



SVD and PCA

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Feature Extraction

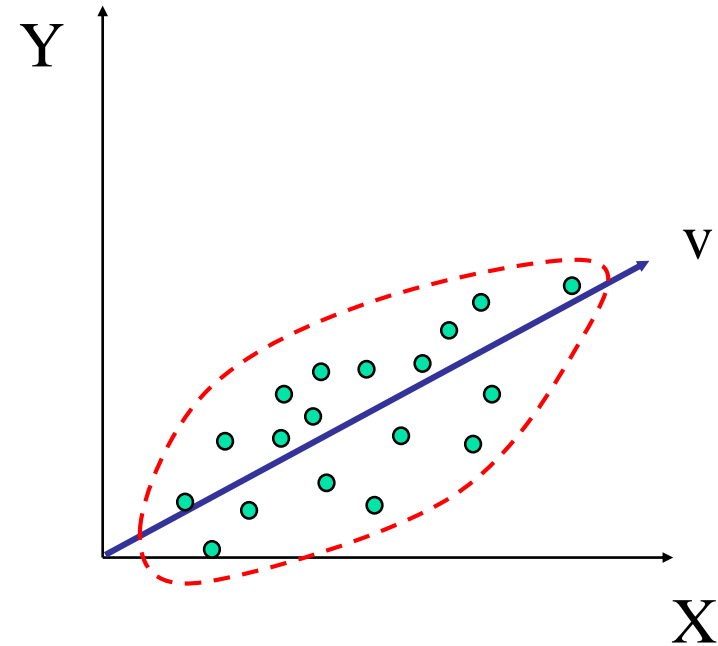
- Create new features (attributes) by combining/mapping existing ones
- Common methods
 - Principle Component Analysis
 - Singular Value Decomposition
- Other compression methods (time-frequency analysis)
 - Fourier transform (e.g. time series)
 - Discrete Wavelet Transform (e.g. 2D images)

Principal Component Analysis (PCA)

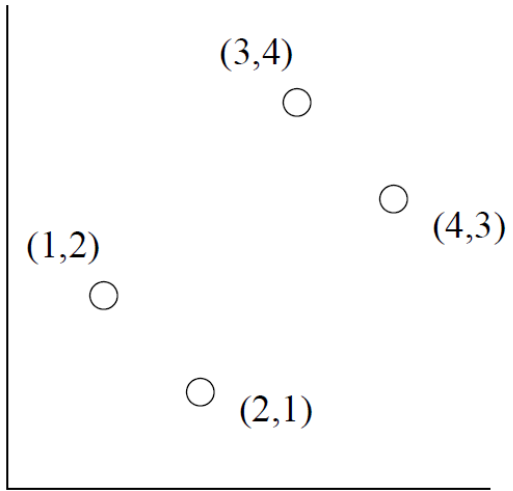
- Principle component analysis: find the dimensions that capture the most variance
 - A linear mapping of the data to a new coordinate system such that the greatest variance lies on the first coordinate (the first principal component), the second greatest variance on the second coordinate, and so on.
- Steps
 - Normalize input data: each attribute falls within the same range
 - Compute k orthonormal (unit) vectors, i.e., *principal components* - each input data (vector) is a linear combination of the k principal component vectors
 - The principal components are sorted in order of decreasing “significance”
 - Weak components can be eliminated, i.e., those with low variance

Dimensionality Reduction: PCA

- Mathematically
 - Compute the covariance matrix
$$\text{Cov}(X, Y) = E[(X - E[X])(Y - E[Y])],$$
 - Find the eigenvectors of the covariance matrix correspond to large eigenvalues $A\mathbf{v} = \lambda\mathbf{v}$.

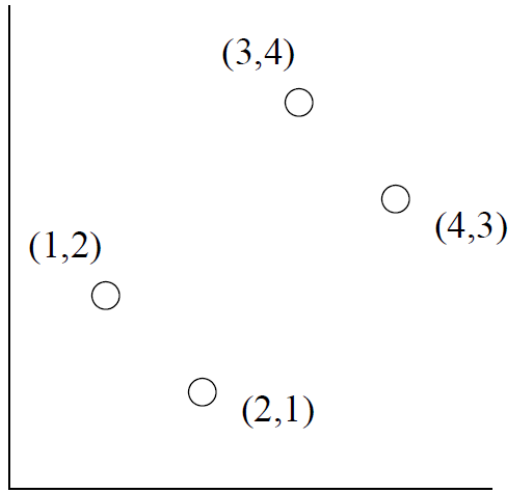


PCA: Illustrative Example



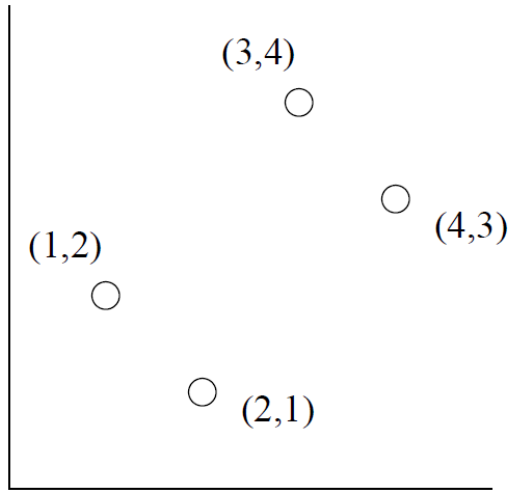
$$M = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix}$$

PCA: Illustrative Example



$$M = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix} \quad M^T M = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 1 & 4 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix} = \begin{bmatrix} 30 & 28 \\ 28 & 30 \end{bmatrix}$$

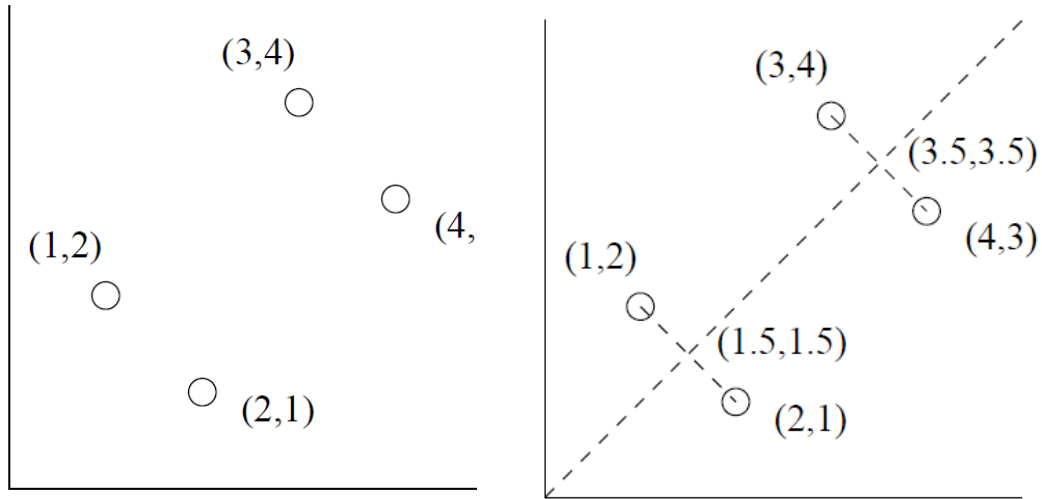
PCA: Illustrative Example



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$$\lambda = 58 \text{ and } \lambda = 2 \quad E = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

PCA: Illustrative Example



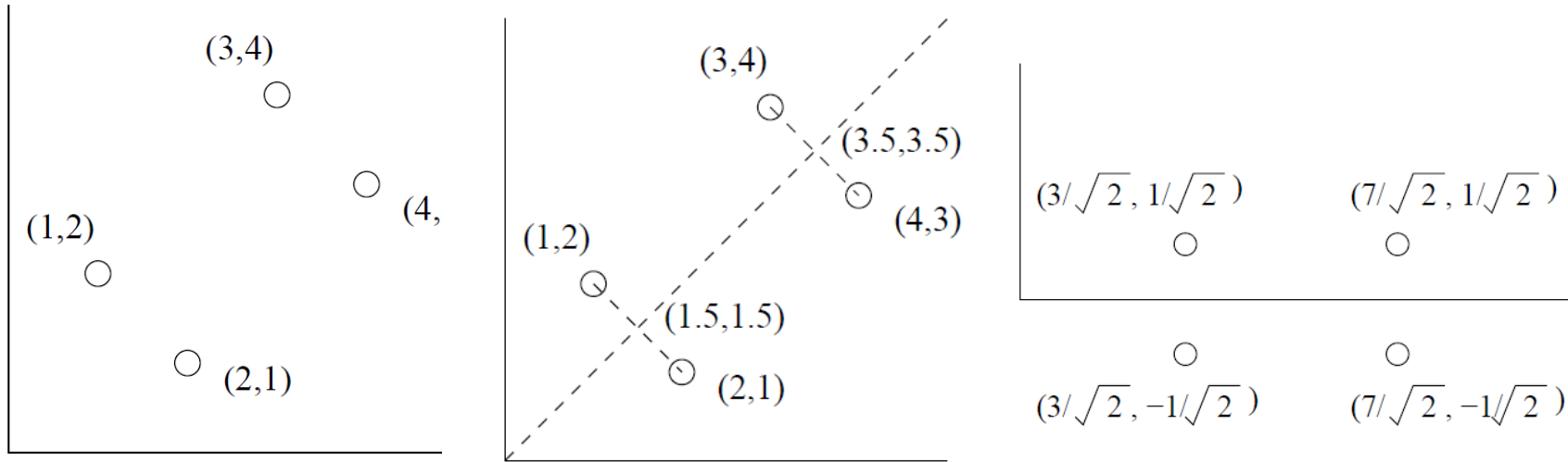
$$M = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix}$$

$$M^T M = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 1 & 4 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix} = \begin{bmatrix} 30 & 28 \\ 28 & 30 \end{bmatrix}$$

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PCA: Illustrative Example



$$M = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix}$$

$$ME = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 3/\sqrt{2} & 1/\sqrt{2} \\ 3/\sqrt{2} & -1/\sqrt{2} \\ 7/\sqrt{2} & 1/\sqrt{2} \\ 7/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}$$

Eigen Decomposition

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$$

$$\mathbf{A} \begin{bmatrix} | & | & & | \\ \mathbf{v}_1 & \mathbf{v}_2 & \dots & \mathbf{v}_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ \mathbf{v}_1 & \mathbf{v}_2 & \dots & \mathbf{v}_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix}$$

$$\mathbf{A}\mathbf{Q} = \mathbf{Q}\mathbf{\Lambda}$$

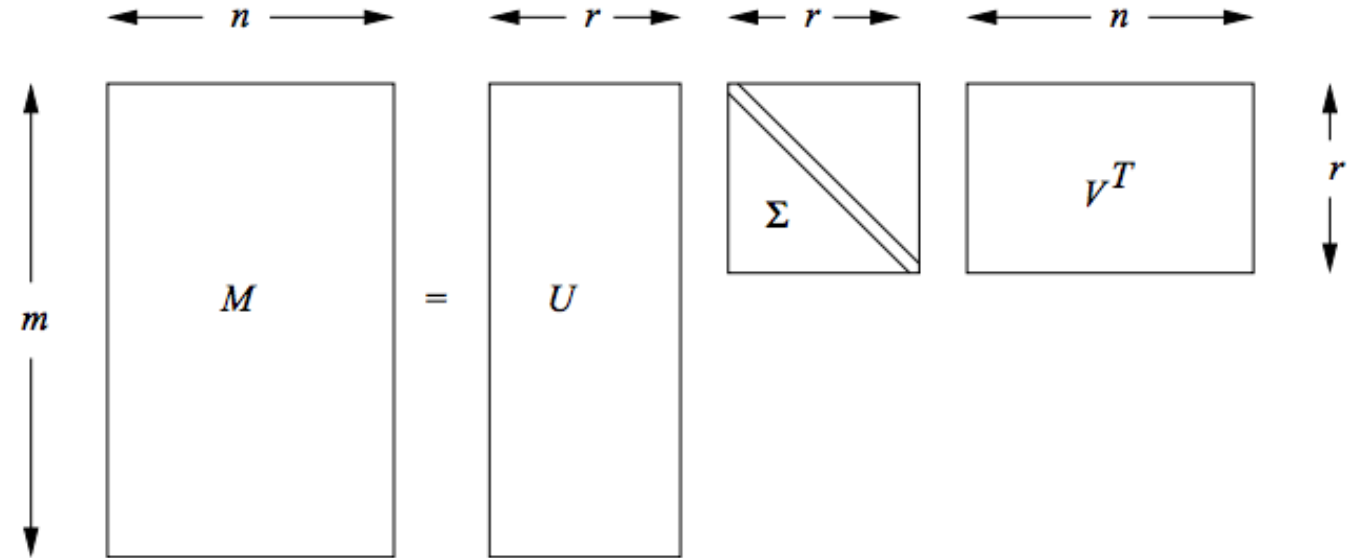
$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^{-1}$$

How the eigenvalues and eigenvectors create a Matrix decomposition.

- \mathbf{Q} is a matrix consisting of the eigenvectors
- $\mathbf{\Lambda}$ is the diagonal matrix containing all the eigenvalues

Singular Value Decomposition (SVD)

$$M = U \Sigma V^T$$



1. U is an $m \times r$ *column-orthonormal matrix*; that is, each of its columns is a unit vector and the dot product of any two columns is 0.
2. V is an $n \times r$ *column-orthonormal matrix*. Note that we always use V in its transposed form, so it is the rows of V^T that are orthonormal.
3. Σ is a diagonal matrix; that is, all elements not on the main diagonal are 0. The elements of Σ are called the *singular values* of M .

Similarity of Eigen and SVD

$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^{-1}$$

$$\mathbf{M} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

- Columns of \mathbf{Q} are eigenvectors
 - $\mathbf{\Lambda}$ contains eigenvalues
 - Columns of \mathbf{u} are left-singular vectors
 - Columns of \mathbf{v} are right-singular vectors
 - $\mathbf{\Sigma}$ contains ordered singular values σ_i
-
- \mathbf{A} must be square and we defined \mathbf{A} as $\mathbf{A} = \mathbf{M}^T \mathbf{M}$.
 - The \mathbf{v}_j are eigenvectors of $\mathbf{M}^T \mathbf{M}$.
 - The \mathbf{u}_i are eigenvectors of $\mathbf{M} \mathbf{M}^T$.
 - The eigenvalues are squares of the singular values. ($\lambda_i = \sigma_i^2$)

AN APPLICATION EXAMPLE.....



FROM::

Dimensionality Reduction: SVD & CUR

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



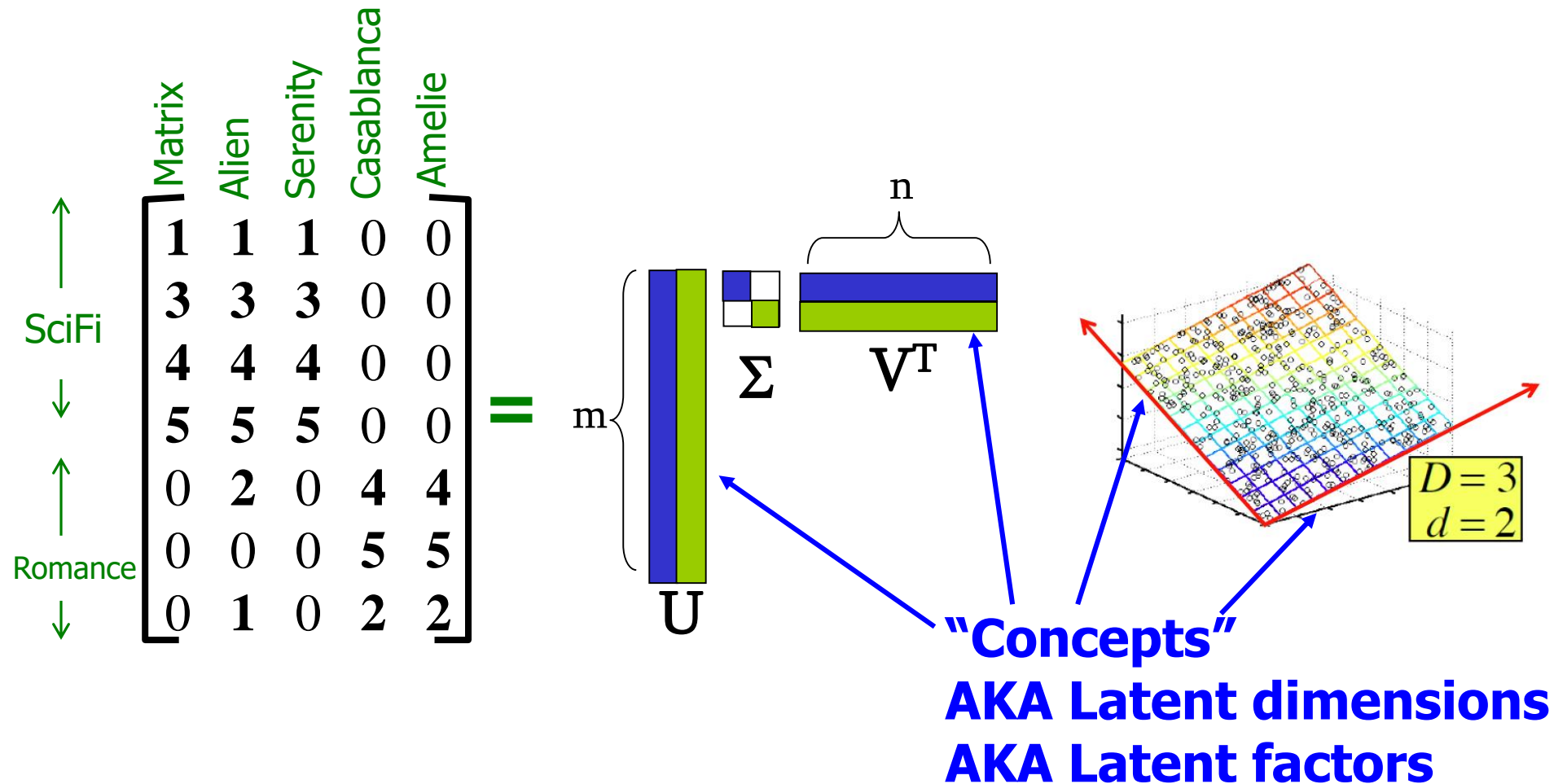
SVD - Properties

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

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

SVD – Example: Users-to-Movies

- Consider a matrix. What does SVD do?



SVD – Example: Users-to-Movies

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

$$\begin{array}{c}
 \begin{array}{c} \uparrow \\ \text{SciFi} \\ \downarrow \\ \uparrow \\ \text{Romance} \\ \downarrow \end{array}
 \begin{array}{c} \text{Matrix} \\ \text{Alien} \\ \text{Serenity} \\ \text{Casablanca} \\ \text{Amelie} \end{array}
 \begin{bmatrix}
 1 & 1 & 1 & 0 & 0 \\
 3 & 3 & 3 & 0 & 0 \\
 4 & 4 & 4 & 0 & 0 \\
 5 & 5 & 5 & 0 & 0 \\
 0 & 2 & 0 & 4 & 4 \\
 0 & 0 & 0 & 5 & 5 \\
 0 & 1 & 0 & 2 & 2
 \end{bmatrix}
 =
 \begin{bmatrix}
 0.13 & 0.02 & -0.01 \\
 0.41 & 0.07 & -0.03 \\
 0.55 & 0.09 & -0.04 \\
 0.68 & 0.11 & -0.05 \\
 0.15 & -0.59 & 0.65 \\
 0.07 & -0.73 & -0.67 \\
 0.07 & -0.29 & 0.32
 \end{bmatrix}
 \times
 \begin{bmatrix}
 12.4 & 0 & 0 \\
 0 & 9.5 & 0 \\
 0 & 0 & 1.3
 \end{bmatrix}
 \times
 \begin{bmatrix}
 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\
 0.12 & -0.02 & 0.12 & -0.69 & -0.69 \\
 0.40 & -0.80 & 0.40 & 0.09 & 0.09
 \end{bmatrix}
 \end{array}$$

SVD – Example: Users-to-Movies

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

Movies

Matrix Alien Serenity Casablanca Amelie

SciFi

Romance

SciFi-concept

Romance-concept

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

SVD – Example: Users-to-Movies

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

Matrix

SciFi

Romance

Alien

Serenity

Casablanca

Amelie

SciFi-concept

Romance-concept

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

SVD – Example: Users-to-Movies

■ $A = U \Sigma V^T$ - example:

Diagram illustrating the SVD decomposition of a user-movie rating matrix A into matrices U , Σ , and V^T .

Matrix A (User-Movie Ratings):

	Matrix	Alien	Serenity	Casablanca	Amelie
SciFi	1	1	1	0	0
	3	3	3	0	0
	4	4	4	0	0
	5	5	5	0	0
Romance	0	2	0	4	4
	0	0	0	5	5
	0	1	0	2	2

Matrix U (User Latent Factors):

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

Matrix Σ (Singular Values):

12.4	0	0
0	9.5	0
0	0	1.3

Matrix V^T (Movie Latent Factors):

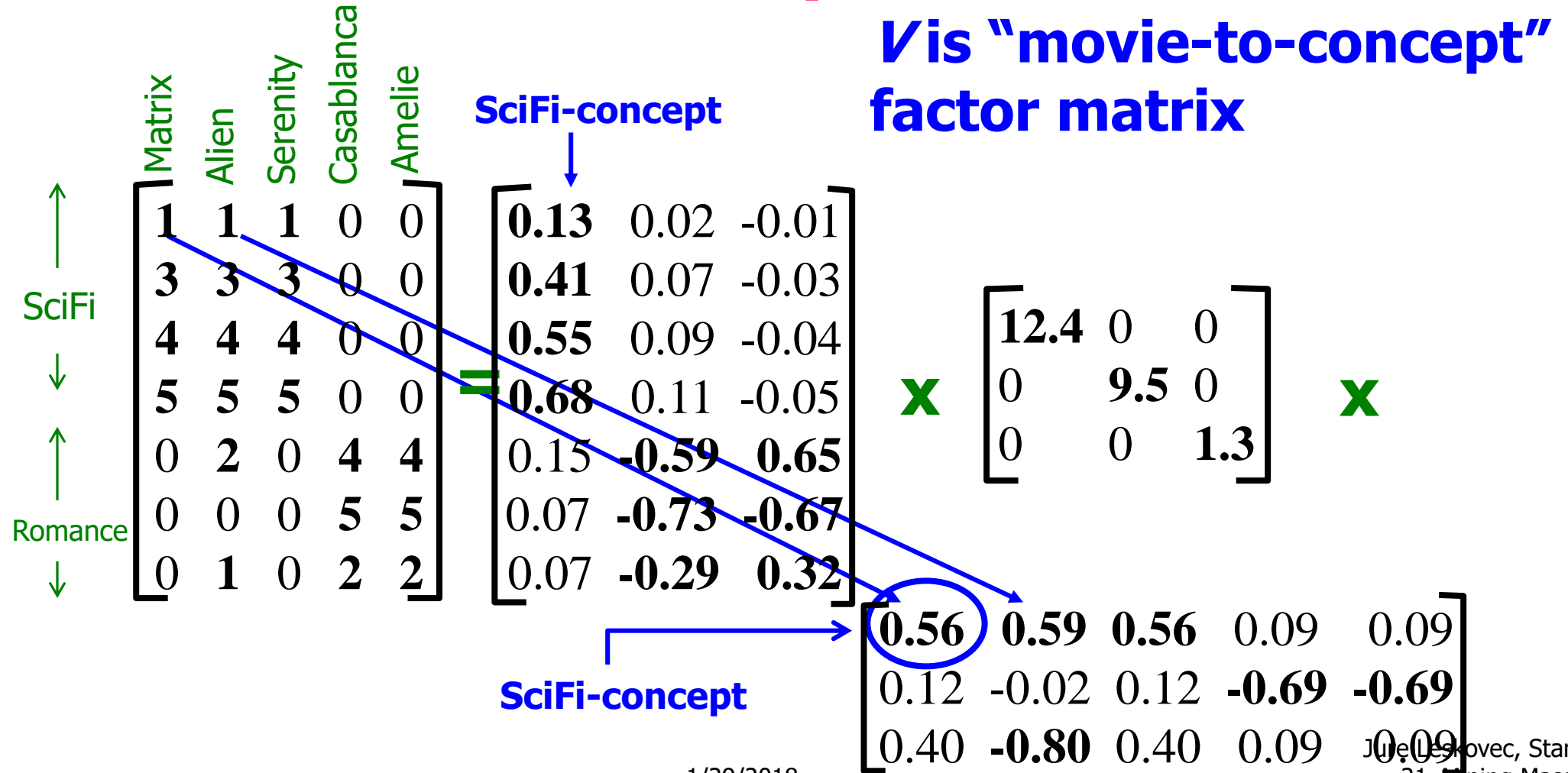
0.56	0.59	0.56	0.09	0.09
0.12	-0.02	0.12	-0.69	-0.69
0.40	-0.80	0.40	0.09	0.09

Annotations:

- SciFi-concept:** Points to the first column of U .
- "strength" of the SciFi-concept:** Points to the value 12.4 in Σ .
- Green 'X' markers:** Indicate the multiplication of U and Σ , and Σ and V^T .
- Green arrows:** Indicate the mapping from the SciFi and Romance rows of A to the corresponding rows in U .

SVD – Example: Users-to-Movies

■ $A = U \Sigma V^T$ - example:



SVD - Interpretation #1

`movies'`, **`users'` and **`concepts'`:****

- U : user-to-concept matrix
- V : movie-to-concept matrix
- Σ : its diagonal elements:
 `strength' of each concept

SVD – Best Low Rank Approx.

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

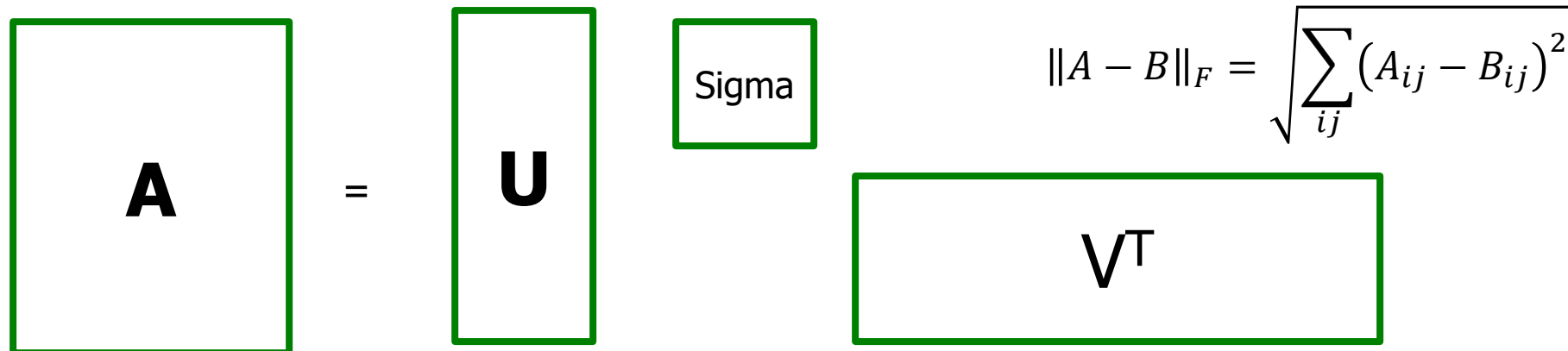


Diagram illustrating the SVD decomposition of matrix A :

$$A = U \Sigma V^T$$

The matrix A is represented by a square box. It is equal to the product of matrix U (a tall vertical rectangle), matrix Σ (a small square box labeled "Sigma"), and matrix V^T (a wide horizontal rectangle). To the right, the Frobenius norm formula is shown:

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

B is best approximation of A:

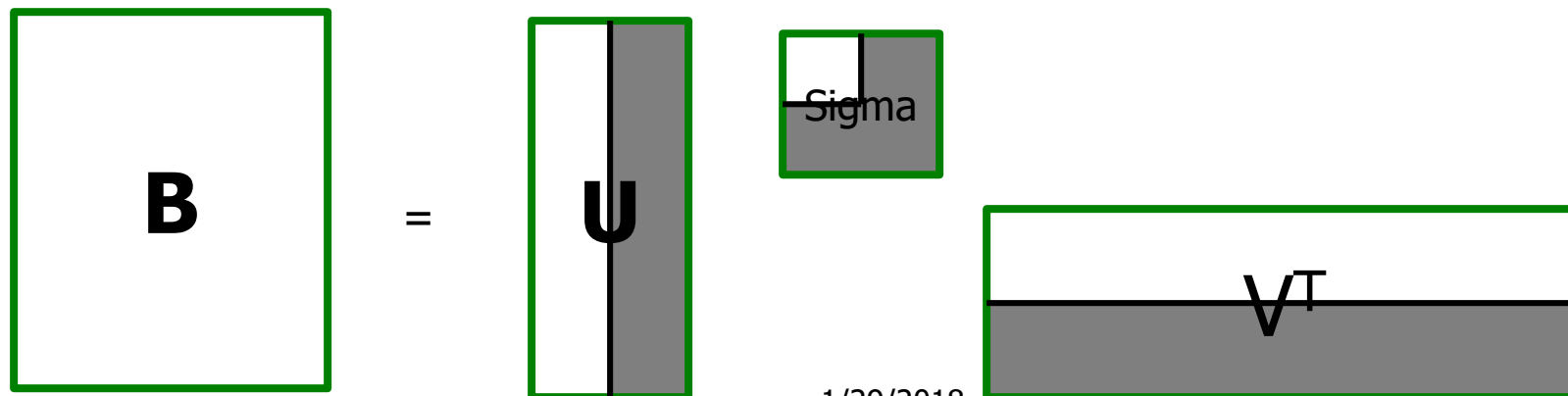


Diagram illustrating the best low-rank approximation B of matrix A :

$$B = U \Sigma_k V^T$$

The matrix B is represented by a square box. It is equal to the product of matrix U (a tall vertical rectangle with a vertical line and a shaded gray area on the right), matrix Σ_k (a small square box labeled "Sigma" with a vertical line and a shaded gray area on the right), and matrix V^T (a wide horizontal rectangle with a horizontal line and a shaded gray area at the bottom). This represents a truncated SVD where only the top k singular values and their corresponding left and right singular vectors are used.



Example of SVD

Case study: How to query?

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

Diagram illustrating the mapping of a query into a concept space for finding users that like 'Matrix'.

The query matrix (Matrix) is shown as a 6x5 matrix, with columns labeled Matrix, Alien, Serenity, Casablanca, and Amelie. The rows are labeled with movie genres: SciFi (rows 1-4) and Romance (rows 5-6).

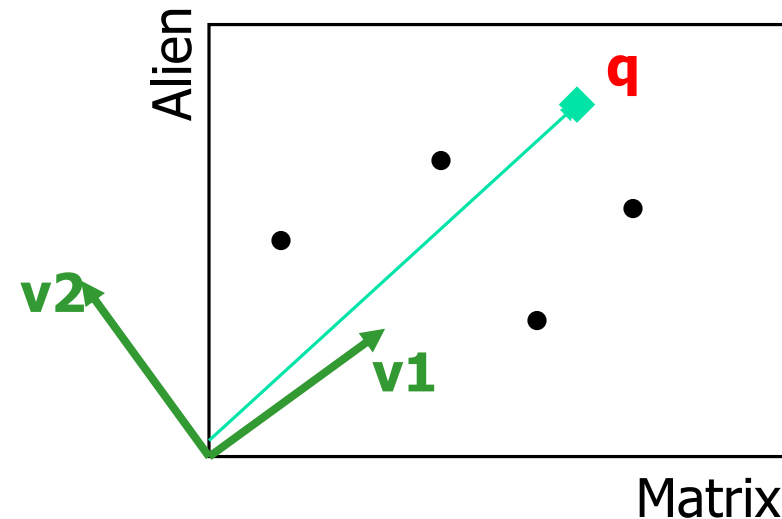
$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} = \begin{bmatrix} 0.13 & 0.02 & -0.01 \\ 0.41 & 0.07 & -0.03 \\ 0.55 & 0.09 & -0.04 \\ 0.68 & 0.11 & -0.05 \\ 0.15 & -0.59 &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

Case study: How to query?

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

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

Project into concept space:
Inner product with each
'concept' vector \mathbf{v}_i

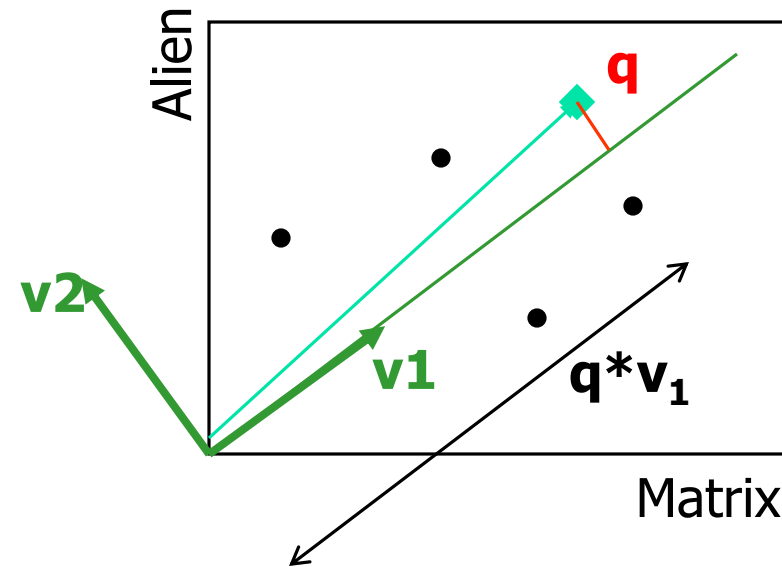


Case study: How to query?

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

Project into concept space:
Inner product with each
'concept' vector \mathbf{v}_i



Case study: How to query?

Compactly, we have:

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

$$\mathbf{q} = \begin{matrix} & \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \\ \begin{matrix} \text{SciFi} \\ \text{Fantasy} \end{matrix} & \begin{bmatrix} 5 & 0 & 0 & 0 & 0 \end{bmatrix} \end{matrix} \times \begin{matrix} \begin{bmatrix} 0.56 & 0.12 \\ 0.59 & -0.02 \\ 0.56 & 0.12 \\ 0.09 & -0.69 \\ 0.09 & -0.69 \end{bmatrix} \\ \text{movie-to-concept} \\ \text{factors (V)} \end{matrix} = \begin{matrix} \text{SciFi-concept} \\ \downarrow \\ \begin{bmatrix} 2.8 & 0.6 \end{bmatrix} \end{matrix}$$

Case study: How to query?

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

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

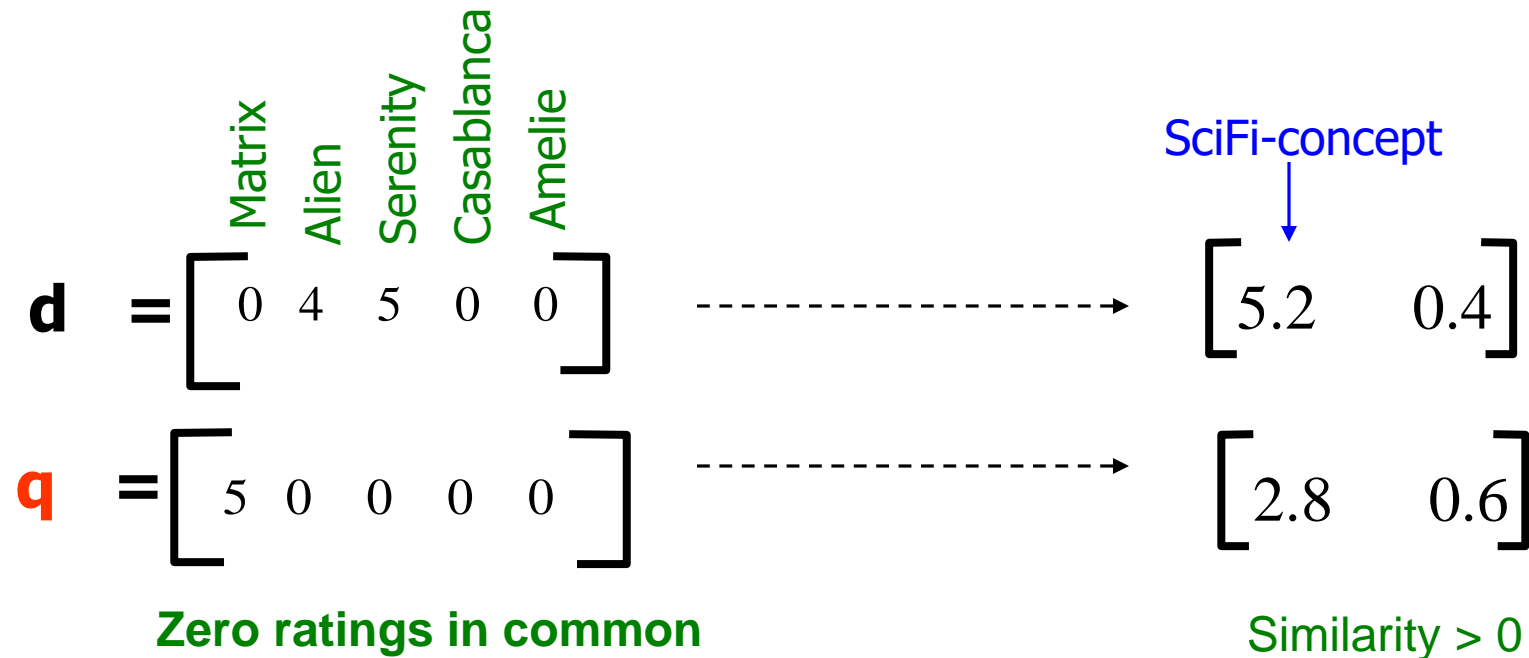
$$\mathbf{q} = \begin{matrix} & \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \\ \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \end{bmatrix} & \times & \begin{bmatrix} 0.56 & 0.12 \\ 0.59 & -0.02 \\ 0.56 & 0.12 \\ 0.09 & -0.69 \\ 0.09 & -0.69 \end{bmatrix} & = & \begin{bmatrix}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

movie-to-concept
factors (V)

SciFi-concept
↓

Case study: How to query?

- **Observation:** User \mathbf{d} that rated (*Alien*, *Serenity*) will be **similar** to user \mathbf{q} that rated (*Matrix*), although \mathbf{d} and \mathbf{q} have **zero ratings in common!**



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!**

