

Introduction to Data Mining

Lecture #21: Dimensionality Reduction

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In This Lecture

- Understand the motivation and applications of dimensionality reduction
- Learn the definition and properties of SVD, one of the most important tools in data mining
- Learn how to interpret the results of SVD, and how to use it for dimensionality reduction



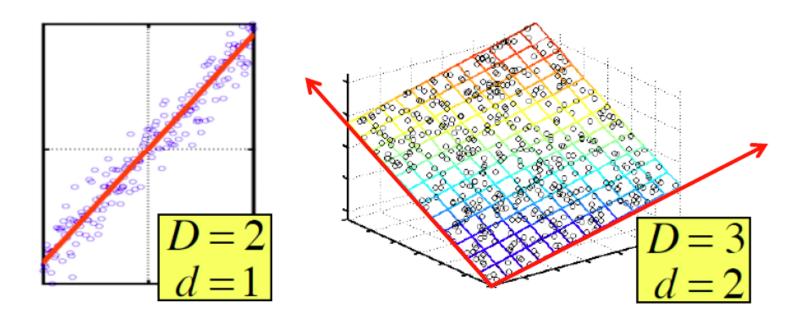
Outline

- **→** □ Overview
 - ☐ Dim. Reduction with SVD

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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{F} r	\mathbf{Sa}	Su
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]

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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 $\mathbf{r} = \mathbf{2}$

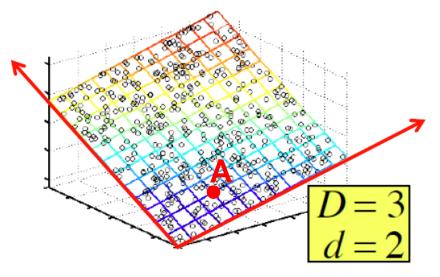
- Why? The first two rows are linearly independent, so the rank is at least 2, but all three rows are linearly dependent (the first is equal to the sum of the second and third) so the rank must be less than 3.
- Why do we care about low rank?
 - We can write A as two "basis" vectors: [1 2 1] [-2 -3 1]
 - 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

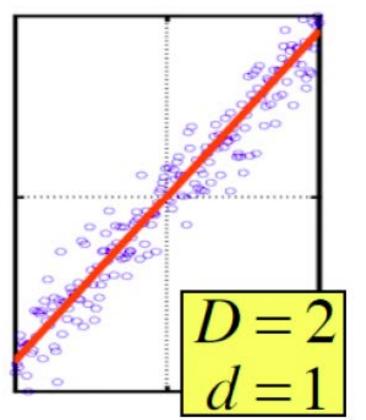


- We can rewrite coordinates more efficiently!
 - Old basis vectors: [1 0 0] [0 1 0] [0 0 1]
 - New basis vectors: [1 2 1] [-2 -3 1]
 - □ Then **A** has new coordinates: [1 0]. **B**: [0 1], **C**: [1 -1]
 - Notice: We reduced the number of coordinates!



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).

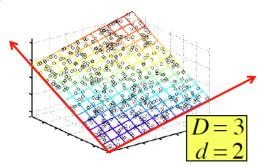
By doing this we incur a bit of **error** as the points do not exactly lie on the line



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



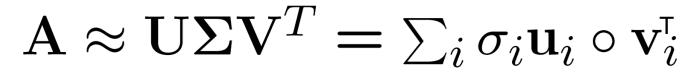
SVD (Singular Value Decomposition)

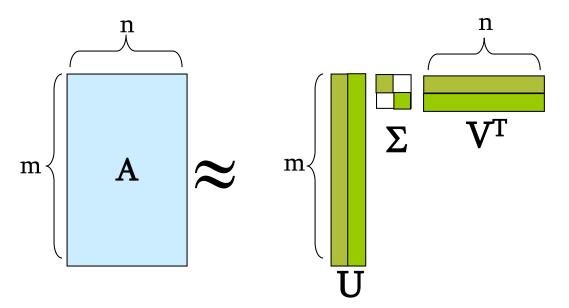
$$\mathbf{A}_{[m \times n]} = \mathbf{U}_{[m \times r]} \mathbf{\Sigma}_{[r \times r]} (\mathbf{V}_{[n \times r]})^{\mathsf{T}}$$

- 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)
- lacksquare 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 (Singular Value Decomposition)

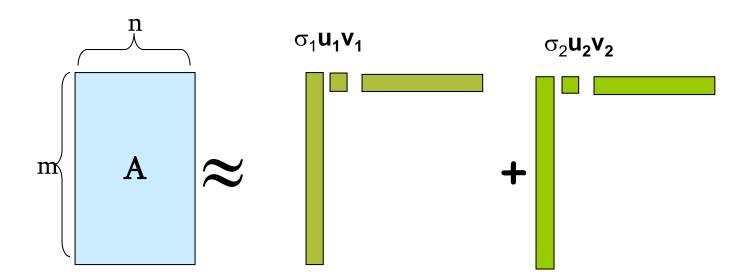






SVD (Singular Value Decomposition)

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



Also called "spectral decomposition"

 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
 - \cup $U^T U = I; V^T V = I (I: identity matrix)$
 - (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

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■ $A = U \Lambda V^T$ - example:

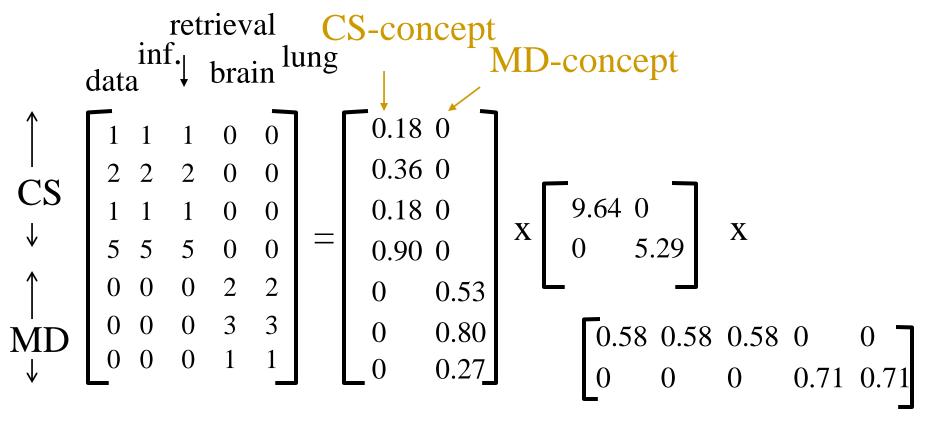
retrieval inf.↓ brain lung

$$= \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix}$$

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■ $A = U \Lambda V^T$ - example:

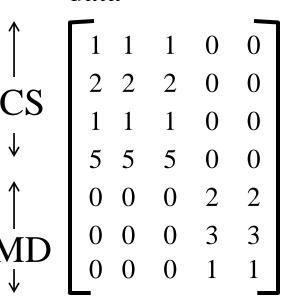




A = **U** Λ **V**^T - example:

doc-to-concept similarity matrix

retrieval CS-concept brain lung MD-concept

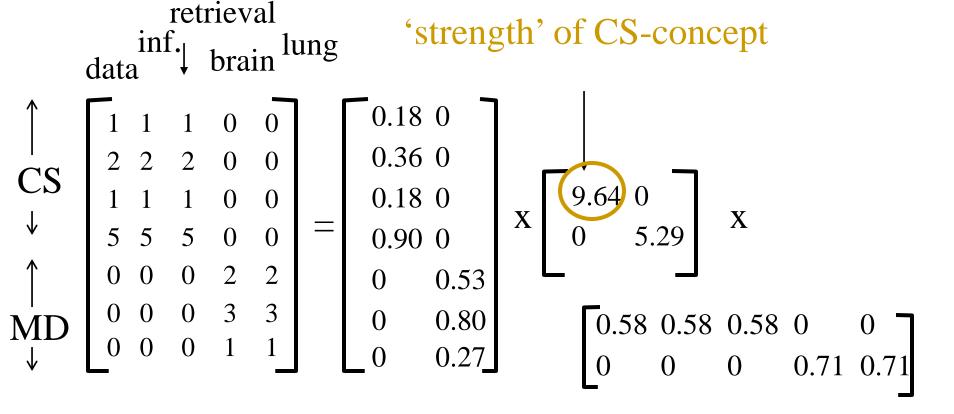


$$\begin{bmatrix}
0.58 & 0.58 & 0.58 & 0 \\
0 & 0 & 0 & 0.71
\end{bmatrix}$$

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■ $A = U \Lambda V^T$ - example:

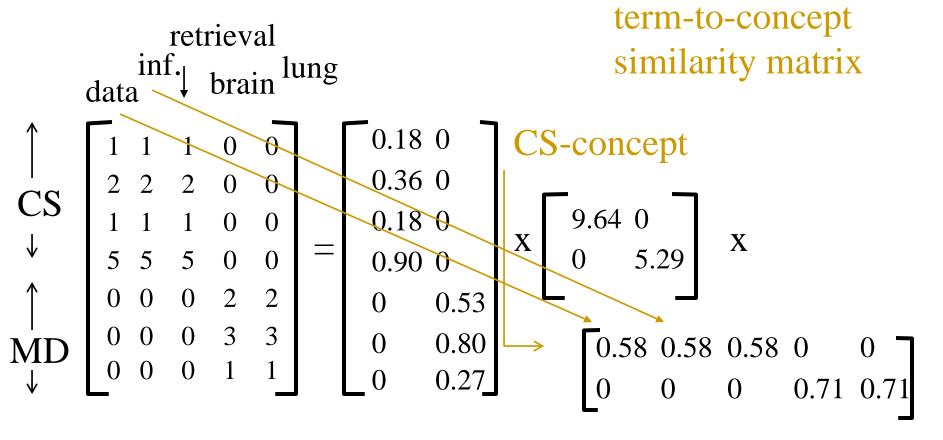


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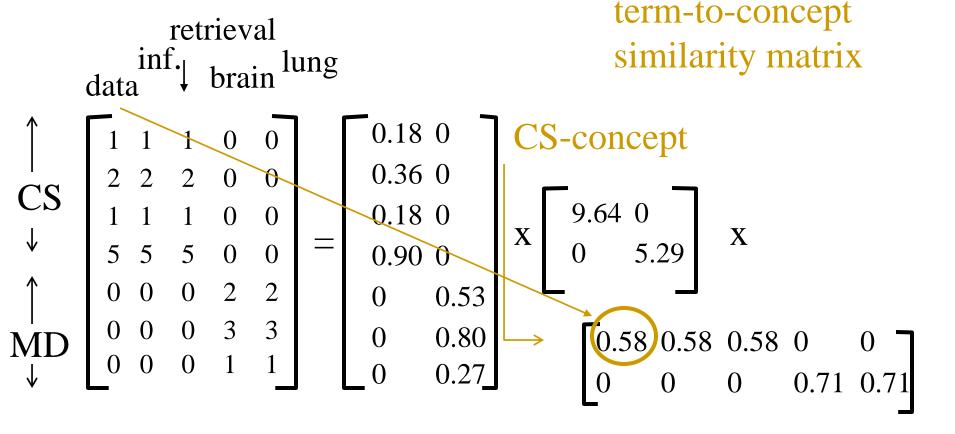


A = **U** Λ **V**^T - example:





A = **U** Λ **V**^T - example:





Outline

Overview





- 'documents', 'terms' and 'concepts':
- **U**: document-to-concept similarity matrix
- V: term-to-concept sim. matrix
- lacktriangle Λ : its diagonal elements: 'strength' of each concept



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'documents', 'terms' and 'concepts':

Q: if A is the document-to-term matrix, what is A<sup>T</sup> A?

A:

Q: A A<sup>T</sup>?

A:
```



'documents', 'terms' and 'concepts':

Q: if A is the document-to-term matrix, what is $A^T A$?

A: term-to-term ([m x m]) similarity matrix

 $Q: A A^T$?

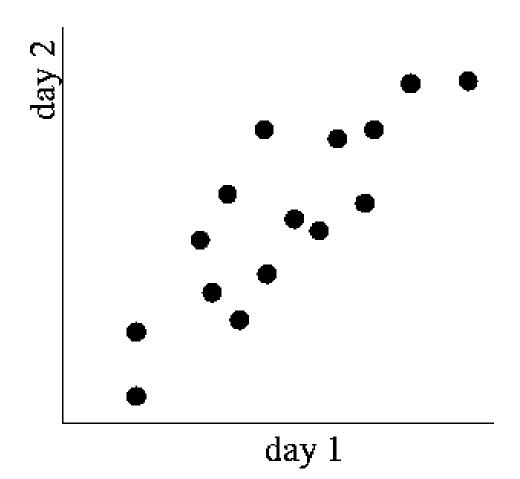
A: document-to-document ([n x n]) similarity matrix



best axis to project on: ('best' = min sum of squares of projection errors)

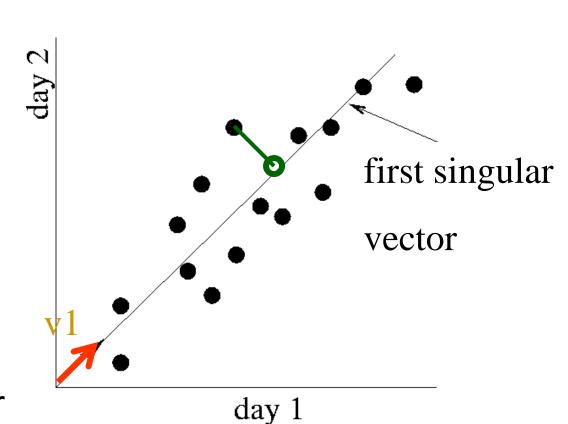


SVD - Motivation





SVD: gives best axis to project



minimum RMS error

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${f Johnson}$	0	0	0	3	3
${f Thompson}$	0	0	0	1	1



■ $A = U \Lambda V^T$ - example:

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix}$$



■ $A = U \Lambda V^T$ - example:

variance ('spread') on the v1 axis

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$



- $A = U \Lambda V^T$ example:
 - ullet **U** $oldsymbol{\Lambda}$ gives the coordinates of the points in the projection axis

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 \\ 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$



- More details
- Q: how exactly is dim. reduction done?

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$



- More details
- Q: how exactly is dim. reduction done?
- A: set the smallest singular values to zero:

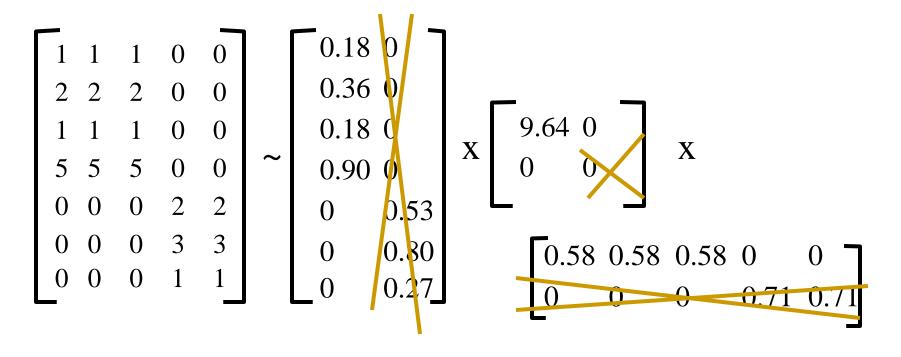
$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 \\ 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$



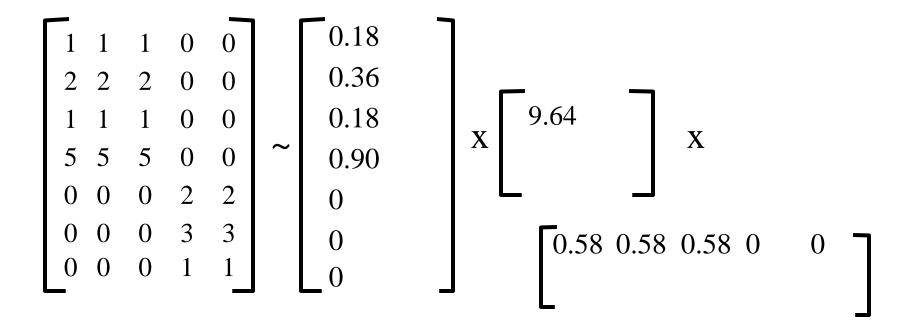
1	1	1	0	0
2	2	2	0	0
1	1	1	0	0
5	5	5	0	0
0	0	0	2	2
0	0	0	3	3
0	0	0	1	1_

```
\begin{array}{c|cccc}
0.18 & 0 \\
0.36 & 0 \\
0.18 & 0 \\
0.90 & 0 \\
0 & 0.53 \\
0 & 0.80 \\
0 & 0.27
\end{array}
```











```
      1
      1
      1
      0
      0

      2
      2
      2
      0
      0

      1
      1
      1
      0
      0

      5
      5
      5
      0
      0

      0
      0
      0
      2
      2

      0
      0
      0
      3
      3

      0
      0
      0
      1
      1
```

```
      1
      1
      1
      0
      0

      2
      2
      2
      0
      0

      1
      1
      1
      0
      0

      5
      5
      5
      0
      0

      0
      0
      0
      0
      0

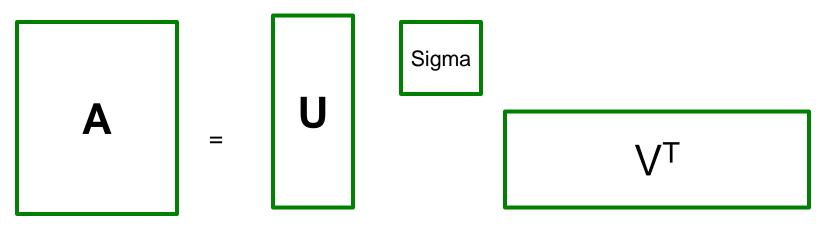
      0
      0
      0
      0
      0

      0
      0
      0
      0
      0

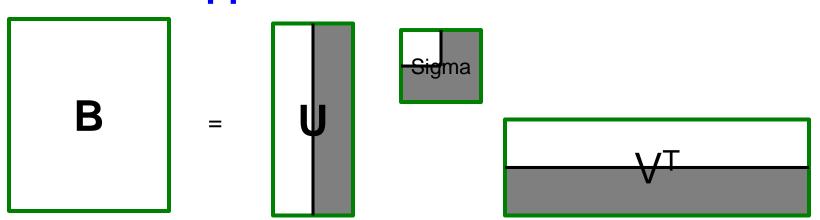
      0
      0
      0
      0
      0
```



SVD – Best Low Rank Approx.



B is best approximation of A





SVD – Best Low Rank Approx.

Theorem:

Let $A = U \sum V^T$ and $B = U S V^T$ where $S = \text{diagonal } r_{x}r$ 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":

 \Box B is a solution to $\min_{B} \|A - B\|_{F}$ where $\operatorname{rank}(B) = k$

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

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



Equivalent:

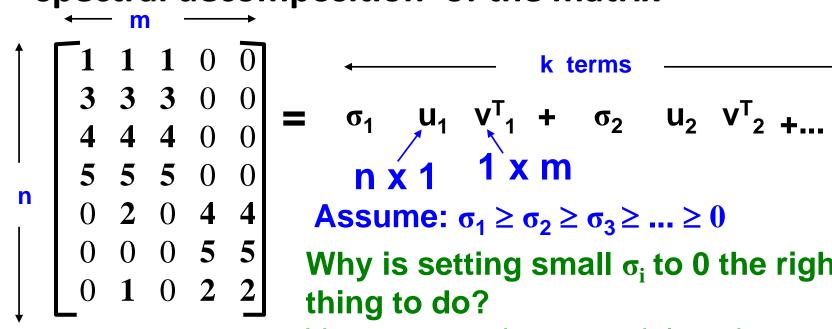
'spectral decomposition' of the matrix:

$$\begin{bmatrix} \mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & 0 \\ \mathbf{3} & \mathbf{3} & \mathbf{3} & 0 & 0 \\ \mathbf{4} & \mathbf{4} & \mathbf{4} & 0 & 0 \\ \mathbf{5} & \mathbf{5} & \mathbf{5} & 0 & 0 \\ 0 & \mathbf{2} & 0 & \mathbf{4} & \mathbf{4} \\ 0 & 0 & 0 & \mathbf{5} & \mathbf{5} \\ 0 & \mathbf{1} & 0 & \mathbf{2} & \mathbf{2} \end{bmatrix} = \begin{bmatrix} \begin{vmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & \mathbf{2} & \mathbf{2} \end{bmatrix} \times \begin{bmatrix} \sigma_1 & 0 & 0 & 0 \\ 0 & 1 & 0 & \mathbf{2} & \mathbf{2} \end{bmatrix} \times \begin{bmatrix} \sigma_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{5} & \mathbf{5} \\ 0 & 1 & 0 & \mathbf{2} & \mathbf{2} \end{bmatrix}$$



Equivalent:

'spectral decomposition' of the matrix



$$= \sigma_1 \quad u_1 \quad v_1^T + \sigma_2 \quad u_2 \quad v_2^T + \dots$$

$$= n \times 1 \quad 1 \times m$$

Why is setting small σ_i to 0 the right

Vectors \mathbf{u}_{i} and \mathbf{v}_{i} are unit length, so $\mathbf{\sigma}_{i}$ scales them.

So, zeroing small σ_i introduces less error.



Q: How many σ_s to keep?

Rule-of-a thumb:

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



SVD - Complexity

- To compute SVD (for n x m matrix):
 - \bigcirc 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 ...



Conclusion

- SVD: $A = U \Sigma V^T$: unique
 - **U**: user-to-concept similarities
 - **V**: movie-to-concept similarities
 - \square Σ : strength of each concept

Dimensionality reduction:

- keep the few largest singular values (80-90% of 'energy')
- SVD: picks up linear correlations



Questions?