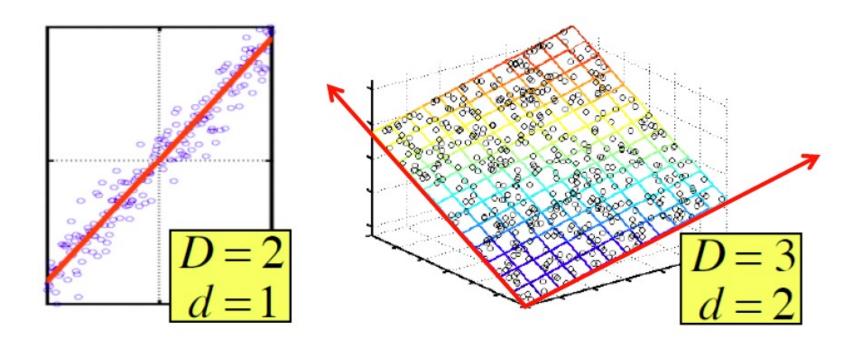
Dimensionality Reduction: SVD

Mining of Massive Datasets Jure Leskovec, Anand Rajaraman, Jeff Ullman Stanford University

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

\mathbf{day}	We	${f Th}$	\mathbf{Fr}	\mathbf{Sa}	$\mathbf{S}\mathbf{u}$
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
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

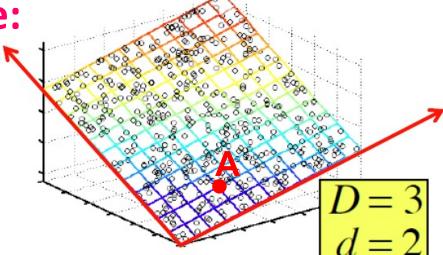
- Q: What is rank of a matrix A?
- A: Number of linearly independent columns of A
- For example:
 - Matrix $\mathbf{A} = \begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$ has rank $\mathbf{r} = \mathbf{2}$
 - Why? The first two rows are linearly independent, so the rank is at least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

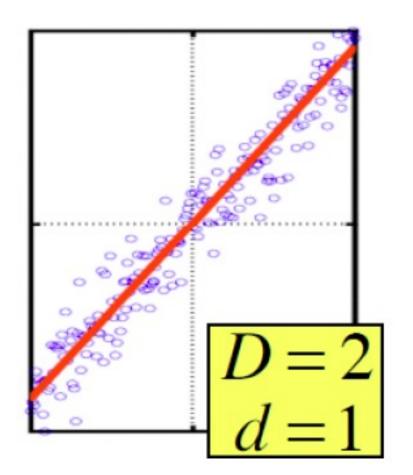
as a matrix: $\begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$ A B C



- 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!



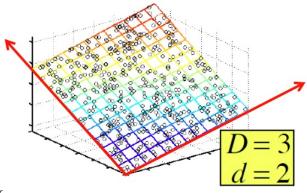
Rather than representing every point with 2 coordinates we represent each point with 1 coordinate (corresponding to the position of the point on the red line).

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

Why Reduce Dimensions?

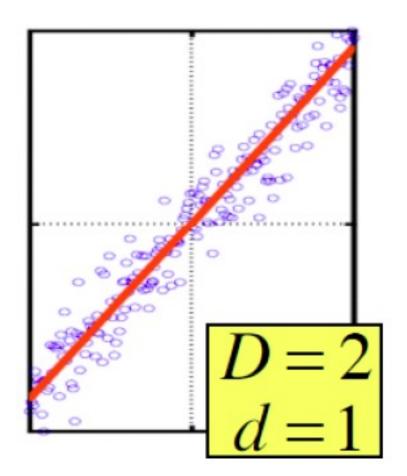
Why reduce dimensions?

- 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



Dimensionality Reduction

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



How to find the axis?

- Singular value decomposition
 - All matrix dimensions

$$X = USV^{T}$$

- Eigenvalue decomposition
 - Square matrix (covariance)

$$\mathbf{C} = \mathbf{V} \mathbf{L} \mathbf{V}^{\mathsf{T}},$$

SVD - Definition

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

- A: Input data matrix
 - m x n matrix (e.g., m users, n movies)
- U: Left singular vectors
 - m x r matrix (m users, 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 movies, r concepts)

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

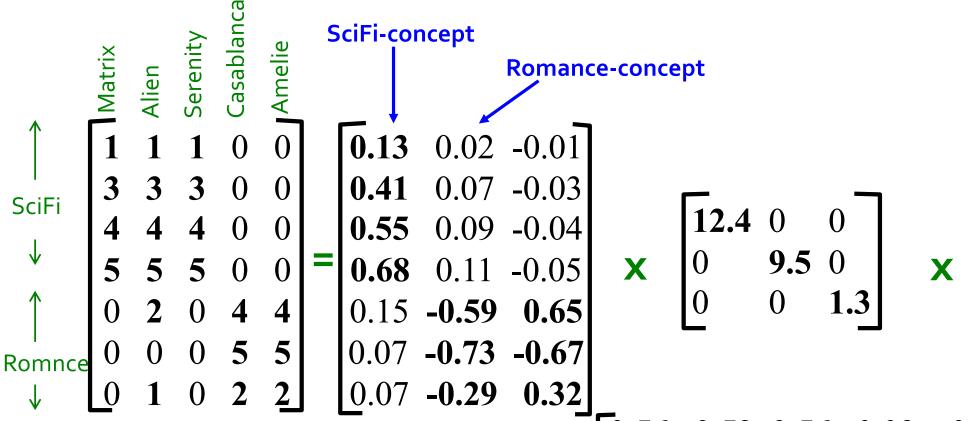
- U, Σ , V: unique
- U, V: column orthonormal
 - $U^T U = I$; $V^T V = I$ (I: identity matrix)
 - (Columns are orthogonal unit vectors)
- Σ: diagonal
 - Entries (singular values) are positive, and sorted in decreasing order ($\sigma_1 \ge \sigma_2 \ge ... \ge 0$)

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

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

Each user is represented by 5 reviews

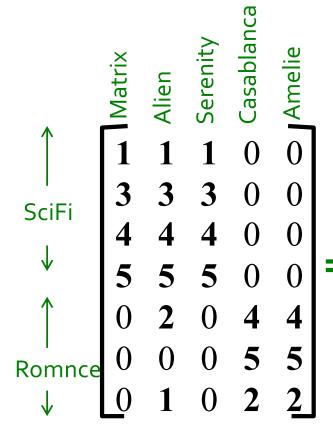
- $A = U \Sigma V^T$ - example: Users to Movies



Each user is represented by 5 reviews

• $A = U \Sigma V^T$ - example:

U is "user-to-concept" similarity matrix



SciFi-concept Romance-concept

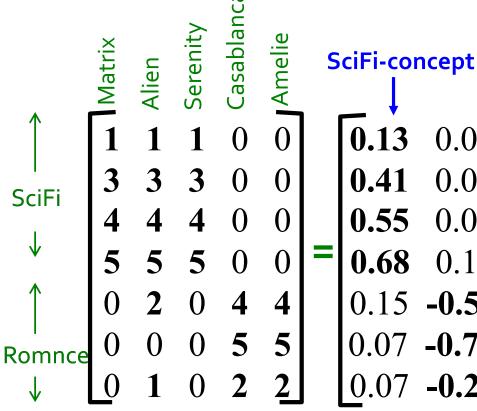
0.13 0.02 -0.01
0.41 0.07 -0.03
0.55 0.09 -0.04
0.68 0.11 -0.05
0.15 -0.59 0.65
0.07 -0.73 -0.67
0.07 -0.29 0.32

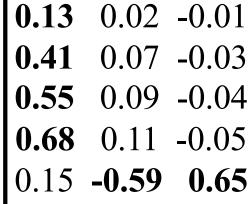
 0.56
 0.59
 0.56
 0.09
 0.09

 0.12
 -0.02
 0.12
 -0.69
 -0.69

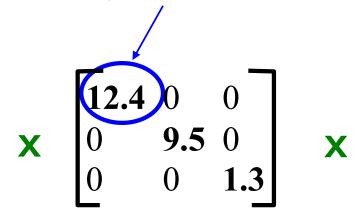
 0.40
 -0.80
 0.40
 0.09
 0.09

• A = U Σ V^T - example:

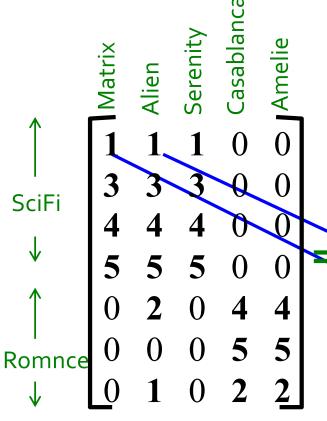




"strength" of the SciFi-concept



• $A = U \Sigma V^T$ - example:



SciFi-concept

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**

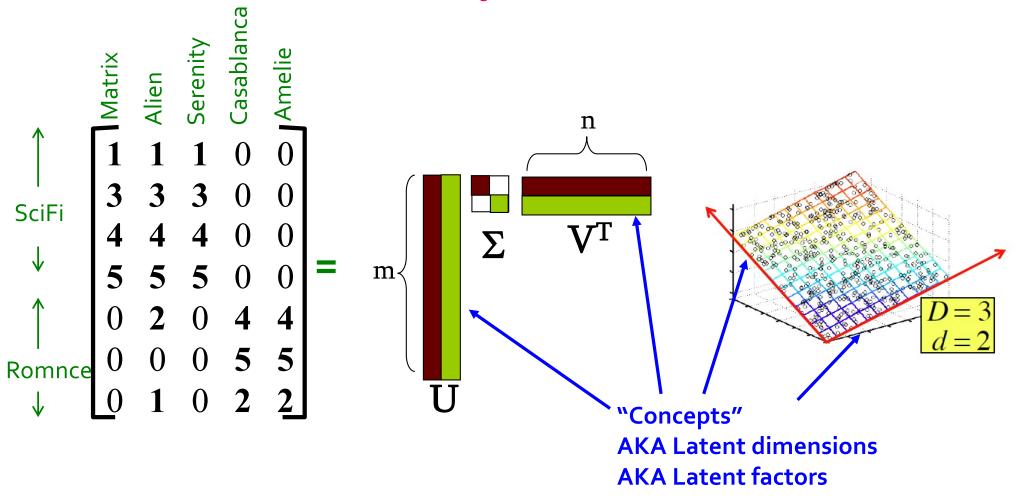
0.07 **-0.29 0.32**

SciFi-concept

V is "movie-to-concept" similarity 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

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

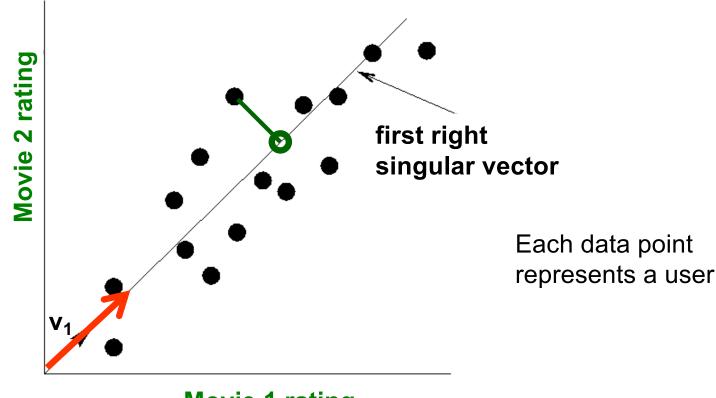


'movies', 'users' and 'concepts':

- 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



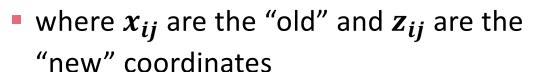
Movie 1 rating

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

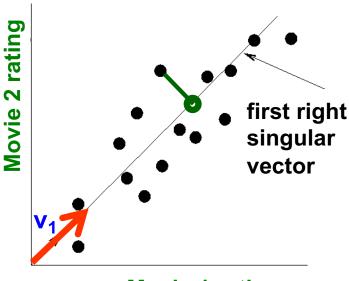
SVD – Dimensionality Reduction

Goal: Minimize the sum of reconstruction errors:

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



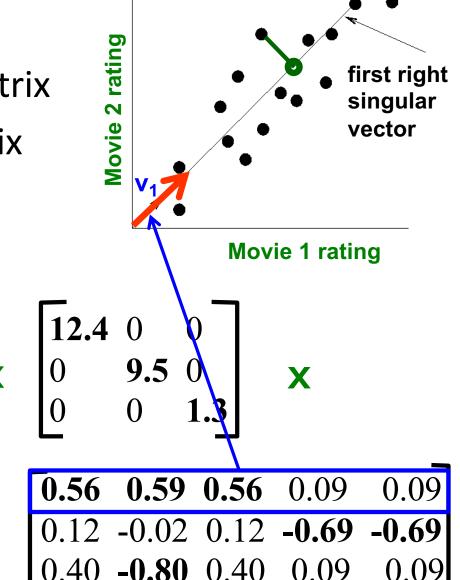
- SVD gives 'best' axis to project on:
 - 'best' = minimizing the reconstruction errors
- In other words, minimum reconstruction error



Movie 1 rating

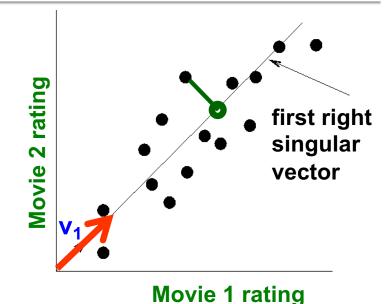
• $A = U \Sigma V^T$ - example:

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

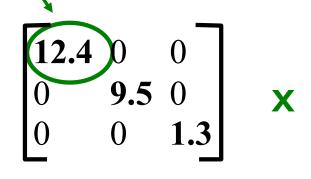


■ A = U Σ V^T - example:

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	



More details

Q: How exactly is dim. reduction done?

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

More details

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

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

More details

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

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

More details

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

```
\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \approx \begin{bmatrix} 0.13 & 0.02 & -0.01 \\ 0.41 & 0.07 & -0.03 \\ 0.55 & 0.09 & -0.04 \\ 0.68 & 0.11 & -0.05 \\ 0.15 & -0.59 & 0.65 \\ 0.07 & -0.73 & -0.67 \\ 0.07 & -0.29 & 0.32 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & \times 3 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & \times 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 & -0.89 & 0.40 & 0.09 & 0.09 \end{bmatrix}
```

More details

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

A user is represented by 5 ratings

Projection: A user is represented by 2 concepts

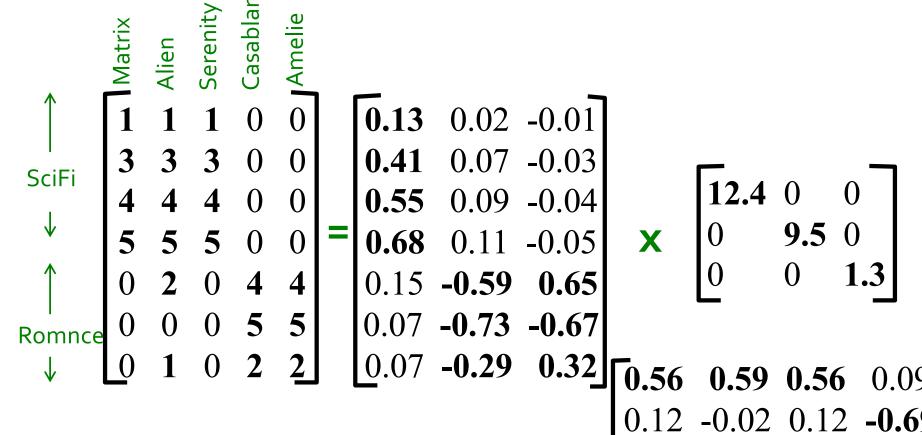
$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \approx$$

$$\mathbf{x} \begin{bmatrix} \mathbf{12.4} & 0 \\ 0 & \mathbf{9.5} \end{bmatrix} \mathbf{x}$$

Two Axis: Sci-Fi and Romance

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

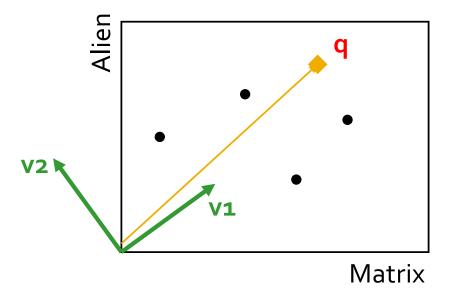


J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, http://www.mmds.or

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

This query also represents a user who likes Matrix, and the goal is to find users with a similar taste

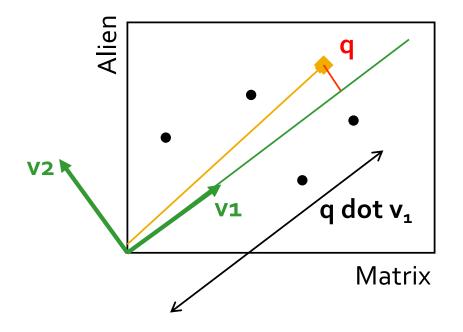
Project into concept space: Inner product with each 'concept' vector v_i



V1 and V2 are concepts

- 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.:

movie-to-concept similarities (V)

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.:

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

movie-to-concept similarities (V)

SciFi-concept
$$= \begin{bmatrix} 5.2 & 0.4 \end{bmatrix}$$

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!

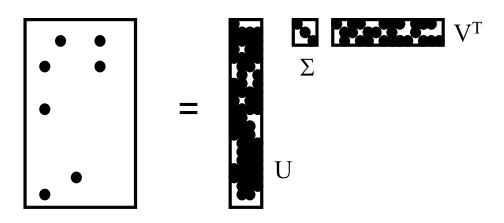
$$\mathbf{d} = \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \\ 5 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad \begin{array}{c} \text{SciFi-concept} \\ \text{SciFi-concept} \\ \text{SciFi-concept} \\ \text{SciFi-concept} \\ \text{SciFi-concept} \\ \text{SciFi-concept} \\ \text{Similarity} \neq 0 \\ \text{Similarity}$$

J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, http://www.mmds.org

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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!



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

- 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