Dimensionality Reduction: SVD & CUR

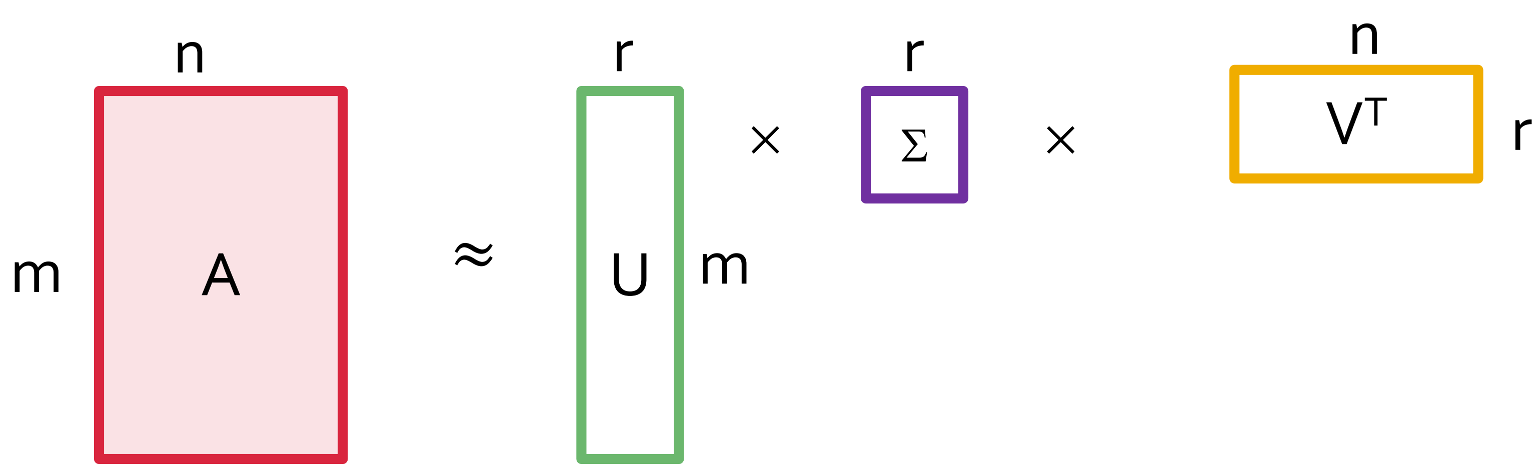
CS547 Machine Learning for Big Data

Tim Althoff

PAUL G. ALLEN SCHOOL
OF COMPUTER SCIENCE & ENGINEERING

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



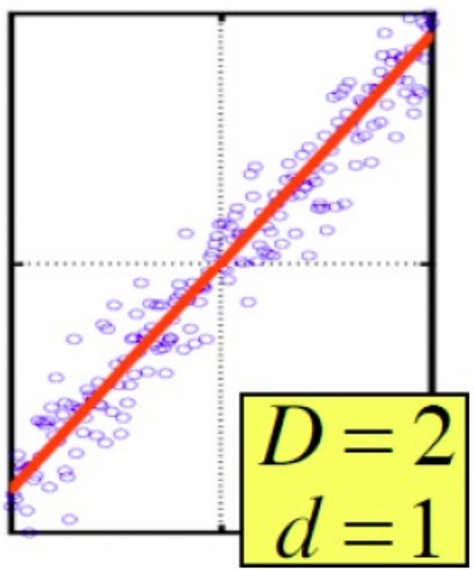
Dimensionality Reduction

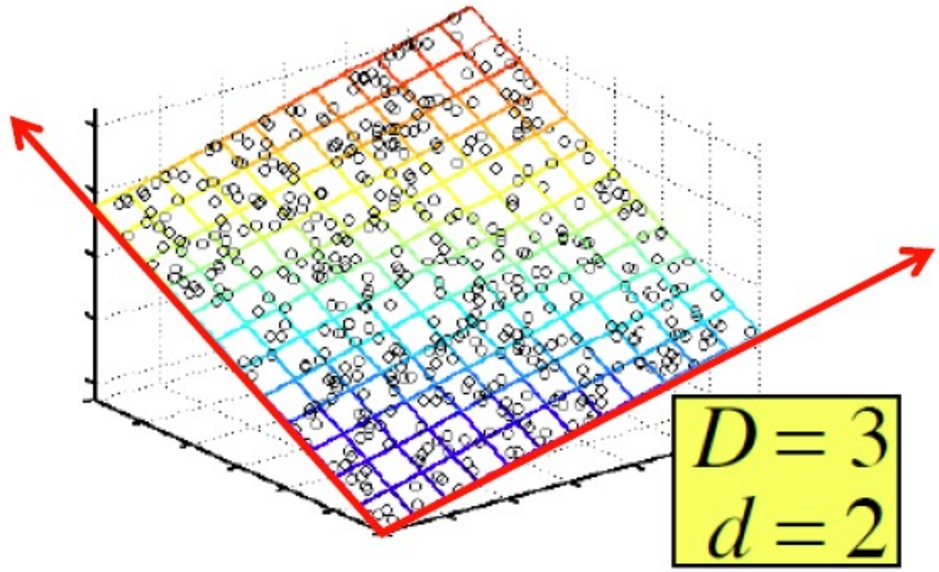
- **Compress / reduce dimensionality:**
  - 10^6 rows; 10^3 columns; no updates
  - Random access to any cell(s); **small error: OK**

day / customer	We 7/10/96	Th 7/11/96	Fr 7/12/96	Sa 7/13/96	Su 7/14/96	New representation
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



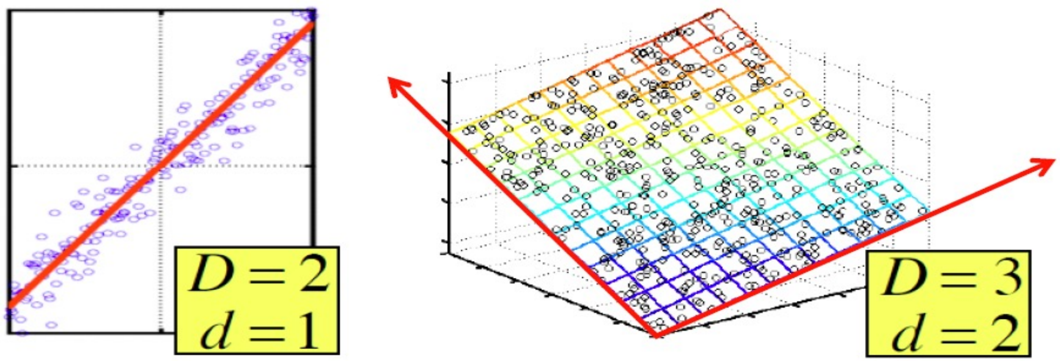


There are hidden, or **latent factors, latent dimensions** that – to a close approximation – explain why the values are as they appear in the data matrix

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 remaining variance is very low

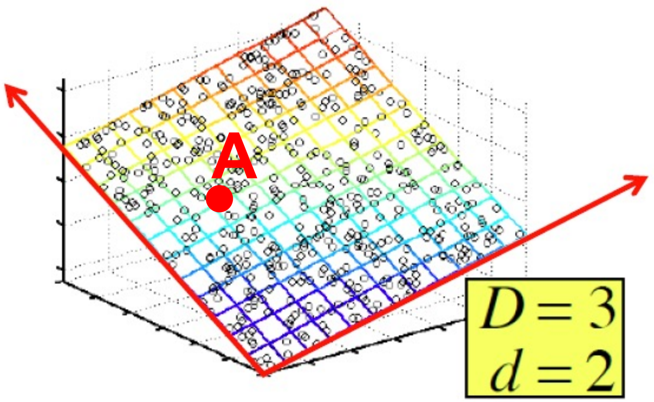


Rank is "Dimensionality"

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

1 row per point:

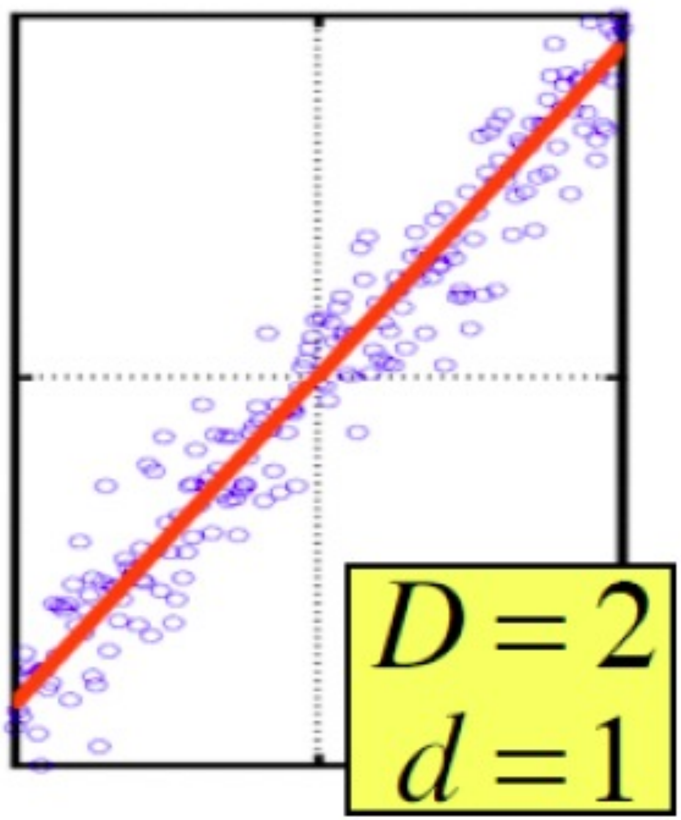
$$\begin{array}{c l} \begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix} & \begin{array}{l} \text{A} \\ \text{B} \\ \text{C} \end{array} \end{array}$$



- **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!**



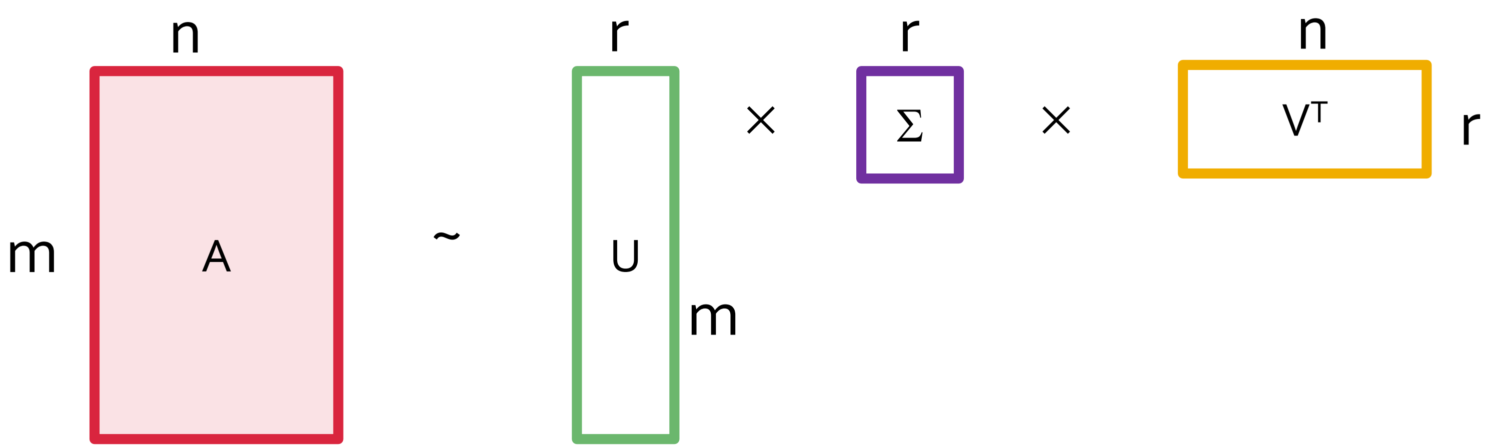
Rather than representing every point with 2 coordinates we represent each point with 1 coordinate (corresponding to the position of the point on the red line).

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

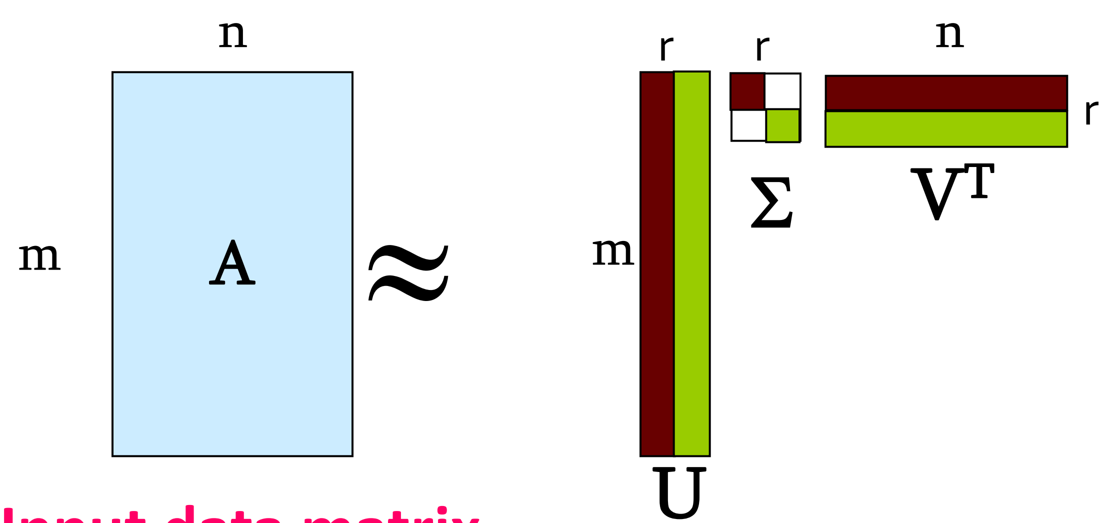
- **Gives a decomposition of any matrix into a product of three matrices:**



- 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

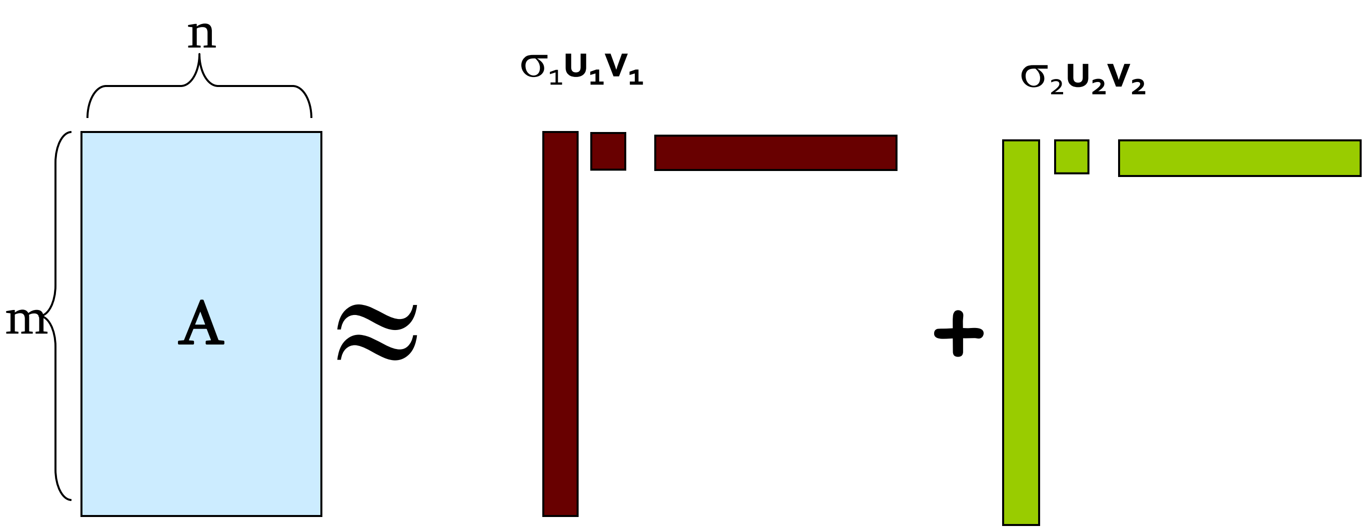
$$\mathbf{A} \approx \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T = \sum_i \sigma_i \mathbf{u}_i \circ \mathbf{v}_i^{\mathsf{T}}$$



- **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)

SVD

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



σ_i … scalar
u_i … vector
v_i … vector

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

SVD – Properties

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

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

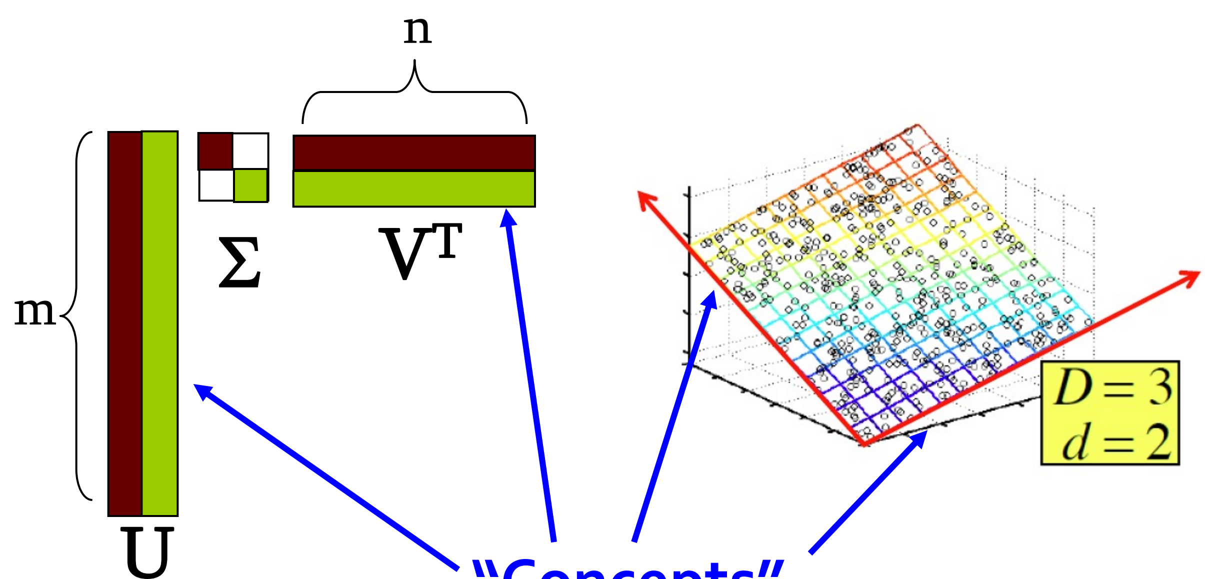
* Up to permutations for redundant singular values and orientation of singular vectors (details)

SVD – Example: Users-to-Movies

- **Consider a matrix. What does SVD do?**

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

=



"Concepts"
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		
	3	3	3		
	4	4	4		
	5	5	5		
Romance		2		4	4
				5	5
		1		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

x

12		
	9.5	
		1.3

x

0.56	0.59	0.56	0.09	0.09
0.12	-0.02	0.12	-0.69	-0.69
0.4	-0.8	0.4	0.09	0.09

SVD – Example: Users-to-Movies

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

SciFi-concept

Romance-concept

$$
\begin{array}{c|ccccc|}
 & \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \\
\hline
\text{SciFi} & 1 & 1 & 1 & & \\
 & 3 & 3 & 3 & & \\
 & 4 & 4 & 4 & & \\
 & 5 & 5 & 5 & & \\
\text{Romance} & & 2 & & 4 & 4 \\
 & & & & 5 & 5 \\
 & & 1 & & 2 & 2 \\
\hline
\end{array}
=
\begin{array}{|ccc|}
\hline
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
0.68 & 0.11 & -0.05 \\
0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32 \\
\hline
\end{array}
\times
\begin{array}{|ccc|}
\hline
12 & & \\
 & 9.5 & \\
 & & 1.3 \\
\hline
\end{array}
\times
\begin{array}{|ccccc|}
\hline
0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
0.4 & -0.8 & 0.4 & 0.09 & 0.09 \\
\hline
\end{array}
$$

SVD – Example: Users-to-Movies

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

U is "user-to-concept" factor matrix

SciFi-concept

Romance-concept

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

$$
= \begin{bmatrix} 0.13 & 0.02 & -0.01 \\ 0.41 & 0.07 & -0.03 \\ 0.55 & 0.09 & -0.04 \\ 0.68 & 0.11 & -0.05 \\ 0.15 & -0.59 & 0.65 \\ 0.07 & -0.73 & -0.67 \\ 0.07 & -0.29 & 0.32 \end{bmatrix}
\times
\begin{bmatrix} 12 & & \\ & 9.5 & \\ & & 1.3 \end{bmatrix}
\times
\begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\ 0.4 & -0.8 & 0.4 & 0.09 & 0.09 \end{bmatrix}
$$

SVD – Example: Users-to-Movies

- **A = U Σ V^T - example:**

SciFi-concept

“strength” of the SciFi-concept

A:

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

=

U:

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

x

Σ:

12		
	9.5	
		1.3

x

V^T:

0.56	0.59	0.56	0.09	0.09
0.12	-0.02	0.12	-0.69	-0.69
0.4	-0.8	0.4	0.09	0.09

SVD – Example: Users-to-Movies

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

V is "movie-to-concept" factor matrix

SciFi-concept

SciFi-concept

$$
\begin{array}{c}
\\
\text{SciFi} \\ \\ \\ \\
\text{Romance} \\ \\ \\
\end{array}
\begin{array}{ccccc}
\text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \\
1 & 1 & 1 & & \\
3 & 3 & 3 & & \\
4 & 4 & 4 & & \\
5 & 5 & 5 & & \\
 & 2 & & 4 & 4 \\
 & & & 5 & 5 \\
 & 1 & & 2 & 2
\end{array}
=
\begin{bmatrix}
\boxed{0.13} & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
0.68 & 0.11 & -0.05 \\
0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32
\end{bmatrix}
\times
\begin{bmatrix}
12 & & \\
 & 9.5 & \\
 & & 1.3
\end{bmatrix}
\times
\begin{bmatrix}
0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
0.4 & -0.8 & 0.4 & 0.09 & 0.09
\end{bmatrix}
$$

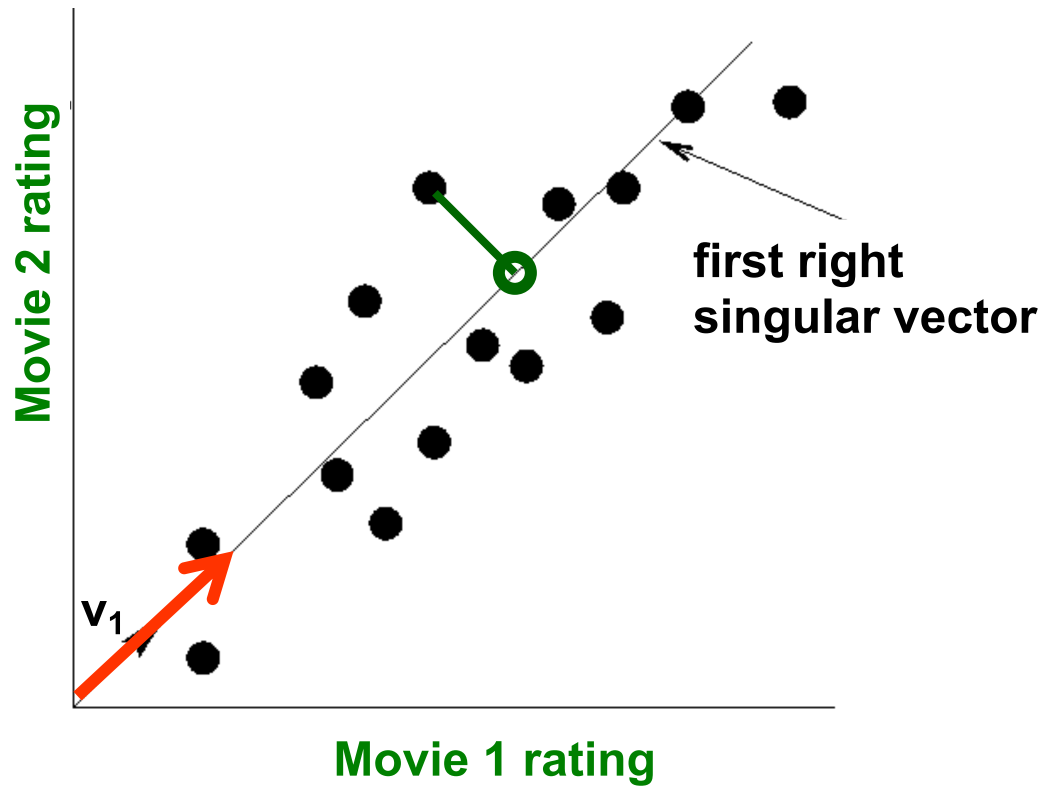
SVD – Interpretation #1

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

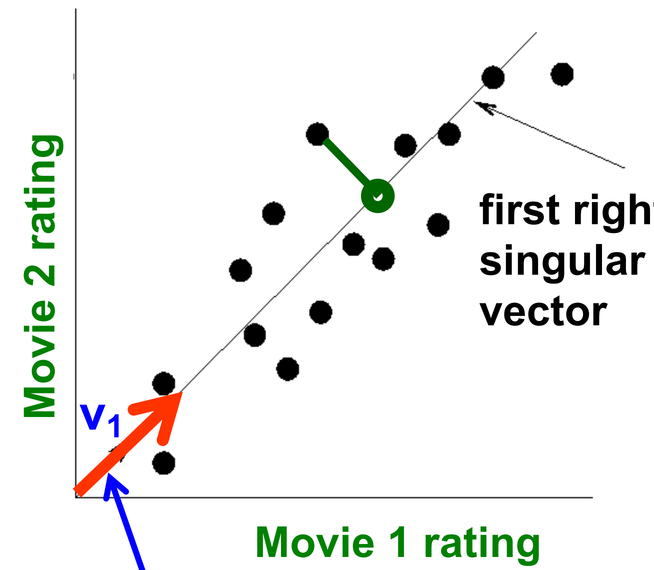
SVD – Dimensionality Reduction



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

SVD – Dimensionality Reduction

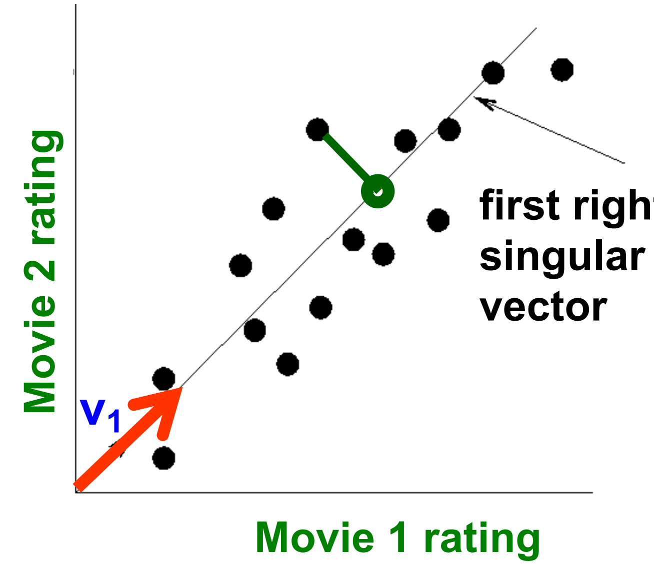
- **$A = U \Sigma V^T$ - example:**
  - **V**: “movie-to-concept” matrix
  - **U**: “user-to-concept” matrix



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

SVD – Dimensionality Reduction

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



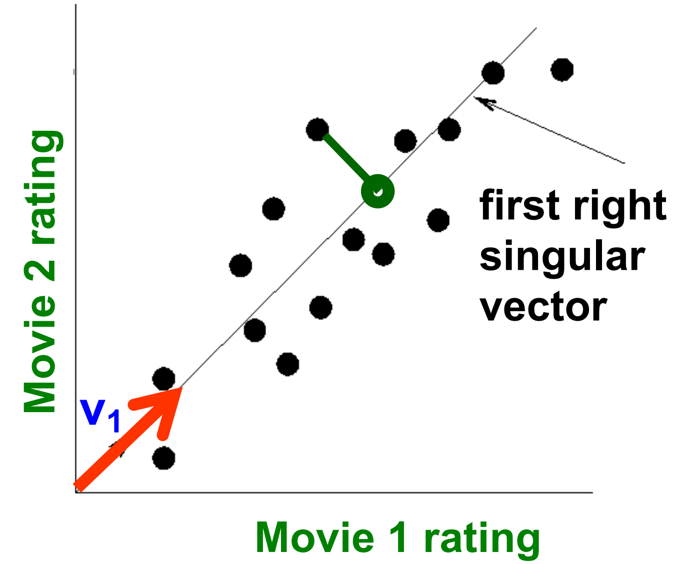
variance ('spread') on the v_1 axis

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

SVD – Dimensionality Reduction

$A = U \Sigma V^T$ - 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

$U \Sigma$:

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

SVD – Interpretation #2

More details

- Q: **How is dim. reduction done?**

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

SVD – Interpretation #2

More details

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

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

SVD – Interpretation #2

More details

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

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

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

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

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

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

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

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

Reconstructed data matrix B

Reconstruction Error is quantified by the Frobenius norm:

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

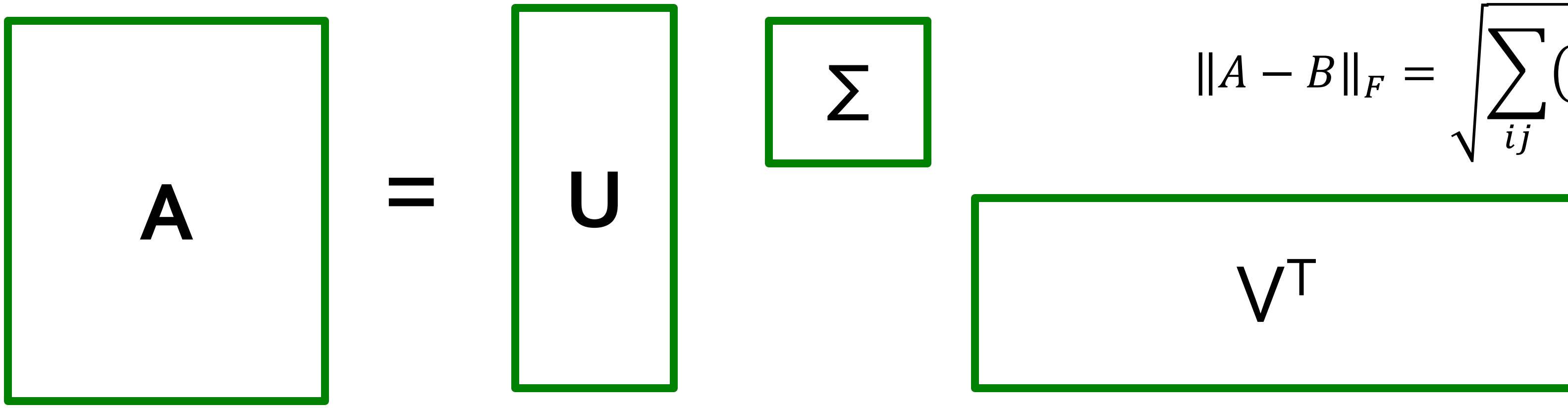
$$\|A-B\|_F = \sqrt{\Sigma_{ij} (A_{ij}-B_{ij})^2}$$

is "small"

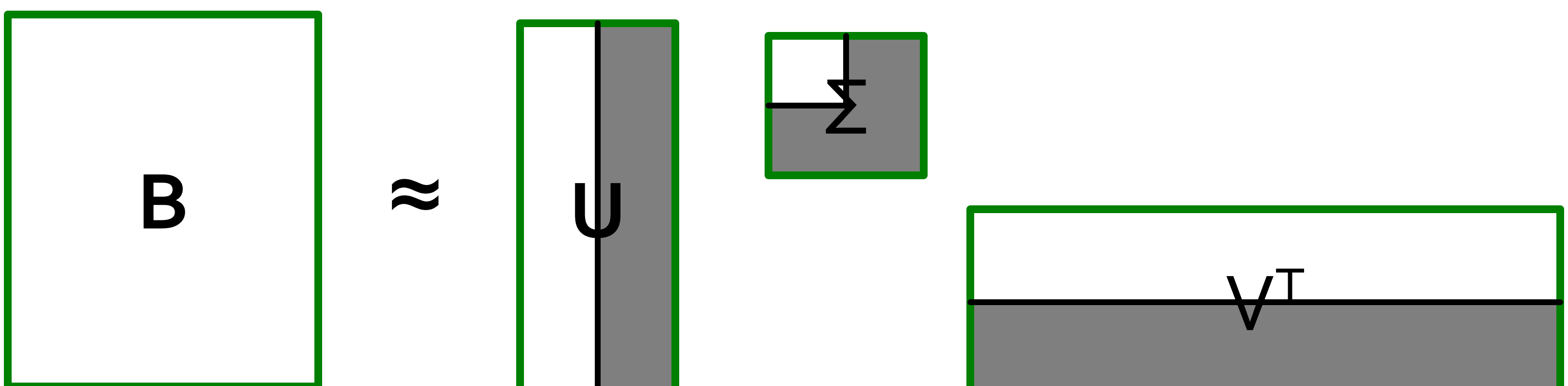
SVD – Best Low Rank Approx.

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

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



B is best approximation of A:



SVD – Conclusions so far

- SVD: **A= U Σ 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?**
- 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" $\boldsymbol{x}_0$
  - Construct $\boldsymbol{x}_{k+1} = \frac{M\boldsymbol{x}_k}{||M\boldsymbol{x}_k||}$ for $k = 0, 1, \ldots$
    - || … || denotes the Frobenius norm
  - Stop when consecutive $\boldsymbol{x}_k$ show little change

Example: Iterative Eigenvector

$$M = \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix} \quad \mathbf{x}_0 = \begin{matrix} 1 \\ 1 \end{matrix}$$

$$\frac{M\mathbf{x}_0}{||M\mathbf{x}_0||} = \begin{bmatrix} 3 \\ 5 \end{bmatrix} / \sqrt{34} = \begin{bmatrix} 0.51 \\ 0.86 \end{bmatrix} = \mathbf{x}_1$$

$$\frac{M\mathbf{x}_1}{||M\mathbf{x}_1||} = \begin{bmatrix} 2.23 \\ 3.60 \end{bmatrix} / \sqrt{17.93} = \begin{bmatrix} 0.53 \\ 0.85 \end{bmatrix} = \mathbf{x}_2$$

…..

Finding the Principal Eigenvalue

- Once you have the principal eigenvector $\boldsymbol{x}$, you find its eigenvalue λ by $\lambda = \boldsymbol{x}^T M \boldsymbol{x}$.
  - In proof: We know $\boldsymbol{x}\lambda = M\boldsymbol{x}$ if λ is the eigenvalue; multiply both sides by $\boldsymbol{x}^T$ on the left.
  - Since $\boldsymbol{x}^T\boldsymbol{x} = 1$ we have $\lambda = \boldsymbol{x}^T M \boldsymbol{x}$

- **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 $\boldsymbol{x}$:

$$M^{*} := M - \lambda\, x\, x^{T}$$

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

- **Example:**

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

How to Compute the SVD

- **Start by supposing** $\boldsymbol{A = U\Sigma V^T}$
- $A^T = (U\Sigma V^T)^T = (V^T)^T\Sigma^T U^T = V\Sigma U^T$
  - **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
- $\boldsymbol{A^T A = V\Sigma U^T U\Sigma V^T = V\Sigma^2 V^T}$
  - **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
- $\boldsymbol{A^T A V = V\Sigma^2 V^T V = V\Sigma^2}$
  - **Why?** V is also orthonormal

Computing the SVD –(2)

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

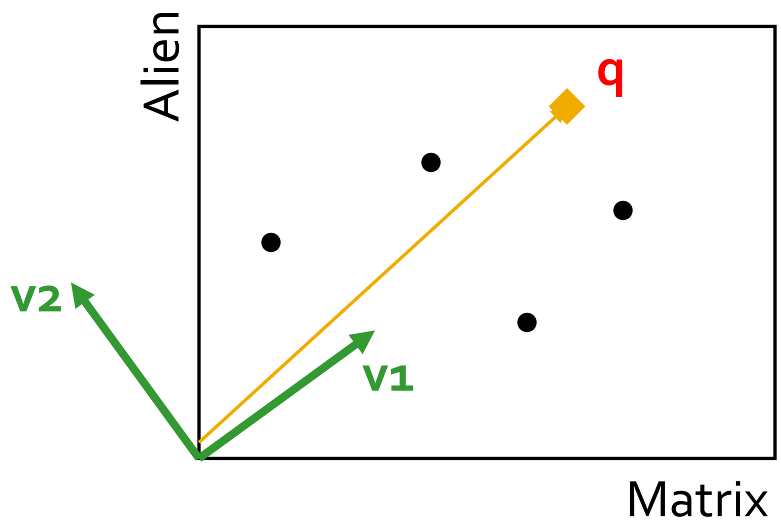
- **Q: Find users that like 'Matrix'**
- **A: Map query into a 'concept space' – how?**

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

Case study: How to query?

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

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



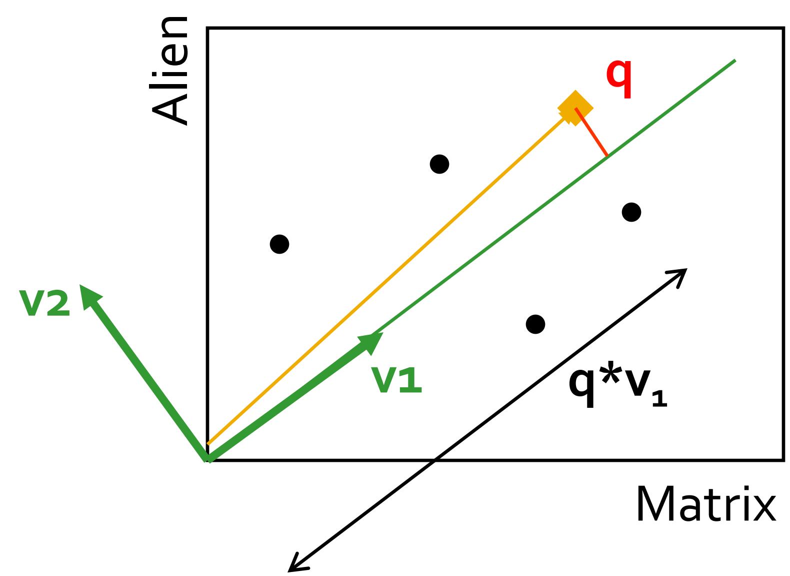
Project into concept space:
Inner product with each 'concept' vector $\mathbf{v}_i$

Case study: How to query?

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

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

Project into concept space:
Inner product with each 'concept' vector $\mathbf{v_i}$



Case study: How to query?

Compactly, we have:

$q_{concept} = q\ V$

E.g.:

$$
q = \begin{array}{c} \begin{array}{ccccc} \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \end{array} \\ \begin{bmatrix} 5 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array} \times \underbrace{\begin{bmatrix} 0.56 & 0.12 \\ 0.59 & -0.02 \\ 0.56 & 0.12 \\ 0.09 & -0.69 \\ 0.09 & -0.69 \end{bmatrix}}_{\text{movie-to-concept factors (V)}} = \begin{array}{c} \text{SciFi-concept} \\ \begin{bmatrix} 2.8 & 0.6 \end{bmatrix} \end{array}
$$

Case study: How to query?

- **How would the user *d* that rated ('Alien', 'Serenity') be handled?**
  $\mathbf{d_{concept} = d\ V}$

E.g.:

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

movie-to-concept factors (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**!

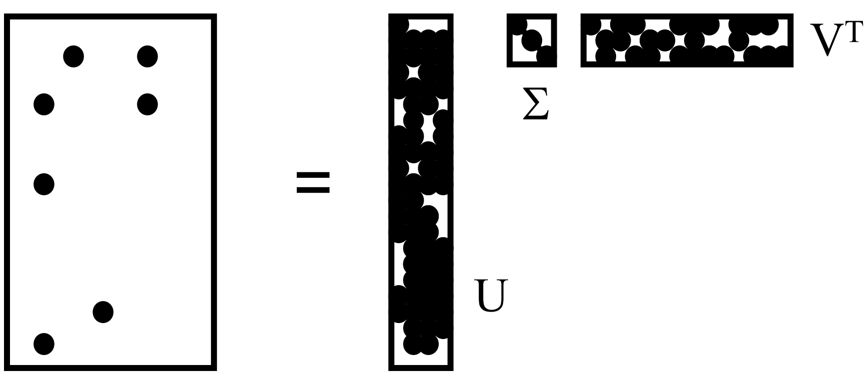
$$
\begin{array}{cc}
 & \begin{array}{ccccc} \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \end{array} \\
\mathbf{d} = & \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \end{bmatrix} \\
\mathbf{q} = & \begin{bmatrix} 5 & 0 & 0 & 0 & 0 \end{bmatrix}
\end{array}
\quad
\begin{array}{c}
\\
\dashrightarrow \\
\dashrightarrow
\end{array}
\quad
\begin{array}{c}
\begin{array}{cc} \text{SciFi-concept} & \end{array} \\
\begin{bmatrix} 5.2 & 0.4 \end{bmatrix} \\
\begin{bmatrix} 2.8 & 0.6 \end{bmatrix}
\end{array}
$$

Zero ratings in common

Similarity > 0

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!**



CUR Decomposition

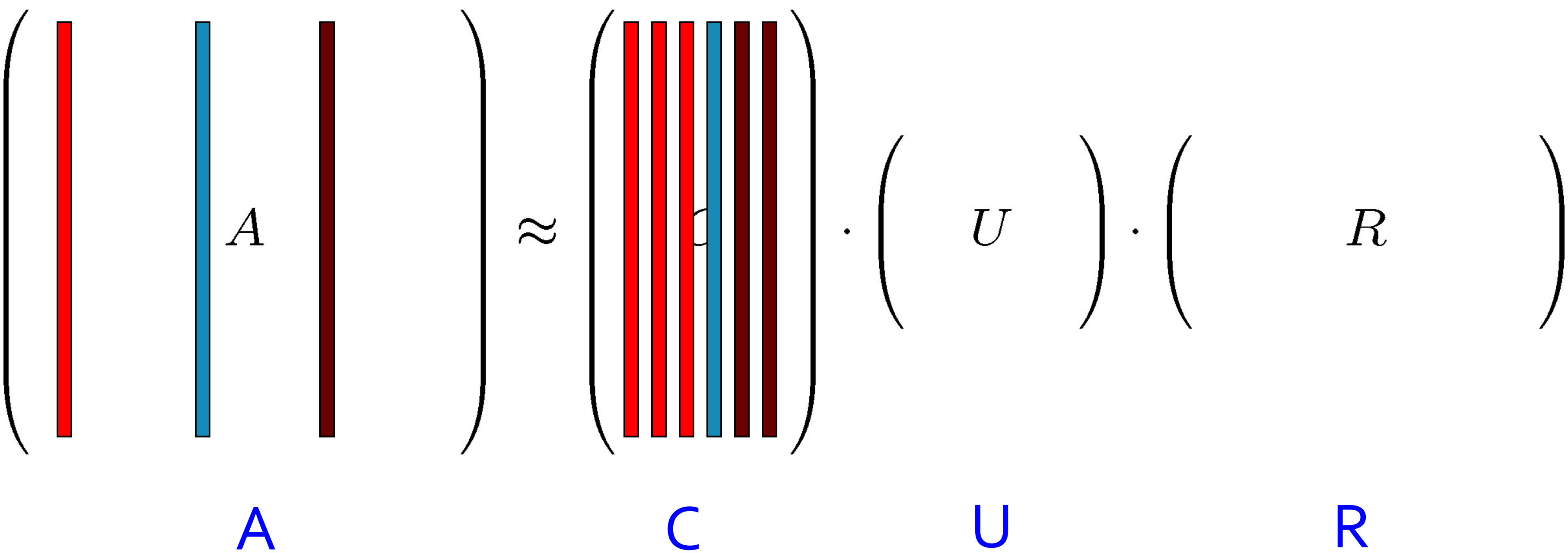
Sparsity

- 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:
$\|X\|_F = \sqrt{\Sigma_{ij} X_{ij}^2}$

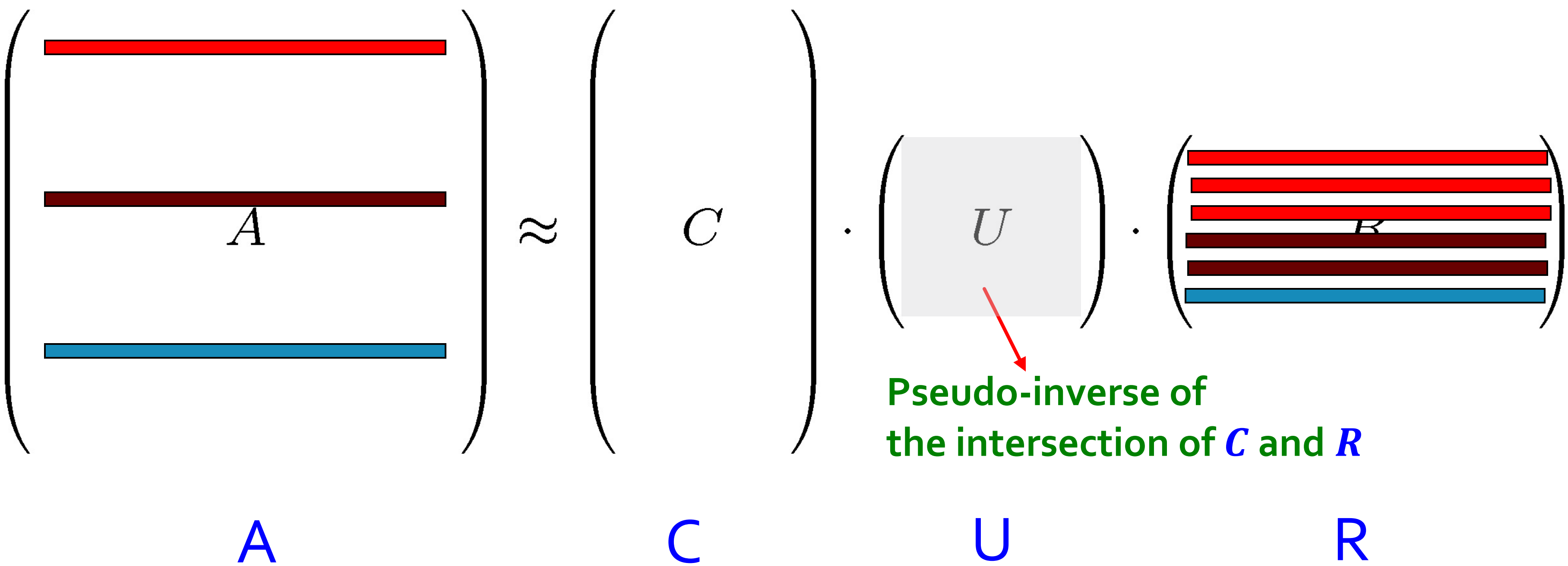
- **Goal: Express A as a product of matrices C, U, R**
  Make $\|A - C \cdot U \cdot R\|_F$ small
- **"Constraints" on C and R:**



CUR Decomposition

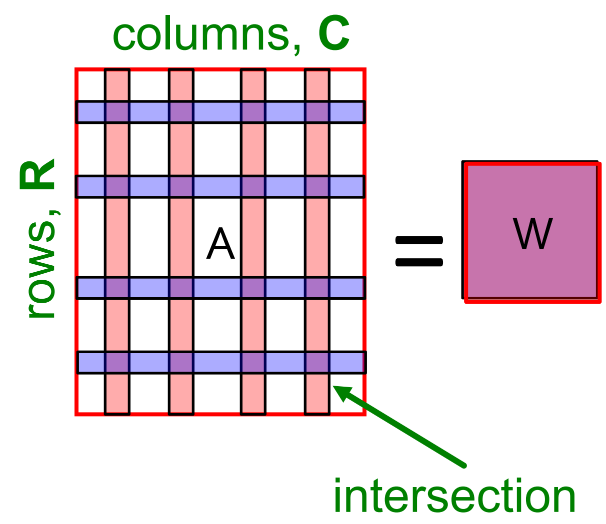
Frobenius norm:
$\|X\|_F = \sqrt{\Sigma_{ij} X_{ij}^2}$

- **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:**



Computing U

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



Why the intersection? These are high magnitude numbers

Why pseudoinverse works?

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

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

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

Thus, if **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 non-uniform 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):**

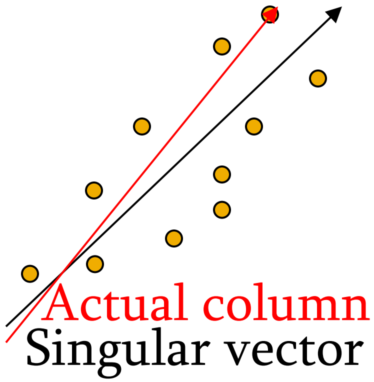
Input: matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, sample size c

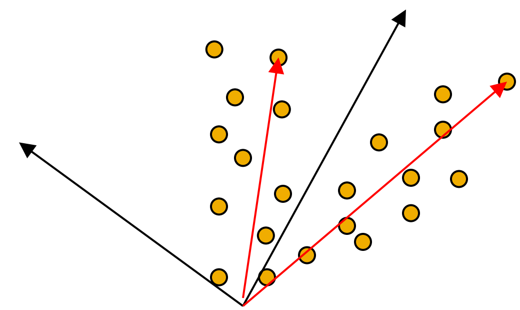
Output: $\mathbf{C}_d \in \mathbb{R}^{m \times c}$

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)

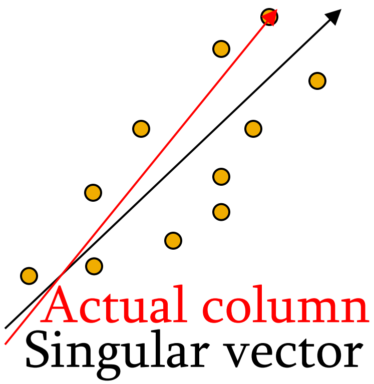
CUR: Provably good approx. to SVD

- **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** $U = W^+$
- **Then:** $\underbrace{\left\|A - CUR\right\|_F}_{\text{CUR error}} \leq (2+\varepsilon)\underbrace{\left\|A - A_K\right\|_F}_{\text{SVD error}}$
  with probability 98%

In practice:
Pick 4*k* 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

sparse and small

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

Huge but sparse   Big and dense

dense but small

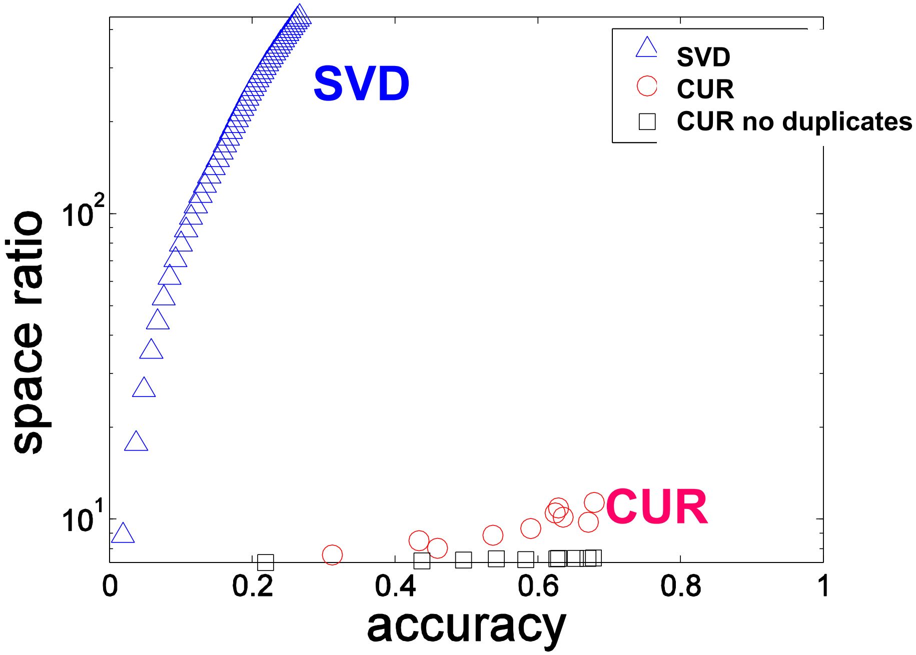
$$\text{CUR:} \quad A \approx C\, U\, R$$

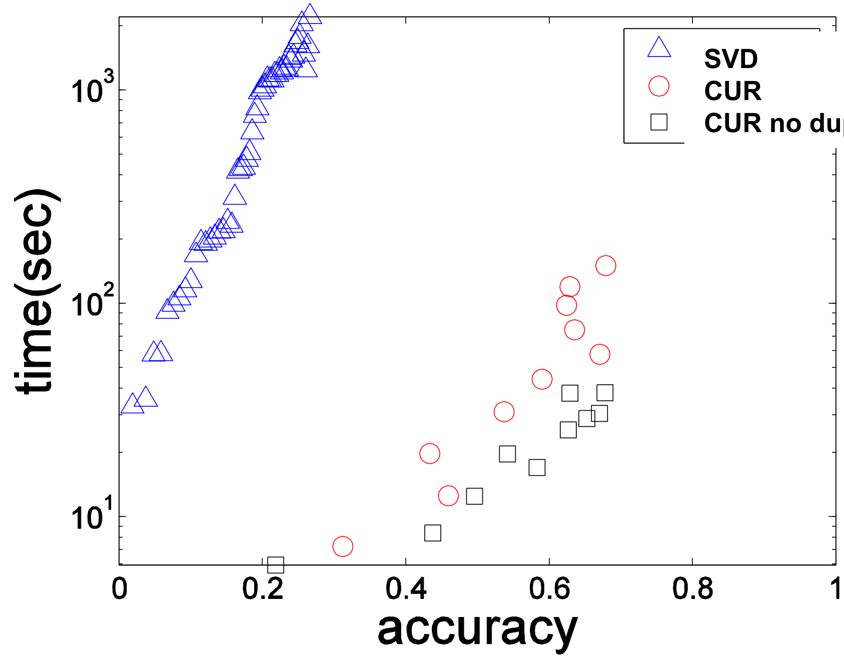
Huge but sparse   Big but sparse

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.