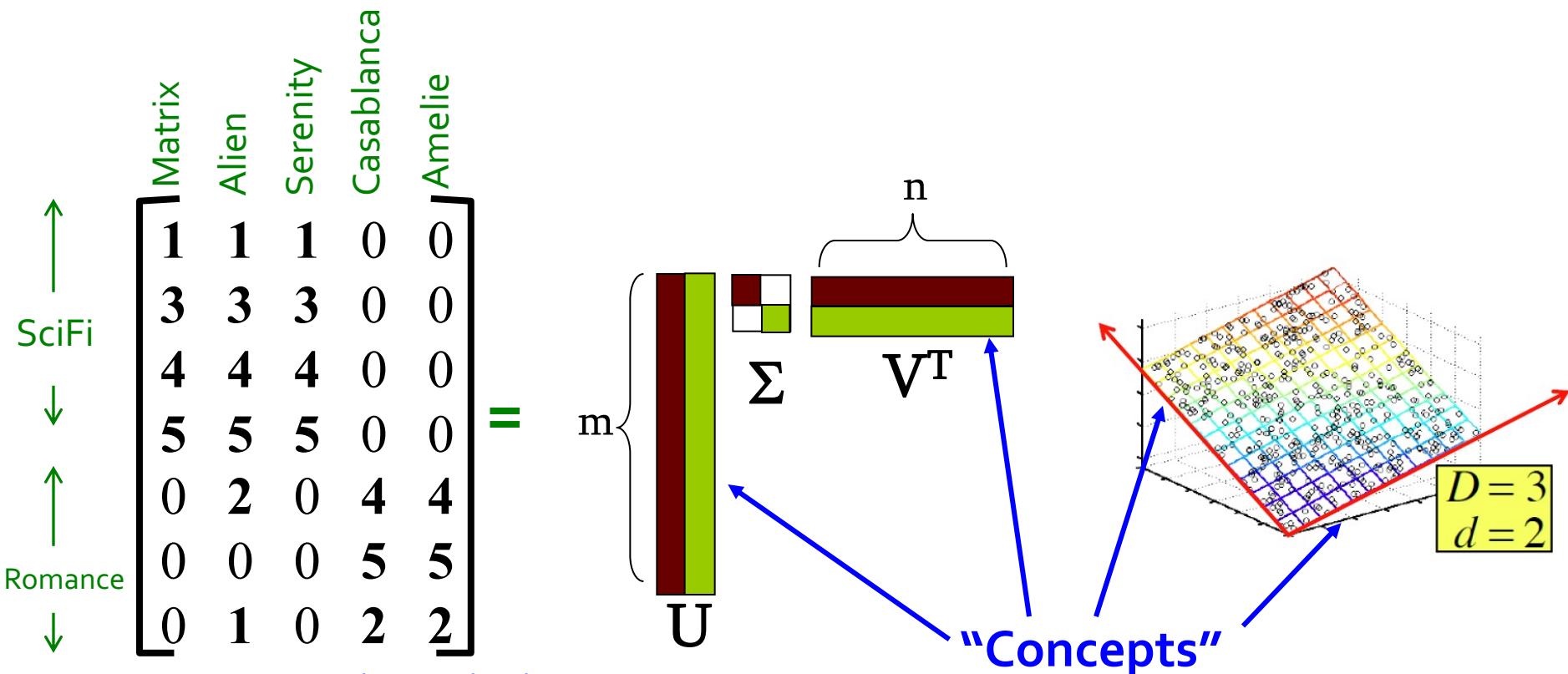
It is **always** possible to decompose a real matrix \mathbf{A} into $\mathbf{A} = \mathbf{U} \Sigma \mathbf{V}^T$, where

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

Nice proof of uniqueness: https://www.cs.cornell.edu/courses/cs322/2008sp/stuff/TrefethenBau_Lec4_SVD.pdf

SVD – Example: Users-to-Movies

- Consider a matrix. What does SVD do?



Ratings matrix where each column corresponds to a movie and each row to a user. First 4 users prefer SciFi, while others prefer Romance.

AKA Latent dimensions
AKA Latent factors

SVD – Example: Users-to-Movies

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

Matrix

	Alien	Serenity	Casablanca	Amelie
SciFi	1 1 1 0 0	0.13 0.02 -0.01		
↓	3 3 3 0 0	0.41 0.07 -0.03		
↑	4 4 4 0 0	0.55 0.09 -0.04		
Romance	5 5 5 0 0	0.68 0.11 -0.05		
↓	0 2 0 4 4	0.15 -0.59 0.65		
	0 0 0 5 5	0.07 -0.73 -0.67		
	0 1 0 2 2	0.07 -0.29 0.32		

=

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		

×

12.4 0 0		
0 9.5 0		
0 0 1.3		

×

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 3 4 5 0 0	1 3 4 5 2 0	0 0 0 0 4 5	0 0 0 0 4 5
Romance	0 0 0 0 1	0 0 0 0 0	2 5 5 5 2	2 2 2 2 2

$=$

	SciFi-concept	Romance-concept
SciFi	0.13 0.41 0.55 0.68 0.15 0.07 0.07	0.02 0.07 0.09 0.11 -0.59 -0.73 -0.29
Romance	-0.01 -0.03 -0.04 -0.05 0.65 -0.67 0.32	

\times

	12.4	0	0
SciFi	0	9.5	0
Romance	0	0	1.3

\times

	0.56	0.59	0.56	0.09	0.09
SciFi	0.12	-0.02	0.12	-0.69	-0.69
Romance	0.40	-0.80	0.40	0.09	0.09

SVD – Example: Users-to-Movies

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

U is “user-to-concept” factor matrix

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

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

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

SVD – Example: Users-to-Movies

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

Matrix

	Alien	Serenity	Casablanca	Amelie	
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

$=$

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

"strength" of the SciFi-concept

\times

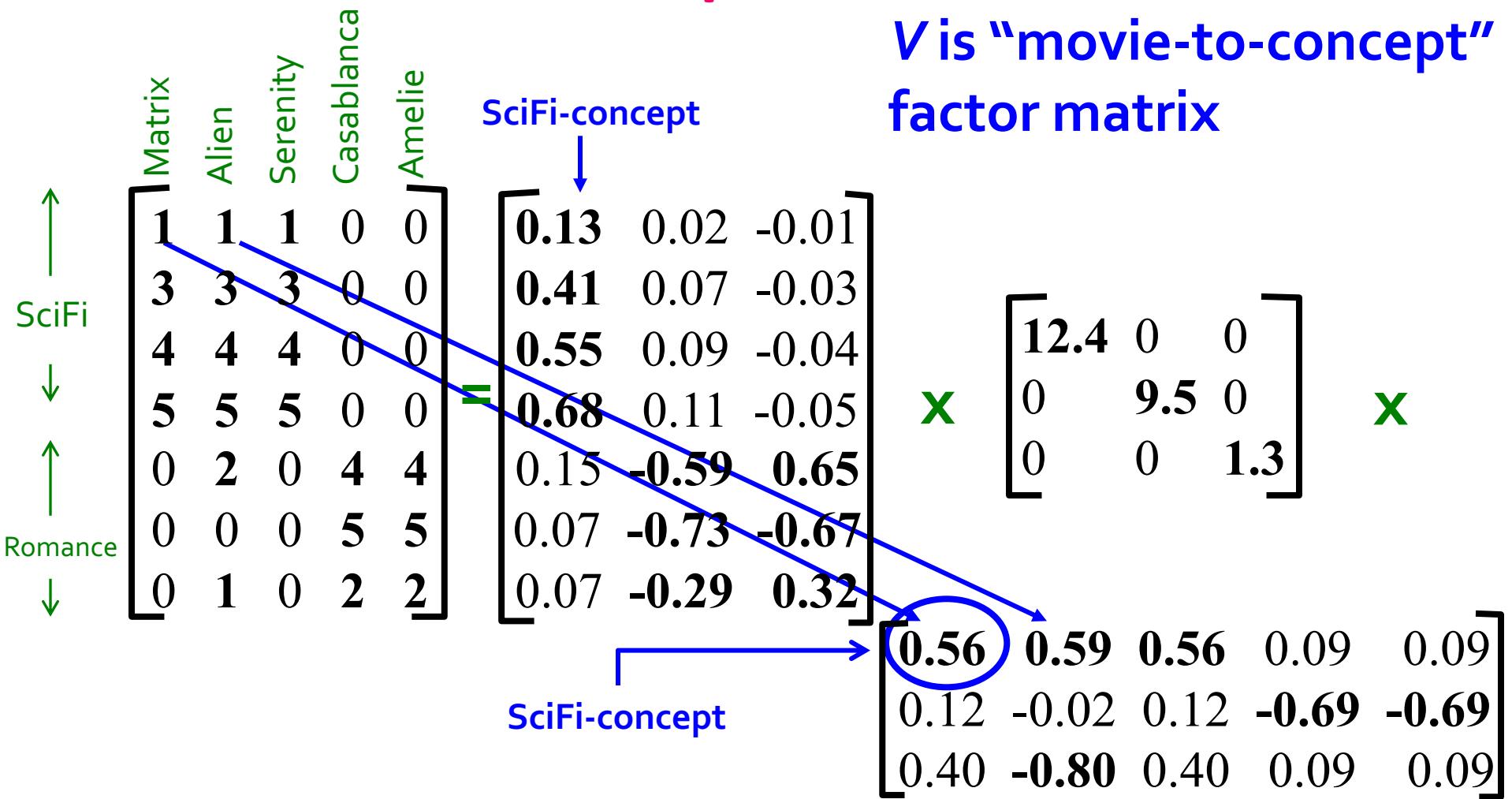
12.4	0	0
0	9.5	0
0	0	1.3

\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:



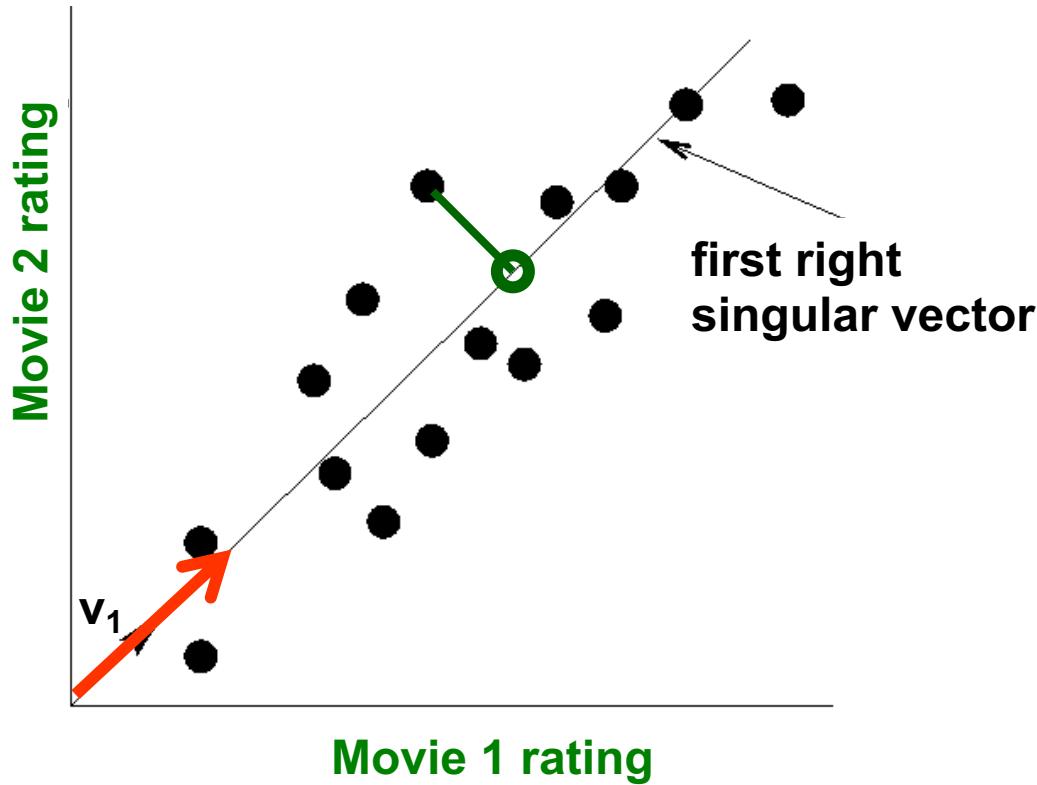
SVD – Interpretation #1

Movies, users and concepts:

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

Dimensionality Reduction with SVD

SVD – Dimensionality Reduction



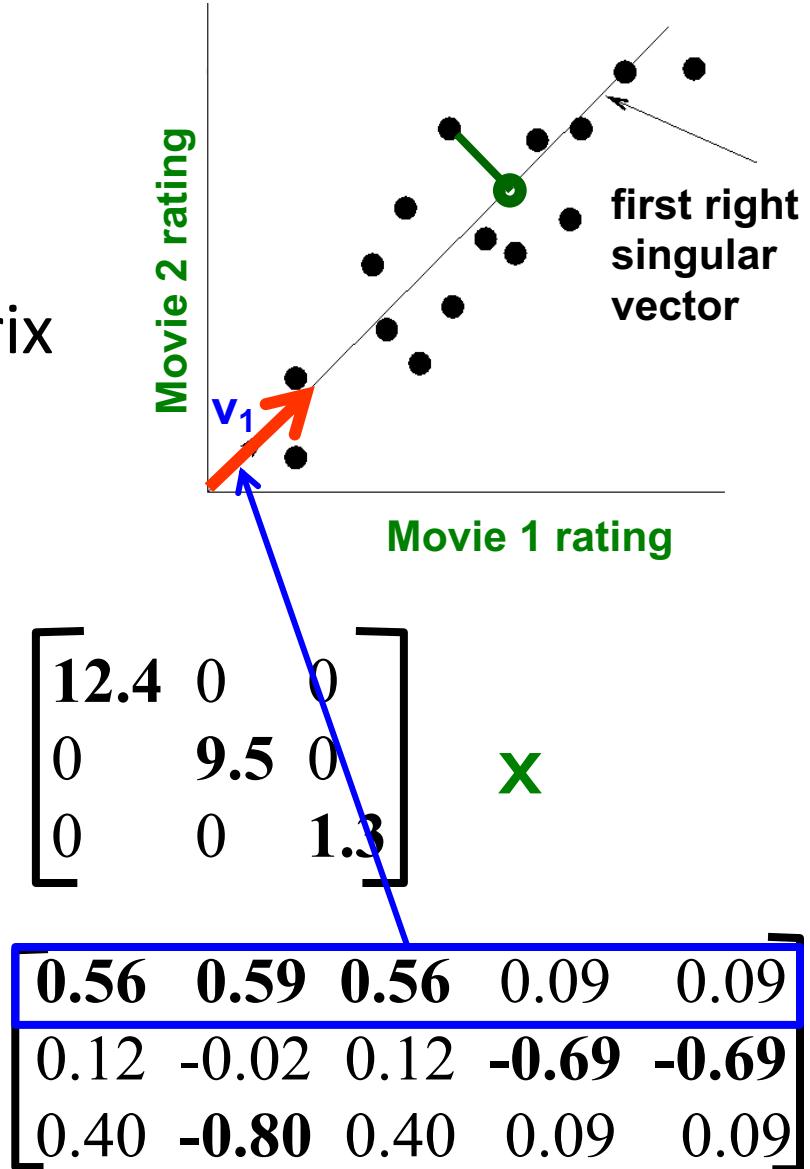
- Instead of using two coordinates (x, y) to describe point positions, let's use only one coordinate
- Point's position is its location along vector v_1

SVD – Dimensionality Reduction

■ $A = U \Sigma V^T$ - example:

- U : “user-to-concept” matrix
- V : “movie-to-concept” matrix

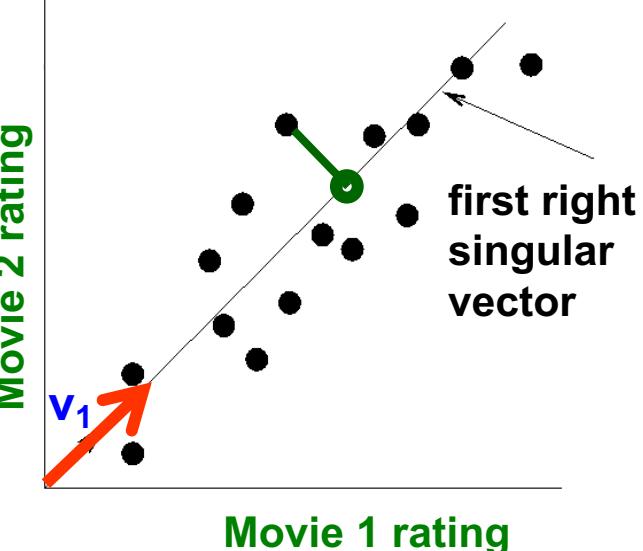
$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} = \begin{bmatrix} 0.13 & 0.02 & -0.01 \\ 0.41 & 0.07 & -0.03 \\ 0.55 & 0.09 & -0.04 \\ 0.68 & 0.11 & -0.05 \\ 0.15 & -0.59 &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



SVD – Dimensionality Reduction

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

variance ('spread')
on the v_1 axis



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

The matrix multiplication shows the decomposition of the original rating matrix into three components: U , Σ , and V^T . The matrix Σ contains the singular values, with the largest value circled in green. A green arrow points from this circled value to the scatter plot, indicating its variance ('spread') on the v_1 axis.

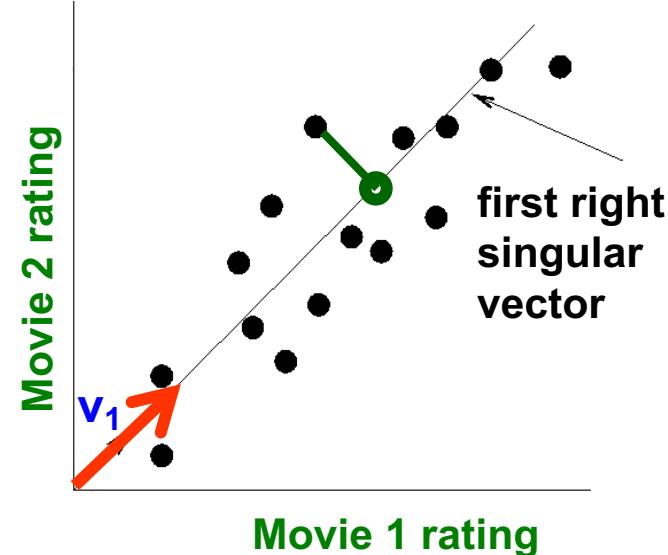
SVD – Dimensionality Reduction

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



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 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

More details

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

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

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

SVD – Interpretation #2

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

More details

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

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

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

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The larger the rank the more accurate the approximation

More details

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

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

Reconstructed
data matrix B

Reconstruction Error is quantified by the Frobenius norm:

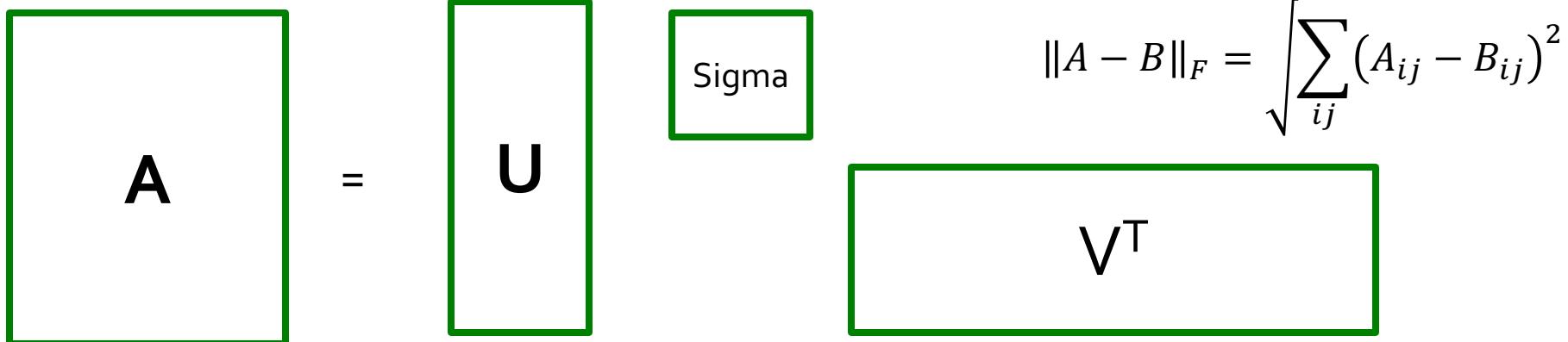
$$\|M\|_F = \sqrt{\sum_{ij} M_{ij}^2}$$

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

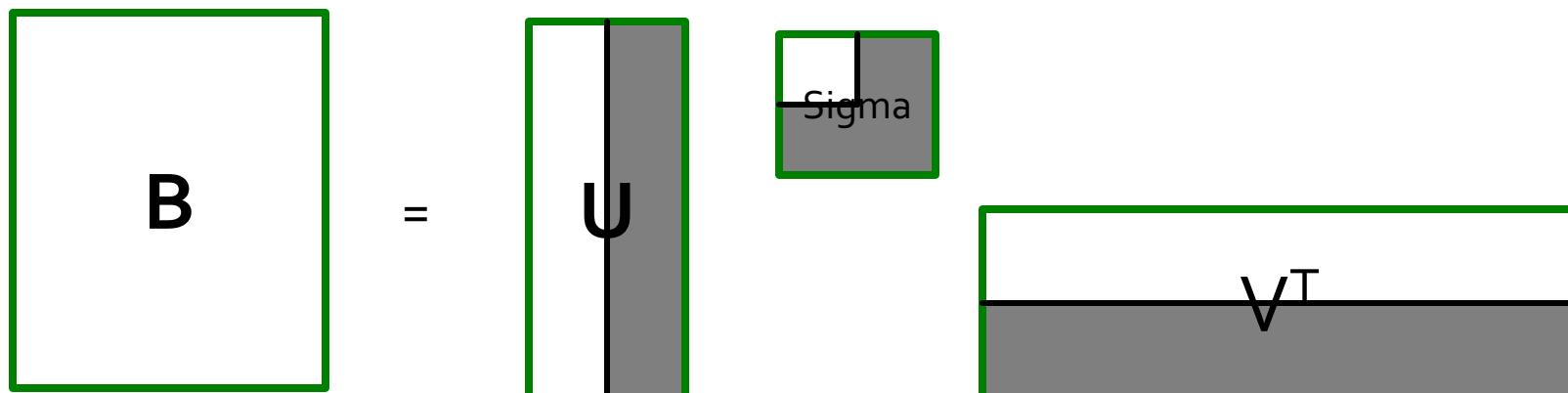
is “small”

SVD – Best Low Rank Approx.

- Fact: SVD gives ‘best’ axis to project on:
 - ‘best’ = minimizing the sum of reconstruction errors

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


B is best approximation of A:

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


SVD – Conclusions so far

- **SVD: $A = U \Sigma V^T$: unique**
 - U : user-to-concept factors
 - V : movie-to-concept factors
 - Σ : strength of each concept
- **Q: So what's a good value for r (# of latent factors)?**
- Let the *energy* of a set of singular values be the sum of their squares.
- Pick r so the retained singular values have at least 90% of the total energy.
- **Back to our example:**
 - With singular values 12.4, 9.5, and 1.3, total energy = 245.7
 - If we drop 1.3, whose square is only 1.7, we are left with energy 244, or over 99% of the total

How to Compute SVD

Finding Eigenpairs

- How do we actually 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 “guess eigenvector” \mathbf{x}_0
 - Construct $\mathbf{x}_{k+1} = \frac{M\mathbf{x}_k}{\|M\mathbf{x}_k\|}$ for $k = 0, 1, \dots$
 - $\| \dots \|$ denotes the Frobenius norm
 - Stop when consecutive \mathbf{x}_k show little change

Example: Iterative Eigenvector

$$M = \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix} \quad x_0 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\frac{Mx_0}{\|Mx_0\|} = \begin{bmatrix} 3 \\ 5 \end{bmatrix} / \sqrt{34} = \begin{bmatrix} 0.51 \\ 0.86 \end{bmatrix} = x_1$$

$$\frac{Mx_1}{\|Mx_1\|} = \begin{bmatrix} 2.23 \\ 3.60 \end{bmatrix} / \sqrt{17.93} = \begin{bmatrix} 0.53 \\ 0.85 \end{bmatrix} = x_2$$

.....

Finding the Principal Eigenvalue

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

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

Finding More Eigenpairs

- Eliminate the portion of the matrix M that can be generated by the first eigenpair, λ and x :

$$M^* := M - \lambda x x^T$$

- Recursively find the principal eigenpair for M^* , eliminate the effect of that pair, and so on

- **Example:**

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

How to Compute the SVD

- Start by supposing $A = U\Sigma V^T$
- $A^T = (U\Sigma V^T)^T = (V^T)^T \Sigma^T U^T = V \Sigma U^T$
 - Why? (1) Rule for transpose of a product; (2) the transpose of the transpose and the transpose of a diagonal matrix are both the identity functions
- $A^T A = V \Sigma U^T U \Sigma V^T = V \Sigma^2 V^T$
 - Why? U is orthonormal, so $U^T U$ is an identity matrix
 - Also note that Σ^2 is a diagonal matrix whose i -th element is the square of the i -th element of Σ
- $A^T A V = V \Sigma^2 V^T V = V \Sigma^2$
 - Why? V is also orthonormal

Computing the SVD –(2)

- Since $\mathbf{A}^T \mathbf{A} = \mathbf{V} \Sigma^2 \mathbf{V}^T \rightarrow \mathbf{A} \mathbf{A}^T \mathbf{V} = \mathbf{V} \Sigma^2$
 - Note that therefore the i -th column of \mathbf{V} is an eigenvector of $\mathbf{A}^T \mathbf{A}$, and its eigenvalue is the i -th element of Σ^2
- Thus, we can find \mathbf{V} and Σ by finding the eigenpairs for $\mathbf{A}^T \mathbf{A}$
 - Once we have the eigenvalues in Σ^2 , we can find the singular values by taking the square root of these eigenvalues
- Symmetric argument, $\mathbf{A} \mathbf{A}^T$ gives us \mathbf{U}

SVD – Complexity

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

Example of SVD

Case study: How to query?

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

$$\begin{array}{c} \text{↑ SciFi} \\ \text{↓} \\ \text{↑ Romance} \\ \text{↓} \end{array} \begin{matrix} \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \\ \left[\begin{matrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{matrix} \right] & = & \left[\begin{matrix} 0.13 & 0.02 & -0.01 \\ 0.41 & 0.07 & -0.03 \\ 0.55 & 0.09 & -0.04 \\ 0.68 & 0.11 & -0.05 \\ 0.15 & -0.59 & 0.65 \\ 0.07 & -0.73 & -0.67 \\ 0.07 & -0.29 & 0.32 \end{matrix} \right] & \times & \left[\begin{matrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 1.3 \end{matrix} \right] & \times \\ \end{array}$$

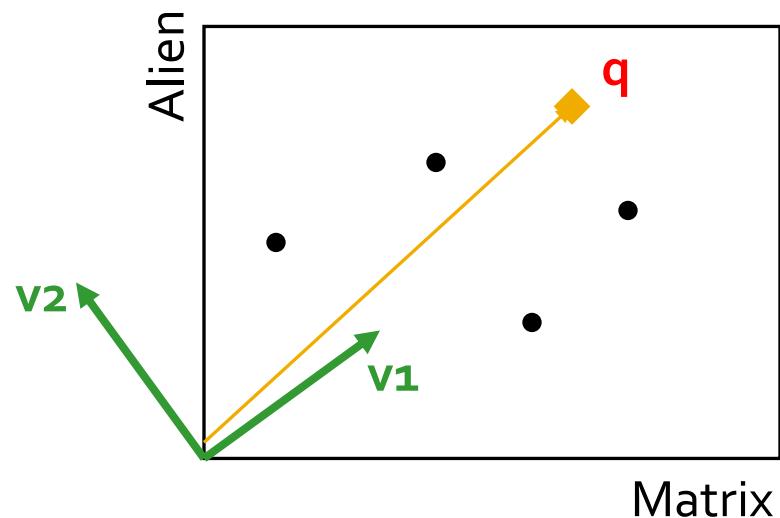
0.56 0.59 0.56 0.09 0.09
0.12 -0.02 0.12 -0.69 -0.69
0.40 -0.80 0.40 0.09 0.09

Case study: How to query?

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

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

Project into concept space:
Inner product with each
'concept' vector v_i

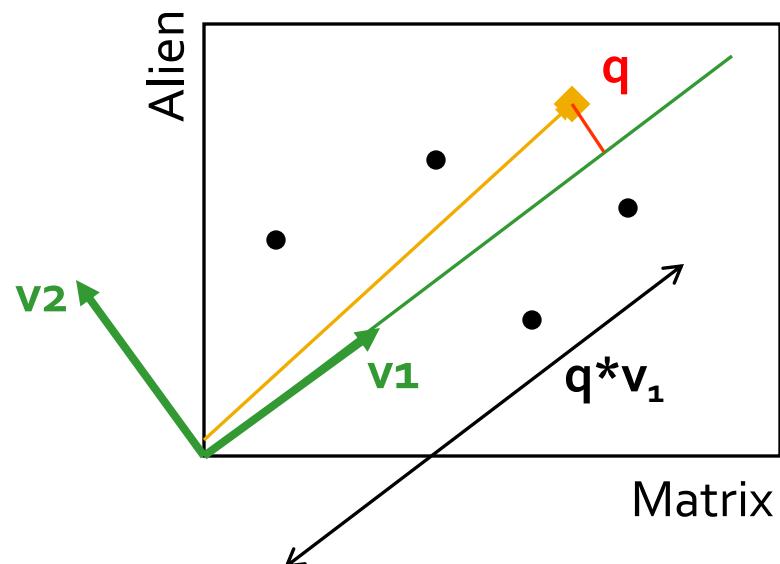


Case study: How to query?

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Project into concept space:
Inner product with each
'concept' vector v_i



Case study: How to query?

Compactly, we have:

$$q_{\text{concept}} = q \mathbf{V}$$

E.g.:

$$q = \begin{bmatrix} \text{Matrix} \\ \text{Alien} \\ \text{Serenity} \\ \text{Casablanca} \\ \text{Amelie} \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.12 \\ 0.59 & -0.02 \\ 0.56 & 0.12 \\ 0.09 & -0.69 \\ 0.09 & -0.69 \end{bmatrix}$$

movie-to-concept
factors (\mathbf{V})

SciFi-concept

$= \begin{bmatrix} 2.8 & 0.6 \end{bmatrix}$

Case study: How to query?

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

$$d_{\text{concept}} = d V$$

E.g.:

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

movie-to-concept factors (V)

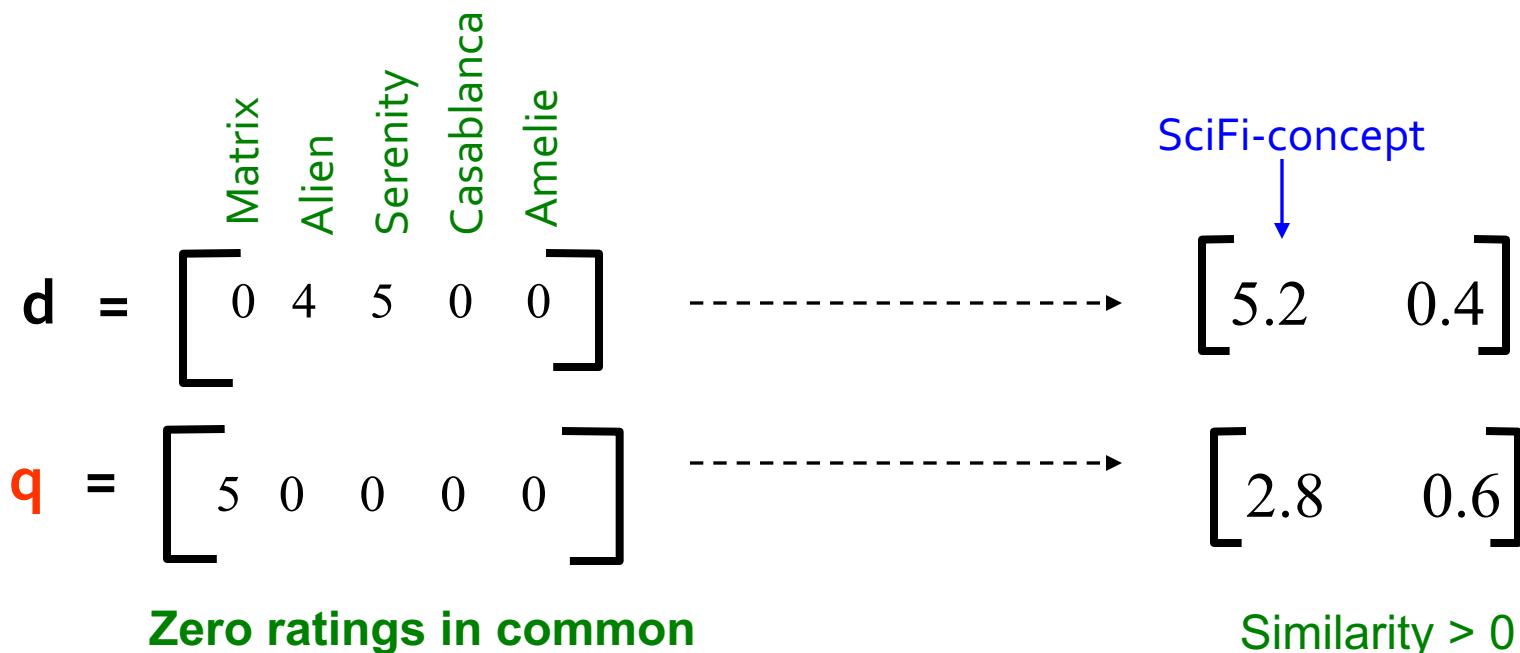
$$= \begin{bmatrix} 0.56 & 0.12 \\ 0.59 & -0.02 \\ 0.56 & 0.12 \\ 0.09 & -0.69 \\ 0.09 & -0.69 \end{bmatrix}$$

SciFi-concept

$$= \begin{bmatrix} 5.2 \\ 0.4 \end{bmatrix}$$

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!**



SVD: Drawbacks

- + **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!**

$$\begin{matrix} \bullet & \bullet \\ \bullet & \bullet \\ \bullet & \\ \bullet & \bullet \end{matrix} = \begin{matrix} \Sigma \\ U \end{matrix} \begin{matrix} V^T \\ \Sigma \end{matrix}$$

CUR Decomposition

Sparsity

- It is common for the matrix A that we wish to decompose to be very sparse
- But U and V from a SVD decomposition will **not** be sparse
- CUR decomposition solves this problem by using only (randomly chosen) rows and columns of A

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 :

$$\begin{pmatrix} & & \\ & A & \\ & & \end{pmatrix} \approx \begin{pmatrix} & & \\ & C & \\ & & \end{pmatrix} \cdot \begin{pmatrix} & \\ & U \\ & \end{pmatrix} \cdot \begin{pmatrix} & \\ & R \\ & \end{pmatrix}$$

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 :

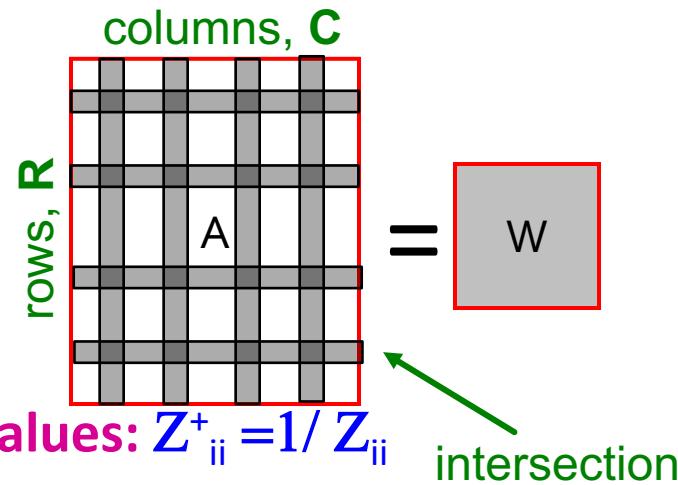
$$\begin{pmatrix} \text{Red row} \\ \text{Dark Brown row} \\ A \\ \text{Blue row} \end{pmatrix} \approx \begin{pmatrix} C \end{pmatrix} \cdot \begin{pmatrix} U \end{pmatrix} \cdot \begin{pmatrix} \text{Red row} \\ \text{Red row} \\ R \\ \text{Dark Brown row} \\ \text{Dark Brown row} \\ \text{Blue row} \end{pmatrix}$$

A C U R

Pseudo-inverse of
the intersection of C and R

Computing U

- Let \mathbf{W} be the “intersection” of sampled columns \mathbf{C} and rows \mathbf{R}
- Def:** \mathbf{W}^+ is the **pseudoinverse**
 - Let SVD of $\mathbf{W} = \mathbf{X} \mathbf{Z} \mathbf{Y}^T$
 - Then: $\mathbf{W}^+ = \mathbf{Y} \mathbf{Z}^+ \mathbf{X}^T$
 - \mathbf{Z}^+ : **reciprocals of non-zero singular values**: $Z_{ii}^+ = 1/Z_{ii}$
- Let: $\mathbf{U} = \mathbf{Y} (\mathbf{Z}^+)^2 \mathbf{X}^T$



Why the intersection? These are high magnitude numbers

Why pseudoinverse works?

$$\mathbf{W} = \mathbf{X} \mathbf{Z} \mathbf{Y}^T \text{ then } \mathbf{W}^{-1} = (\mathbf{Y}^T)^{-1} \mathbf{Z}^{-1} \mathbf{X}^{-1}$$

Due to orthonormality: $\mathbf{X}^{-1} = \mathbf{X}^T$, $\mathbf{Y}^{-1} = \mathbf{Y}^T$

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

Thus, if \mathbf{W} is nonsingular, pseudoinverse is the true inverse

Which Rows and Columns?

- To decrease the expected error between A and its decomposition, we must pick rows and columns in a nonuniform manner
- The **importance** of a row or column of A is the **square of its Frobenius norm**
 - That is, the sum of the squares of its elements.
- When picking rows and columns, the probabilities must be proportional to importance
- **Example:** [3,4,5] has importance 50, and [3,0,1] has importance 10, so pick the first 5 times as often as the second

CUR: Row Sampling Algorithm

■ Sampling columns (similarly for rows):

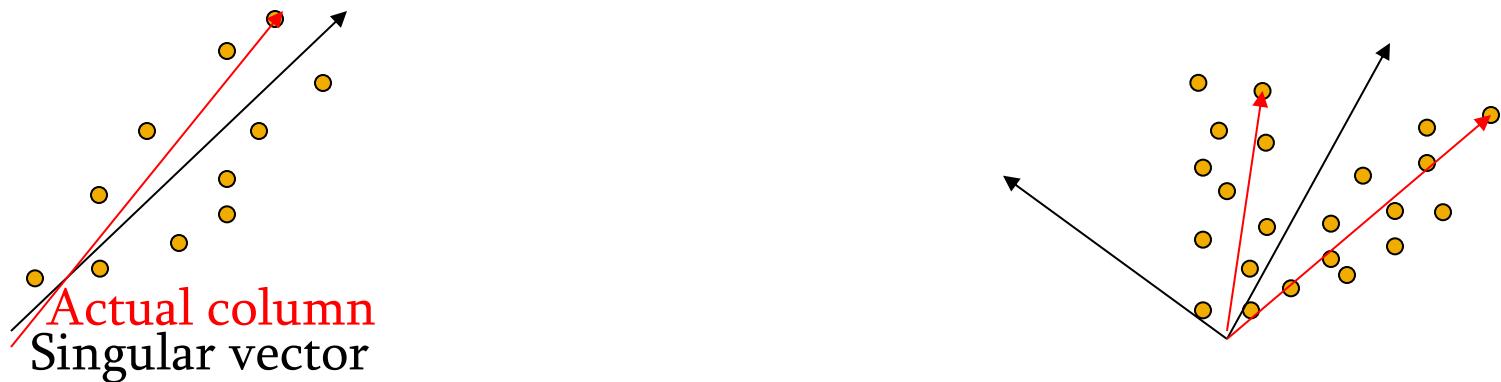
Input: matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, sample size c

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 $\mathbf{C}_d(:, i) = \mathbf{A}(:, j) / \sqrt{cP(j)}$

Note this is a randomized algorithm, same column can be sampled more than once

Intuition



- **Rough and imprecise intuition behind CUR**
 - CUR is more likely to pick points away from the origin
 - Assuming smooth data with no outliers these are the directions of maximum variation
- **Example:** Assume we have 2 clouds at an angle
 - SVD dimensions are orthogonal and thus will be in the middle of the two clouds
 - CUR will find the two clouds (but will be redundant)

CUR: Provably good approx. to SVD

- For example:

- Select $c = O\left(\frac{k \log k}{\varepsilon^2}\right)$ columns of A using **ColumnSelect algorithm** (slide 56)
- Select $r = O\left(\frac{k \log k}{\varepsilon^2}\right)$ rows of A using **RowSelect algorithm** (slide 56)
- Set $U = Y (Z^+)^2 X^T$
- Then: $\left| \left| A - CUR \right| \right|_F \stackrel{\text{CUR error}}{\leq} (2 + \varepsilon) \left| \left| A - A_K \right| \right|_F \stackrel{\text{SVD error}}{\leq}$
with probability 98%

In practice: Pick $4k$ cols/rows for a “rank-k” approximation

CUR: Pros & Cons

+ Easy interpretation

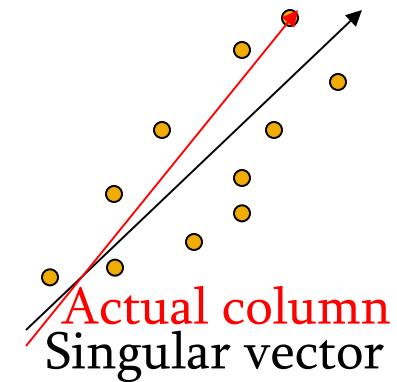
- Since the basis vectors are actual columns and rows

+ Sparse basis

- Since the basis vectors are actual columns and rows

- Duplicate columns and rows

- Columns of large norms will be sampled many times



SVD vs. CUR

$$\text{SVD: } A = U \Sigma V^T$$

Huge but sparse

sparse and small

Big and dense

$$\text{CUR: } A = C U R$$

Huge but sparse

Big but sparse

dense but small

SVD vs. CUR: Simple Experiment

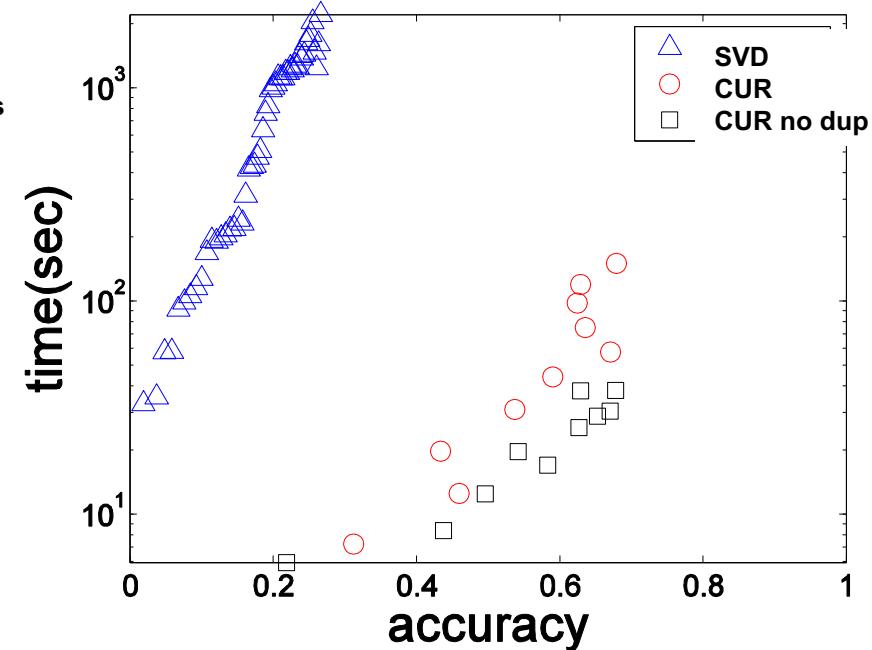
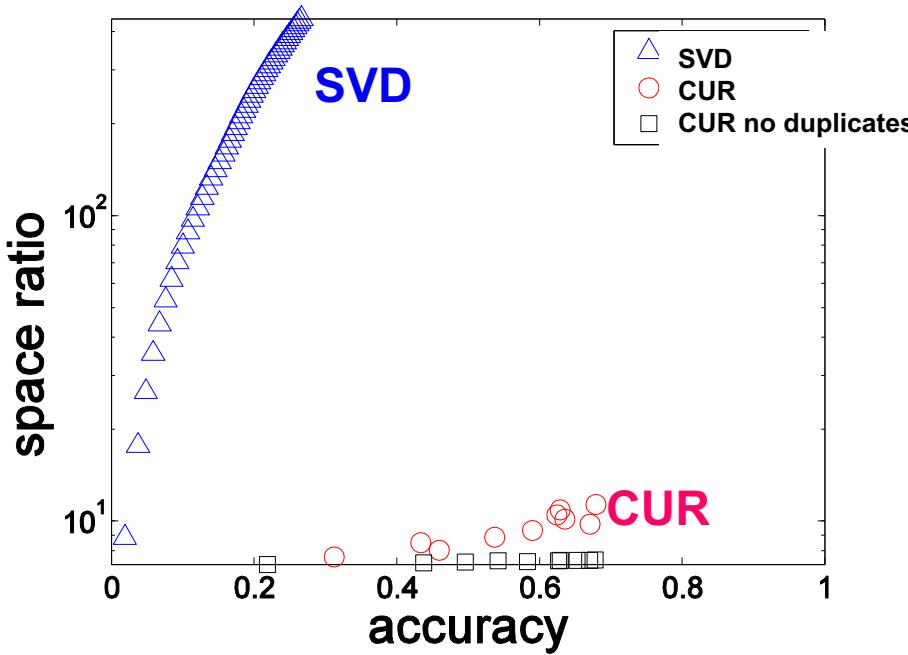
- **DBLP bibliographic data**

- 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:**
 - #output matrix entries / #input matrix entries
- **CPU time**

Sun, Faloutsos: *Less is More: Compact Matrix Decomposition for Large Sparse Graphs*, SDM '07.