Dimensionality Reduction: SVD & CUR

CS246: Mining Massive Datasets
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http://cs246.stanford.edu

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
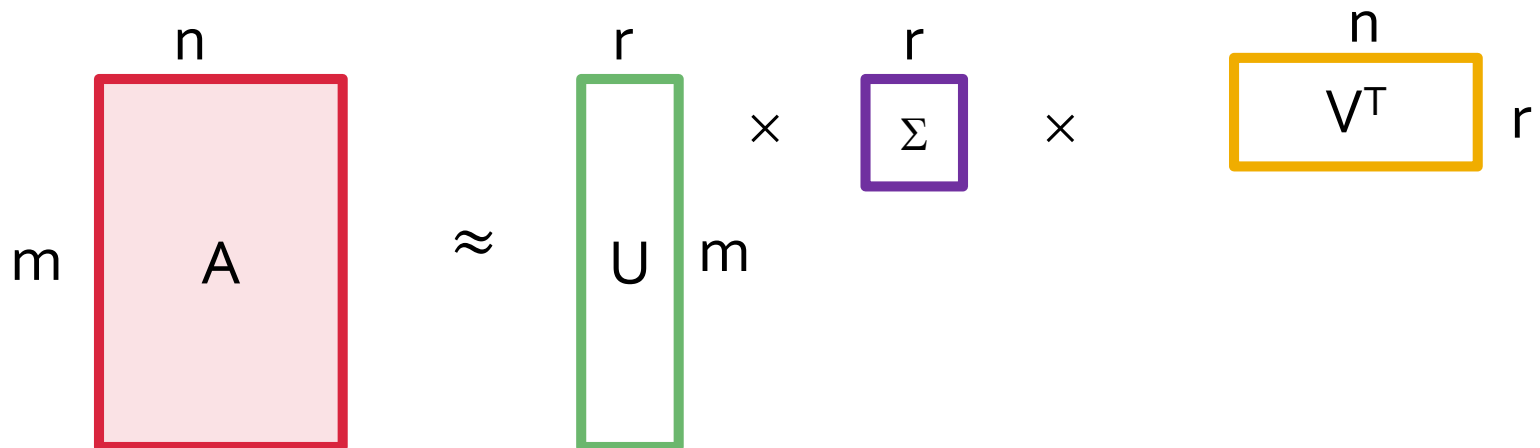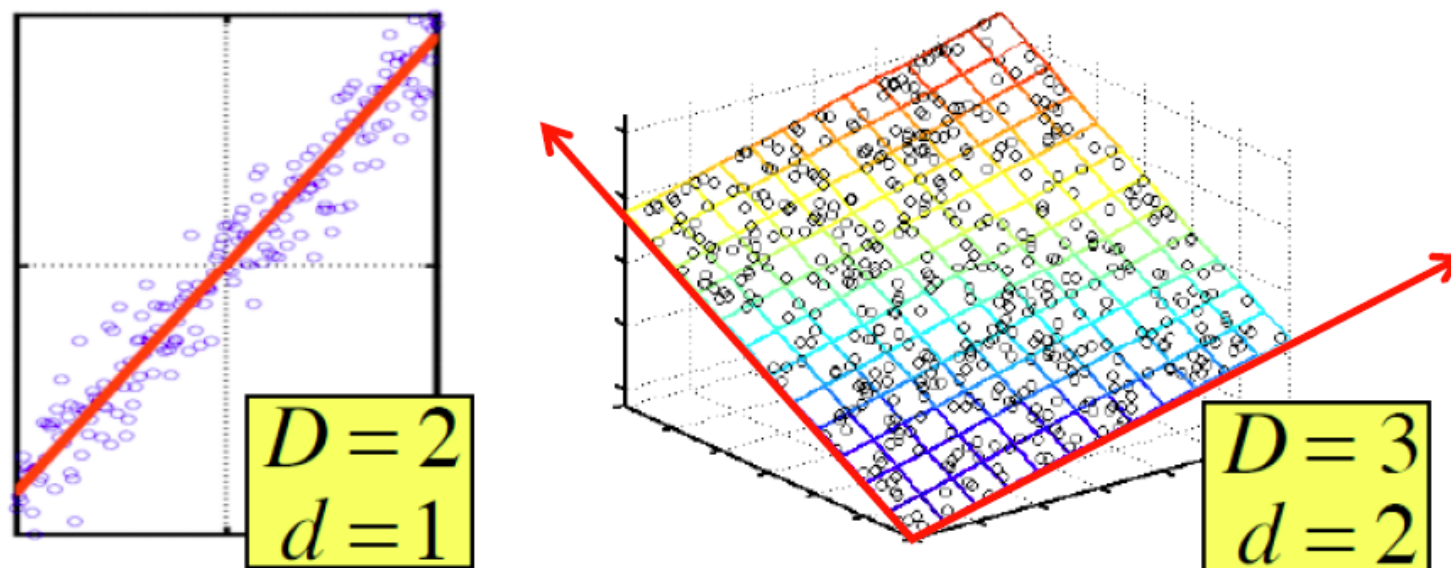
Dimensionality Reduction

- **Compress / reduce dimensionality:**

  - 10^6 rows; 10^3 columns; no updates

  - Random access to any cell(s); **small error: OK**

day customer	Wc 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

$$D = 2$$
$$d = 1$$

$$D = 3$$
$$d = 2$$

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
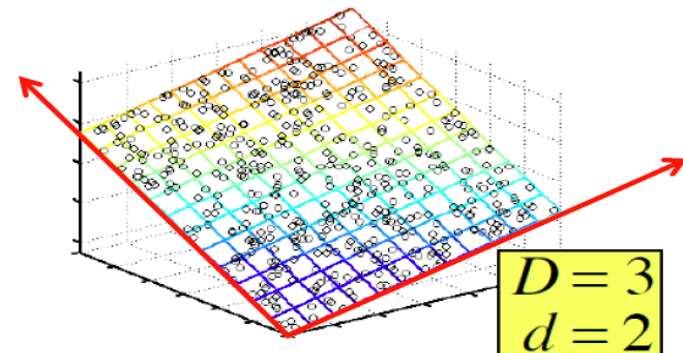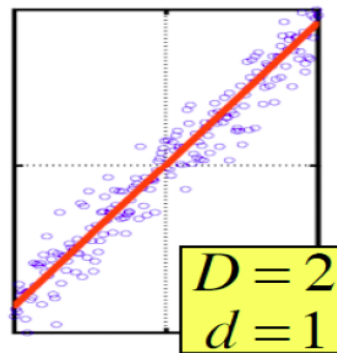
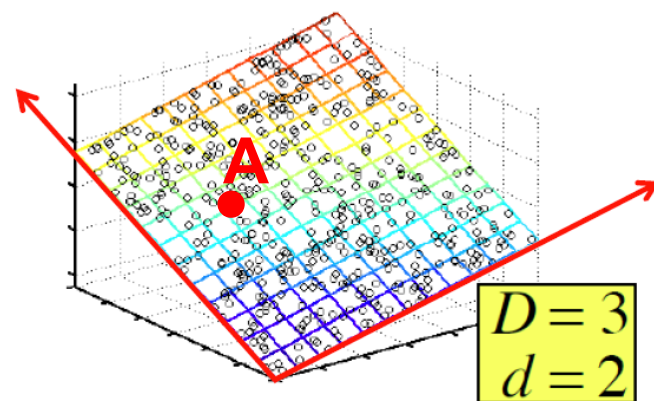# Rank is "Dimensionality"

- **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:

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

    $D = 3$
    $d = 2$

- **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!**

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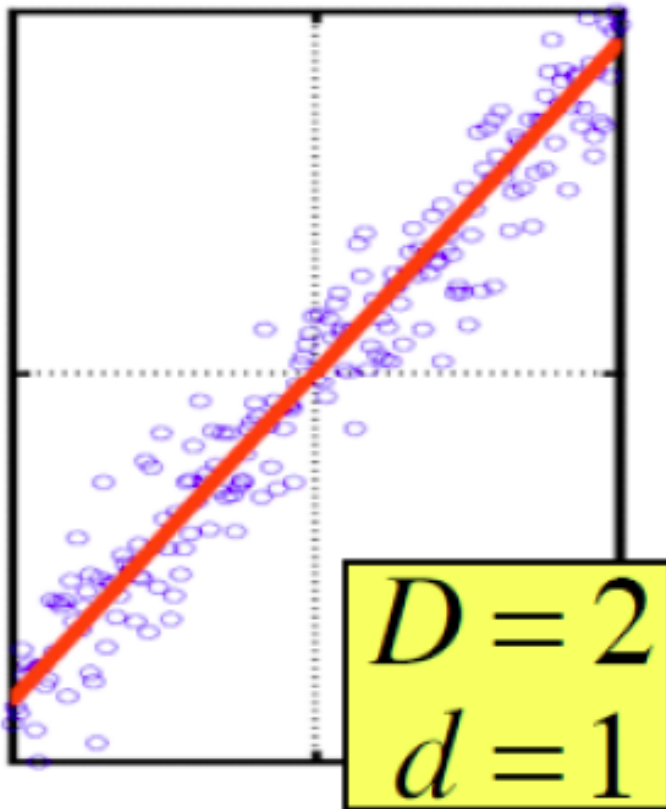
Rather than representing every point with 2 coordinates we represent each point with 1 coordinate (corresponding to the position of the point on the red line).

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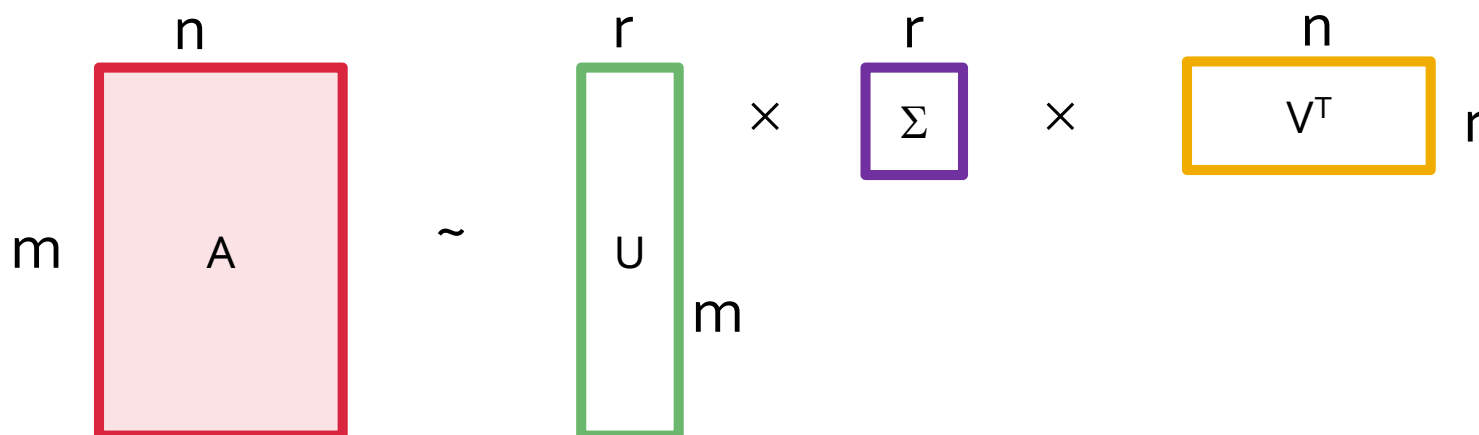
- There are strong constraints on the form of each of these matrices
    - Results in a unique decomposition
- From this decomposition, you can choose any number r of intermediate concepts (latent factors) in a way that minimizes the reconstruction error

SVD – Definition

$$\mathbf{A} \approx \mathbf{U\Sigma V}^T = \sum_i \sigma_i \mathbf{u}_i \circ \mathbf{v}_i^{\mathsf{T}}$$
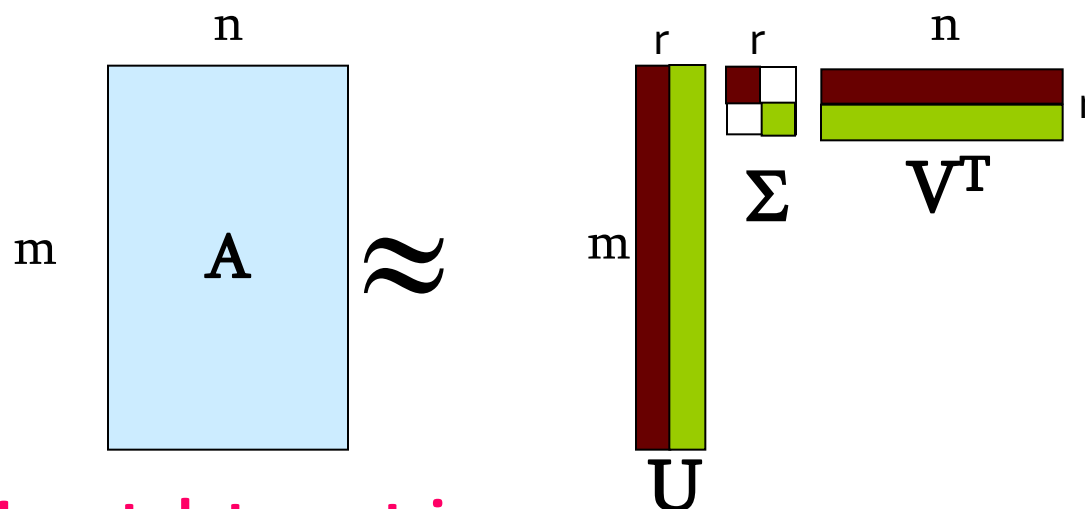
- **A**: **Input data matrix**
  - m x n matrix (e.g., m documents, n terms)
- **U**: **Left singular vectors**
  - m x r matrix (m documents, r concepts)
- Σ: **Singular values**
  - r x r diagonal matrix (strength of each 'concept')
    (r : rank of the matrix **A**)
- **V**: **Right singular vectors**
  - n x r matrix (n terms, r concepts)

SVD

$$\mathbf{A} \approx \mathbf{U\Sigma V}^T = \sum_i \sigma_i \mathbf{u}_i \circ \mathbf{v}_i^\mathsf{T}$$
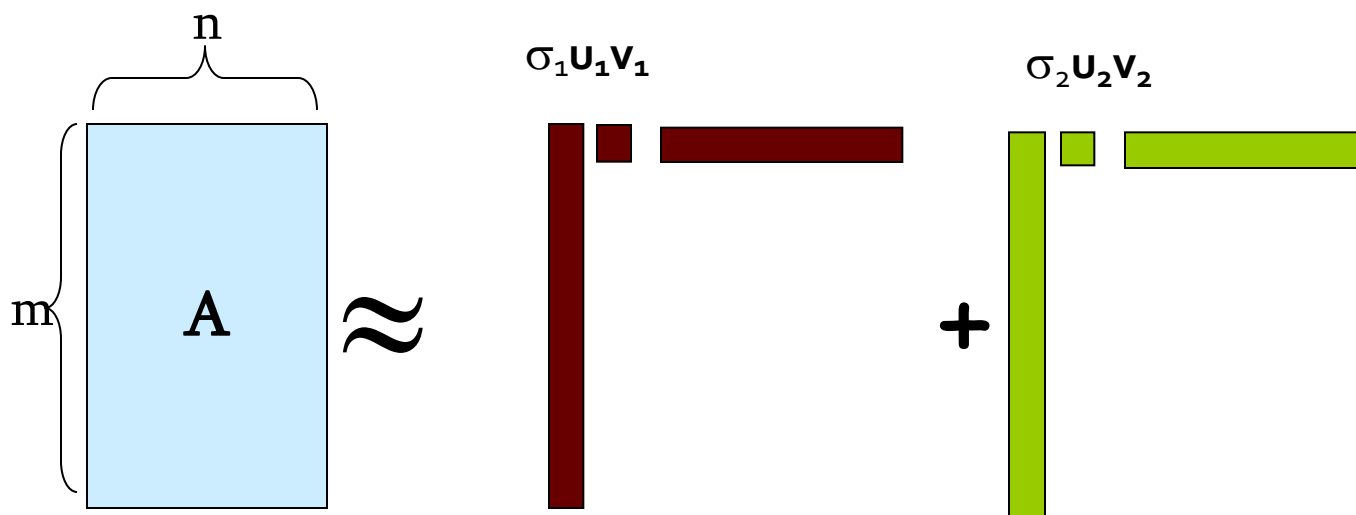
If we set $\sigma_2 = 0$, then the green columns may as well not exist.

σ_i … scalar
u_i … vector
v_i … vector

SVD – Properties

It is **always** possible to decompose a real matrix 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 non-negative, and sorted in decreasing order ($\sigma_1 \geq \sigma_2 \geq ... \geq 0$)

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

- **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.

"Concepts"
AKA Latent dimensions
AKA Latent factors

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

$D = 3$
$d = 2$
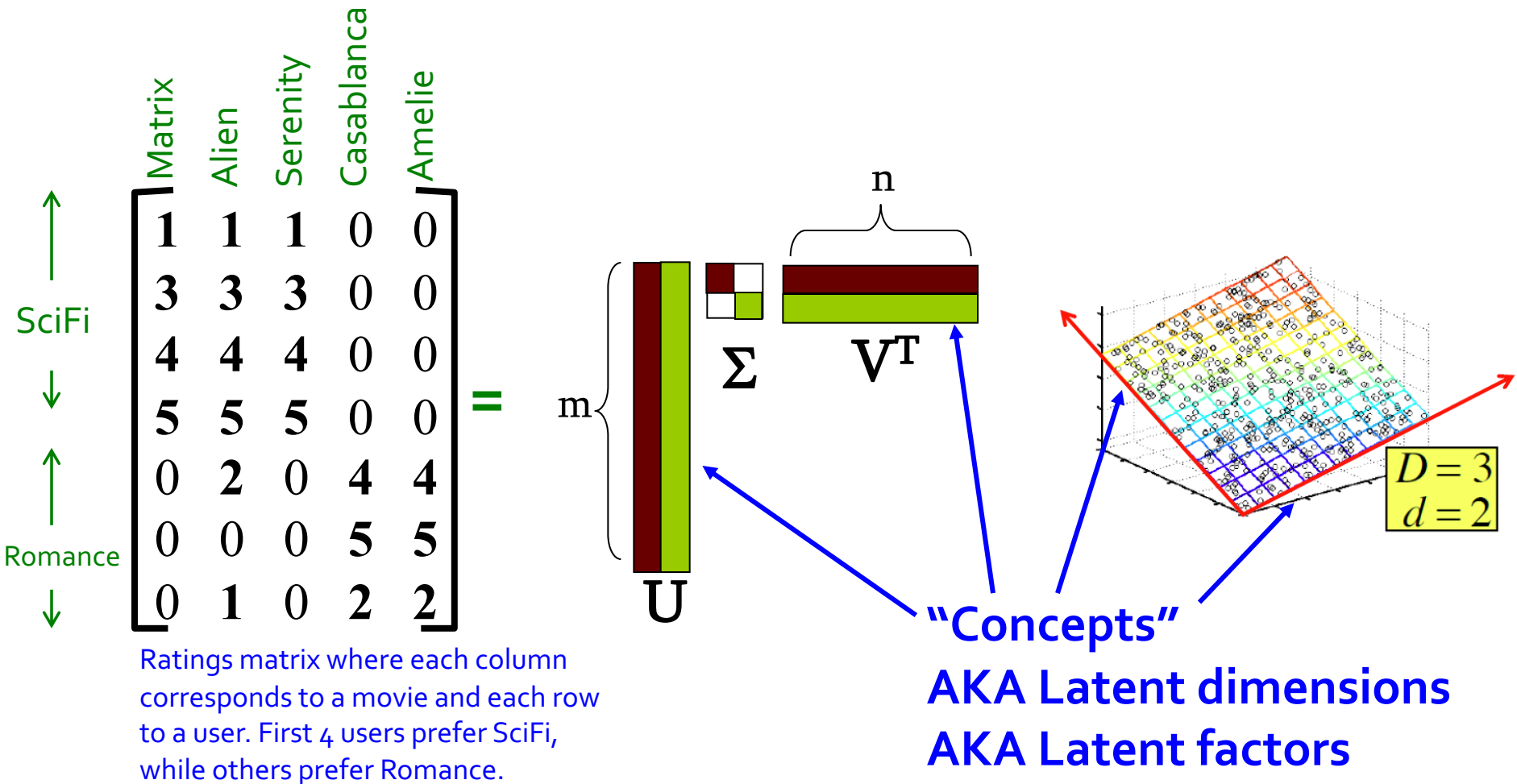
- **A = U Σ V^T - example: Users to Movies**

	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

=

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

12.4	0	0
0	**9.5**	0
0	0	**1.3**

X

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

A = U Σ V^T - example: Users to Movies

SciFi-concept

Romance-concept

SciFi

Romance

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

Column labels: Matrix, Alien, Serenity, Casablanca, Amelie

- **A = U Σ V^T - example:** *U* is "user-to-concept" factor matrix

SciFi-concept   Romance-concept

SciFi

Romance

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

(Movie labels: Matrix, Alien, Serenity, Casablanca, Amelie)

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

- **A = U Σ V^T - example:**

$$
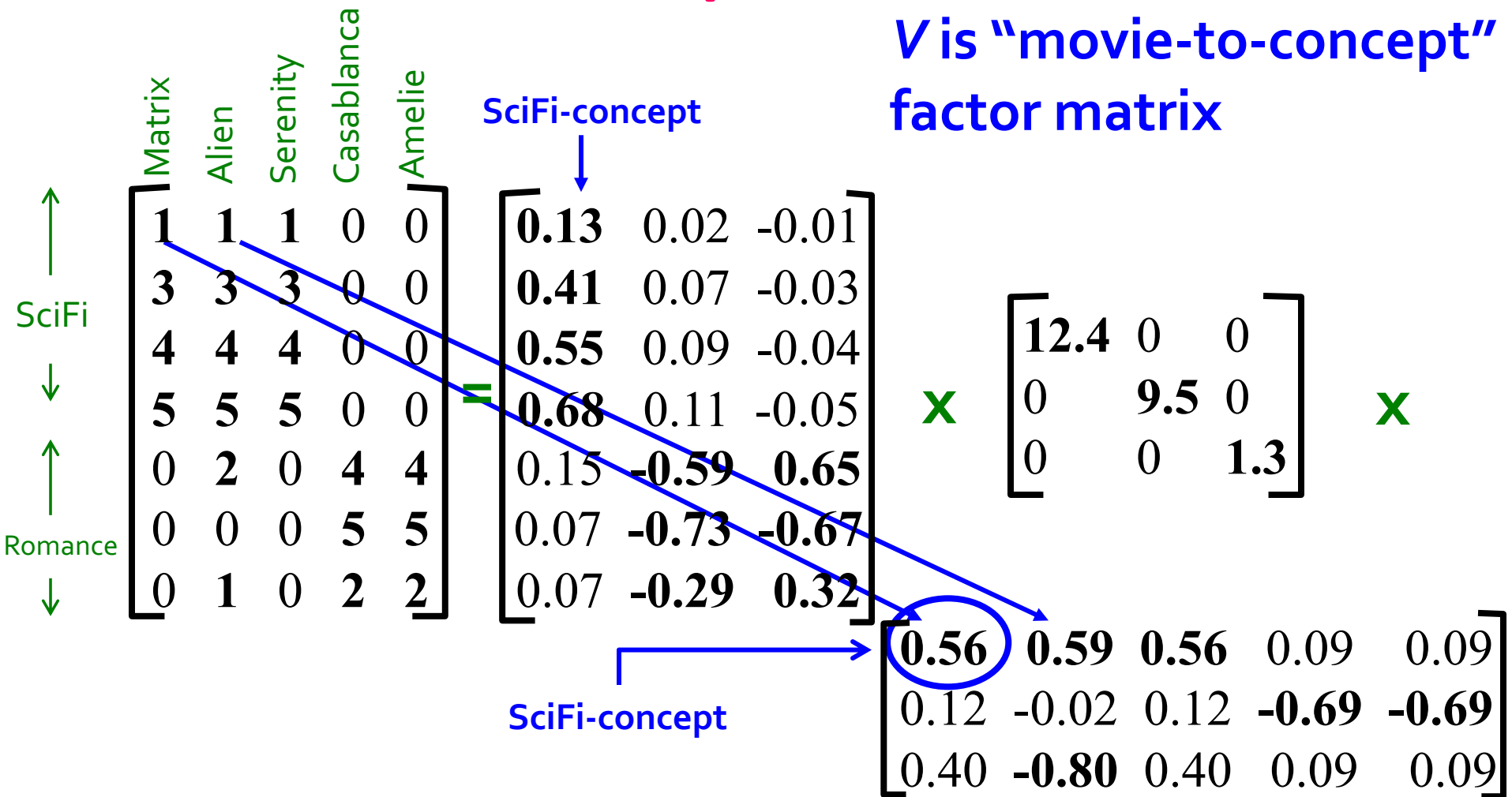\begin{array}{c}
\text{SciFi} \\[2em]
\text{Romance}
\end{array}
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2
\end{bmatrix}
=
\begin{bmatrix}
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
0.55 & 0.09 & -0.04 \\
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0.15 & -0.59 & 0.65 \\
0.07 & -0.73 & -0.67 \\
0.07 & -0.29 & 0.32
\end{bmatrix}
\times
\begin{bmatrix}
12.4 & 0 & 0 \\
0 & 9.5 & 0 \\
0 & 0 & 1.3
\end{bmatrix}
\times
$$

(Columns of A: Matrix, Alien, Serenity, Casablanca, Amelie)

SciFi-concept

"strength" of the SciFi-concept

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

A = U Σ Vᵀ - example:

V is "movie-to-concept" factor matrix

SciFi-concept

	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

$=$

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

SciFi-concept

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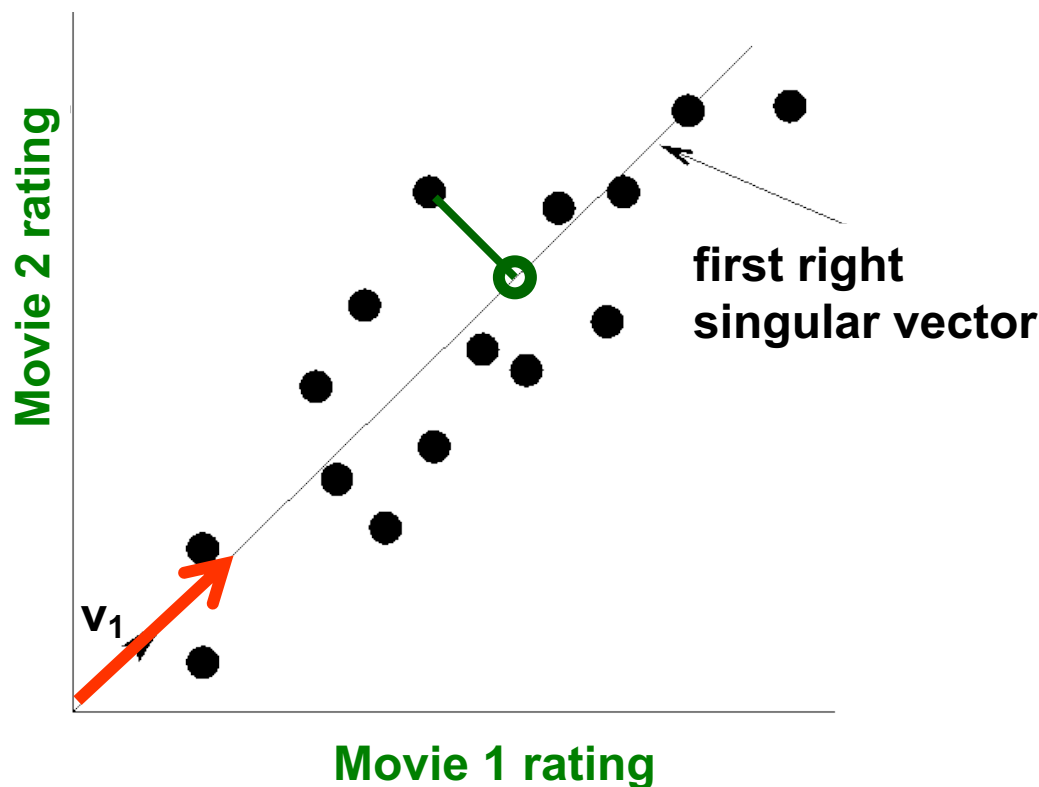
- Instead of using two coordinates (x, y) to describe point positions, let's use only one coordinate
- Point's position is its location along vector v_1
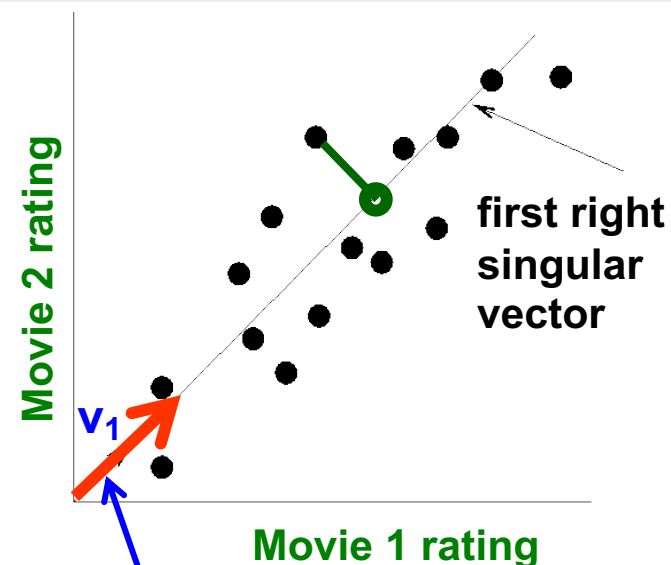
SVD – Dimensionality Reduction

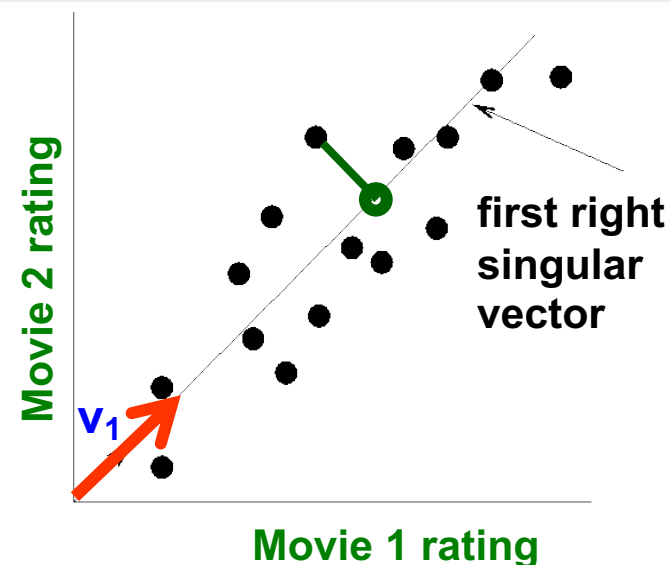- ## A = U Σ V^T - example:
  - **U**: "user-to-concept" matrix
  - **V**: "movie-to-concept" matrix

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

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

Movie 2 rating

Movie 1 rating

first right singular vector

v_1

- **A = U Σ V^T - example:**

Movie 2 rating

first right singular vector

v_1

Movie 1 rating

**variance ('spread')
on the v_1 axis**

$$
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2
\end{bmatrix}
=
\begin{bmatrix}
0.13 & 0.02 & -0.01 \\
0.41 & 0.07 & -0.03 \\
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\end{bmatrix}
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\begin{bmatrix}
12.4 & 0 & 0 \\
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\end{bmatrix}
\times
$$

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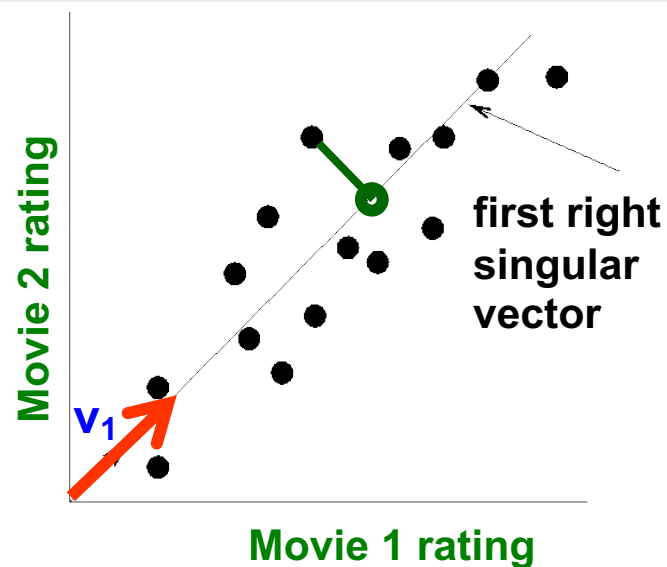0.40 & -0.80 & 0.40 & 0.09 & 0.09
\end{bmatrix}
$$

SVD – Dimensionality Reduction

A = U Σ Vᵀ - example:

- **U Σ:** Gives the coordinates of the points in the projection axis

Movie 2 rating

first right singular vector

v_1

Movie 1 rating

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix}$$

Projection of users on the "Sci-Fi" axis
U Σ:

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

More details

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

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

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

SVD – Interpretation #2

More details

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

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

SVD – Interpretation #2

More details

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

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

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**

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

SVD – Interpretation #2

More details

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

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

SVD – Interpretation #2

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:

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

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

is "small"

SVD – Best Low Rank Approx.

- **Fact: SVD gives 'best' axis to project on:**
  - '**best**' = minimizing the sum of reconstruction errors
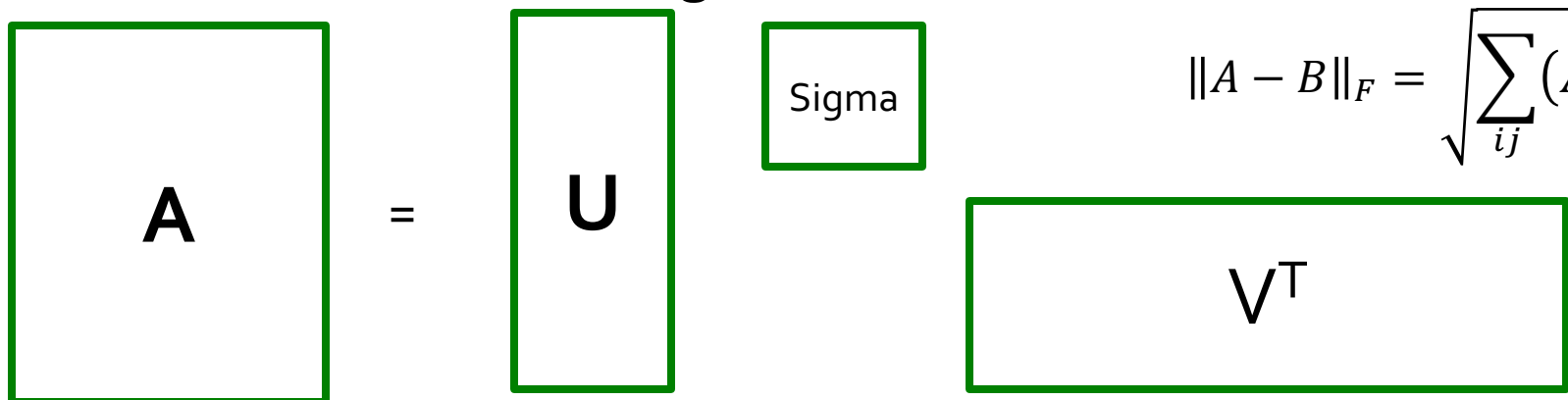
$$\|A - B\|_F = \sqrt{\sum_{ij}(A_{ij} - B_{ij})^2}$$

A = U × Sigma × V^T

B is best approximation of A:
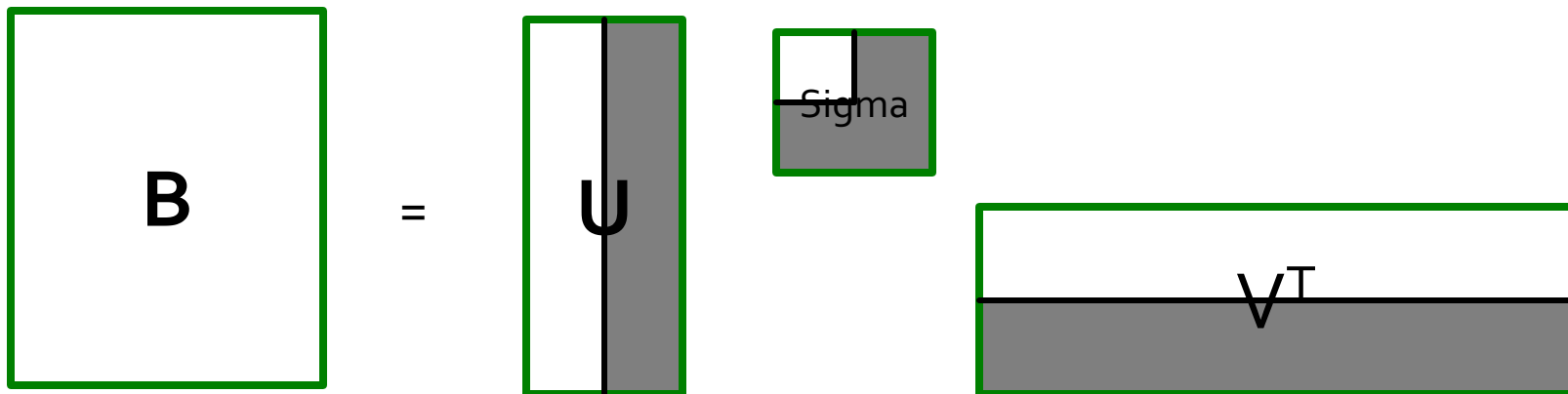
B = U × Sigma × V^T

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 (# 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" $\boldsymbol{x}_0$
  - Construct $\boldsymbol{x}_{k+1} = \dfrac{M\boldsymbol{x_k}}{||M\boldsymbol{x_k}||}$ for $k = 0, 1, \dots$
    - $|| \dots ||$ denotes the Frobenius norm
  - Stop when consecutive $\boldsymbol{x}_k$ show little change

Example: Iterative Eigenvector

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

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

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

…..

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 $\boldsymbol{x}^T = [0.53, 0.85]$, 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:**

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

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)

- Starting with $(A^TA)V = V\Sigma^2$

  - **Note** that therefore the i-th column of V is an eigenvector of A^TA, and its eigenvalue is the i-th element of Σ^2

- Thus, we can find V and Σ by finding the eigenpairs for A^TA

  - 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

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

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

Columns: Matrix, Alien, Serenity, Casablanca, Amelie

SciFi — Romance

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

$$q = \begin{bmatrix} 5 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Matrix Alien Serenity Casablanca Amelie

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

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

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

Project into concept space:
Inner product with each 'concept' vector v_i
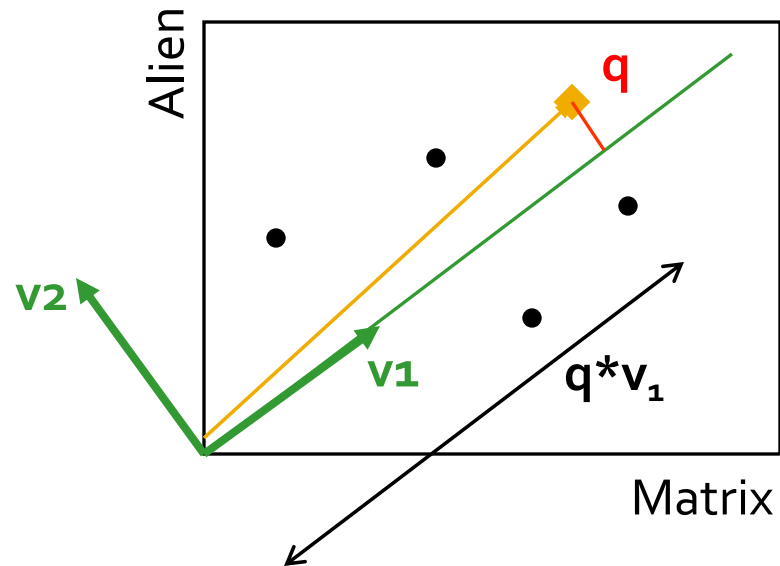
Compactly, we have:

$q_{concept} = q\ V$

E.g.:

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

$$
q = \begin{bmatrix} 5 & 0 & 0 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.12 \\ 0.59 & -0.02 \\ 0.56 & 0.12 \\ 0.09 & -0.69 \\ 0.09 & -0.69 \end{bmatrix} = \begin{bmatrix} 2.8 & 0.6 \end{bmatrix}
$$

SciFi-concept

movie-to-concept factors (V)

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

E.g.:

$$d = \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.12 \\ 0.59 & -0.02 \\ 0.56 & 0.12 \\ 0.09 & -0.69 \\ 0.09 & -0.69 \end{bmatrix} = \begin{bmatrix} 5.2 & 0.4 \end{bmatrix}$$

Columns of d: Matrix, Alien, Serenity, Casablanca, Amelie

SciFi-concept

movie-to-concept factors (V)

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**!

SciFi-concept

$$d = \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \end{bmatrix} \dashrightarrow \begin{bmatrix} 5.2 & 0.4 \end{bmatrix}$$

$$q = \begin{bmatrix} 5 & 0 & 0 & 0 & 0 \end{bmatrix} \dashrightarrow \begin{bmatrix} 2.8 & 0.6 \end{bmatrix}$$

(columns: Matrix, Alien, Serenity, Casablanca, Amelie)

Zero ratings in common

Similarity > 0
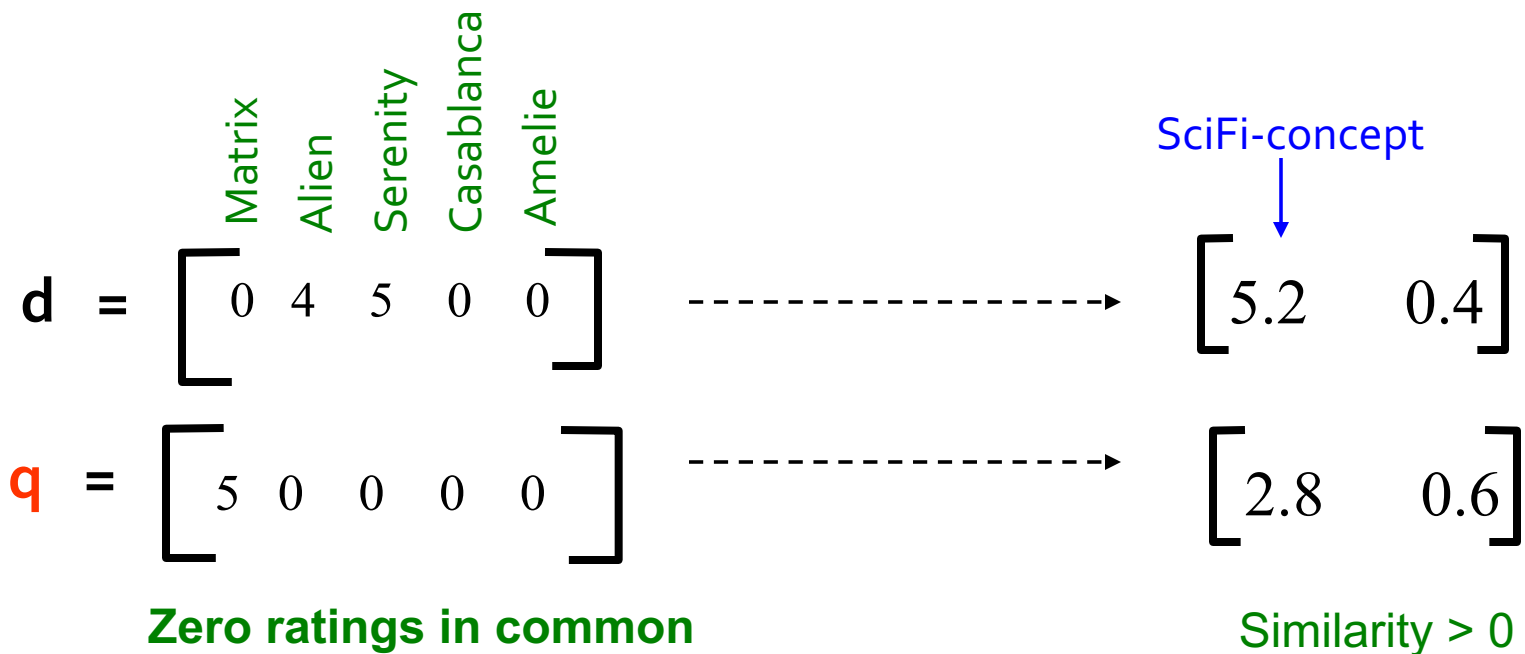
SVD: Drawbacks

+ **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!**
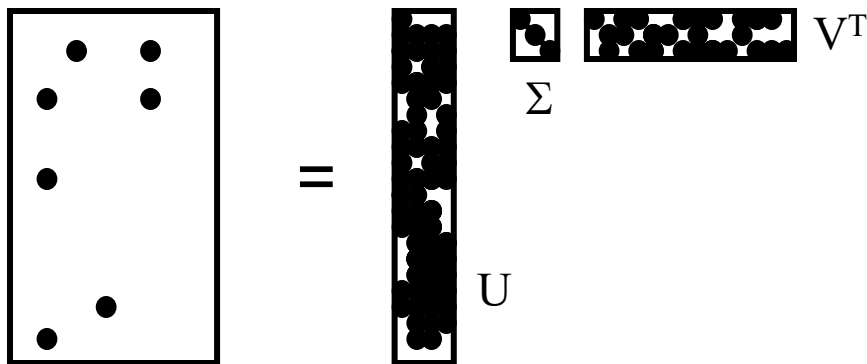
CUR Decomposition

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

- **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:**

$$A \approx C \cdot U \cdot R$$

A   C   U   R

CUR Decomposition

- **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:**

$A \approx C \cdot U \cdot R$

Pseudo-inverse of the intersection of C and R

A   C   U   R

Computing U

- Let W be the "intersection" of sampled columns C and rows R

- **Def: W^+ is the pseudoinverse**

  - Let SVD of $W = X\,Z\,Y^T$

  - **Then: $W^+ = Y\,Z^+\,X^T$**

    - Z^+: **reciprocals of non-zero singular values:** $Z^+_{ii} = 1/Z_{ii}$

- **Let: $U = Y\,(Z^+)^2 X^T$**

columns, **C**

rows, **R**

A = W
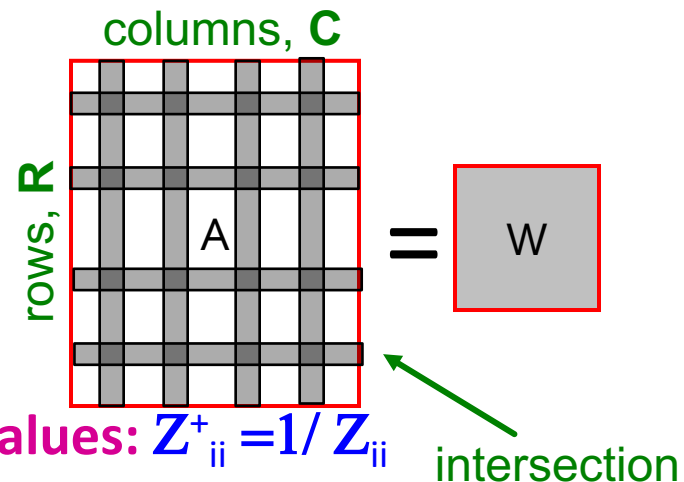
intersection

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 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

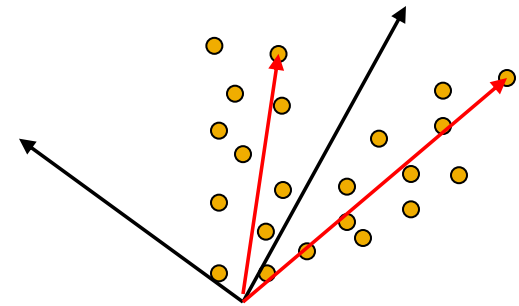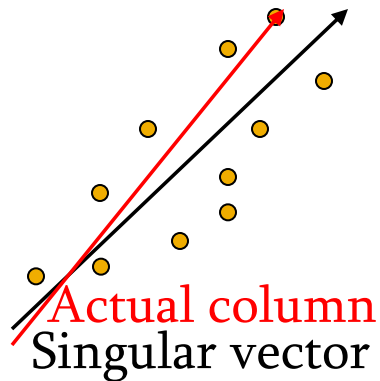- **Sampling columns (similarly for rows):**

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

Actual column
Singular vector

- **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 $c = O\left(\dfrac{k \log k}{\varepsilon^2}\right)$ columns of A using ColumnSelect algorithm (slide 56)**

  - **Select $r = O\left(\dfrac{k \log k}{\varepsilon^2}\right)$ rows of A using RowSelect algorithm (slide 56)**

  - **Set $U = Y\,(Z^+)^2 X^T$**

- **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 4k cols/rows for a "rank-k" approximation

CUR: Pros & Cons

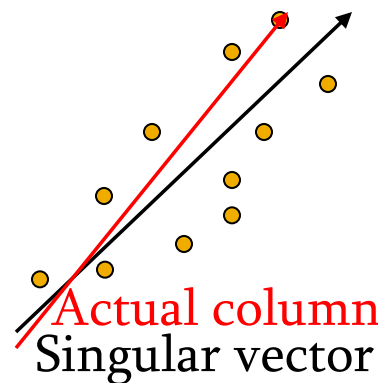+ **Easy interpretation**

  - 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

Actual column
Singular vector

SVD vs. CUR

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

sparse and small

Huge but sparse

Big and dense

CUR: $A = C U R$

dense but small

Huge but sparse

Big but sparse

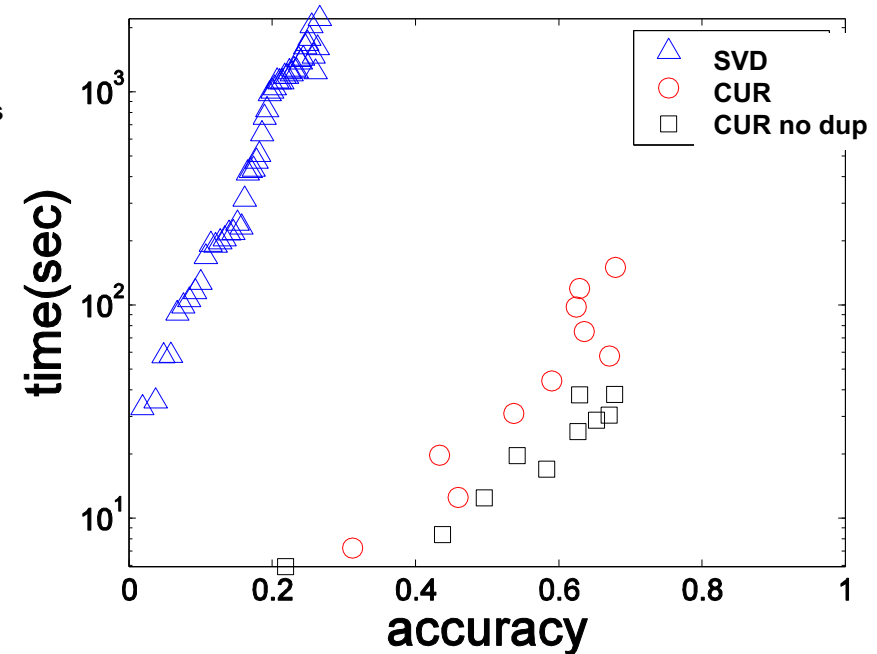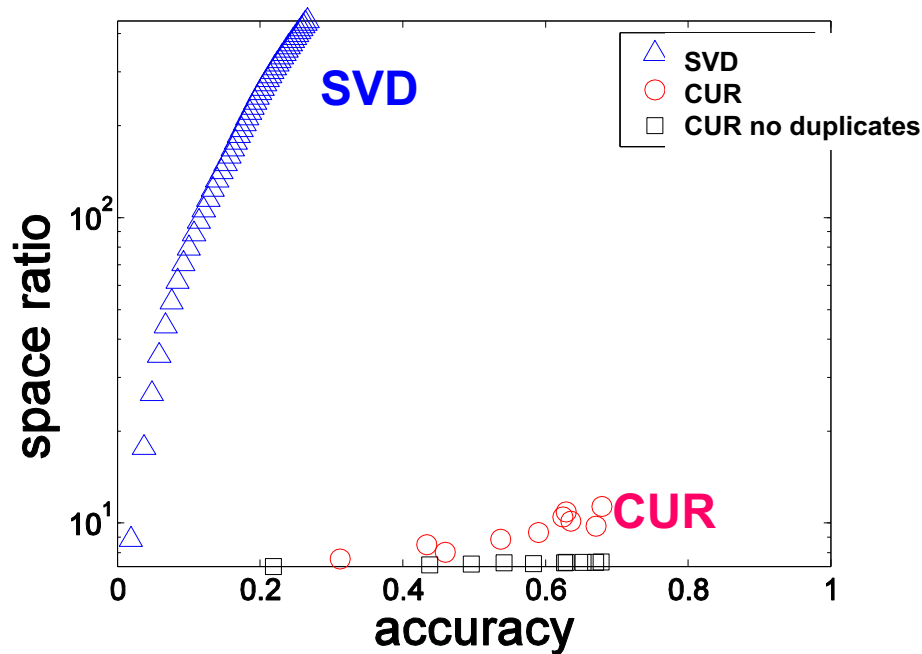# SVD vs. CUR: Simple Experiment

- ## 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.