

DATA MINING

DIMENSIONALITY REDUCTION

PCA – SVD

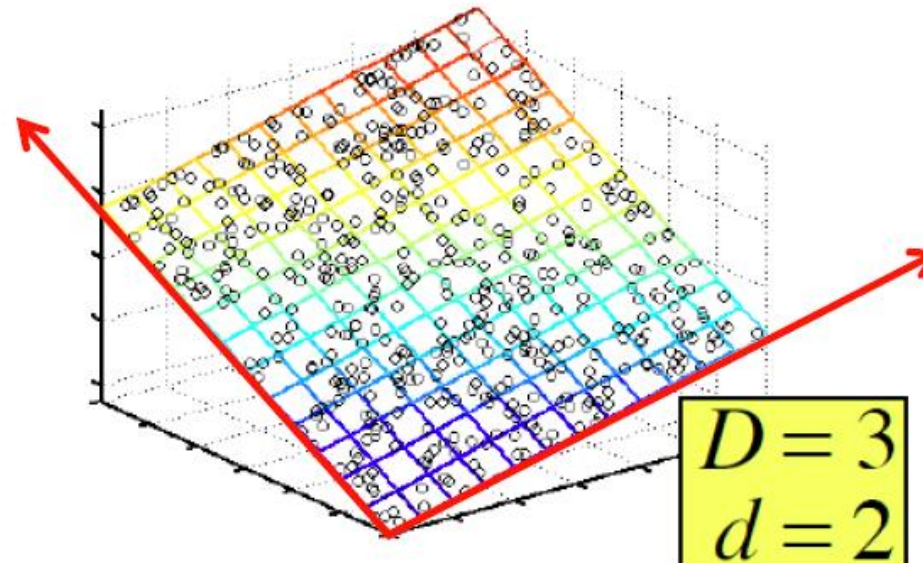
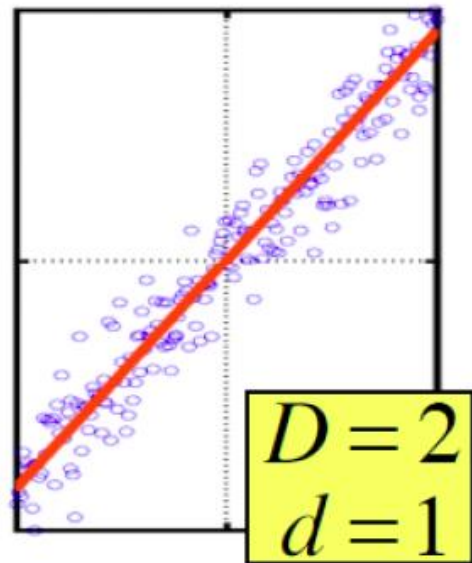
(Thanks to Jure Leskovec, Evimaria Terzi)

The curse of dimensionality

- Real data usually have **thousands**, or **millions** of dimensions
 - E.g., web documents, where the dimensionality is the vocabulary of words
 - Facebook graph, where the dimensionality is the number of users
- Huge number of dimensions causes problems
 - Data becomes very **sparse**, some algorithms become meaningless (e.g. density-based clustering)
 - The **complexity** of several algorithms depends on the dimensionality and they become infeasible (e.g. nearest neighbor search).

Dimensionality Reduction

- Usually the data can be described with fewer dimensions, without losing much of the information in the data.
 - The data reside in a space of lower dimensionality



Example

TID	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	B1	B2	B3	B4	B5	B6	B7	B8	B9	B10	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10
1	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1
12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1
13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1
14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1

- In this data matrix the dimension is essentially 3
 - There are three types of products and three types of users

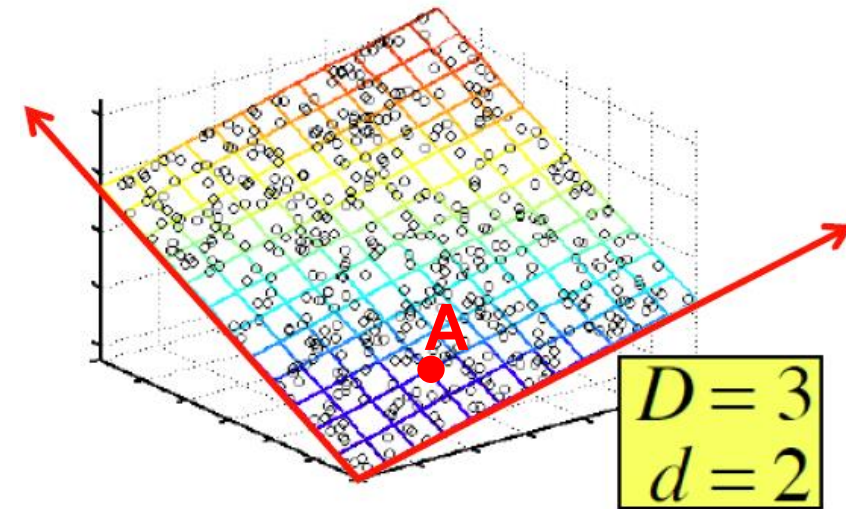
Example

- **Cloud of points 3D space:**

- Think of point positions as a matrix:

1 row per point:

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



- **We can rewrite coordinates more efficiently!**

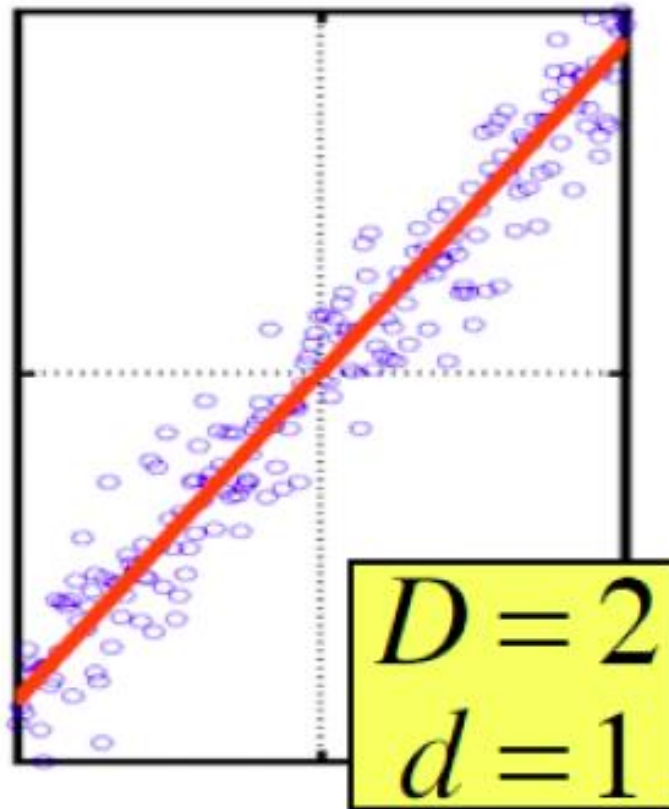
- Old basis vectors: $[1 \ 0 \ 0]$ $[0 \ 1 \ 0]$ $[0 \ 0 \ 1]$
- **New basis vectors: $[1 \ 2 \ 1]$ $[-2 \ -3 \ 1]$**
- Then **A** has new coordinates: $[1 \ 0]$. **B**: $[0 \ 1]$, **C**: $[1 \ -1]$
 - **Notice: We reduced the number of coordinates!**

Dimensionality Reduction

- Find the “true dimension” of the data
 - In reality, things are never as clear and simple as in this example, but we can still reduce the dimension.
- Essentially, we assume that some of the data is useful signal and some data is noise, and that we can approximate the useful part with a lower dimensionality space.
 - Dimensionality reduction does not just reduce the amount of data, it often brings out the useful part of the data

Dimensionality Reduction

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

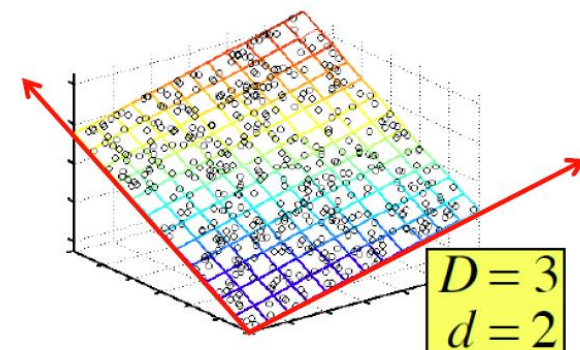


Rather than representing every point with 2 coordinates we represent each point with 1 coordinate (corresponding to the position of the point on the red line).

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

Why Reduce Dimensions?

- **Discover hidden correlations/topics**
 - E.g., in documents, words that occur commonly together
- **Remove redundant and noisy features**
 - E.g., in documents, not all words are useful
- **Interpretation and visualization**
- **Easier storage and processing of the data**



Data in the form of a matrix

- We are given n objects and d attributes describing the objects. Each object has d numeric values describing it.
- We will represent the data as a $n \times d$ real matrix A .
 - We can now use tools from linear algebra to process the data matrix
- Our goal is to produce a new $n \times k$ matrix B such that
 - It preserves as much of the information in the original matrix A as possible
 - It reveals something about the structure of the data in A

Example: Document matrices

d terms
(e.g., theorem, proof, etc.)

n documents

A

A_{ij} = frequency of the j -th term in the i -th document

Find subsets of terms that bring documents together

Example: Recommendation systems

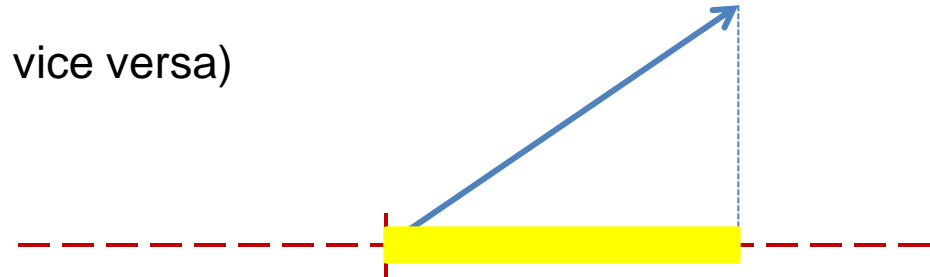
$$\begin{matrix} & \text{d movies} \\ \text{n customers} & \left(\begin{matrix} A \\ A_{ij} = \text{rating of } j\text{-th} \\ \text{product by the } i\text{-th} \\ \text{customer} \end{matrix} \right) \end{matrix}$$

Find subsets of movies that capture the behavior of the customers

Linear algebra

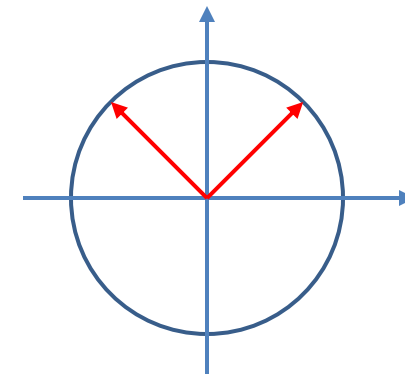
- We assume that vectors are **column vectors**.
- We use v^T for the **transpose** of vector v (**row vector**)
- **Dot product**: $u^T v$ ($1 \times n, n \times 1 \rightarrow 1 \times 1$)
 - The dot product is the **projection** of vector v on u (and vice versa)

$$[1, 2, 3] \begin{bmatrix} 4 \\ 1 \\ 2 \end{bmatrix} = 12$$



- $u^T v = \|v\| \|u\| \cos(u, v)$
 - If $\|u\| = 1$ (**unit vector**) then $u^T v$ is the **projection length** of v on u
 - If $\|u\| = \|v\| = 1$ then $u^T v$ is the **cosine similarity** of v and u

- $[-1, 2, 3] \begin{bmatrix} 4 \\ -1 \\ 2 \end{bmatrix} = 0$: **orthogonal** vectors
 - **Orthonormal** vectors: two **unit** vectors that are **orthogonal**



Matrices

- An $n \times m$ matrix A is a collection of n row vectors and m column vectors

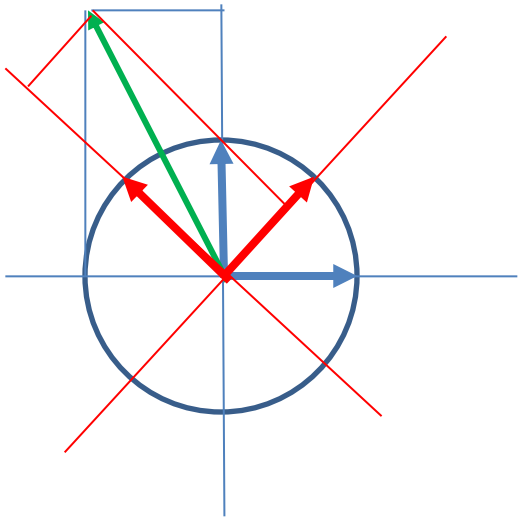
$$A = \begin{bmatrix} | & | & | \\ a_1 & a_2 & a_3 \\ | & | & | \end{bmatrix} \quad A = \begin{bmatrix} - & \alpha_1^T & - \\ - & \alpha_2^T & - \\ - & \alpha_3^T & - \end{bmatrix}$$

- Matrix-vector multiplication
 - Right multiplication Au : projection of u onto the row vectors of A , or projection of row vectors of A onto u .
 - Left-multiplication $u^T A$: projection of u onto the column vectors of A , or projection of column vectors of A onto u
- Example:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

Change of basis

- By default a vector is expressed in the axis-aligned basis.
 - For example, for vector $[-1, 2]$ we have:
 - $\begin{bmatrix} -1 \\ 2 \end{bmatrix} = -1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + 2 \begin{bmatrix} 0 \\ 1 \end{bmatrix}$
- With a projection we can change the basis over which a vector is expressed.



$$\begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix} \begin{bmatrix} -1 \\ 2 \end{bmatrix} = \begin{bmatrix} \frac{3\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} \end{bmatrix}$$

Rank

- **Row space** of A: The set of vectors that can be written as a linear combination of the **rows** of A
 - All vectors of the form $v = u^T A$
- **Column space** of A: The set of vectors that can be written as a linear combination of the **columns** of A
 - All vectors of the form $v = Au$.
- **Rank** of A: the number of **linearly independent** row (or column) vectors
 - These vectors define a **basis** for the row (or column) space of A
 - All vectors in the row (column) space are linear combinations of the basis vectors
- **Example**
 - Matrix $A = \begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix}$ has rank **r=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.

Rank-1 matrices

- In a rank-1 matrix, all columns (or rows) are multiples of the same column (or row) vector

$$A = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 4 & -2 \\ 3 & 6 & -3 \end{bmatrix}$$

- All **rows** are multiples of $r^T = [1, 2, -1]$
- All **columns** are multiples of $c = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$
- **External product:** uv^T ($n \times 1, 1 \times m \rightarrow n \times m$)
 - The resulting $n \times m$ has **rank** 1: all rows (or columns) are **linearly dependent**
 - $A = cr^T$

Eigenvectors

- (Right) Eigenvector of matrix A : a vector v such that $Av = \lambda v$
- λ : eigenvalue of eigenvector v
- A square symmetric matrix A of rank r , has r orthonormal eigenvectors u_1, u_2, \dots, u_r with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_r$.
- Eigenvectors define an orthonormal basis for the column space of A
- We can write:

$$A = U\Lambda U^T$$
$$A = \lambda_1 u_1 u_1^T + \lambda_2 u_2 u_2^T + \dots + \lambda_r u_r u_r^T$$

Singular Value Decomposition

$$A = U \Sigma V^T = [u_1, u_2, \dots, u_r] \begin{bmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_r \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_r^T \end{bmatrix}$$

$[n \times m] = [n \times r] [r \times r] [r \times m]$
 r : rank of matrix A

- $\sigma_1, \geq \sigma_2 \geq \dots \geq \sigma_r$: singular values of matrix A
- u_1, u_2, \dots, u_r : left singular vectors of A
- v_1, v_2, \dots, v_r : right singular vectors of A

$$A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \dots + \sigma_r u_r v_r^T$$

Singular Value Decomposition

- The left singular vectors U are an orthonormal basis for the column space of A .
- The right singular vectors V are an orthonormal basis for the row space of A .
- If A has rank r , then A can be written as the sum of r rank-1 matrices
- There are r “linear components/trends” (axes) in A .
 - Linear component: vector v along which the row vectors of A tend to be aligned
 - Strength of the i -th linear trend: $\|Av_i\| = |\sigma_i|$

- Property of SVD:

$$v_1 = \arg \max_{v: \|v\|=1} \|Av\|$$

Symmetric matrices

- Special case: A is **symmetric** positive definite matrix

$$A = \lambda_1 u_1 u_1^T + \lambda_2 u_2 u_2^T + \cdots + \lambda_r u_r u_r^T$$

- $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r \geq 0$: **Eigenvalues** of A are also the singular values
- u_1, u_2, \dots, u_r : **Eigenvectors** of A are also the left and right singular vectors

Singular Values and Eigenvalues

- Singular Value Decomposition

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

- The **left singular vectors** of A are also the eigenvectors of the (symmetric) matrix AA^T

$$AA^T = U\Sigma^2 U^T$$

- The **right singular vectors** of A are also the eigenvectors of the (symmetric) matrix $A^T A$

$$A^T A = V\Sigma^2 V^T$$

- The **singular values** of matrix A are also the square roots of eigenvalues of AA^T and $A^T A$

$$\lambda_i(A^T A) = \lambda_i(AA^T) = \sigma_i^2$$

SVD properties

- Singular Value Decomposition has three useful properties that we will study now:
 - It provides the important (**principal**) directions (dimensions) in the data – **Principal Component Analysis**
 - It provides the best **low rank approximation** for our matrix
 - It minimizes the reconstruction error (squared distance between real data points and their estimates)

Principal Component Analysis

- Goal: reduce the dimensionality while preserving the “information in the data”.
- In the new space we want to:
 - Maximize the amount of information
 - Minimize redundancy – remove the redundant dimensions
 - Minimize the noise in the data.

Variability

- Information in the data: **variability** in the data
 - We measure variability using the **covariance matrix**.
 - Sample variance for variable X:

$$\sigma_X^2 = \frac{1}{N} \sum_i (x_i - \mu_X)(x_i - \mu_X) = \frac{1}{N} (x - \mu_X)^T (x - \mu_X)$$

- Sample covariance of variables X and Y

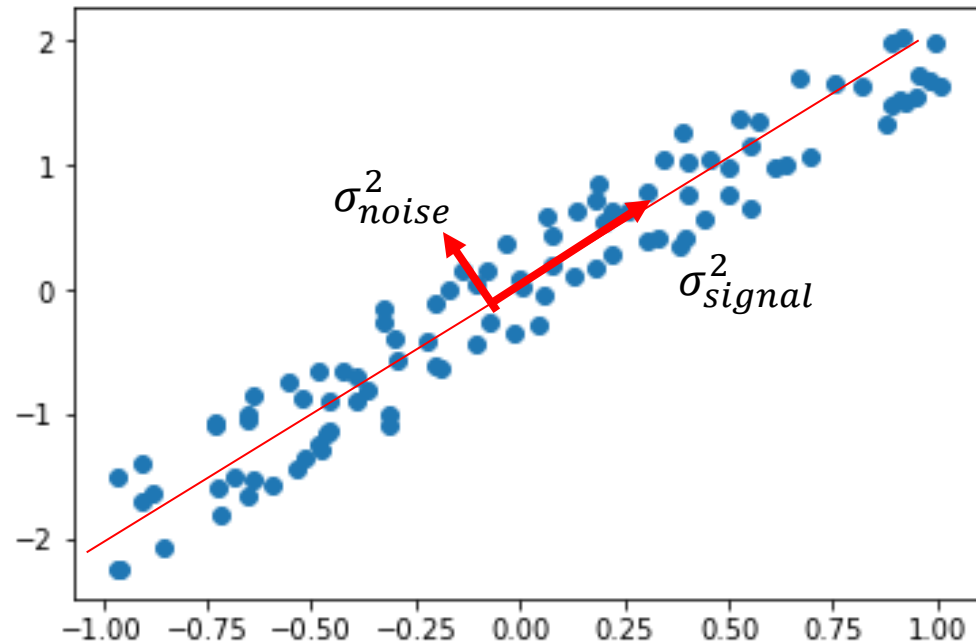
$$\sigma_{XY}^2 = \frac{1}{N} \sum_i (x_i - \mu_X) (y_i - \mu_Y) = \frac{1}{N} (x - \mu_X)^T (y - \mu_Y)$$

- **High variance** σ_X^2 means **high information** in dimension (attribute) X
 - We want to maximize the **signal-to-noise ratio** $\frac{\sigma_{signal}^2}{\sigma_{noise}^2}$
- **High co-variance** σ_{XY}^2 means high correlation between attributes X,Y, and thus **high redundancy**.
 - Ideally we want $\sigma_{XY}^2 = 0$ for all pairs X,Y

Example

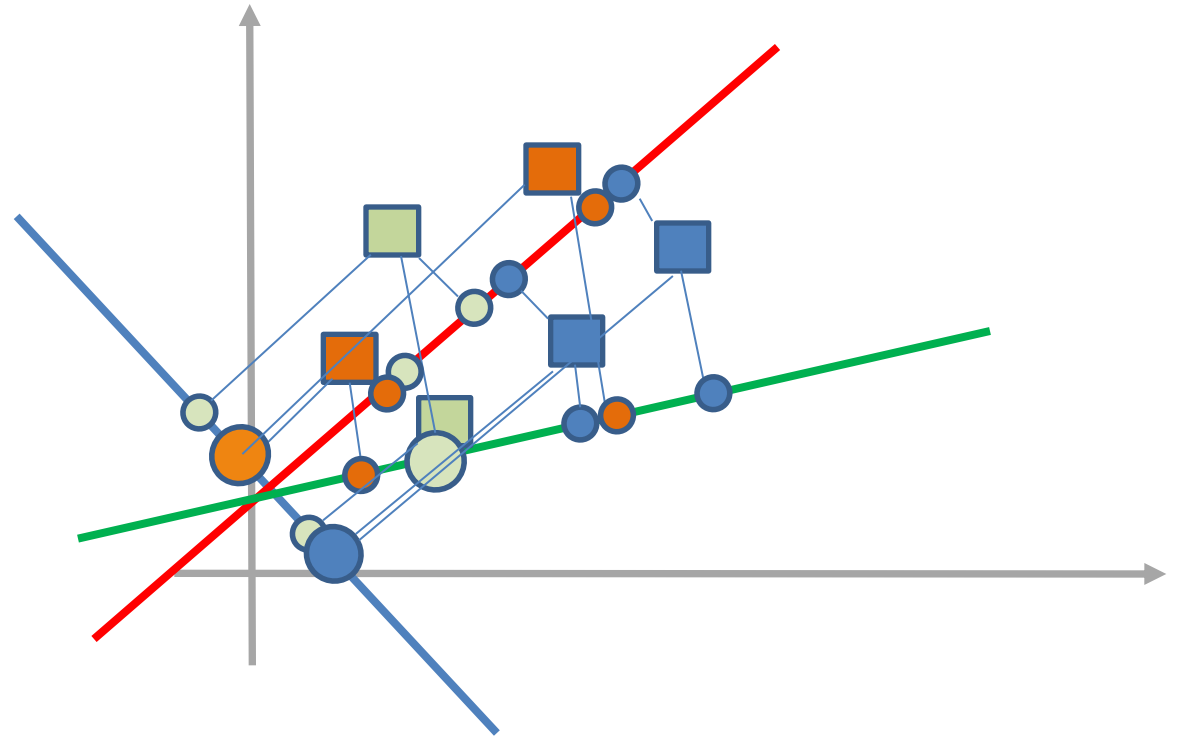
- In the data below the data are essentially one-dimensional, but what is the axis we should use?
 - The direction in which the variance is **maximized**.

The variance along the direction **orthogonal** to the main direction is small and captures the noise in the data



Example

- Which direction is best to project?



- Note that in the case of blue and green directions we have points that are far falling on each other.
- The red maximizes the variance, which gives more information

Covariance matrix

- We are given the data matrix A , with n rows and m columns, where the rows correspond to data samples over a set of features defined by the columns.
- Remove the **mean** of each **column** from the column vectors to get the **centered** matrix \bar{A}
- The matrix $C = \bar{A}^T \bar{A}$ is proportional to the **covariance matrix** of the **column** vectors of \bar{A} .
- We want to change the basis of the data so that the matrix becomes diagonal
 - All the values are in the diagonal and the off-diagonal entries are zero

PCA: Principal Component Analysis

- We will project the **rows** of matrix \bar{A} onto a **new** set of **attributes** (dimensions) such that:
 - The attributes have **zero covariance** to each other (they are **orthogonal**)
 - Each attribute captures **the most remaining variance** in the data, while orthogonal to the existing attributes
 - The first attribute should capture the most variance in the data
- For matrix A , the variance of the rows of A when projected to vector v is given by $\sigma^2 = \left\| \bar{A}v \right\|^2$
 - The **first right singular vector** of \bar{A} maximizes σ^2 !

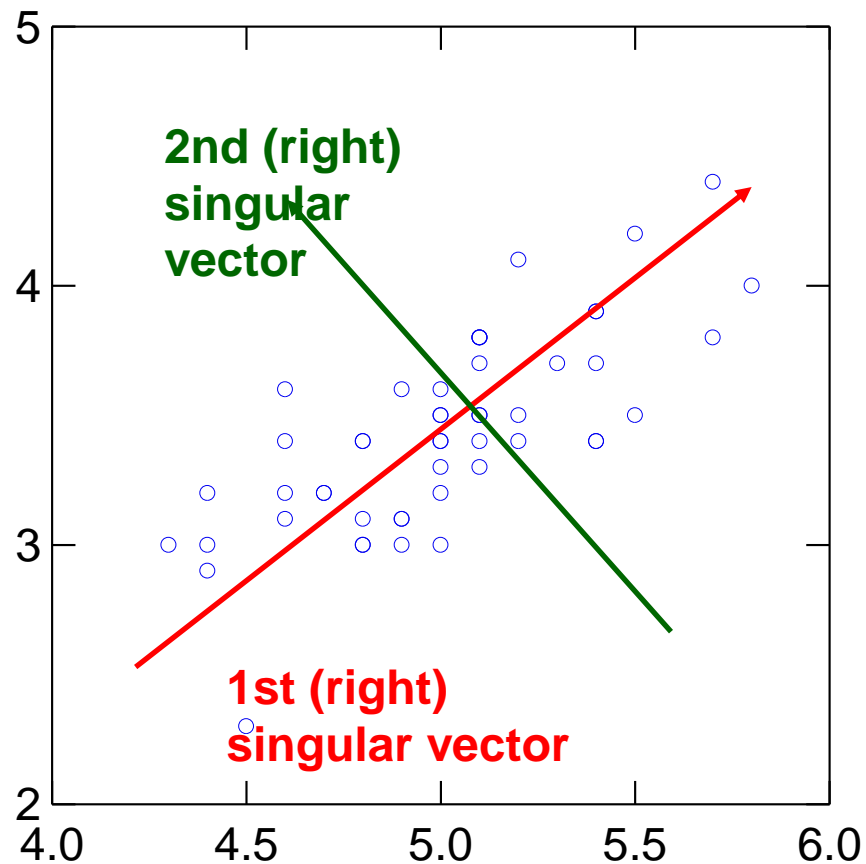
PCA and SVD

- PCA is a special case of SVD on the **centered matrix**.
- After projecting the centered matrix \bar{A} to the singular vectors in V we have that the covariance matrix of the new dataset $\bar{A}V$ is:

$$(\bar{A}V)^T (\bar{A}V) = \Sigma$$

- We have achieved to make the matrix diagonal!
- **Dimensionality reduction**: Don't keep all the singular vectors in V just the k first ones.

PCA



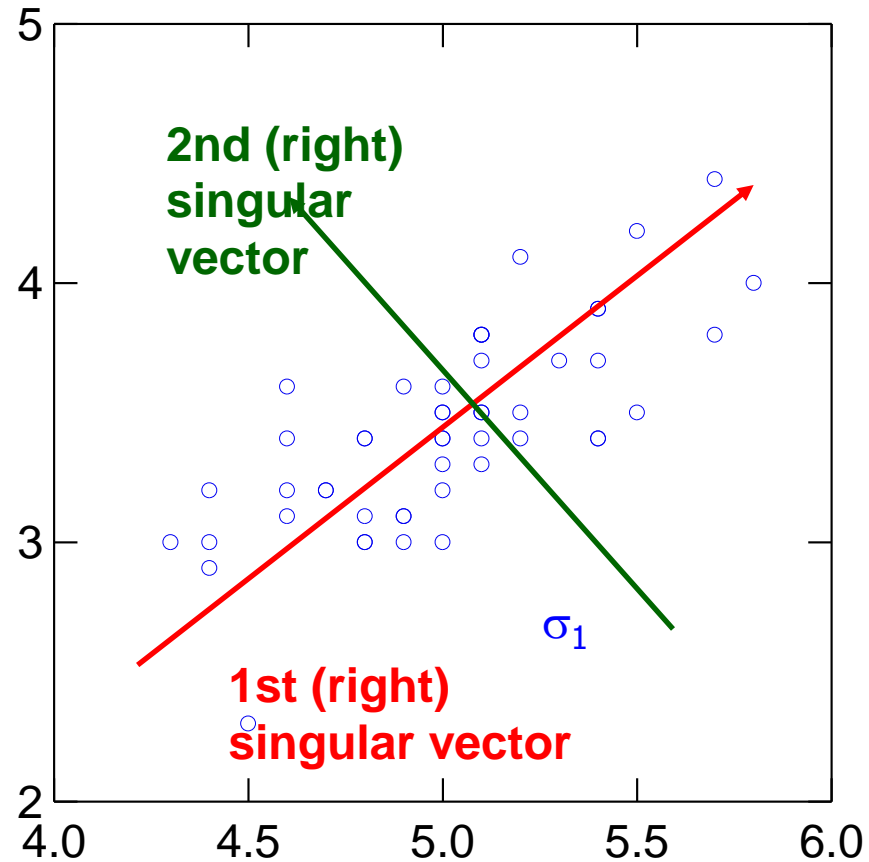
Input: 2-d dimensional points

Output:

1st (right) singular vector:
direction of maximal variance,

2nd (right) singular vector:
direction of maximal variance,
after removing the projection of
the data along the first singular
vector.

Singular values



σ_1 : measures data variance along the first singular vector.

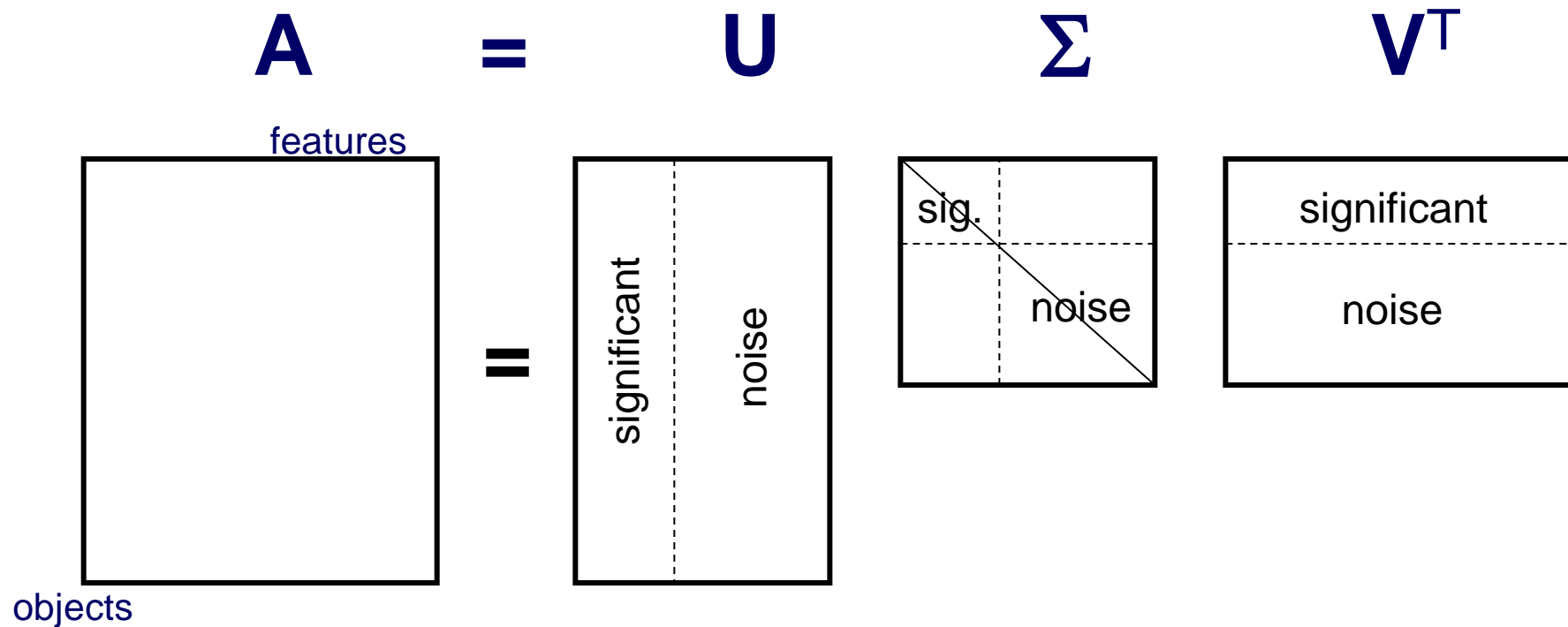
σ_2 : measures how much of the data variance is explained by the second singular vector.

Singular values tell us something about the variance

- The variance in the direction of the **k**-th principal component is given by the corresponding singular value σ_k^2
- Singular values can be used to estimate how many components to keep
- **Rule of thumb:** keep enough to explain **85%** of the variation:

$$\frac{\sum_{j=1}^k \sigma_j^2}{\sum_{j=1}^n \sigma_j^2} \approx 0.85$$

SVD and Rank-**k** approximations



We keep the k most important singular vectors

The matrix $U_k \Sigma_k V_k^T$ is a **rank- k approximation** of A

The idea is that this is the part that has the useful information and noise is removed

This is also the **best** rank- k approximation (closest to the original A)

Rank-**k** approximations (A_k)

$$\begin{pmatrix} A_k \\ n \times d \end{pmatrix} = \begin{pmatrix} U_k \\ n \times k \end{pmatrix} \cdot \begin{pmatrix} \Sigma_k \\ k \times k \end{pmatrix} \cdot \begin{pmatrix} V_k^T \\ k \times d \end{pmatrix}$$

U_k : orthogonal matrix containing the top **k** left singular vectors of **A**.

V_k : orthogonal matrix containing the top **k** right singular vectors of **A**.

Σ_k : diagonal matrix containing the top **k** singular values of **A**

A_k is a rank-k approximation of **A**

A_k is the **best** approximation of **A**

SVD as an optimization

- The **rank-k approximation** matrix A_k produced by the top-k singular vectors of A **minimizes** the **Frobenious norm** of the difference with the matrix A

$$A_k = \arg \min_{B: \text{rank}(B)=k} \|A - B\|_F^2$$

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

Explanation: The (i, j) cell in A_k is close on average with the (i, j) cell of A

What does this mean?

- We can **project** the row (and column) vectors of the matrix A into a **k-dimensional space** and preserve most of the information
- (**Ideally**) The A_k approximation of matrix A , contains all the **useful information**, and what is discarded is noise
- (**Ideally**) The k dimensions reveal **latent features/aspects/topics** of the term (document) space.

Latent factor model

- Rows (columns) are linear combinations of **k latent factors**
 - E.g., in our extreme document example there are two factors
- Some **noise** is added to this rank-k matrix resulting in higher rank
- SVD retrieves the latent factors (hopefully).

An (extreme) example

- User-Movie matrix
 - Blue and Red rows (columns) are **linearly dependent**

$$A = \begin{bmatrix} \text{Blue} & \text{White} \\ \text{White} & \text{Red} \end{bmatrix}$$

- There are two **prototype** users (vectors of movies): blue and red
 - To describe the data is enough to describe the two **prototypes**, and the **projection weights** for each row
- **A** is a **rank-2** matrix

$$A = [w_1, w_2] \begin{bmatrix} d_1^T \\ d_2^T \end{bmatrix}$$



SVD – Example: Users-to-Movies

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

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	0	0	4	4
	0	0	0	5	5
	0	0	0	2	2

Matrix U (User Latent Factors):

0.14	0.00
0.42	0.00
0.56	0.00
0.70	0.00
0.00	0.60
0.00	0.75
0.00	0.30

Matrix Σ (Singular Values):

12.4	0
0	9.5

Matrix V^T (Movie Latent Factors):

0.58	0.58	0.58	0.00	0.00
0.00	0.00	0.00	0.71	0.71

The decomposition is shown as:

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

SVD – Example: Users-to-Movies

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

Diagram illustrating the SVD decomposition for a Users-to-Movies matrix A .

The matrix A (Users to Movies) is shown with rows representing movies and columns representing users. The rows are labeled with movie titles: Matrix, Alien, Serenity, Casablanca, and Amelie. The columns are labeled with user ratings: 1, 3, 4, 5, 0, 0, 0, 0, 0, 0, 0, 2, 2.

The matrix A is decomposed into three matrices: U (user-to-concept similarity matrix), Σ (singular values), and V^T (movie-to-concept similarity matrix).

The matrix U is shown as a 5x2 matrix with columns labeled "SciFi-concept" and "Romance-concept". The values are:

	SciFi-concept	Romance-concept
Matrix	0.14	0.00
Alien	0.42	0.00
Serenity	0.56	0.00
Casablanca	0.70	0.00
Amelie	0.00	0.60

The matrix Σ is shown as a 2x2 matrix with diagonal elements 12.4 and 9.5.

The matrix V^T is shown as a 5x2 matrix with columns labeled "SciFi" and "Romance". The values are:

	SciFi	Romance
Matrix	0.58	0.00
Alien	0.58	0.00
Serenity	0.58	0.00
Casablanca	0.00	0.71
Amelie	0.00	0.71

The decomposition is shown as:

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

Annotations: The value 0.14 in the U matrix is circled in red. The value 0.75 in the V^T matrix is circled in red. A green box contains the text: U is "user-to-concept" similarity (or importance) matrix.

SVD – Example: Users-to-Movies

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

Diagram illustrating the SVD decomposition for a Users-to-Movies matrix A .

The matrix A (Users to Movies) is shown with rows representing movies (Matrix, Alien, Serenity, Casablanca, Amelie) and columns representing users (SciFi, Romance). The matrix is:

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

The matrix A is decomposed into three matrices:

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

Where:

- U is the "movie to concept" similarity (or importance) matrix.
- Σ is the diagonal matrix of singular values.
- V^T is the "movie to concept" similarity (or importance) matrix.

The matrix U is:

$$U = \begin{bmatrix} 0.14 & 0.00 \\ 0.42 & 0.00 \\ 0.56 & 0.00 \\ 0.70 & 0.00 \\ 0.00 & 0.60 \\ 0.00 & 0.75 \\ 0.00 & 0.30 \end{bmatrix}$$

The matrix Σ is:

$$\Sigma = \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix}$$

The matrix V^T is:

$$V^T = \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.71 & 0.71 \end{bmatrix}$$

The matrix V^T is circled in red, indicating it is the "movie to concept" similarity (or importance) matrix.

SVD – Example: Users-to-Movies

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

Diagram illustrating the SVD decomposition of a Users-to-Movies matrix A .

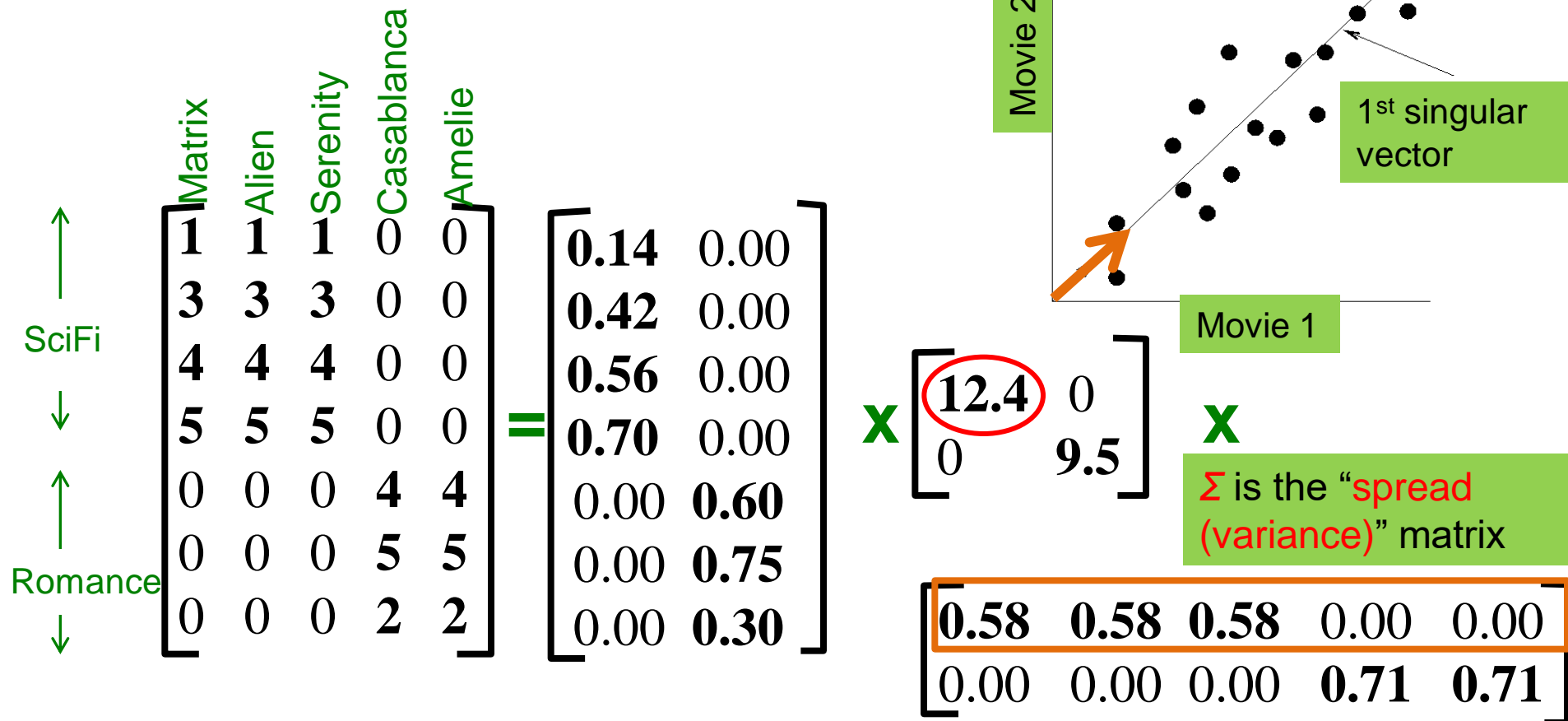
The matrix A (Users to Movies) is shown with rows representing movies and columns representing users. The rows are labeled with movie titles: Matrix, Alien, Serenity, Casablanca, and Amelie. The columns are labeled with user names: Matrix, Alien, Serenity, Casablanca, and Amelie. The matrix is annotated with "SciFi" (up arrow) and "Romance" (down arrow) on the left, and "SciFi-concept" (down arrow) and "Romance-concept" (down arrow) on the right.

$$\begin{bmatrix}
 1 & 1 & 1 & 0 & 0 \\
 3 & 3 & 3 & 0 & 0 \\
 4 & 4 & 4 & 0 & 0 \\
 5 & 5 & 5 & 0 & 0 \\
 0 & 0 & 0 & 4 & 4 \\
 0 & 0 & 0 & 5 & 5 \\
 0 & 0 & 0 & 2 & 2
 \end{bmatrix}
 =
 \begin{bmatrix}
 0.14 & 0.00 \\
 0.42 & 0.00 \\
 0.56 & 0.00 \\
 0.70 & 0.00 \\
 0.00 & 0.60 \\
 0.00 & 0.75 \\
 0.00 & 0.30
 \end{bmatrix}
 \times
 \begin{bmatrix}
 12.4 & 0 \\
 0 & 9.5
 \end{bmatrix}
 \times
 \begin{bmatrix}
 0.58 & 0.58 & 0.58 & 0.00 & 0.00 \\
 0.00 & 0.00 & 0.00 & 0.71 & 0.71
 \end{bmatrix}$$

Σ is the "concept strength" matrix

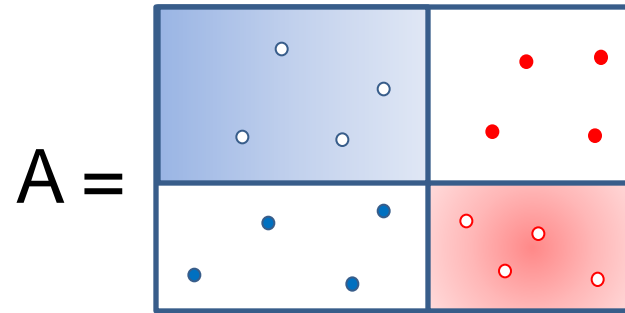
SVD – Example: Users-to-Movies

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



An (more realistic) example

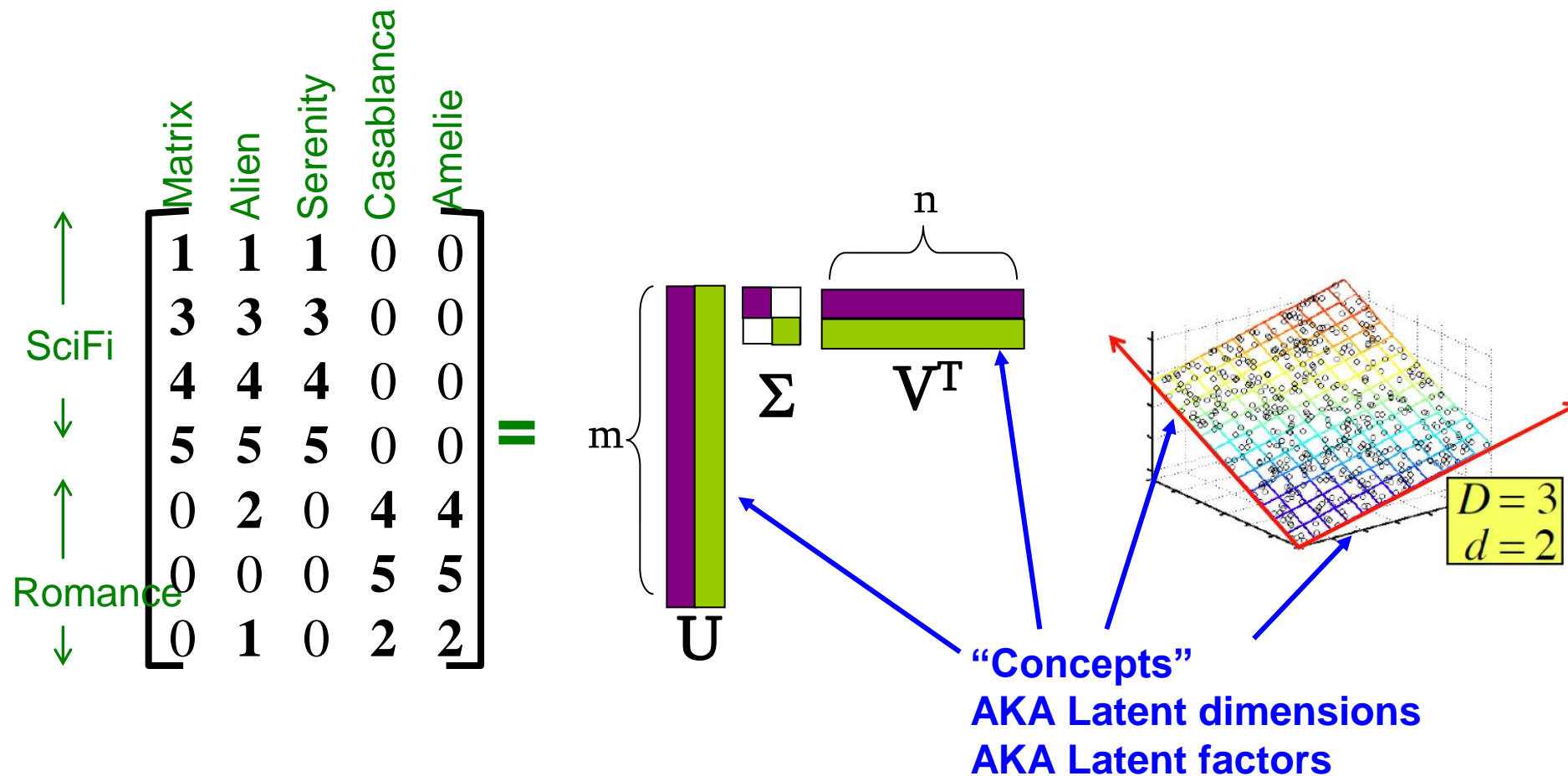
- User-Movie matrix



- There are two prototypes of users and movies but they are **noisy**
 - Missing ratings
 - Ratings out of “character”
- This is the usual case for real data (lots of missing entries)

SVD – Example: Users-to-Movies

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



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

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

Matrix A (Users to Movies):

	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
Rom	0	2	0	4	4
	0	0	0	5	5
	0	1	0	2	2

Matrix U (User Latent Space):

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 Space):

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 .
- Romance-concept:** Points to the second column of U .
- Green box:** The first two vectors are more or less unchanged.
- Green arrows:** Indicate the mapping from the original matrix A to the latent space matrices U and V^T .

SVD – Example: Users-to-Movies

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

SciFi \uparrow
 \downarrow
 Rom \uparrow
 \downarrow

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

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

The third vector has a very low singular value

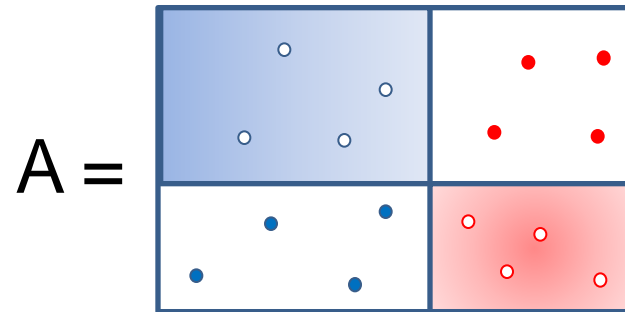
SVD - Interpretation

‘**movies**’, ‘**users**’ and ‘**concepts**’:

- U : user-to-concept similarity matrix
- V : movie-to-concept similarity matrix
- Σ : its diagonal elements:
 ‘**strength**’ of each concept

Rank-k approximation

- In this User-Movie matrix



- We have more than two singular vectors, but the **strongest** ones are still about the two types.
 - The third models the **noise** in the data
- By keeping the two **strongest singular vectors** we obtain most of the information in the data.
 - This is the **rank-2 approximation** of the matrix A

Example

More details

- **Q:** How exactly is dim. reduction done?
- **A: Compute SVD**

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

Example

More details

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

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

Example

More details

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

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

Example

More details

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

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

Note: In the original image, the third column of the second matrix and the third row of the third matrix are crossed out with red lines, indicating they are the smallest singular values being set to zero.

Example

More details

- **Q:** How exactly is dim. reduction done?
- **A:** Keep the new representation of the users-movies

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \approx \begin{bmatrix} 0.13 & -0.02 \\ 0.41 & -0.07 \\ 0.55 & -0.09 \\ 0.68 & -0.11 \\ 0.15 & 0.59 \\ 0.07 & 0.73 \\ 0.07 & 0.29 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \times \begin{bmatrix} 0.56 & 0.59 & 0.56 & 0.09 & 0.09 \\ -0.12 & 0.02 & -0.12 & 0.69 & 0.69 \end{bmatrix}$$

Example

More details

- **Q:** How exactly is dim. reduction done?
- **A:** Compute new matrix that approximates the original (w/o noise)

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \approx \begin{bmatrix} 0.92 & 0.95 & 0.92 & 0.01 & 0.01 \\ 2.91 & 3.01 & 2.91 & -0.01 & -0.01 \\ 3.90 & 4.04 & 3.90 & 0.01 & 0.01 \\ 4.82 & 5.00 & 4.82 & 0.03 & 0.03 \\ 0.70 & 0.53 & 0.70 & 4.11 & 4.11 \\ -0.69 & 1.34 & -0.69 & 4.78 & 4.78 \\ 0.32 & 0.23 & 0.32 & 2.01 & 2.01 \end{bmatrix}$$

Frobenius norm:

$$\|M\|_F = \sqrt{\sum_{ij} M_{ij}^2}$$

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

is “small”

SVD for matrix reconstruction

- We will now see how we can use the fact that SVD gives the best rank- k approximation for a data matrix A .
- The idea is that we assume that the “true” matrix is rank- k , and rank is increased due to noise
- We use SVD to find the best rank- k approximation for A , and thus the best approximation of the “true” matrix

Application: Recommender systems

- Data: Users rating movies
 - Sparse and often noisy
- Assumption: There are k basic **user profiles**, and each user is a **linear combination** of these profiles
 - E.g., action, comedy, drama, romance
 - Each user is a weighted combination of these profiles
- Assumption: The matrix with the **true preferences** of the users for the movies is a rank- k matrix A_k

Model-based Recommendation Systems

- What we observe is \tilde{A} a **noisy**, and **incomplete** version matrix A_k
- Given matrix \tilde{A} and we would like to get the missing ratings that A_k would produce
- **Algorithm**: compute the **rank-k approximation** \tilde{A}_k of matrix \tilde{A} and predict for user u and movie m , the value $\tilde{A}_k[m, u]$.
 - The rank-k approximation \tilde{A}_k is **provably** close to the ideal matrix A_k (under some model assumptions for the missing and noisy entries)
- **Model-based** collaborative filtering

Example

Missing ratings and noise

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 3 & 3 & 0 & 0 \\ 4 & 4 & 0 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} = \begin{bmatrix} 0.14 & -0.06 & -0.04 \\ 0.30 & -0.11 & -0.61 \\ 0.43 & -0.16 & 0.76 \\ 0.74 & -0.31 & -0.18 \\ 0.15 & 0.53 & 0.02 \\ 0.07 & 0.70 & -0.03 \\ 0.07 & 0.27 & 0.01 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 1.3 \end{bmatrix} \times \begin{bmatrix} 0.51 & 0.66 & 0.44 & 0.23 & 0.23 \\ -0.24 & -0.13 & -0.21 & 0.66 & 0.66 \\ 0.59 & 0.08 & -0.80 & 0.01 & 0.01 \end{bmatrix}$$

Example

Missing ratings and noise

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 3 & 3 & 0 & 0 \\ 4 & 4 & 0 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} = \begin{bmatrix} 0.14 & -0.06 & -0.04 \\ 0.30 & -0.11 & -0.61 \\ 0.43 & -0.16 & 0.76 \\ 0.74 & -0.31 & -0.18 \\ 0.15 & 0.53 & 0.02 \\ 0.07 & 0.70 & -0.03 \\ 0.07 & 0.27 & 0.01 \end{bmatrix} \times \begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 1.3 \end{bmatrix} \times \begin{bmatrix} 0.51 & 0.66 & 0.44 & 0.23 & 0.23 \\ -0.24 & -0.13 & -0.21 & 0.66 & 0.66 \\ 0.59 & 0.08 & -0.80 & 0.01 & 0.01 \end{bmatrix}$$

The matrix multiplication is shown with various annotations:

- Blue '0' in the first row of the first matrix.
- Red '2' in the fifth row of the first matrix.
- Red '1' in the seventh row of the first matrix.
- Red '0' in the third row of the first matrix.
- Red '0.61' in the second row of the second matrix.
- Red '0.76' in the third row of the second matrix.
- Red '0.18' in the fourth row of the second matrix.
- Red '0.01' in the seventh row of the second matrix.
- Red '1.3' in the third row of the third matrix.
- Red lines crossing out the third column of the second matrix and the third row of the third matrix.
- Green 'x' marks between the second and third matrices.

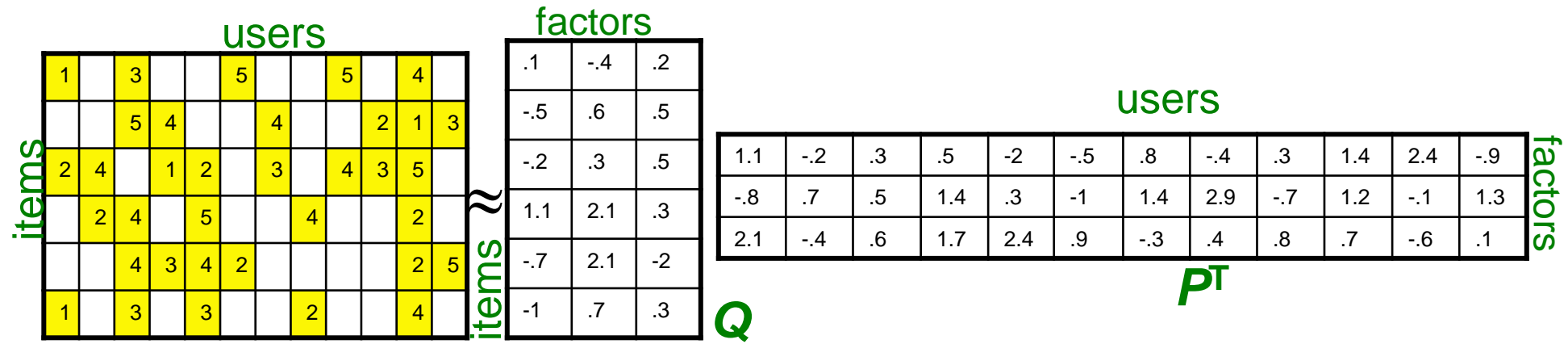
Example

- Reconstruction of missing ratings

$$\begin{bmatrix} 0.96 & 1.14 & 0.82 & -0.01 & -0.01 \\ 1.94 & 2.32 & 1.66 & 0.07 & 0.07 \\ 2.77 & 3.32 & 2.37 & 0.08 & 0.08 \\ 4.84 & 5.74 & 4.14 & -0.08 & 0.08 \\ 0.40 & 1.42 & 0.33 & 4.06 & 4.06 \\ -0.42 & 0.63 & -0.38 & 4.92 & 4.92 \\ 0.20 & 0.71 & 0.16 & 2.03 & 2.03 \end{bmatrix}$$

- This is the rank-2 approximation of the input matrix

Latent Factor Models



- SVD also considers entries that are missing!
- Use specialized methods to find P , Q

- $$\min_{P, Q} \sum_{(i, x) \in R} (r_{xi} - q_i^T \cdot p_x)^2$$

$$\hat{r}_{xi} = q_i^T \cdot p_x$$

- **Note:**

- We don't require cols of P , Q to be orthogonal/unit length
- P , Q map users/movies to a latent space

Latent factors

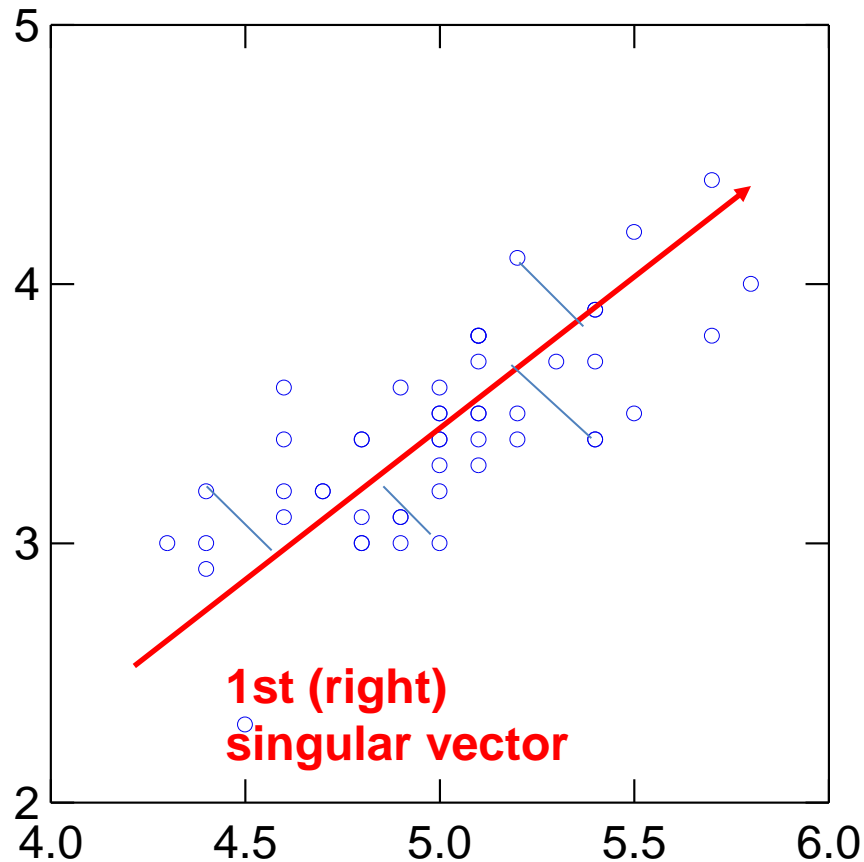
- We can define latent factor models that apply the same idea in different ways
 - Probabilistic/Generative models.
- The latent factor methods work well in practice, and they are employed by most sophisticated recommendation systems
- Today there is also a lot of deep learning involved

Another Application

- **Latent Semantic Indexing (LSI):**
 - Apply PCA on the **document-term** matrix, and index the k-dimensional vectors
 - When a query comes, **project** it onto the k-dimensional space and compute **cosine similarity** in this space
 - Principal components capture main **topics**, and enrich the document representation

Another property of PCA/SVD

- The chosen vectors are such that minimize the **sum of square differences** between the data vectors and the low-dimensional projections



**SVD is “the Rolls-Royce and the Swiss
Army Knife of Numerical Linear
Algebra.”***

***Dianne O’Leary, MMDS ’06**

Other dimensionality reduction techniques

- **Multidimensional Scaling**

- You are given pairwise distances between objects
- Find a low-dimensional representation of the objects (2D for visualization) such that you approximate the distances as well as possible

- **Embeddings:**

- Use a very simplistic, high-dimensional representation of the data (e.g., one-hot encoding)
- Consider a prediction problem (e.g., predict the context words) and pass the data through a multi-layer neural network.
- Use the input of the last layer as the representation

Computation of eigenvectors

- Consider a symmetric square matrix M
- Power-method:
 - Start with the vector v of all 1's
 - Compute $v = Mv$
 - Normalize by the length of v
 - Repeat until the vector does not change
- This will give us the first eigenvector.
- The first eigenvalue is $\lambda = v^T M v$
- For the second one, compute the first eigenvector of the matrix $M^* = M - \lambda v v^T$

Computing singular vectors

- Compute the eigenvectors and eigenvalues of the matrices MM^T and $M^T M$