WANTED

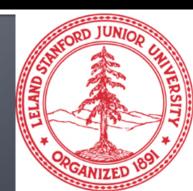
Graders

We need help grading the problem sets. Grading is paid 15\$/h. If interested send us email.

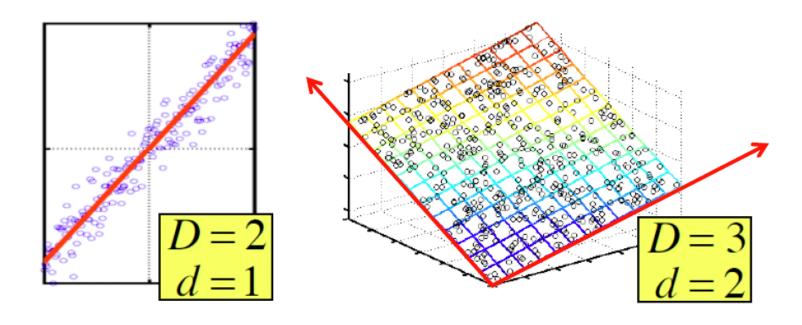
MERLU OCOLES CALWEL

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

\mathbf{day}	We	${ m Th}$	\mathbf{F} r	$\mathbf{S}\mathbf{a}$	$\mathbf{S}\mathbf{u}$
customer	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
\mathbf{Smith}	0	0	0	2	2
$_{ m Johnson}$	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

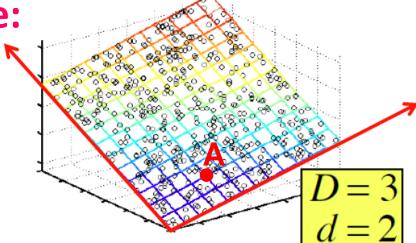
- Q: What is rank of a matrix A?
- A: Number of linearly independent rows of A
- For example:
 - Matrix $\mathbf{A} = \begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$ has rank $\mathbf{r} = \mathbf{2}$
 - Why? The first two rows are linearly independent, so the rank is at least 2, 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

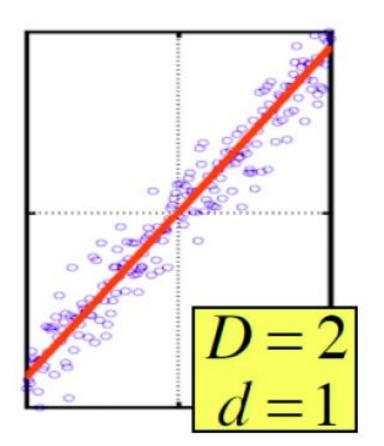
as a matrix: $\begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$ A B C



- 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 coordinates!

Dimensionality Reduction

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



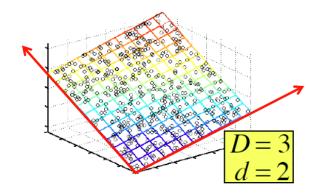
Rather than representing every point with 2 coordinates we represent each point with 1 coordinate (corresponding to the position of the point on the red line).

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



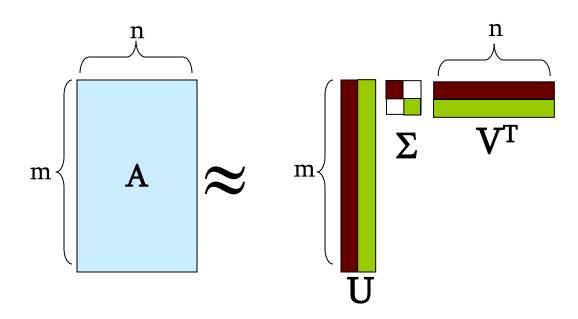
SVD - Definition

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

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

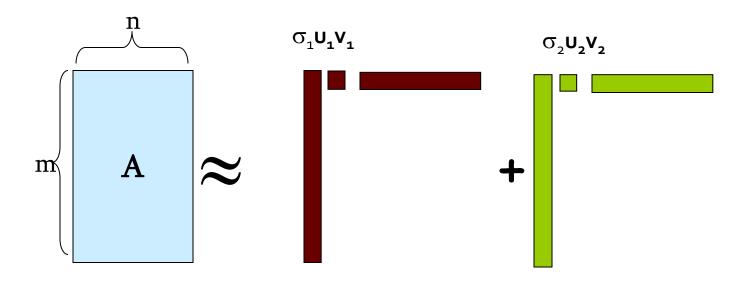
SVD

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



SVD

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



 σ_i ... scalar u_i ... vector v_i ... vector

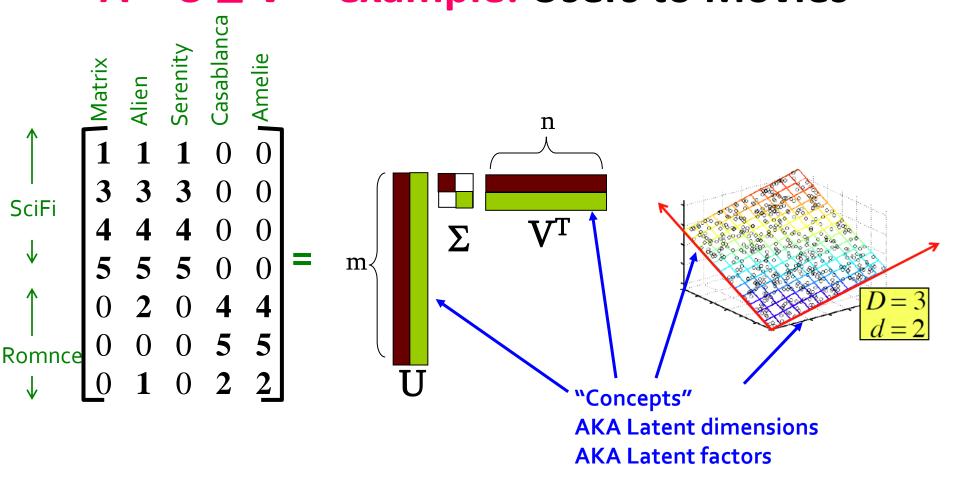
SVD - Properties

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

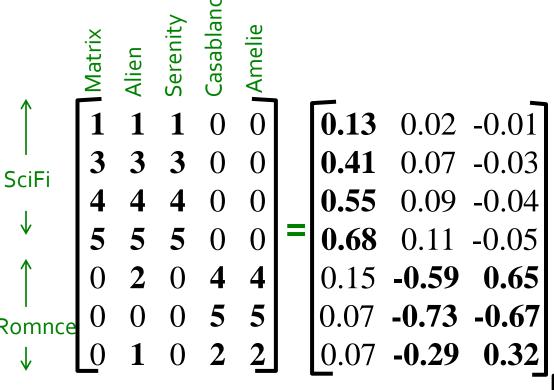
- **U**, Σ, *V*: unique
- U, V: column orthonormal
 - $U^T U = I$; $V^T V = I$ (I: identity matrix)
 - (Columns are orthogonal unit vectors)
- Σ: diagonal
 - Entries (singular values) are positive, and sorted in decreasing order $(\sigma_1 \ge \sigma_2 \ge ... \ge 0)$

Nice proof of uniqueness: http://www.mpi-inf.mpg.de/~bast/ir-seminar-ws04/lecture2.pdf

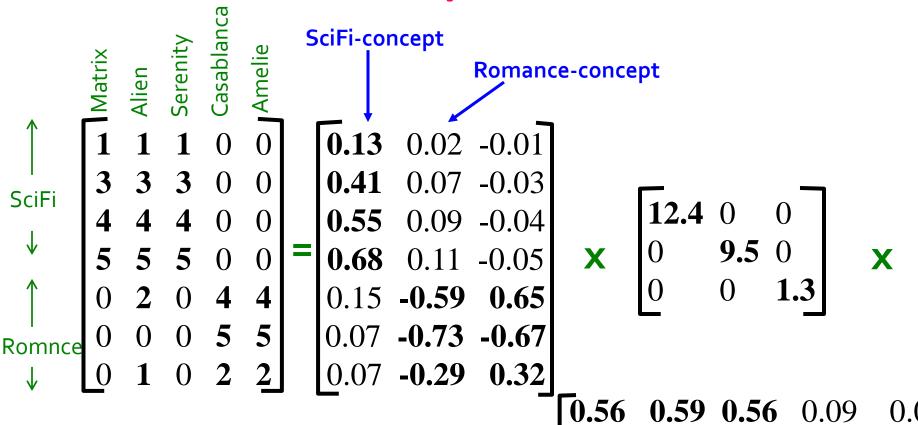
■ A = U Σ V^T - example: Users to Movies



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



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



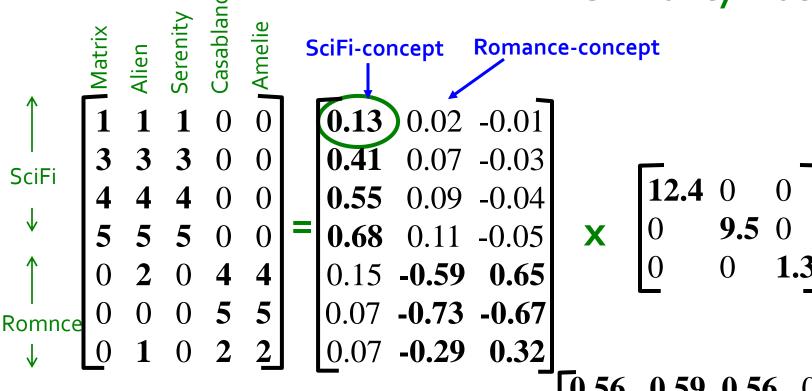
1/26/2015

-0.02 0.12 -0.69 -0.69

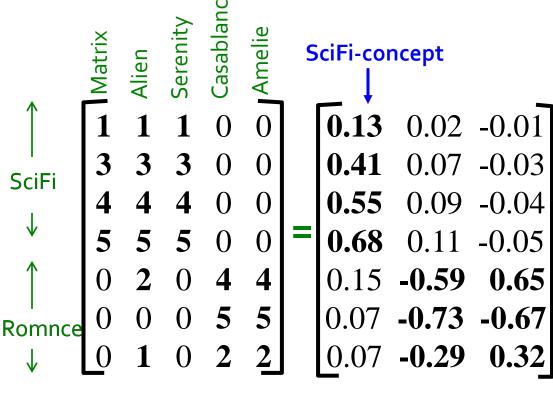
-0.80 0.40

■ $A = U \Sigma V^T$ - example:

U is "user-to-concept" similarity matrix



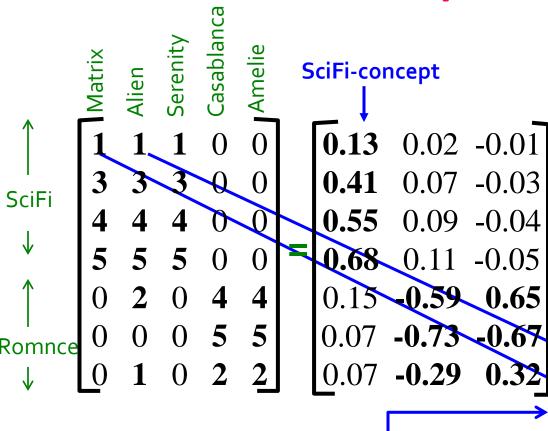
■ A = U Σ V^T - example:



"strength" of the SciFi-concept

(12.4)0 0
0 9.5 0
0 0 1.3

• $A = U \Sigma V^T$ - example:



V is "movie-to-concept" similarity matrix

$$\begin{array}{c|cccc}
\mathbf{X} & \begin{bmatrix}
\mathbf{12.4} & 0 & 0 \\
0 & \mathbf{9.5} & 0 \\
0 & 0 & \mathbf{1.3}
\end{bmatrix} \quad \mathbf{X}$$

0.56 0.59 0.56 0.09 0.09 0.12 -0.02 0.12 **-0.69** -**0.69**

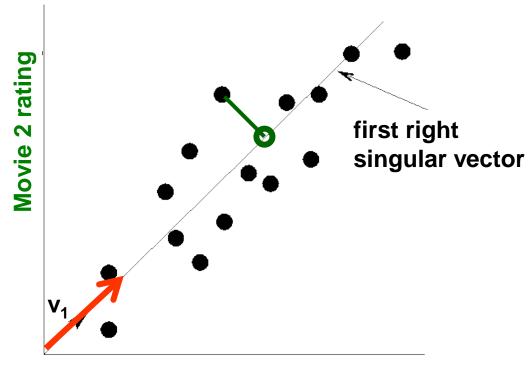
0.40 **-0.80** 0.40 0.09 0.09

'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



Movie 1 rating

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

SVD – Dimensionality Reduction

Goal: Minimize the sum of reconstruction errors:

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

first right singular vector

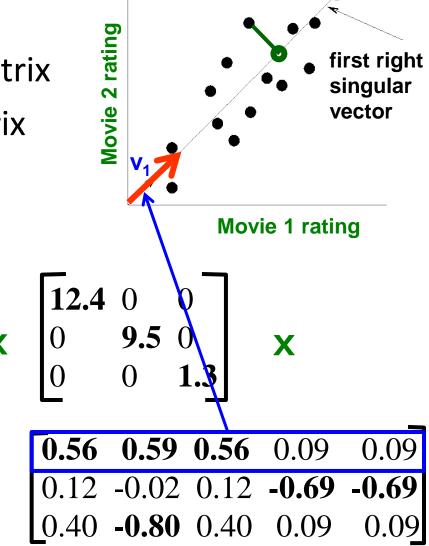
• where x_{ij} are the "old" and z_{ij} are the "new" coordinates

Movie 1 rating

- SVD gives 'best' axis to project on:
 - 'best' = minimizing the sum of reconstruction errors
- In other words, minimum reconstruction error

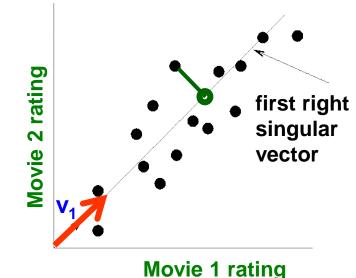
• $A = U \Sigma V^T$ - example:

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

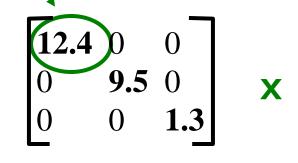




variance ('spread') on the v₁ axis

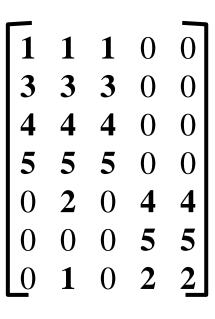


1	1	1	0	0	
3	3	3	0	0	
4	4	4	0	0	
5	5	5	0	0	=
0	2	0	4	4	
0	0	0	5	5	
0	1	0	2	2	

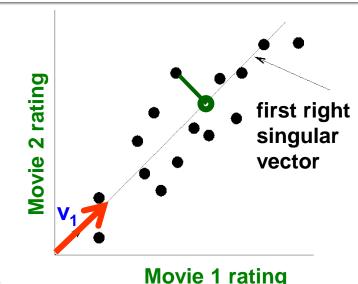


$A = U \Sigma V^{T}$ - example:

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



Projection of users on the "Sci-Fi" axis $(U \Sigma)^T$:



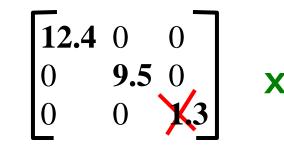
			_
ſ	1.61	0.19	-0.01
	5.08	0.66	-0.03
	6.82	0.85	-0.05
	8.43	1.04	-0.06
	1.86	-5.60	0.84
	0.86	-6.93	-0.87
L	0.86	-2.75	0.41

More details

Q: How exactly is dim. reduction done?

12.4 0 0 0 9.5 0 0 0 1.3

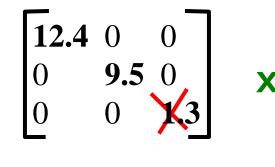
- Q: How exactly is dim. reduction done?
- A: Set smallest singular values to zero

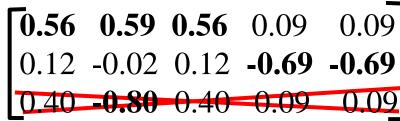


- Q: How exactly is dim. reduction done?
- A: Set smallest singular values to zero

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

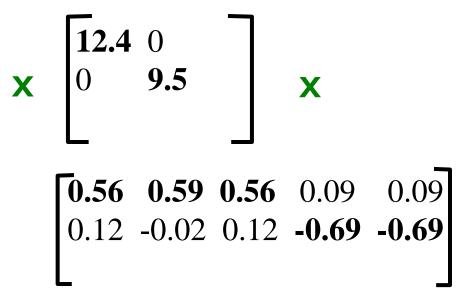
- Q: How exactly is dim. reduction done?
- A: Set smallest singular values to zero





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- 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
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the approximation

More details

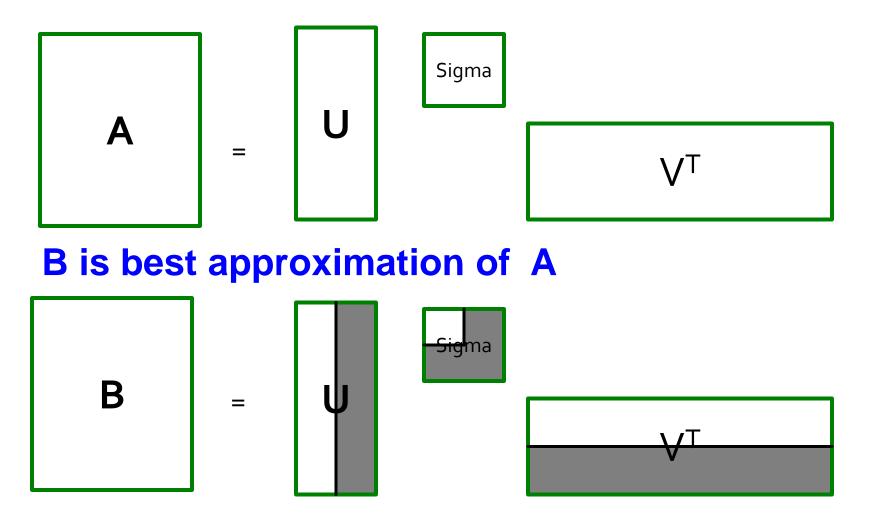
- Q: How exactly is dim. reduction done?
- A: Set smallest singular values to zero

Frobenius norm:

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

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

SVD – Best Low Rank Approx.



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 $\operatorname{rank}(B)=k$

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

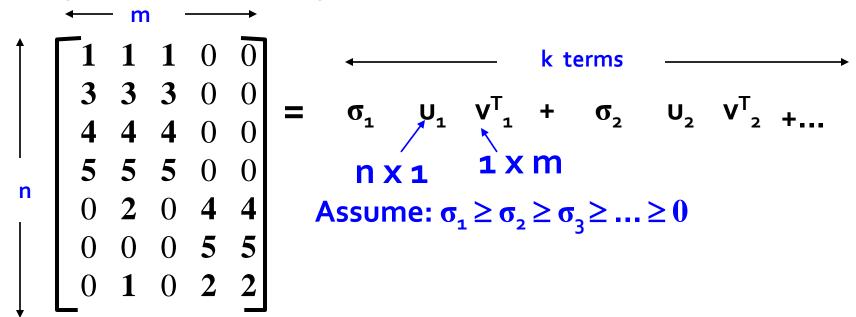
$$||A - B||_F = \sqrt{\sum_{ij} (A_{ij} - B_{ij})^2}$$

Equivalent:

'spectral decomposition' of the matrix:

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'spectral decomposition' of the matrix



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 (rather than large) σ_i introduces less error.

Q: How many σ_s to keep?

A: Rule-of-a thumb:

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

SVD - Complexity

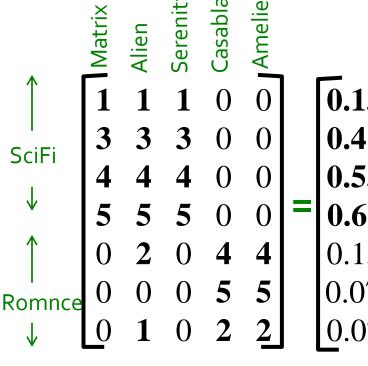
- To compute SVD:
 - O(nm²) or O(n²m) (whichever is less)
- But:
 - Less work, if we just want singular values
 - or if we want first k singular vectors
 - or if the matrix is sparse
- Implemented in linear algebra packages like
 - LINPACK, Matlab, SPlus, Mathematica ...

SVD - Conclusions so far

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

Example of SVD & Conclusion

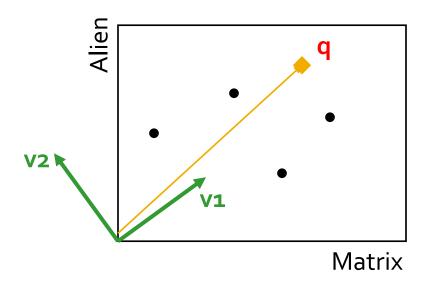
- Q: Find users that like 'Matrix'
- A: Map query into a 'concept space' how?



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

Project into concept space:

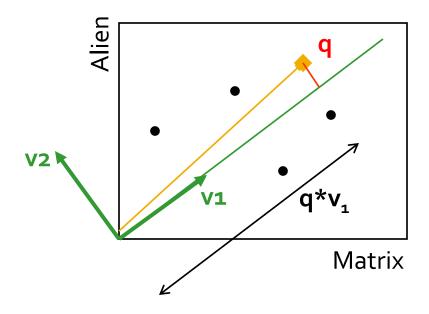
Inner product with each 'concept' vector **v**_i



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

Project into concept space:

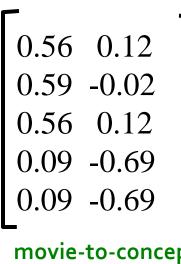
Inner product with each 'concept' vector $\mathbf{v_i}$



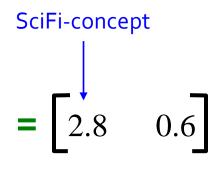
Compactly, we have:

$$q_{concept} = q V$$

E.g.:



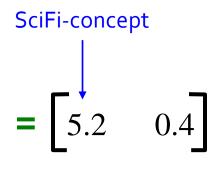
movie-to-concept similarities (V)



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

$$d_{concept} = d V$$

E.g.:

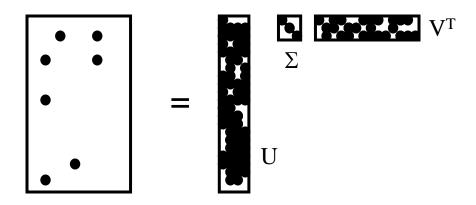


Observation: User d that rated ('Alien', 'Serenity') will be similar to user q that rated ('Matrix'), although d and q have zero ratings in common!

$$\mathbf{d} = \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \\ 5 & 0 & 0 & 0 & 0 \end{bmatrix} \quad \begin{array}{c} \text{SciFi-concept} \\ \text{SciFi-concept} \\ \text{SciFi-concept} \\ \text{Similarity} > 0 \\ \text{Similarit$$

SVD: Drawbacks

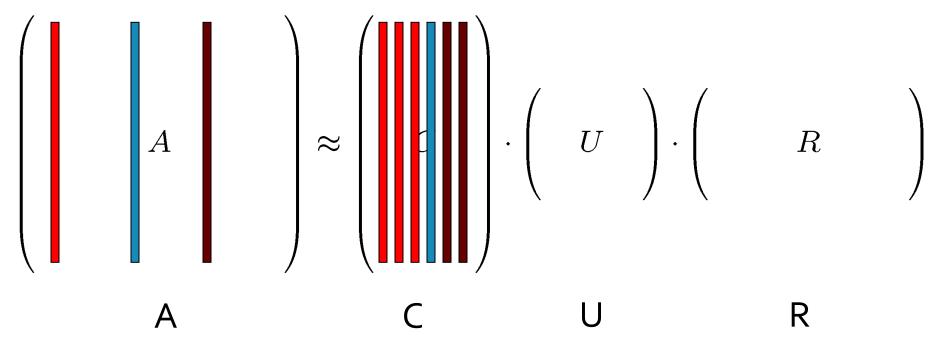
- Optimal low-rank approximation in terms of Frobenius norm
- Interpretability problem:
 - A singular vector specifies a linear combination of all input columns or rows
- Lack of sparsity:
 - Singular vectors are dense!



CUR Decomposition

CUR Decomposition

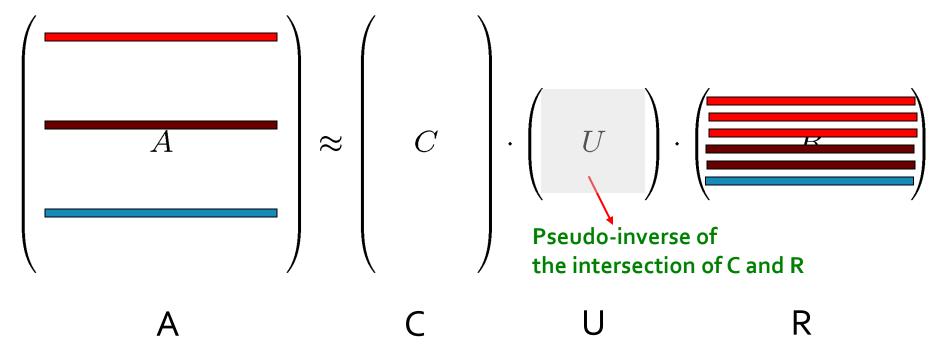
- Goal: Express A as a product of matrices C,U,R
 Make ||A-C·U·R||_F small
- "Constraints" on C and R:



CUR Decomposition

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

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



CUR: How it Works

Sampling columns (similarly for rows):

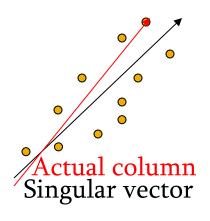
Input: matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, sample size c

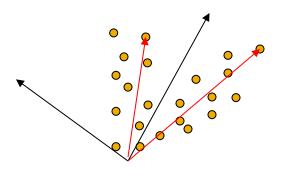
Output: $\mathbf{C}_d \in \mathbb{R}^{m \times c}$

- 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

Intuition



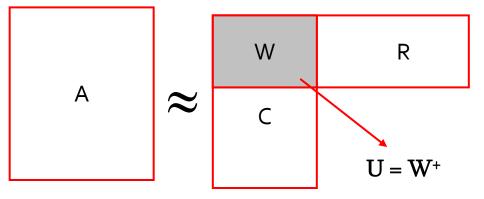


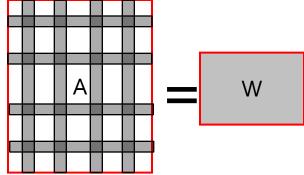
Rough and imprecise intuition behind CUR

- 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)

Computing U

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





Why the intersection?

these are high magnitude numbers

Why pseudoinverse works?

W = X Z Ythen $W^{-1} = Y^{-1} Z^{-1} X^{-1}$ 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 $c = O\left(\frac{k \log k}{\epsilon^2}\right)$ columns of A using ColumnSelect algorithm
- Select $r = O\left(\frac{k \log k}{\epsilon^2}\right)$ rows of A using ColumnSelect algorithm

• Set
$$U = W^+_{CUR error}$$

• Set
$$U = W^+_{\text{CUR error}}$$
 SVD error
• 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

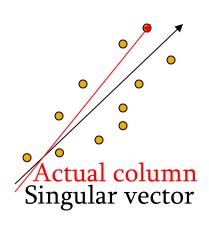
Since the basis vectors are actual columns and rows

Sparse basis

Since the basis vectors are actual columns and rows

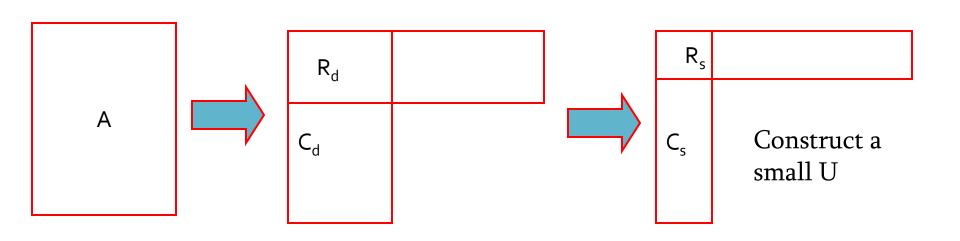


 Columns of large norms will be sampled many times

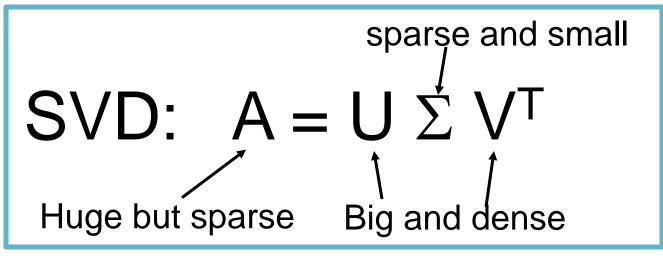


Solution

- 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

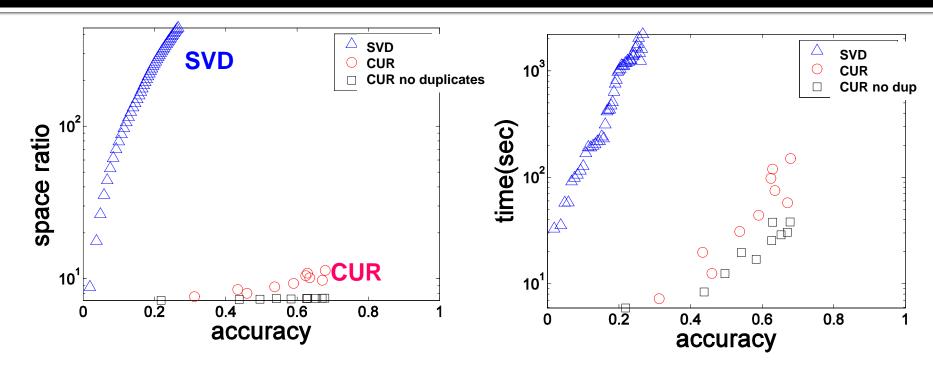


SVD vs. CUR: Simple Experiment

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:

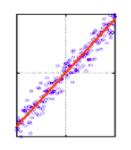
- 1 relative sum squared errors
- Space ratio:
 - #output matrix entries / #input matrix entries
- CPU time

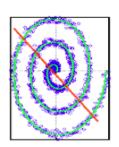
Sun, Faloutsos: Less is More: Compact Matrix Decomposition for Large Sparse Graphs, SDM '07.

What about linearity assumption?

SVD is limited to linear projections:

 Lower-dimensional linear projection that preserves Euclidean distances

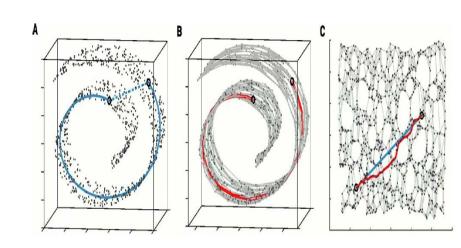




- Non-linear methods: Isomap
 - Data lies on a nonlinear low-dim curve aka manifold
 - Use the distance as measured along the manifold

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)