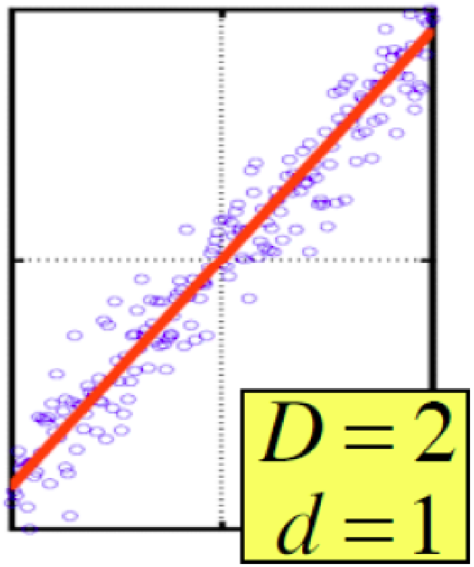
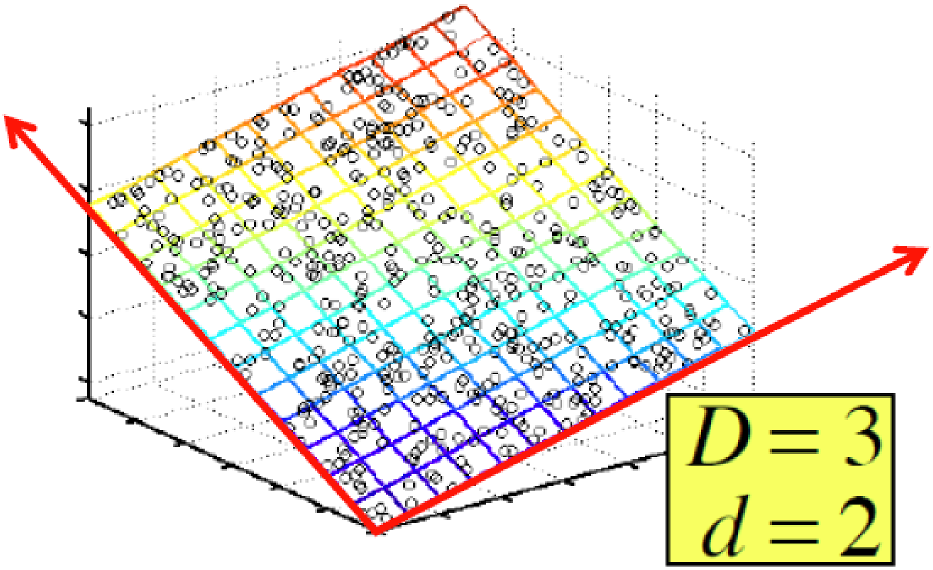
Dimensionality Reduction: SVD & CUR

CS246: Mining Massive Datasets
Jure Leskovec, Stanford University
http://cs246.stanford.edu

Dimensionality Reduction





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

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
ABC Inc.	1	1	1	0	0
DEF Ltd.	2	2	2	0	0
GHI Inc.	1	1	1	0	0
KLM Co.	5	5	5	0	0
Smith	0	0	0	2	2
Johnson	0	0	0	3	3
Thompson	0	0	0	1	1

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

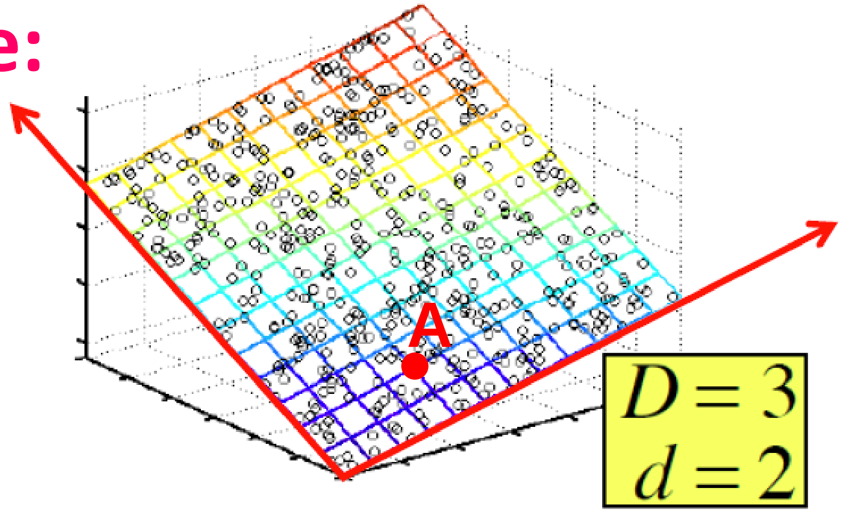
Rank of a Matrix

- **Q:** What is **rank** of a matrix **A**?
- **A:** Number of **linearly independent** columns of **A**
- **For example:**
  - Matrix **A** = $\begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$ has rank **r=2**
    - **Why?** The first two rows are linearly independent, so the rank is at least 2, but all three rows are linearly dependent (the first is equal to the sum of the second and third) so the rank must be less than 3.
- **Why do we care about low rank?**
  - We can write **A** as two "basis" vectors: [1 2 1] [-2 -3 1]
  - And new coordinates of : [1 0] [0 1] [1 1]

Rank is "Dimensionality"

- **Cloud of points 3D space:**
  - Think of point positions as a matrix:

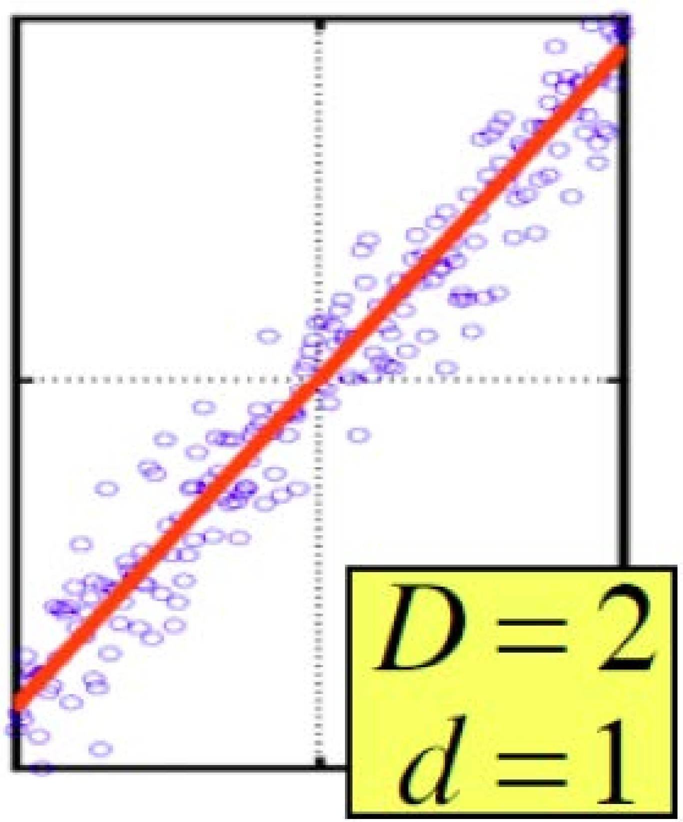
    1 row per point:
    $$\begin{array}{c} \begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix} \end{array} \begin{array}{c} \text{A} \\ \text{B} \\ \text{C} \end{array}$$



- **We can rewrite coordinates more efficiently!**
  - Old coordinate system: [1 0 0] [0 1 0] [0 0 1]
  - **New coordinate system: [1 2 1] [-2 -3 1]**
  - Then **A** has new coordinates: [1 0]. **B**: [0 1], **C**: [1 1]
    - **Notice: We reduced the number of coordinates!**

Dimensionality Reduction

- **Goal of dimensionality reduction is to discover the axis of data!**



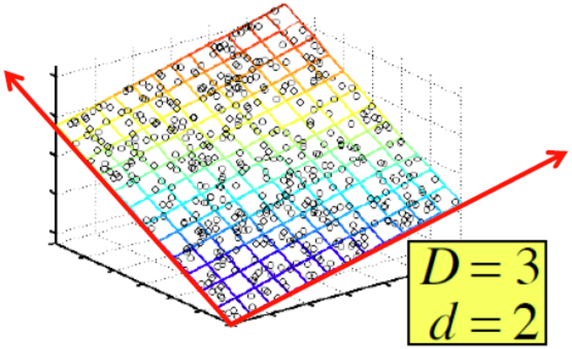
Rather than representing every point with 2 coordinates we represent each point with 1 coordinate (corresponding to the position of the point on the red line).

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

Why Reduce Dimensions?

Why reduce dimensions?

- **Discover hidden correlations/topics**
  - Words that occur commonly together
- **Remove redundant and noisy features**
  - Not all words are useful
- **Interpretation and visualization**
- **Easier storage and processing of the data**



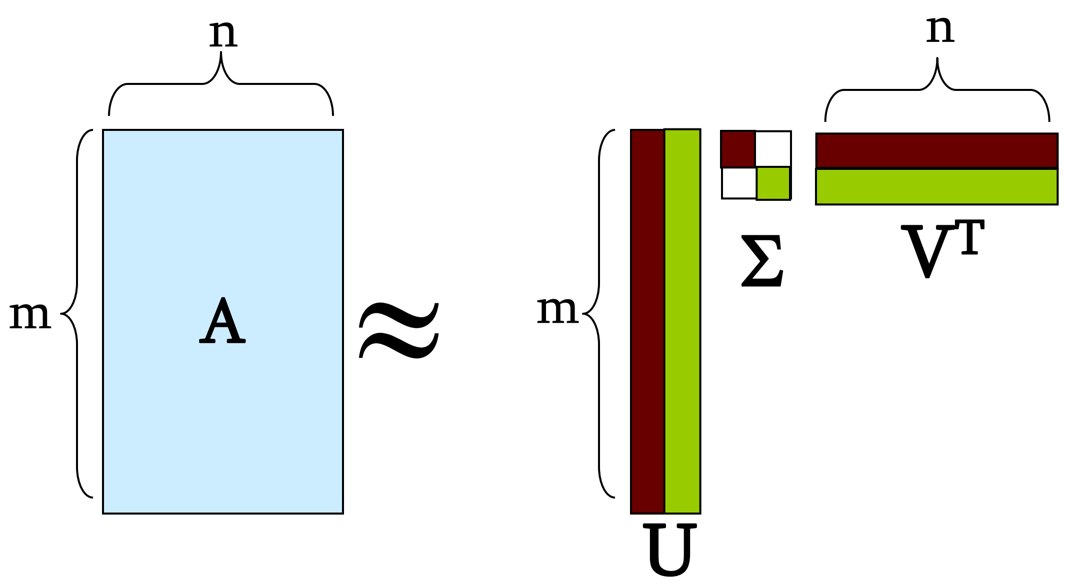
SVD - Definition

$$\mathbf{A}_{[m \times n]} = \mathbf{U}_{[m \times r]} \, \boldsymbol{\Sigma}_{[r \times r]} \, (\mathbf{V}_{[n \times r]})^{\mathrm{T}}$$

- **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)

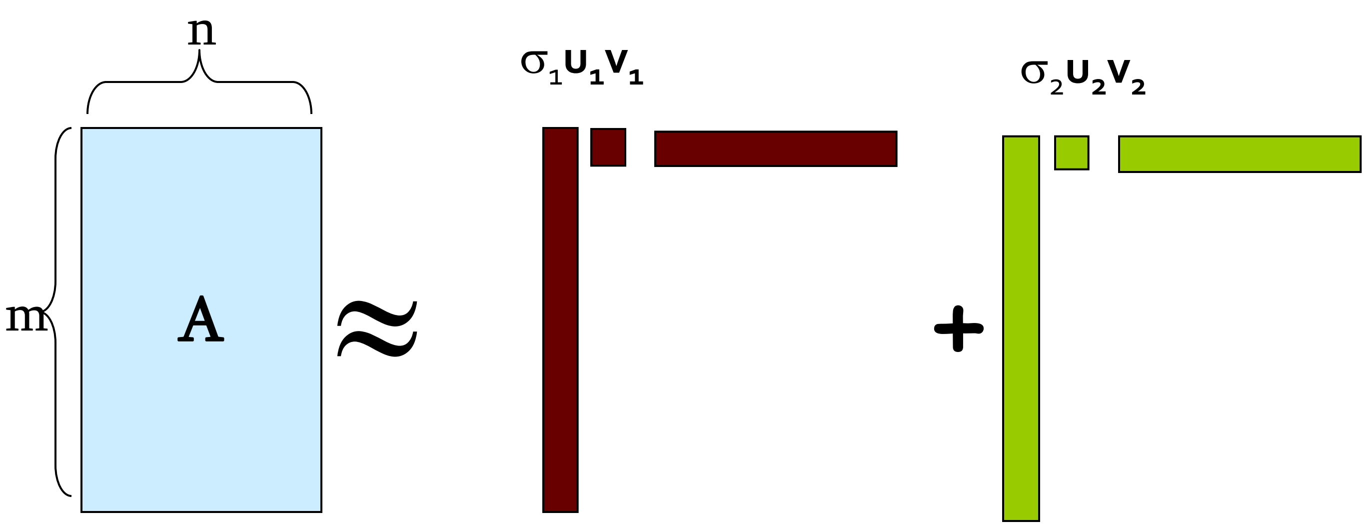
SVD

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



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

SVD - Properties

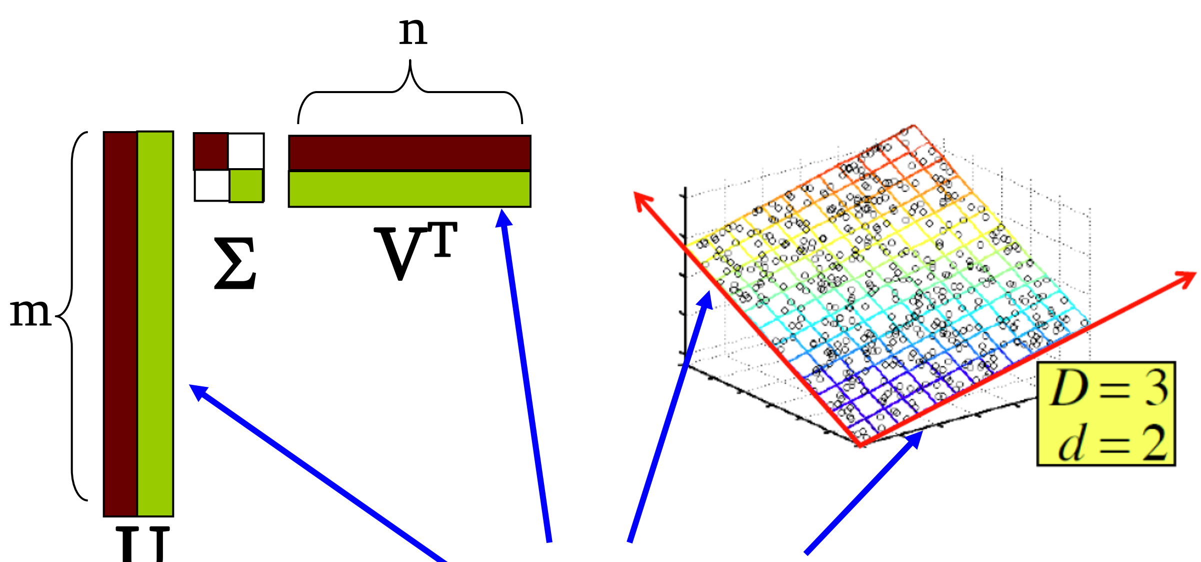
It is **always** possible to decompose a real matrix $\boldsymbol{A}$ into $\boldsymbol{A = U\, \Sigma\, V^T}$, where

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

SVD – Example: Users-to-Movies

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

$$\begin{array}{cc} & \begin{array}{ccccc} \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \end{array} \\ \begin{array}{c} \uparrow \\ \text{SciFi} \\ \downarrow \\ \\ \uparrow \\ \text{Romnce} \\ \downarrow \end{array} & \left[\begin{array}{ccccc} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{array}\right] \end{array} =$$



"Concepts"
AKA Latent dimensions
AKA Latent factors

SVD – Example: Users-to-Movies

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

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

SVD – Example: Users-to-Movies

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

SciFi-concept

Romance-concept

$$
\begin{array}{c|c}
 & \begin{array}{ccccc} \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \end{array} \\
\begin{array}{c} \\ \\ \text{SciFi} \\ \\ \\ \text{Romnce} \\ \\ \end{array} &
\begin{bmatrix}
\mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & 0 \\
\mathbf{3} & \mathbf{3} & \mathbf{3} & 0 & 0 \\
\mathbf{4} & \mathbf{4} & \mathbf{4} & 0 & 0 \\
\mathbf{5} & \mathbf{5} & \mathbf{5} & 0 & 0 \\
0 & \mathbf{2} & 0 & \mathbf{4} & \mathbf{4} \\
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\end{array}
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0.40 & \mathbf{-0.80} & 0.40 & 0.09 & 0.09
\end{bmatrix}
$$

SVD – Example: Users-to-Movies

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

U is "user-to-concept" similarity matrix

SciFi-concept Romance-concept

$$
\begin{array}{c}
 \\ \text{SciFi} \\ \\ \\ \text{Romnce} \\ \\ \\
\end{array}
\begin{array}{c}
\begin{array}{ccccc} \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \end{array} \\
\begin{bmatrix}
\mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & 0 \\
\mathbf{3} & \mathbf{3} & \mathbf{3} & 0 & 0 \\
\mathbf{4} & \mathbf{4} & \mathbf{4} & 0 & 0 \\
\mathbf{5} & \mathbf{5} & \mathbf{5} & 0 & 0 \\
0 & \mathbf{2} & 0 & \mathbf{4} & \mathbf{4} \\
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\end{bmatrix}
\end{array}
=
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0.40 & \mathbf{-0.80} & 0.40 & 0.09 & 0.09
\end{bmatrix}
$$

SVD – Example: Users-to-Movies

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

SciFi-concept

"strength" of the SciFi-concept

$$
\begin{array}{c}
\\
\text{SciFi} \\
\\
\\
\text{Romnce} \\
\\
\end{array}
\begin{array}{c}
\begin{array}{ccccc} \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \end{array} \\
\left[\begin{array}{ccccc}
\mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & 0 \\
\mathbf{3} & \mathbf{3} & \mathbf{3} & 0 & 0 \\
\mathbf{4} & \mathbf{4} & \mathbf{4} & 0 & 0 \\
\mathbf{5} & \mathbf{5} & \mathbf{5} & 0 & 0 \\
0 & \mathbf{2} & 0 & \mathbf{4} & \mathbf{4} \\
0 & 0 & 0 & \mathbf{5} & \mathbf{5} \\
0 & \mathbf{1} & 0 & \mathbf{2} & \mathbf{2}
\end{array}\right]
\end{array}
=
\left[\begin{array}{ccc}
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\mathbf{0.55} & 0.09 & -0.04 \\
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0.07 & \mathbf{-0.73} & \mathbf{-0.67} \\
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\end{array}\right]
\times
\left[\begin{array}{ccc}
\mathbf{12.4} & 0 & 0 \\
0 & \mathbf{9.5} & 0 \\
0 & 0 & \mathbf{1.3}
\end{array}\right]
\times
\left[\begin{array}{ccccc}
\mathbf{0.56} & \mathbf{0.59} & \mathbf{0.56} & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & \mathbf{-0.69} & \mathbf{-0.69} \\
0.40 & \mathbf{-0.80} & 0.40 & 0.09 & 0.09
\end{array}\right]
$$

SVD – Example: Users-to-Movies

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

***V* is "movie-to-concept" similarity matrix**

SciFi-concept

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

SciFi-concept

SVD - Interpretation #1

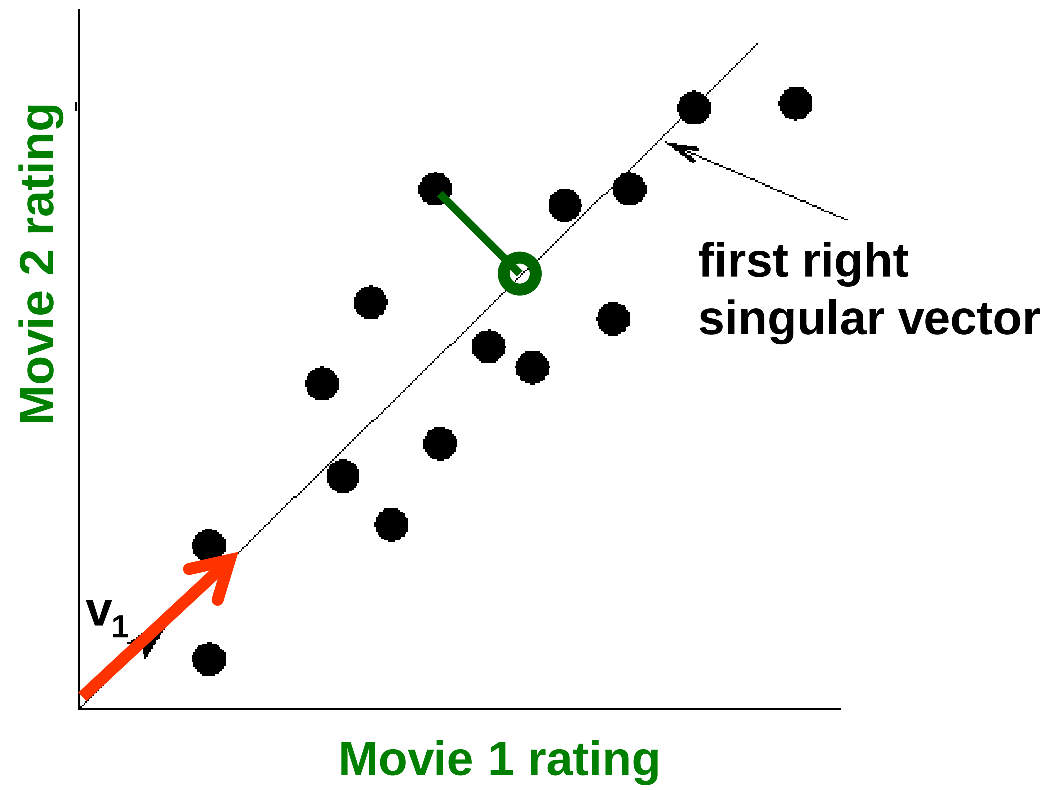
‘**movies**’, ‘**users**’ and ‘**concepts**’:

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

Dimensionality Reduction with SVD

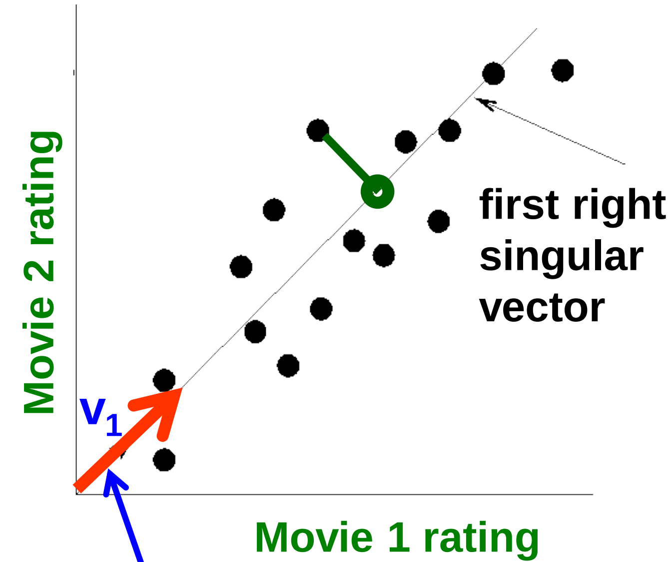
SVD – Dimensionality Reduction

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



SVD - Interpretation #2

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



$$
\begin{bmatrix}
\mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & 0 \\
\mathbf{3} & \mathbf{3} & \mathbf{3} & 0 & 0 \\
\mathbf{4} & \mathbf{4} & \mathbf{4} & 0 & 0 \\
\mathbf{5} & \mathbf{5} & \mathbf{5} & 0 & 0 \\
0 & \mathbf{2} & 0 & \mathbf{4} & \mathbf{4} \\
0 & 0 & 0 & \mathbf{5} & \mathbf{5} \\
0 & \mathbf{1} & 0 & \mathbf{2} & \mathbf{2}
\end{bmatrix}
=
\begin{bmatrix}
\mathbf{0.13} & 0.02 & -0.01 \\
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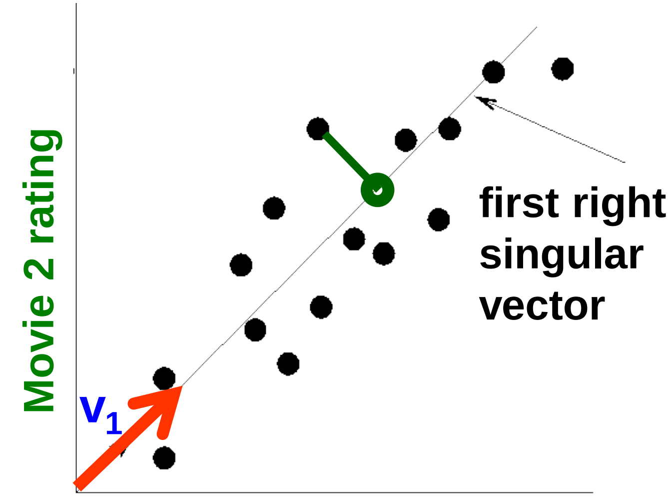
\end{bmatrix}
\times
\begin{bmatrix}
\mathbf{12.4} & 0 & 0 \\
0 & \mathbf{9.5} & 0 \\
0 & 0 & \mathbf{1.3}
\end{bmatrix}
\times
\begin{bmatrix}
\mathbf{0.56} & \mathbf{0.59} & \mathbf{0.56} & 0.09 & 0.09 \\
0.12 & -0.02 & 0.12 & \mathbf{-0.69} & \mathbf{-0.69} \\
0.40 & \mathbf{-0.80} & 0.40 & 0.09 & 0.09
\end{bmatrix}
$$

SVD - Interpretation #2

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



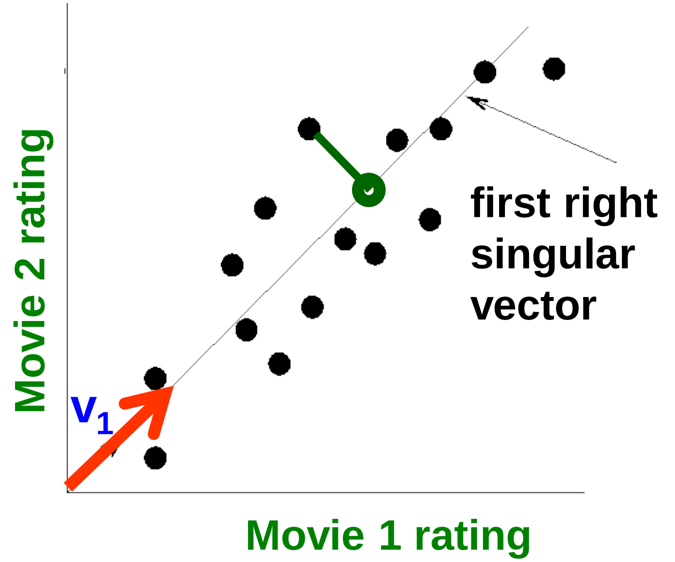
variance ('spread') on the v_1 axis

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

SVD - Interpretation #2

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

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

SVD - Interpretation #2

More details

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

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

SVD - Interpretation #2

More details

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

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

SVD - Interpretation #2

More details

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

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

SVD - Interpretation #2

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

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

More details

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

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

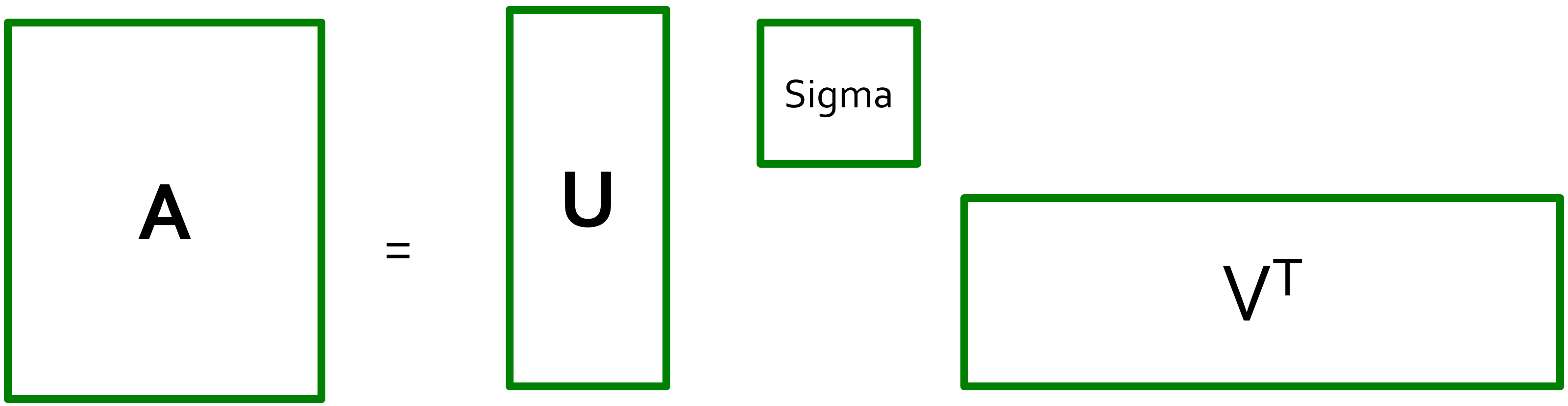
Frobenius norm:

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

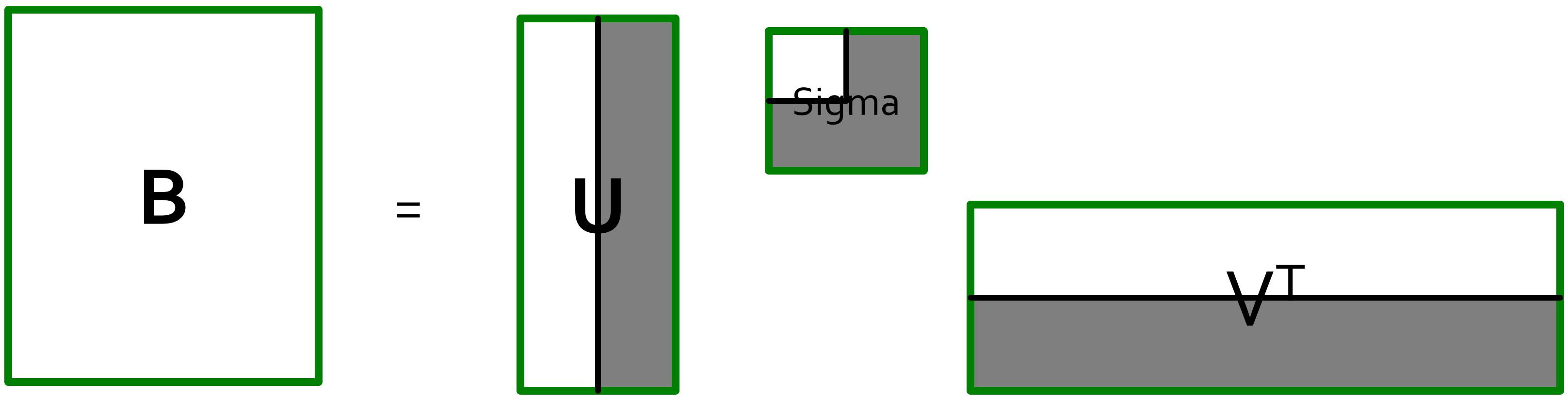
$$\|A-B\|_F = \sqrt{\Sigma_{ij} (A_{ij}-B_{ij})^2}$$

is "small"

SVD – Best Low Rank Approx.



B is best approximation of A

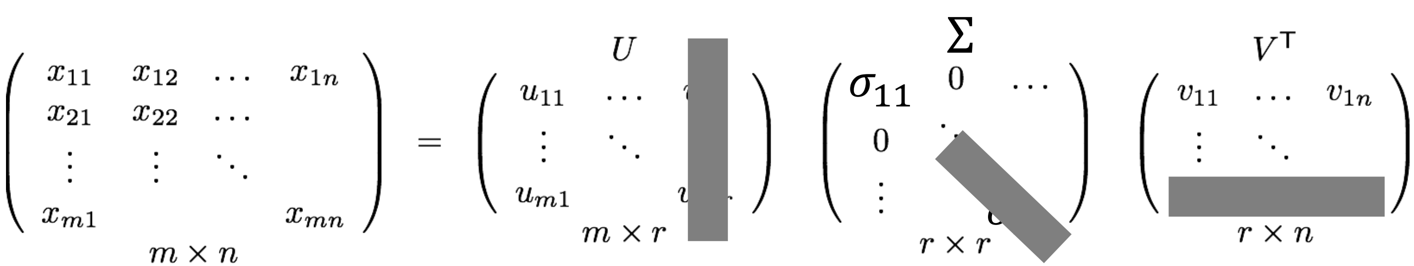


SVD – Best Low Rank Approx.

- **Theorem:**
  Let A = U Σ V^T where Σ: $\sigma_1 \geq \sigma_2 \geq \ldots$, and rank(***A***)=***r***
  then B = U S V^T is a **best** rank(B)=***k*** approx. to ***A***
  - **S = diagonal *n*x*n* matrix** where ***s$_i$*=*σ$_i$*** (*i=1…k*) else ***s$_i$*=0**

What do we mean by "best":

- ***B* is a solution to min$_B$ ‖*A*-*B*‖$_F$ where rank(*B*)=*k***



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

SVD - Interpretation #2

Equivalent:

'spectral decomposition' of the matrix:

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

SVD - Interpretation #2

Equivalent:

'spectral decomposition' of the matrix

$$\begin{array}{cc} & \xleftarrow{\quad m \quad} \\ n & \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \end{array} = \underbrace{\sigma_1 \underset{n \times 1}{u_1} \underset{1 \times m}{v^T_1} + \sigma_2 u_2 v^T_2 + \ldots}_{k \text{ terms}}$$

Assume: $\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \ldots \geq 0$

Why is setting small σ_i to 0 the right thing to do?

Vectors $\mathbf{u_i}$ and $\mathbf{v_i}$ are unit length, so σ_i scales them.

So, zeroing small σ_i introduces less error.

SVD - Interpretation #2

Q: How many σs to keep?

A: Rule-of-a thumb:

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

$$
\begin{array}{c c}
 & \xleftarrow{\quad m \quad} \\
n \updownarrow &
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
3 & 3 & 3 & 0 & 0 \\
4 & 4 & 4 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 2 & 0 & 4 & 4 \\
0 & 0 & 0 & 5 & 5 \\
0 & 1 & 0 & 2 & 2
\end{bmatrix}
\end{array}
= \sigma_1 \quad u_1 \quad v^T_1 \quad + \quad \sigma_2 \quad u_2 \quad v^T_2 \quad + \ldots
$$

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

SVD - Complexity

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

SVD - Conclusions so far

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

Relation to Eigen-decomposition

- **SVD gives us:**
  - $A = U \, \Sigma \, V^T$
- **Eigen-decomposition:**
  - $A = X \, \Lambda \, X^T$
    - A is symmetric
    - U, V, X are orthonormal (**$U^TU=I$**),
    - Λ, Σ are diagonal
- **What is:**
  - $\mathbf{AA^T=}$
  - $\mathbf{A^TA = V\,\Sigma^T\,U^T\,(U\Sigma\,V^T) = V\,\Sigma\Sigma^T\,V^T}$

Relation to Eigen-decomposition

- SVD gives us:
  - $A = U\,\Sigma\,V^T$
- Eigen-decomposition:
  - $A = X\,\Lambda\,X^T$
    - A is symmetric
    - U, V, X are orthonormal ($\mathbf{U^TU=I}$),
    - Λ, Σ are diagonal
- What is:
  - $\mathbf{AA^T = U\Sigma\, V^T(U\Sigma\, V^T)^T = U\Sigma\, V^T(V\Sigma^T U^T) = U\Sigma\Sigma^T\, U^T}$
  - $\mathbf{A^TA = V\,\Sigma^T\,U^T\,(U\Sigma\,V^T) = V\,\Sigma\Sigma^T\,V^T}$

Shows how to compute SVD using eigenvalue decomposition!

$X\ \Lambda\ X^T$

$X\ \Lambda\ X^T$

So, $\lambda_i = \sigma_i^2$

Example of SVD & Conclusion

Case study: How to query?

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

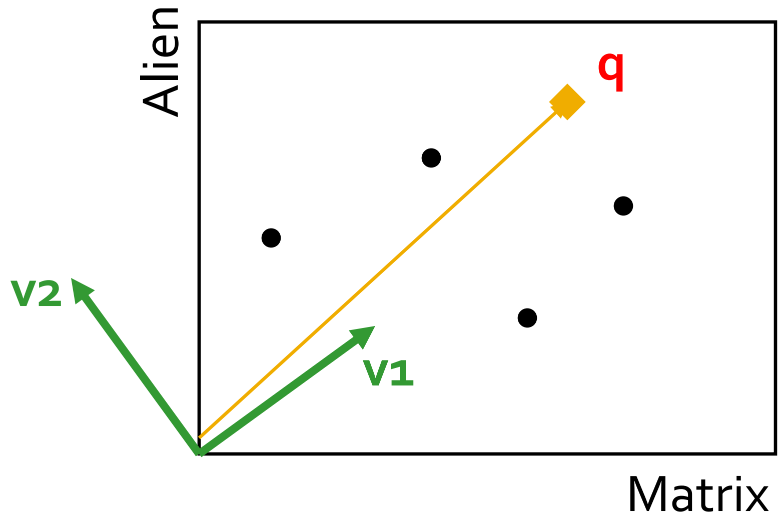
$$
\begin{array}{c}
 \\ \\ \text{SciFi} \\ \\ \\ \text{Romnce} \\ \\
\end{array}
\begin{array}{c}
\begin{array}{ccccc} \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \end{array} \\
\begin{bmatrix}
\mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & 0 \\
\mathbf{3} & \mathbf{3}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

Case study: How to query?

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

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

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

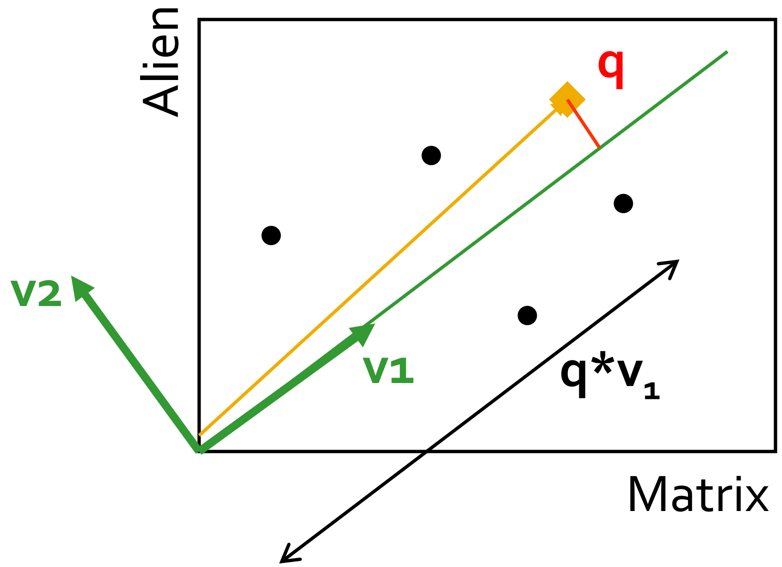


Case study: How to query?

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

$$\begin{array}{cccccc} & \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \\ \mathbf{q} = & \left[5 \right. & 0 & 0 & 0 & \left. 0 \right] \end{array}$$

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.:

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

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

movie-to-concept similarities (V)

Case study: How to query?

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

E.g.:

$$
\begin{array}{c}
\begin{array}{ccccc} \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \end{array} \\
q = \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \end{bmatrix}
\end{array}
\mathbf{x}
\begin{bmatrix} 0.56 & 0.12 \\ 0.59 & -0.02 \\ 0.56 & 0.12 \\ 0.09 & -0.69 \\ 0.09 & -0.69 \end{bmatrix}
= \begin{array}{c} \text{SciFi-concept} \\ \downarrow \\ \begin{bmatrix} 5.2 & 0.4 \end{bmatrix} \end{array}
$$

movie-to-concept similarities (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**!

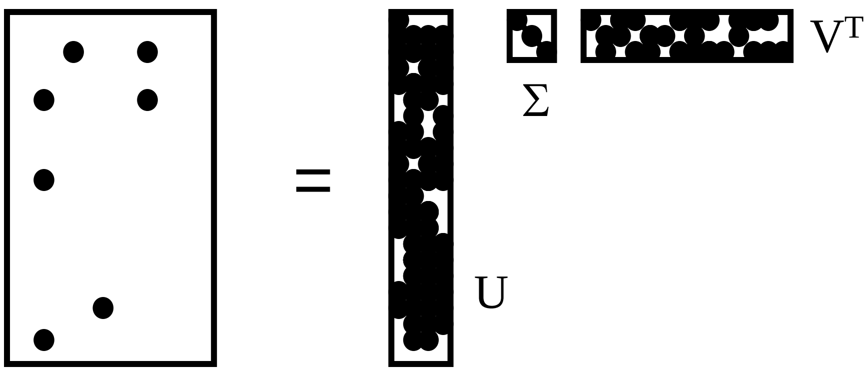
$$
\begin{array}{cc}
 & \begin{array}{ccccc} \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \end{array} \\
\mathbf{d}= & \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \end{bmatrix} \\
\mathbf{q}= & \begin{bmatrix} 5 & 0 & 0 & 0 & 0 \end{bmatrix}
\end{array}
\begin{array}{c} \\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

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!**



Announcements:

- **HW2 has been posted**

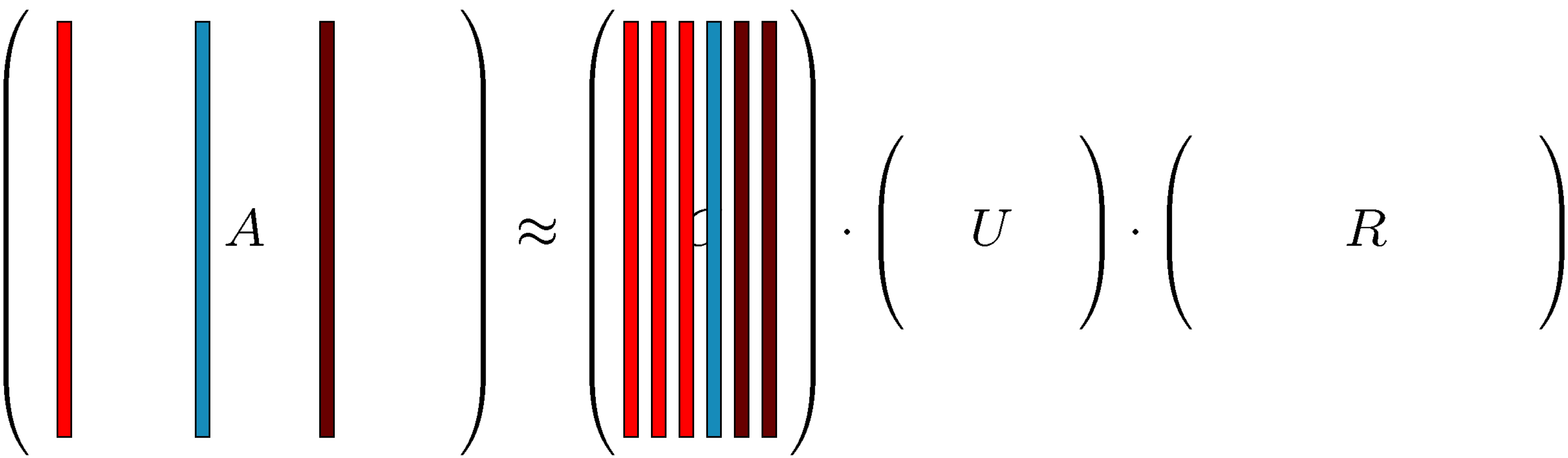
CUR Decomposition

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:**

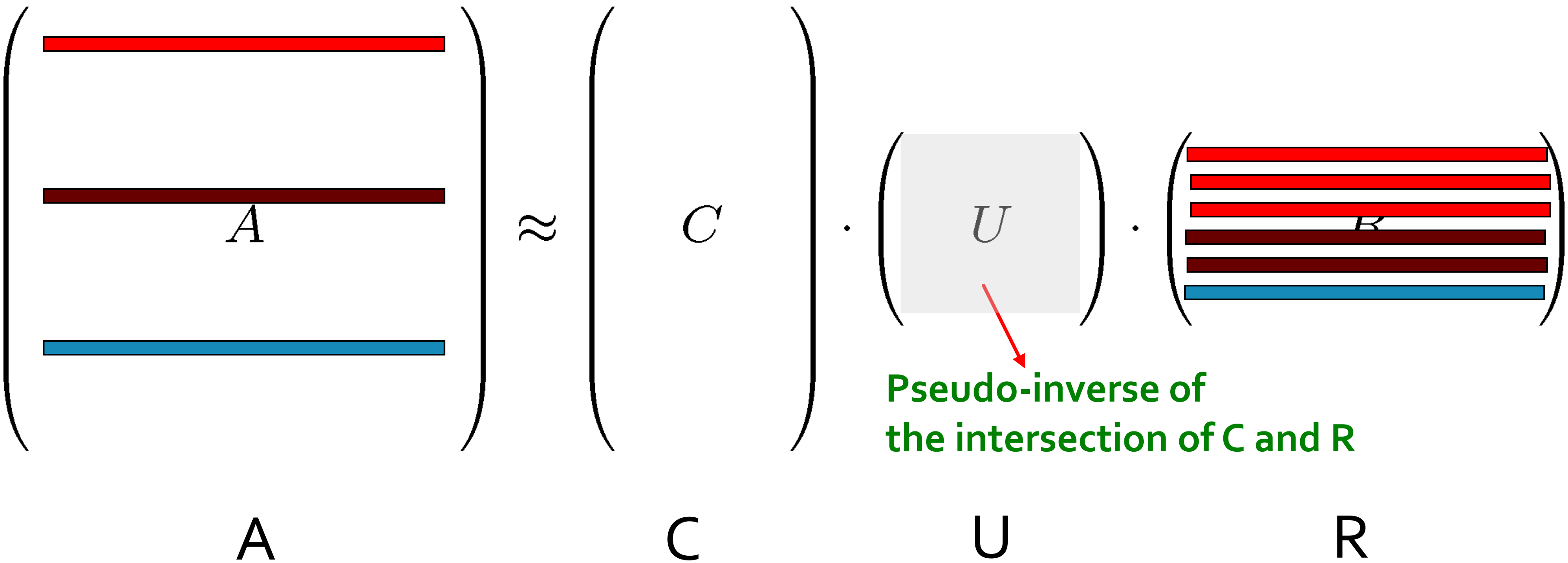


A C U R

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:**



CUR: Provably good approx. to SVD

- **Let:**
  $\mathbf{A_k}$ be the "best" rank $\boldsymbol{k}$ approximation to $\mathbf{A}$ (that is, $\mathbf{A_k}$ is SVD of A)

Theorem [Drineas et al.]
CUR in O(**m·n**) time achieves
- $\|A\text{-}CUR\|_F \leq \|A\text{-}A_k\|_F + \varepsilon\|A\|_F$

with probability at least $1\text{-}\delta$, by picking
- $O(k \log(1/\delta)/\varepsilon^2)$ columns, and
- $O(k^2 \log^3(1/\delta)/\varepsilon^6)$ rows

In practice:
Pick 4*k* cols/rows

CUR: How it Works

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

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

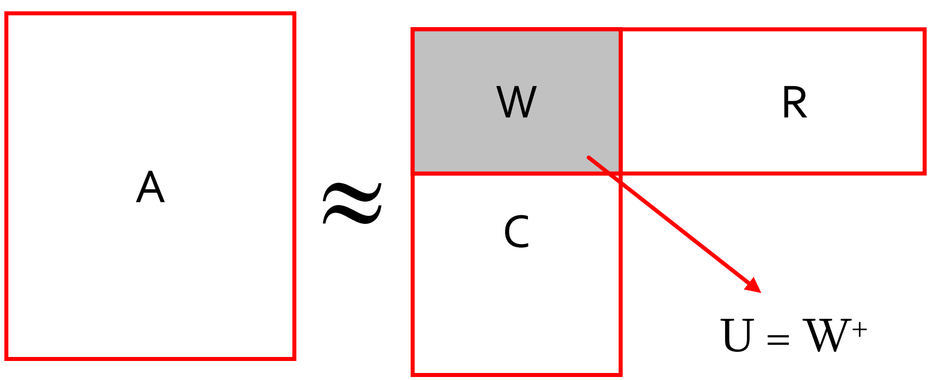
Output: $\mathbf{C}_d \in \mathbb{R}^{m \times c}$

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

Computing U

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



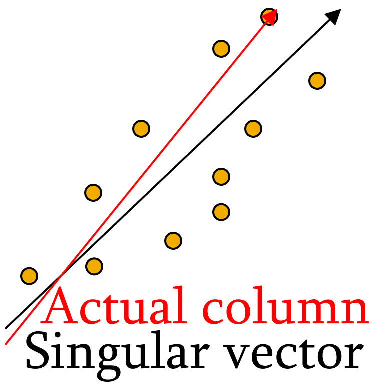
Why pseudoinverse works?
$W = X\,Z\,Y$ then $W^{-1} = X^{-1}\,Z^{-1}\,Y^{-1}$
Due to orthonomality
$X^{-1}=X^T$ and $Y^{-1}=Y^T$
Since Z is diagonal $Z^{-1} = 1/Z_{ii}$
Thus, if **W** is nonsingular, pseudoinverse is the true inverse

CUR: Provably good approx. to SVD

- **For example:**
  - **Select $c = O\left(\frac{k \log k}{\varepsilon^2}\right)$ columns of A using ColumnSelect algorithm**
  - **Select $r = O\left(\frac{k \log k}{\varepsilon^2}\right)$ rows of A using ColumnSelect algorithm**
  - **Set $U = W^+$**
- **Then:** $\|A - CUR\|_F \leq (2 + \epsilon)\, \|A - A_k\|_F$ with probability 98%

CUR: Pros & Cons

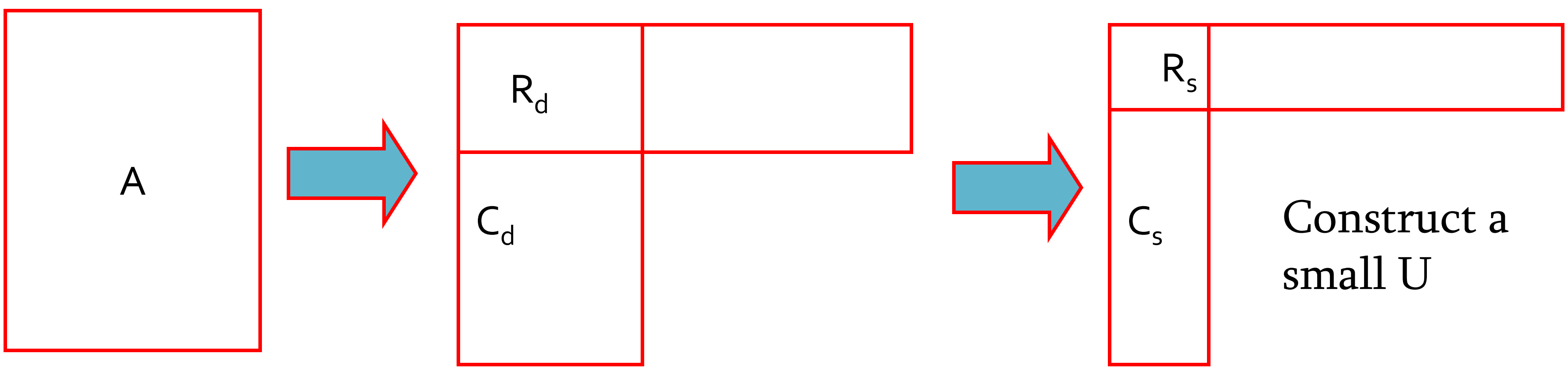
+ **Easy interpretation**
  - Since the basis vectors are actual columns and rows
+ **Sparse basis**
  - Since the basis vectors are actual columns and rows



- **Duplicate columns and rows**
  - Columns of large norms will be sampled many times

Solution

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



SVD vs. CUR

sparse and small

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

Huge but sparse Big and dense

dense but small

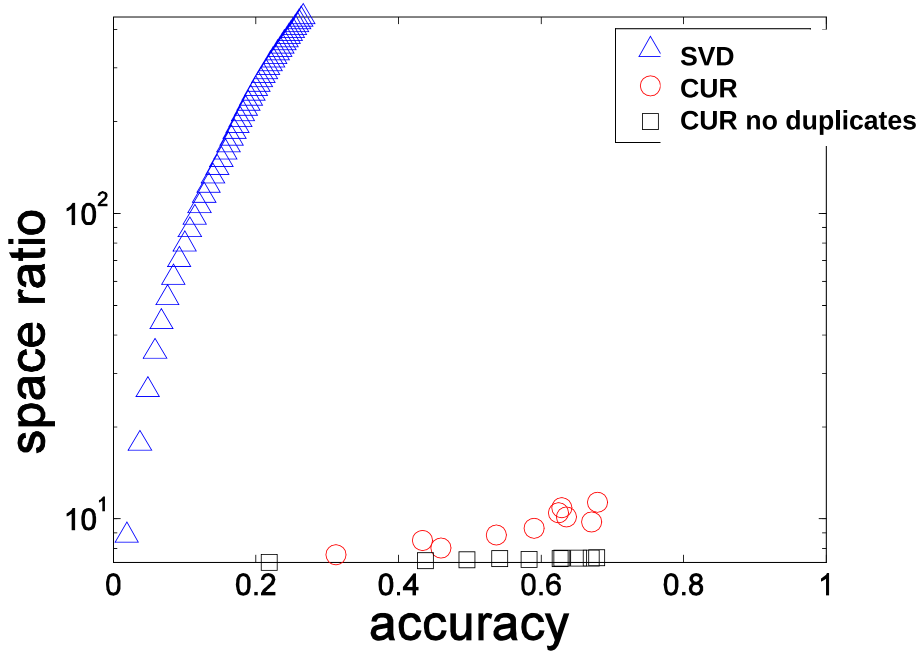
$$\text{CUR:}\quad A = C\,U\,R$$

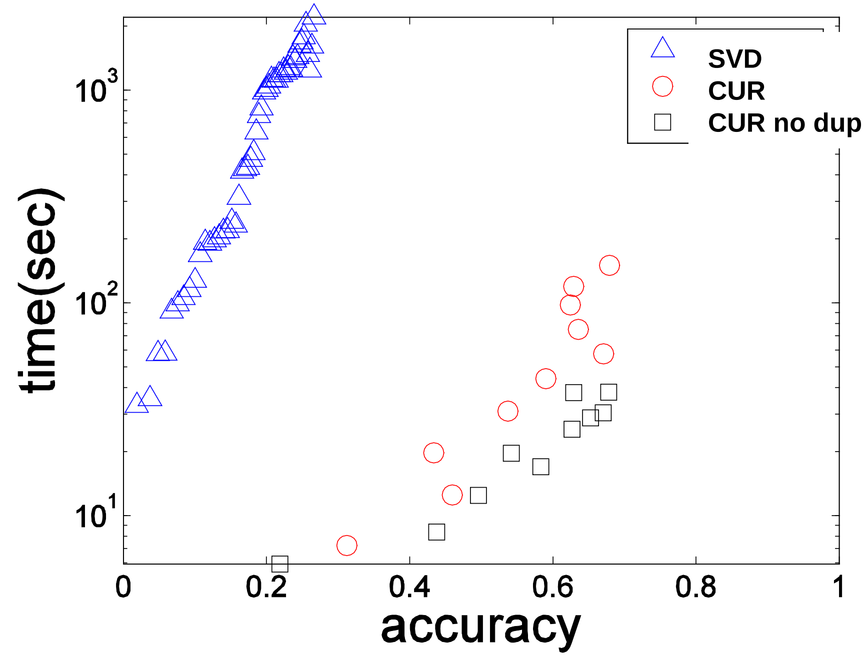
Huge but sparse Big but sparse

Simple Experiment

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

Results: DBLP- big sparse matrix



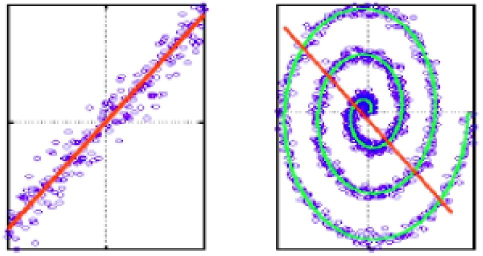


- **Accuracy:**
  - 1 – relative sum squared errors
- **Space ratio:**
  - #output matrix entries / #input matrix entries
- **CPU time**

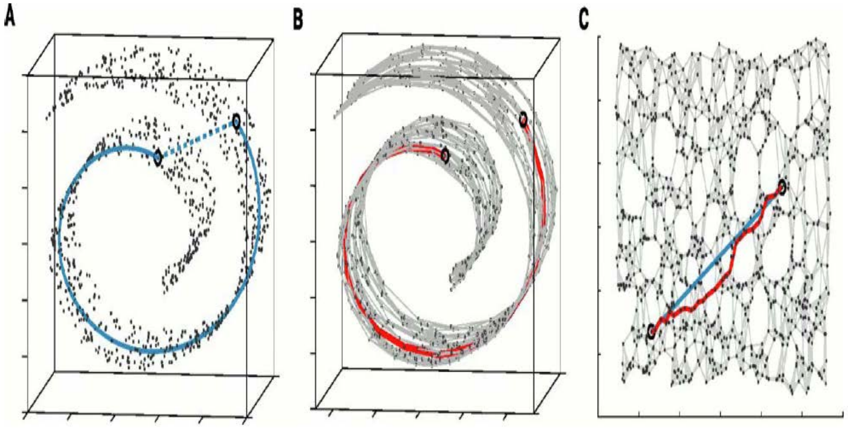
Sun, Faloutsos: *Less is More: Compact Matrix Decomposition for Large Sparse Graphs*, SDM '07.

What about linearity assumption?

- **SVD is limited to linear projections:**
  - Lower-dimensional linear projection that preserves Euclidean distances



- Non-linear methods: **Isomap**
  - Data lies on a nonlinear low-dim curve aka manifold
    - Use the distance as measured along the manifold
  - **How?**
    - Build adjacency graph
    - Geodesic distance is graph distance
    - SVD/PCA the graph pairwise distance matrix



Further Reading: CUR

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