

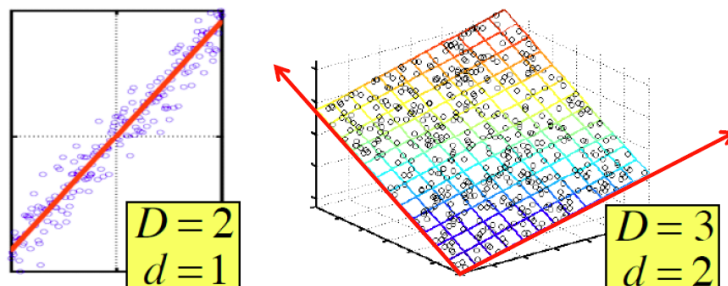
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Dimensionality Reduction: SVD & CUR

Mining of Massive Datasets
Jure Leskovec, Anand Rajaraman, Jeff Ullman
Stanford University
<http://www.mmnds.org>



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**

customer	day	We	Th	Fr	Sa	Su
		7/10/96	7/11/96	7/12/96	7/13/96	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
Johanson		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 $[0\ 0\ 0\ 1\ 1]$

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Rank of a Matrix

- **Q:** What is **rank** of a matrix **A**?
- **A:** Number of **linearly independent** columns of **A**
- **For example:**
 - Matrix $\mathbf{A} = \begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$ 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 : $[1\ 0]$ $[0\ 1]$ $[1\ -1]$

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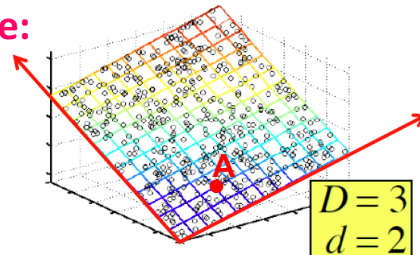
Rank is "Dimensionality"

- Cloud of points 3D space:

- Think of point positions

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

1 row per point:



- We can rewrite coordinates more efficiently!

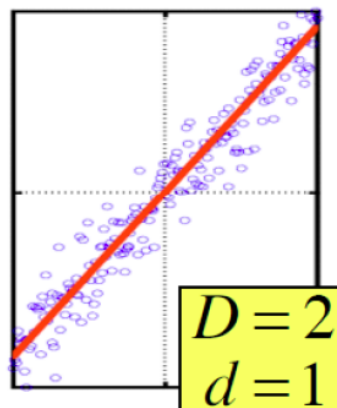
- Old basis vectors: $[1 \ 0 \ 0]$ $[0 \ 1 \ 0]$ $[0 \ 0 \ 1]$
- New basis vectors: $[1 \ 2 \ 1]$ $[-2 \ -3 \ 1]$
- Then **A** has new coordinates: $[1 \ 0]$. **B**: $[0 \ 1]$, **C**: $[1 \ -1]$
 - Notice: We reduced the number of coordinates!

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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

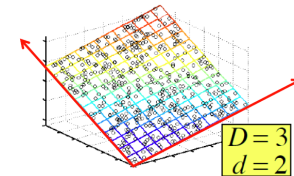
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Why Reduce Dimensions?

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**



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SVD - Definition

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

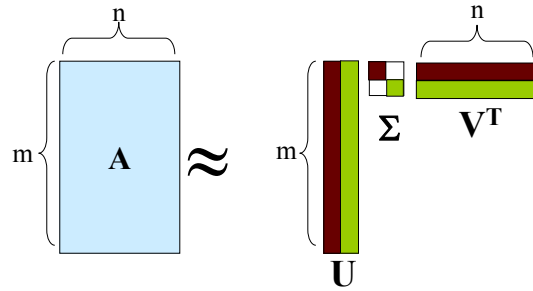
- **A: Input data matrix**
 - $m \times n$ matrix (e.g., m documents, n terms)
- **U: Left singular vectors**
 - $m \times r$ matrix (m documents, r concepts)
- **Σ : Singular values**
 - $r \times r$ diagonal matrix (strength of each 'concept')
 - (r : rank of the matrix **A**)
- **V: Right singular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

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SVD

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

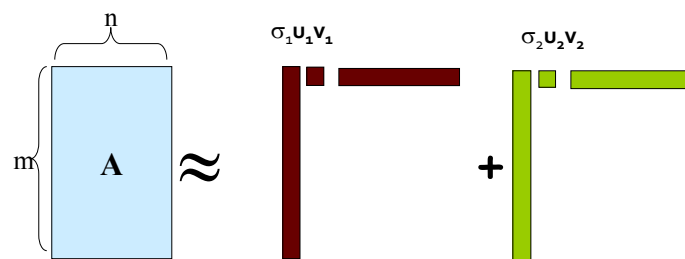


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SVD

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



σ_i ... scalar
 \mathbf{u}_i ... vector
 \mathbf{v}_i ... vector

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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 **positive**, and sorted in decreasing order ($\sigma_1 \geq \sigma_2 \geq \dots \geq 0$)

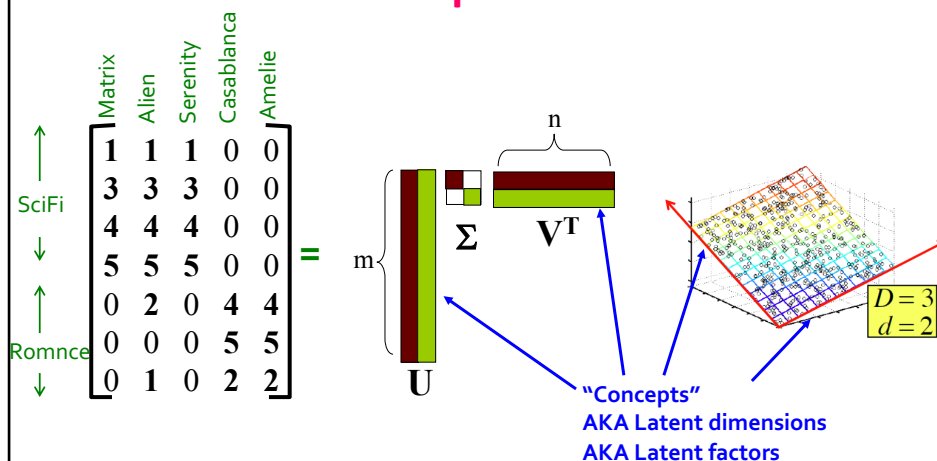
Nice proof of uniqueness: <http://www.mpi-inf.mpg.de/~bast/ir-seminar-wso4/lecture2.pdf>

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SVD – Example: Users-to-Movies

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



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SVD – Example: Users-to-Movies

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

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

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

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SVD – Example: Users-to-Movies

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		0	2	0	4	4		0.15	-0.59	0.65
↑	Romnce	0	0	0	5	5		0.07	-0.73	-0.67
↓		0	1	0	2	2		0.07	-0.29	0.32

SciFi-concept Romance-concept

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

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SVD – Example: Users-to-Movies

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

		Matrix	Alien	Serenity	Casablanca	Amelie		SciFi-concept	Romance-concept	
		1	1	1	0	0	0.13	0.02	-0.01	
↑	SciFi	3	3	3	0	0	0.41	0.07	-0.03	
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↓		0	2	0	4	4	0.15	-0.59	0.65	
		0	0	0	5	5	0.07	-0.73	-0.67	
		0	1	0	2	2	0.07	-0.29	0.32	

=

12.4	0	0
0	9.5	0
0	0	1.3

×

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

×

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SVD – Example: Users-to-Movies

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

		Matrix	Alien	Serenity	Casablanca	Amelie		SciFi-concept	
		1	1	1	0	0	0.13	0.02	-0.01
↑	SciFi	3	3	3	0	0	0.41	0.07	-0.03
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=

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×

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

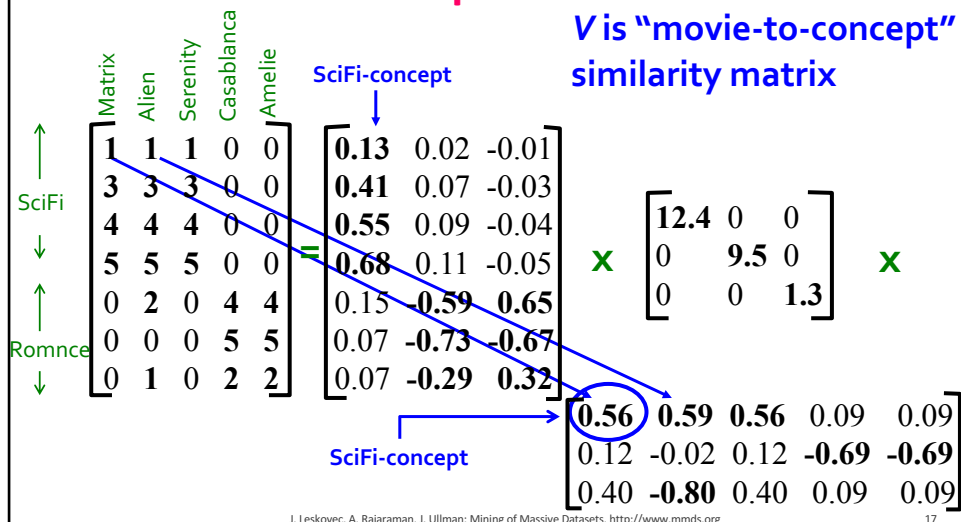
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"strength" of the SciFi-concept

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SVD – Example: Users-to-Movies

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

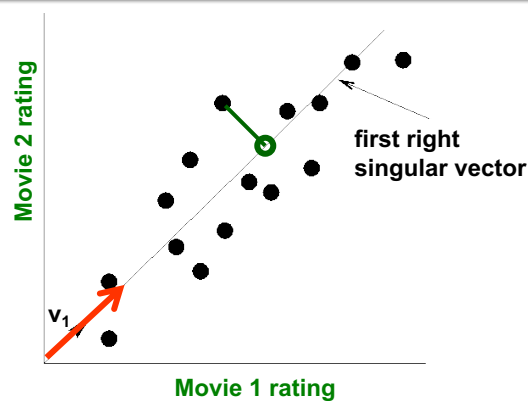


SVD - Interpretation #1

- ‘**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



- Instead of using two coordinates (x, y) to describe point locations, let's use only one coordinate (z)
- Point's position is its location along vector v_1
- How to choose v_1 ? **Minimize reconstruction error**

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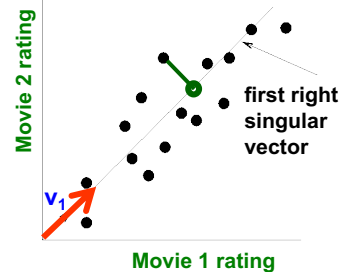
SVD – Dimensionality Reduction

- **Goal:** Minimize the sum of reconstruction errors:

$$\sum_{i=1}^N \sum_{j=1}^D \|x_{ij} - z_{ij}\|^2$$

- where x_{ij} are the “old” and z_{ij} are the “new” coordinates

- **SVD gives ‘best’ axis to project on:**
 - ‘best’ = minimizing the reconstruction errors
- In other words, **minimum reconstruction error**



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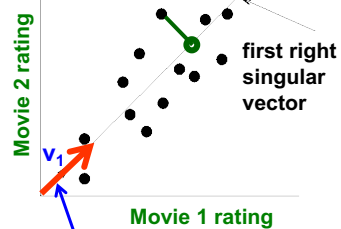
SVD - Interpretation #2

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

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

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

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



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SVD - Interpretation #2

■ $A = U \Sigma V^T$ - example:

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

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variance ('spread') on the v_1 axis

Movie 2 rating

Movie 1 rating

first right singular vector

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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 $(U \Sigma)^T$:

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

Movie 2 rating

Movie 1 rating

first right singular vector

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SVD - Interpretation #2

More details

- Q: How exactly is dim. reduction done?

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

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SVD - Interpretation #2

More details

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

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

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SVD - Interpretation #2

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

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

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

Frobenius norm:

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

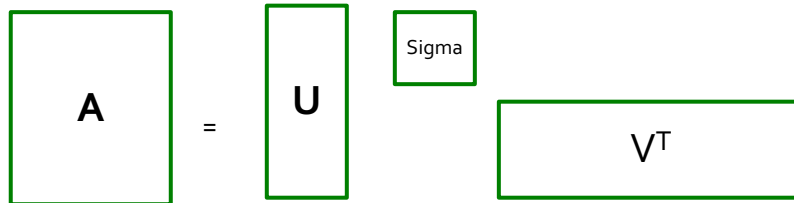
$$\|A-B\|_F = \sqrt{\sum_{ij} (A_{ij}-B_{ij})^2}$$

is "small"

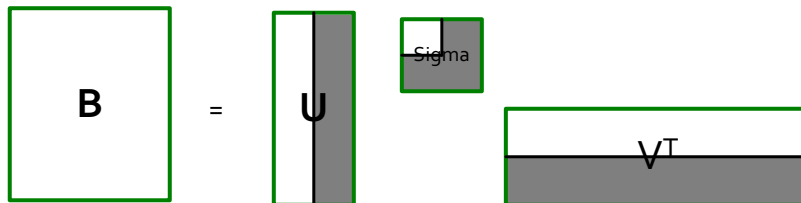
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SVD – Best Low Rank Approx.



B is best approximation of A



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SVD – Best Low Rank Approx.

- **Theorem:**

Let $A = U \Sigma V^T$ and $B = U S V^T$ where

S is **diagonal $r \times r$ matrix** with $s_i = \sigma_i$ ($i=1 \dots k$) else $s_i = 0$
then B is a **best rank(B)= k approx. to A**

What do we mean by “best”:

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

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

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

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SVD – Best Low Rank Approx.

Details!

- Theorem:** Let $A = U \Sigma V^T$ ($\sigma_1 \geq \sigma_2 \geq \dots$, $\text{rank}(A)=r$) then $B = U S V^T$
 - S = diagonal $r \times r$ matrix where $s_i = \sigma_i$ ($i=1 \dots k$) else $s_i=0$ is a best rank- k approximation to A :
 - B is a solution to $\min_B \|A-B\|_F$ where $\text{rank}(B)=k$

$$\begin{pmatrix} x_{11} & x_{12} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \dots & x_{mn} \end{pmatrix}_{m \times n} = \begin{pmatrix} u_{11} & \dots & u_{1r} \\ \vdots & \ddots & \vdots \\ u_{m1} & \dots & u_{mr} \end{pmatrix}_{m \times r} \begin{pmatrix} \sigma_{11} & 0 & \dots \\ 0 & \sigma_{22} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}_{r \times r} \begin{pmatrix} v_{11} & \dots & v_{1n} \\ \vdots & \ddots & \vdots \\ v_{r1} & \dots & v_{rn} \end{pmatrix}_{r \times n}$$

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

SVD – Best Low Rank Approx.

Details!

- We will need 2 facts:**
 - $\|M\|_F = \sum_k (q_{kk})^2$ where $M = P Q R$ is SVD of M

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

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

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

- We apply:**
- P column orthonormal
 - R row orthonormal
 - Q is diagonal

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

SVD – Best Low Rank Approx.

Details!

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

Why?

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

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

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

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

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SVD - Interpretation #2

Equivalent:

'spectral decomposition' of the matrix:

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

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SVD - Interpretation #2

Equivalent:

'spectral decomposition' of the matrix

$$\begin{matrix} \leftarrow m \rightarrow \\ \uparrow n \\ \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \end{matrix} = \begin{matrix} \leftarrow k \text{ terms} \rightarrow \\ \sigma_1 \begin{matrix} \swarrow u_1 \\ n \times 1 \end{matrix} \begin{matrix} \nwarrow v_1^T \\ 1 \times m \end{matrix} + \sigma_2 u_2 v_2^T + \dots \end{matrix}$$

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

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

Vectors u_i and v_i are unit length, so σ_i scales them.

So, zeroing small σ_i introduces less error.

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SVD - Interpretation #2

Q: How many σ_s to keep?

A: Rule-of-a thumb:

keep 80-90% of 'energy' = $\sum_i \sigma_i^2$

$$\begin{matrix} \leftarrow m \rightarrow \\ \uparrow n \\ \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \end{matrix} = \begin{matrix} \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \dots \end{matrix}$$

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

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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 ...

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SVD - Conclusions so far

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

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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 ($U^T U = I$),
 - Λ, Σ are diagonal
- Now let's calculate:
 - $AA^T =$
 - $A^T A = V \Sigma^T U^T (U \Sigma V^T) = V \Sigma \Sigma^T V^T$

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Relation to Eigen-decomposition

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 - Eigen-decomposition:
 - $A = X \Lambda X^T$
 - A is symmetric
 - U, V, X are orthonormal ($U^T U = I$),
 - Λ, Σ are diagonal
 - Now let's calculate:
 - $AA^T = U \Sigma V^T (U \Sigma V^T)^T = U \Sigma V^T (V \Sigma^T U^T) = U \Sigma \Sigma^T U^T$
 - $A^T A = V \Sigma^T U^T (U \Sigma V^T) = V \Sigma \Sigma^T V^T$
- Shows how to compute SVD using eigenvalue decomposition!
- ↓
- $X \Lambda^2 X^T$
- ↓ ↓ ↓
- $X \Lambda^2 X^T$

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SVD: Properties

- $\mathbf{A} \mathbf{A}^T = \mathbf{U} \Sigma^2 \mathbf{U}^T$
- $\mathbf{A}^T \mathbf{A} = \mathbf{V} \Sigma^2 \mathbf{V}^T$
- $(\mathbf{A}^T \mathbf{A})^k = \mathbf{V} \Sigma^{2k} \mathbf{V}^T$
 - E.g.: $(\mathbf{A}^T \mathbf{A})^2 = \mathbf{V} \Sigma^2 \mathbf{V}^T \mathbf{V} \Sigma^2 \mathbf{V}^T = \mathbf{V} \Sigma^4 \mathbf{V}^T$
- $(\mathbf{A}^T \mathbf{A})^k \sim v_1 \sigma_1^{2k} v_1^T$ for $k \gg 1$

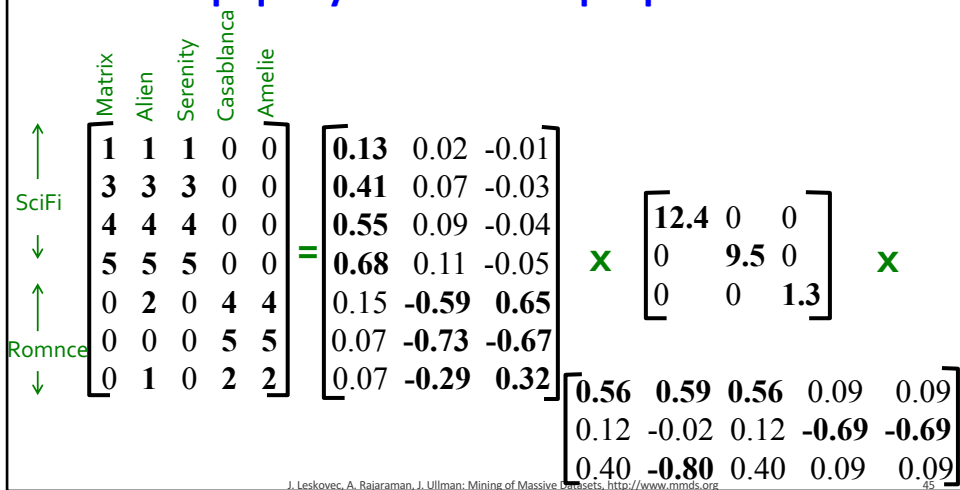
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Example of SVD & Conclusion

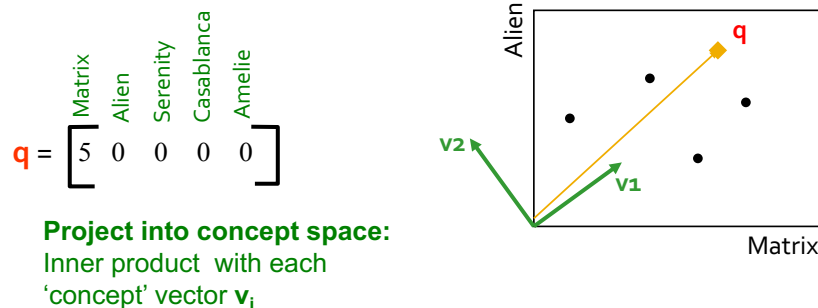
Case study: How to query?

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



Case study: How to query?

- Q: Find users that like 'Matrix'
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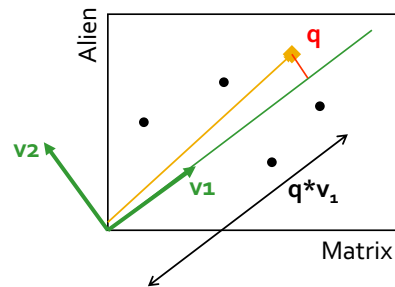


Case study: How to query?

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

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

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



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Case study: How to query?

Compactly, we have:

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

E.g.:

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

movie-to-concept similarities (V)

SciFi-concept
↓
=

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Case study: How to query?

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

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

E.g.:

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

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

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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!**

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

Zero ratings in common Similarity $\neq 0$

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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!**

The diagram shows a matrix with 6 dots (representing a sparse matrix) on the left, followed by an equals sign, and then three matrices on the right: a dense matrix labeled U , a diagonal matrix labeled Σ , and a dense matrix labeled V^T . This illustrates that the singular vectors U and V^T are dense, even when the original matrix is sparse.

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CUR Decomposition

CUR Decomposition

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

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

$$\left(\begin{array}{|c|} \hline A \\ \hline \end{array} \right) \approx \left(\begin{array}{|c|} \hline C \\ \hline \end{array} \right) \cdot \left(\begin{array}{|c|} \hline U \\ \hline \end{array} \right) \cdot \left(\begin{array}{|c|} \hline R \\ \hline \end{array} \right)$$

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CUR Decomposition

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Pseudo-inverse of the intersection of C and R

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CUR: Provably good approx. to SVD

- **Let:**
 \mathbf{A}_k be the “best” rank k approximation to \mathbf{A} (that is, \mathbf{A}_k is SVD of \mathbf{A})

Theorem [Drineas et al.]

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

- $\|\mathbf{A} - \mathbf{CUR}\|_F \leq \|\mathbf{A} - \mathbf{A}_k\|_F + \epsilon \|\mathbf{A}\|_F$

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

- $O(k \log(1/\delta)/\epsilon^2)$ columns, and
- $O(k^2 \log^3(1/\delta)/\epsilon^6)$ rows

In practice:
Pick 4k cols/rows

CUR: How it Works

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

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

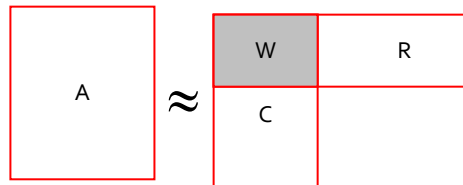
Output: $\mathbf{C}_d \in \mathbb{R}^{m \times c}$

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



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CUR: Provably good approx. to SVD

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

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

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CUR: Pros & Cons

+ Easy interpretation

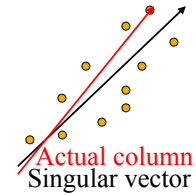
- Since the basis vectors are actual columns and rows

+ Sparse basis

- Since the basis vectors are actual columns and rows

- Duplicate columns and rows

- Columns of large norms will be sampled many times



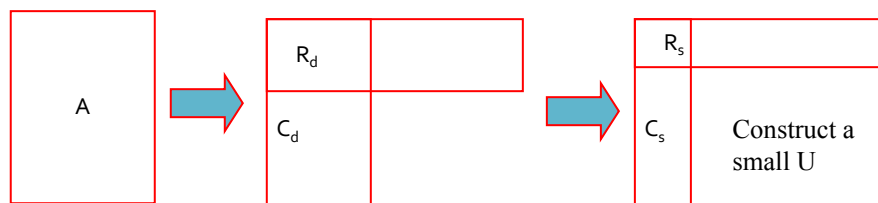
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Solution

■ 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



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SVD vs. CUR

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

sparse and small (pointing to Σ)
 Huge but sparse (pointing to A)
 Big and dense (pointing to U and V^T)

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

dense but small (pointing to U)
 Huge but sparse (pointing to A)
 Big but sparse (pointing to C and R)

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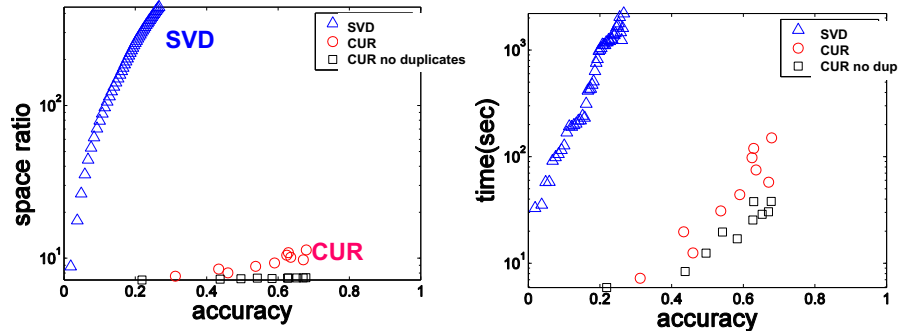
SVD vs. CUR: Simple Experiment

- **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?

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Results: DBLP- big sparse matrix



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

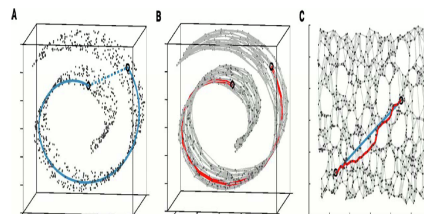
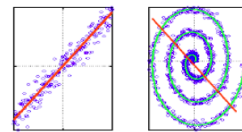
Sun, Faloutsos: *Less is More: Compact Matrix Decomposition for Large Sparse Graphs*, SDM '07.

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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



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Further Reading: CUR

- Drineas et al., *Fast Monte Carlo Algorithms for Matrices III: Computing a Compressed Approximate Matrix Decomposition*, SIAM Journal on Computing, 2006.
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