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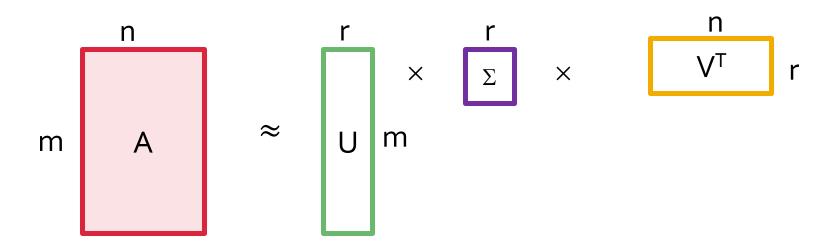
Dimensionality Reduction: SVD & CUR

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



Reducing Matrix Dimension

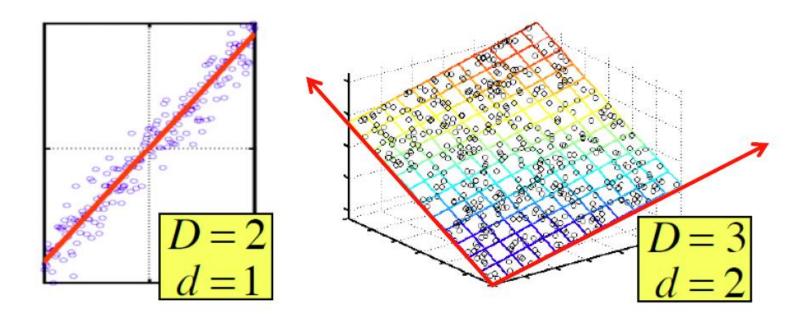
- Often, our data can be represented by an m-by-n matrix
- And this matrix can be closely approximated by the product of three matrices that share a small common dimension r



- Compress / reduce dimensionality:
 - 10⁶ rows; 10³ columns; no updates
 - Random access to any cell(s); small error: OK

day	We	${f Th}$	\mathbf{Fr}	\mathbf{Sa}	$\mathbf{S}\mathbf{u}$	New
customer	7/10/96	7/11/96	7/12/96	7/13/96	7/14/96	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]
\mathbf{Smith}	0	0	0	2	2	[0 2]
Johnson	0	0	0	3	3	[0 3]
Thompson	0	0	0	1	1	[0 1]

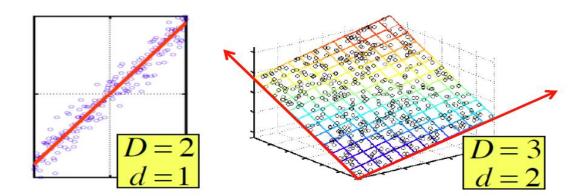
Note: The above matrix is really "2-dimensional." All rows can be reconstructed by scaling [1 1 1 0 0] or [0 0 0 1 1]



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

The axes of these dimensions can be chosen by:

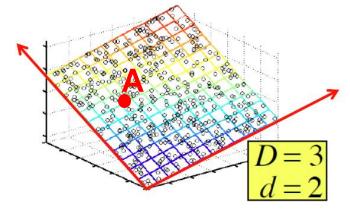
- The first dimension is the direction in which the points exhibit the greatest variance
- The second dimension is the direction, orthogonal to the first, in which points show the 2nd greatest variance
- And so on..., until you have enough dimensions that variance is really low



Rank is "Dimensionality"

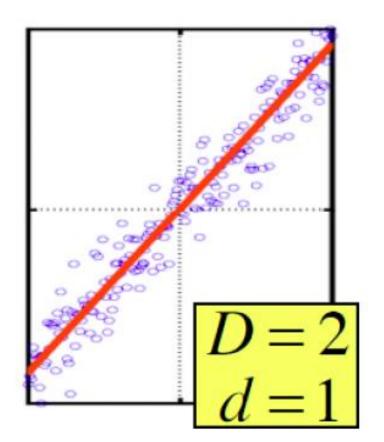
- Q: What is rank of a matrix A?
- A: Number of linearly independent rows of A
- Cloud of points in 3D space:

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



- We can rewrite coordinates more efficiently!
 - Old basis vectors: [1 0 0] [0 1 0] [0 0 1]
 - New basis vectors: [1 2 1] [-2 -3 1]
 - Then A has new coordinates: [1 0], B: [0 1], C: [1 -1]
 - Notice: We reduced the number of dimensions/coordinates!

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



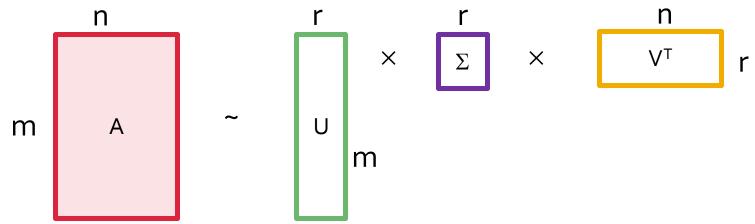
Rather than representing every point with 2 coordinates we represent each point with 1 coordinate (corresponding to the position of the point on the red line).

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

SVD: Singular Value Decomposition

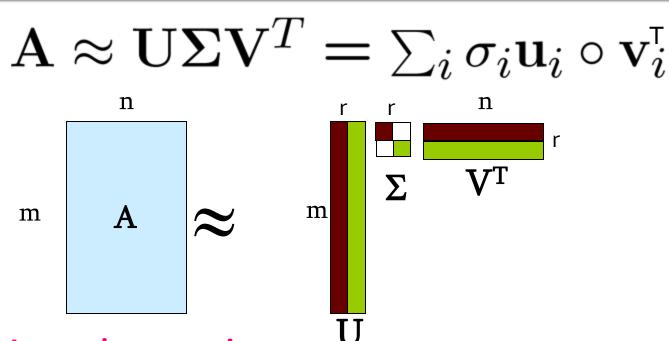
Reducing Matrix Dimension

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



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

SVD – Definition



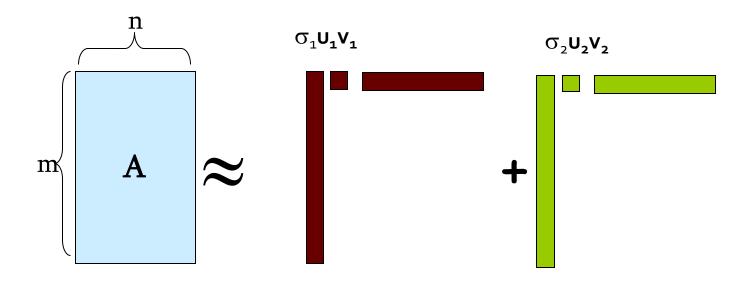
- A: Input data matrix
 - $\mathbf{m} \times \mathbf{n}$ matrix (e.g., m documents, n terms)
- U: Left singular vectors
 - m x r matrix (m documents, r concepts)
- Σ : Singular values
 - r x r diagonal matrix (strength of each 'concept') (r: rank of the matrix A)
- V: Right singular vectors
- n x r matrix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

 1/20/22 n x r matrix (n terms, r concepts)

 Les kovec, Stanford CS246: Mining Massive Datasets

SVD

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



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

σ_i ... scalar

u_i ... vector

v_i ... vector

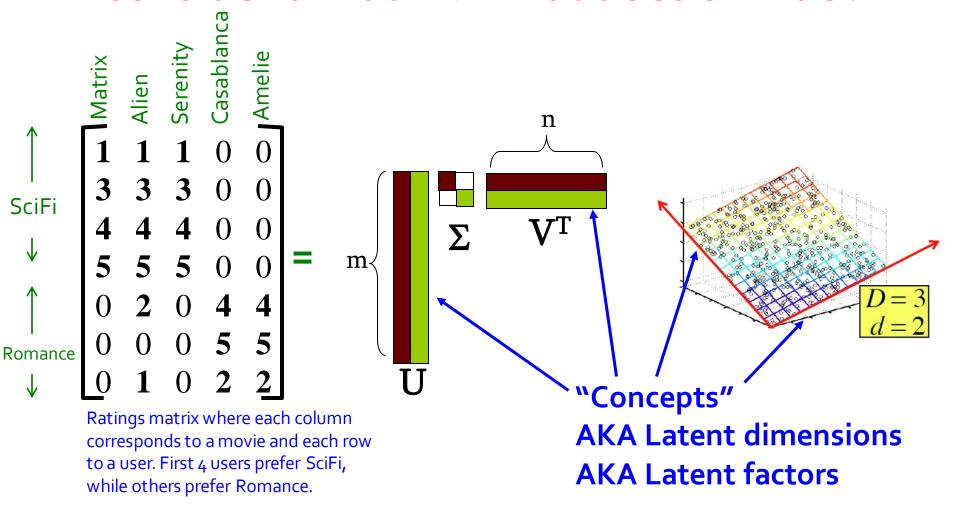
SVD – Properties

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

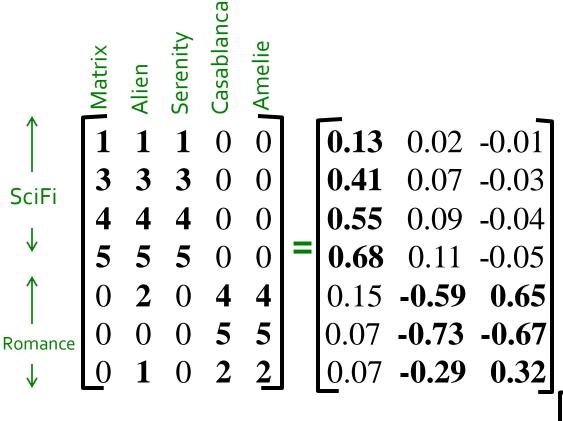
- **U**, Σ, **V**: unique
- U, V: column orthonormal
 - $U^T U = I$; $V^T V = I$ (I: identity matrix)
 - (Columns are orthogonal unit vectors)
- Σ: diagonal
 - Entries (singular values) are non-negative, and sorted in decreasing order $(\sigma_1 \ge \sigma_2 \ge ... \ge 0)$

Nice proof of uniqueness: https://www.cs.cornell.edu/courses/cs322/2008sp/stuff/TrefethenBau Lec4 SVD.pdf

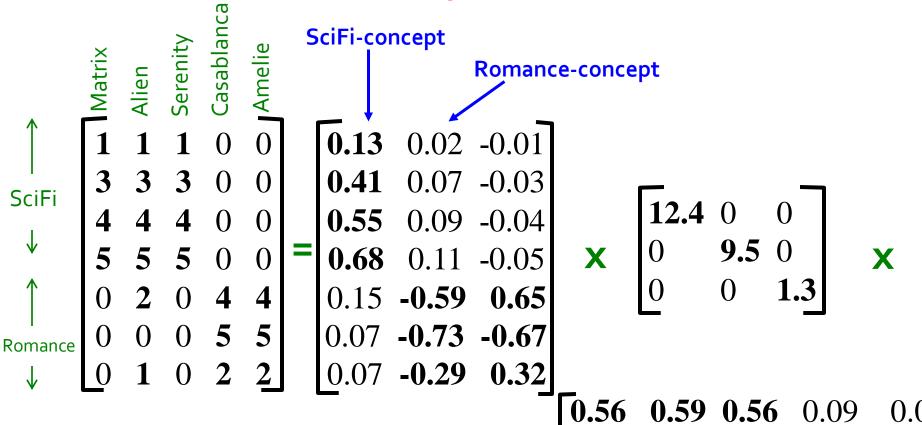
Consider a matrix. What does SVD do?



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



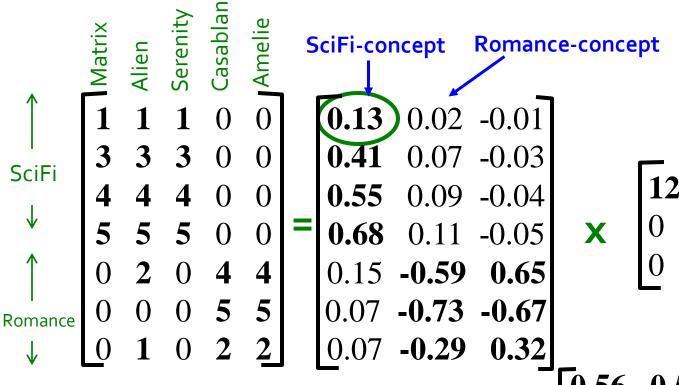
■ A = U Σ V^T - example: Users to Movies



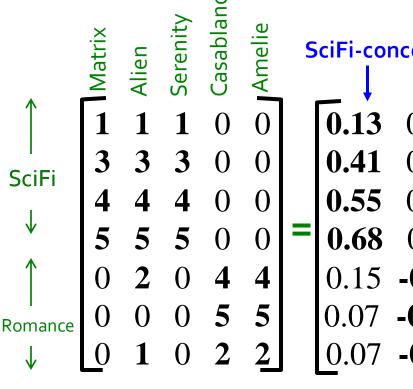
-0.02 0.12 **-0.69**

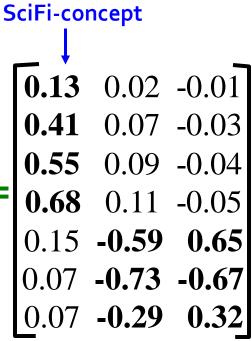
■ A = U $\sum V^T$ - example:

U is "user-to-concept" factor matrix

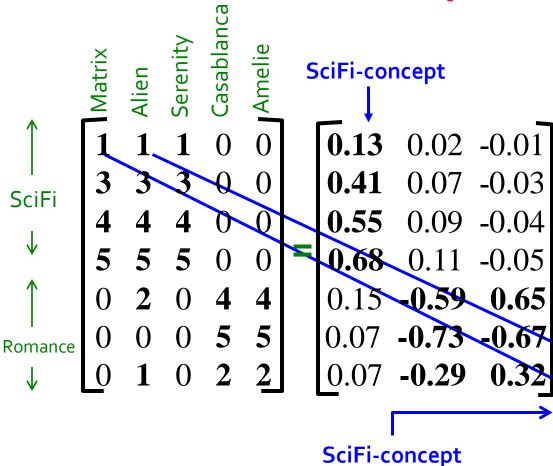


• $A = U \Sigma V^T$ - example:





• $A = U \Sigma V^T$ - example:



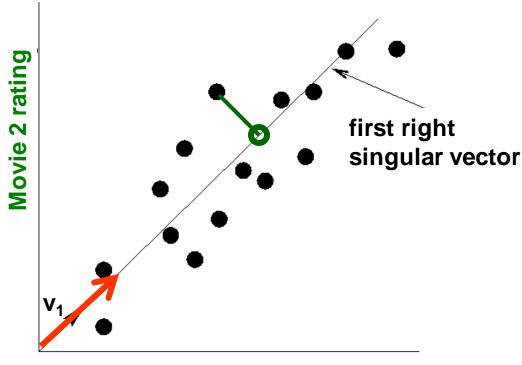
V is "movie-to-concept" factor matrix

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

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

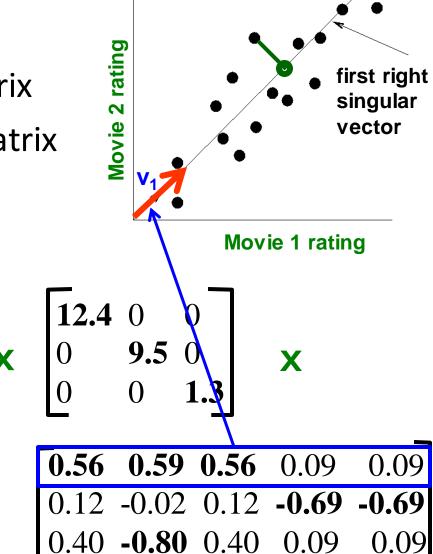


Movie 1 rating

- 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 $oldsymbol{v_1}$

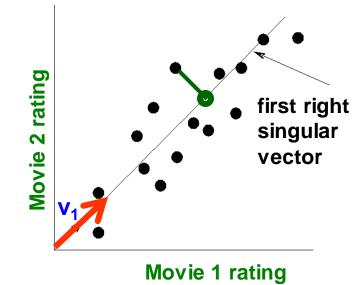
• $A = U \Sigma V^T$ - example:

- U: "user-to-concept" matrix
- V: "movie-to-concept" matrix

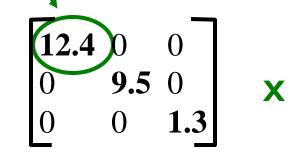




variance ('spread') on the v₁ axis

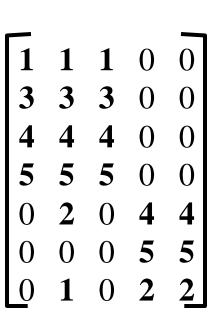


1	1	1	0	0
3	3	1 3 4 5	0	0
4	4	4	0	0
5	5	5	0	0

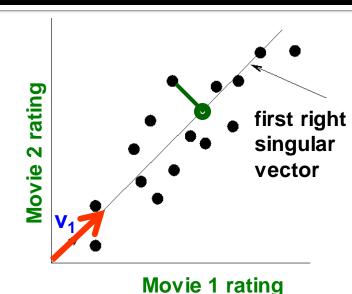


$A = U \Sigma V^{T}$ - example:

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



Projection of users on the "Sci-Fi" axis $U\Sigma$:



		_
1.61	0.19	-0.01
5.08	0.66	-0.03
6.82	0.85	-0.05
8.43	1.04	-0.06
1.86	-5.60	0.84
0.86	-6.93	-0.87
0.86	-2.75	0.41

More details

Q: How is dim. reduction done?

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

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- A: Set smallest singular values to zero

```
\begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 13 \end{bmatrix}
```

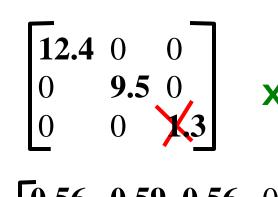
```
      0.56
      0.59
      0.56
      0.09
      0.09

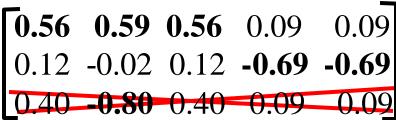
      0.12
      -0.02
      0.12
      -0.69
      -0.69

      0.40
      -0.80
      0.40
      0.09
      0.09
```

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

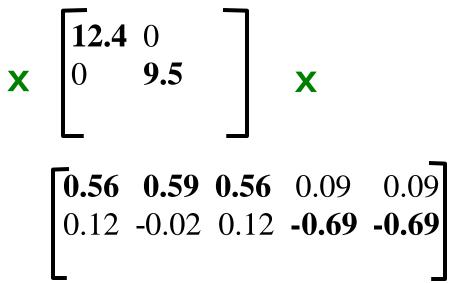
- Q: How exactly is dim. reduction done?
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This is Rank 2 approximation to A. We could also do Rank 1 approx. The larger the rank the more accurate the approximation.

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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

Reconstructed data matrix B

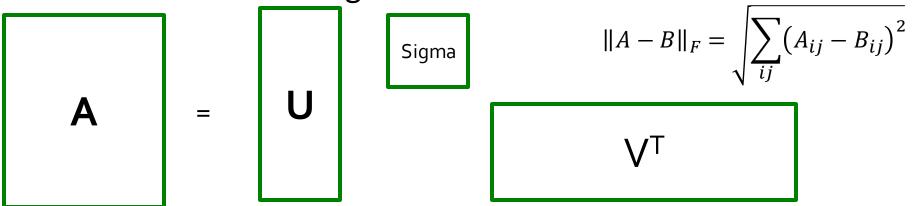
Reconstruction Error is quantified by the Frobenius norm:

$$\|\mathbf{M}\|_{\mathrm{F}} = \sqrt{\Sigma_{\mathrm{ij}} \, \mathbf{M}_{\mathrm{ij}}}^2$$

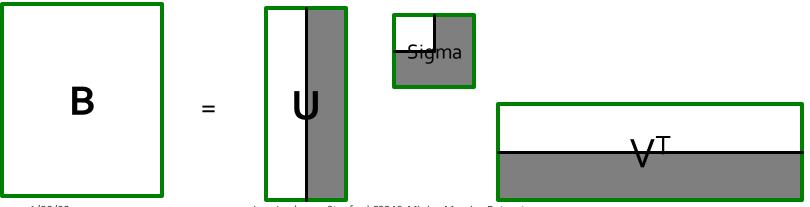
$$\|A - B\|_{F} = \sqrt{\sum_{ij} (A_{ij} - B_{ij})^{2}}$$
 is "small"

SVD – Best Low Rank Approx.

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



B is best approximation of A:



SVD – Best Low Rank Approx.

Theorem:

Let $A = U \sum V^T$ and $B = U \sum V^T$ where $S = diagonal r_{x}r$ matrix with $s_i = \sigma_i$ (i = 1...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 $\operatorname{rank}(B) = k$

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

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

SVD – Conclusions so far

- SVD: $A = U \Sigma V^T$: unique
 - U: user-to-concept factors
 - V: movie-to-concept factors
 - ullet 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
 - lacksquare M is $\emph{symmetric}$ if $m_{ij} = m_{ji}$ for all i and j
- Method:
 - Start with any "guess eigenvector" x₀
 - Construct $x_{k+1} = \frac{Mx_k}{||Mx_k||}$ for k = 0, 1, ...
 - | | ... | denotes the Frobenius norm
 - Stop when consecutive x_k show little change

Example: Iterative Eigenvector

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

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

$$\frac{\mathbf{M}\mathbf{x}_1}{||\mathbf{M}\mathbf{x}_1||} = \begin{bmatrix} 2.23 \\ 3.60 \end{bmatrix} / \sqrt{17.9}3 = \begin{bmatrix} 0.53 \\ 0.85 \end{bmatrix} = \mathbf{x}_2$$

.

Finding the Principal Eigenvalue

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

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

Finding More Eigenpairs

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

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

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

Example:

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

How to Compute the SVD

- Start by supposing $A = U \Sigma V^T$
- $A^T = (U\Sigma V^T)^T = (V^T)^T \Sigma^T U^T = V\Sigma U^T$
 - Why? (1) Rule for transpose of a product; (2) the transpose of the transpose and the transpose of a diagonal matrix are both the identity functions
- $A^TA = V \Sigma U^T U \Sigma V^T = V \Sigma^2 V^T$
 - Why? U is orthonormal, so U^TU 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
- $A^TAV = V\Sigma^2V^TV = V\Sigma^2$
 - Why? V is also orthonormal

Computing the SVD -(2)

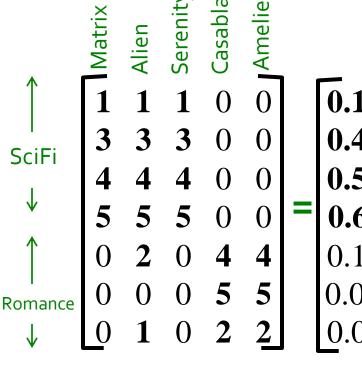
- Since $A^TA = V\Sigma^2V^T \rightarrow ATAV = V\Sigma^2$
 - Note that therefore the i-th column of V is an eigenvector of A^TA , and its eigenvalue is the i-th element of Σ^2
- Thus, we can find V and Σ by finding the eigenpairs for A^TA
 - Once we have the eigenvalues in Σ^2 , we can find the singular 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(nm²) or O(n²m) (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

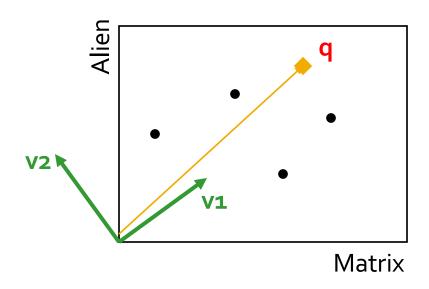
- Q: Find users that like 'Matrix'
- A: Map query into a 'concept space' how?



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Project into concept space:

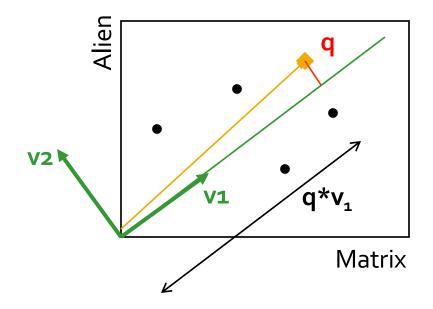
Inner product with each 'concept' vector **v**_i



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

Project into concept space:

Inner product with each 'concept' vector **v**_i



Compactly, we have:

$$q_{concept} = q V$$

E.g.:

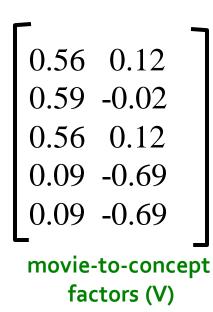
SciFi-concept
$$= \begin{bmatrix} 2.8 & 0.6 \end{bmatrix}$$

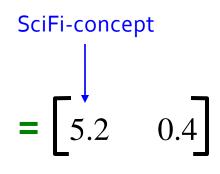
How would the user d that rated ('Alien', 'Serenity') be handled?

$$d_{concept} = d V$$

E.g.:

$$d = \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.12 \\ 0.59 & -0.02 \\ 0.56 & 0.12 \\ 0.00 & 0.60 \end{bmatrix}$$





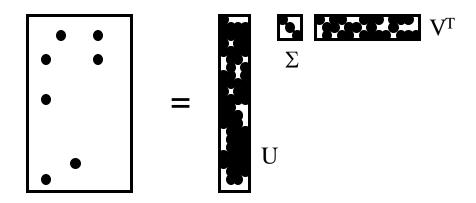
Observation: User d that rated ('Alien', 'Serenity') will be similar to user q that rated ('Matrix'), although d and q have zero ratings in common!

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!



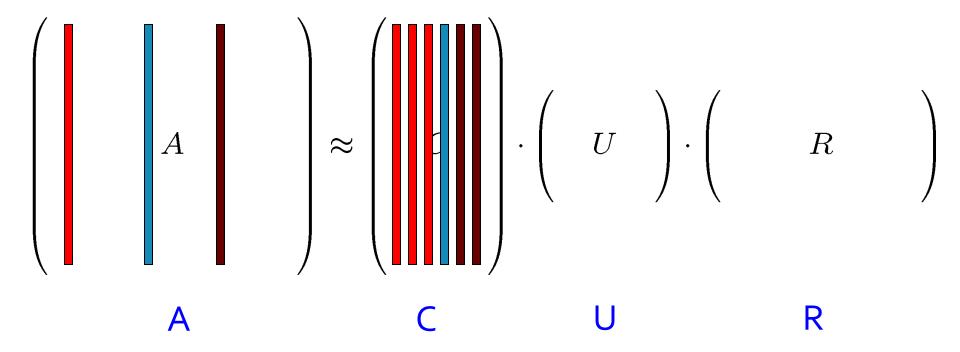
CUR Decomposition

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

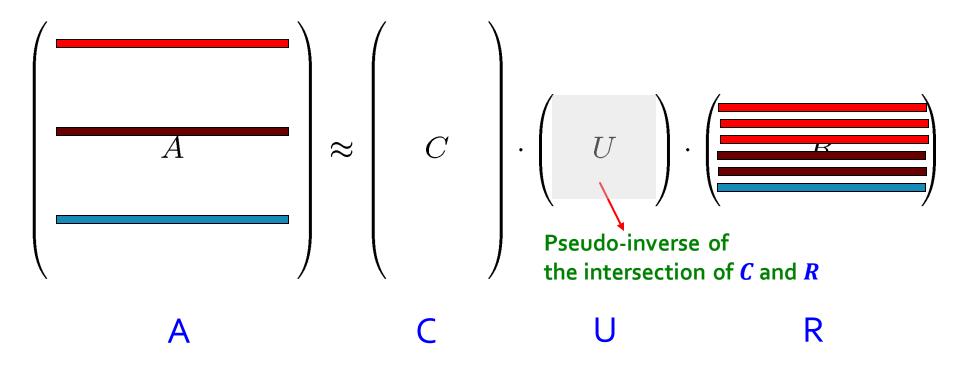
- Goal: Express A as a product of matrices C, U, R Make $\|A C \cdot U \cdot R\|_F$ small
- "Constraints" on C and R:



CUR Decomposition

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

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



Computing U

- Let W be the "intersection" of sampled columns
 - C and rows R
- Def: W⁺ is the pseudoinverse
 - Let SVD of $W = XZY^T$
 - Then: $W^{+} = Y Z^{+} X^{T}$



columns, C

~

70WS,

• Let: $U = Y(Z^+)^2 X^T$

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: $X^{-1} = X^T$, $Y^{-1} = Y^T$

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

Thus, if W is nonsingular, pseudoinverse is the true inverse

W

Which Rows and Columns?

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

CUR: Row Sampling Algorithm

Sampling columns (similarly for rows):

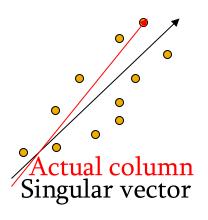
Input: matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, sample size c

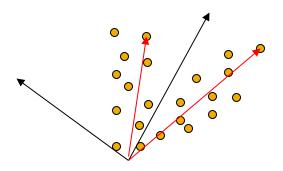
Output: $\mathbf{C}_d \in \mathbb{R}^{m \times c}$

- 1. for x = 1 : n [column distribution]
- 2. $P(x) = \sum_{i} \mathbf{A}(i, x)^{2} / \sum_{i,j} \mathbf{A}(i, j)^{2}$
- 3. for i = 1 : c [sample columns]
- 4. Pick $j \in 1 : n$ based on distribution P(x)
- 5. Compute $\mathbf{C}_d(:,i) = \mathbf{A}(:,j)/\sqrt{cP(j)}$

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

Intuition





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

CUR: Provably good approx. to SVD

For example:

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

In practice: Pick 4k cols/rows for a "rank-k" approximation

CUR: Pros & Cons

+ Easy interpretation

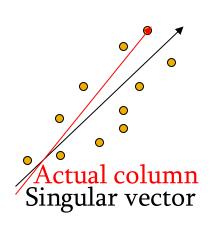
Since the basis vectors are actual columns and rows

+ Sparse basis

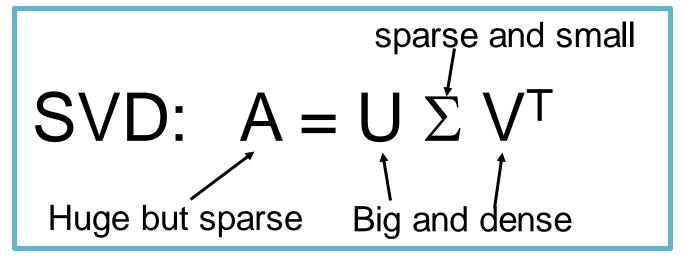
 Since the basis vectors are actual columns and rows

Duplicate columns and rows

 Columns of large norms will be sampled many times



SVD vs. CUR



CUR:
$$A = CUR$$

Huge but sparse

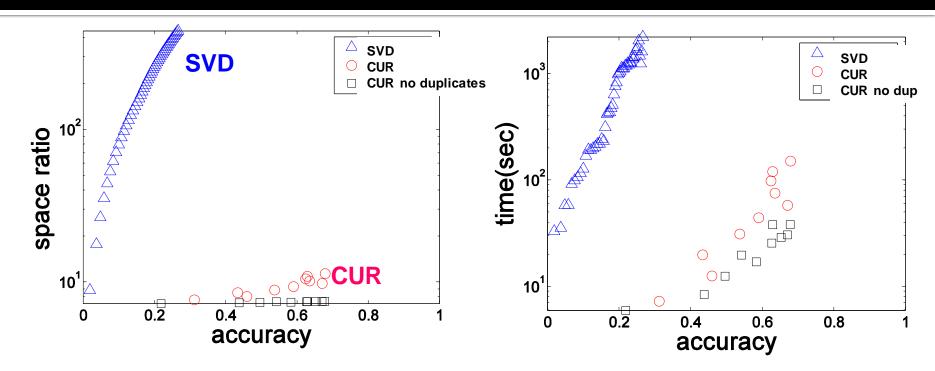
Big but sparse

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.