

# COMP7180 - Lecture 4

## Dimensionality Reduction (Feature Extraction) – Part II

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# Summary of Eigenvalues and Eigenvectors

- Eigenvalue equation  $\mathbf{Ax} = \lambda\mathbf{x}$ : An **eigenvector**  $\mathbf{x}$  lies along the same line as  $\mathbf{Ax}$ , the **eigenvalue** is  $\lambda$ .
- If  $\mathbf{Ax} = \lambda\mathbf{x}$ , then  $(\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = 0$  and  $\mathbf{A} - \lambda\mathbf{I}$  is singular and  $\det(\mathbf{A} - \lambda\mathbf{I}) = 0$ .
- If  $\mathbf{Ax} = \lambda\mathbf{x}$ , the eigenvalues of  $\mathbf{A}^k$  and  $(\mathbf{A} + c\mathbf{I})$  are  $\lambda^k$  and  $\lambda + c$ , with the same eigenvectors of  $\mathbf{A}$ .
- The sum of the eigenvalues  $\lambda$ 's equals the sum down the main diagonal of  $\mathbf{A}$  (the trace). The product of the  $\lambda$ 's equals the determinant of  $\mathbf{A}$ .
- If the  $n$  by  $n$  matrix  $\mathbf{A}$  has  $n$  linearly independent eigenvectors  $\mathbf{x}_1, \dots, \mathbf{x}_n$ , eigen-decomposition of  $\mathbf{A}$  is  $\mathbf{A} = \mathbf{X}\mathbf{\Lambda}\mathbf{X}^{-1}$ .
- The powers of  $\mathbf{A}$  are  $\mathbf{A}^k = \mathbf{X}\mathbf{\Lambda}^k\mathbf{X}^{-1}$ . The eigenvectors in  $\mathbf{X}$  are unchanged.
- Eigen-decomposition for symmetric matrix  $\mathbf{S}$  becomes  $\mathbf{S} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$  with an orthonormal eigenvector matrix  $\mathbf{Q}$ .

# Singular Value Decomposition (SVD)

# Singular Value Decomposition

- The eigenvalue decomposition requires square matrices. It would be useful to perform a decomposition on general matrices.
- The singular value decomposition (SVD) of a matrix is a central matrix decomposition method in linear algebra. It has been referred to as the “fundamental theorem of linear algebra” because it can be applied to all matrices, not only to square matrices, and it always exists.

# SVD - Definition

- The Singular value decomposition (SVD) of a rectangular matrix  $\mathbf{A}^{m \times n}$

$$\begin{array}{c} \mathbf{A} \\ m \times n \end{array} = \begin{array}{c} \mathbf{U} \\ m \times m \end{array} \begin{array}{c} \mathbf{\Sigma} \\ m \times n \end{array} \begin{array}{c} \mathbf{V}^T \\ n \times n \end{array}$$

$$\begin{array}{c} \mathbf{A} \\ m \times n \end{array} = \begin{array}{c} \mathbf{U} \\ m \times r \end{array} \begin{array}{c} \mathbf{\Sigma} \\ r \times r \end{array} \begin{array}{c} \mathbf{V}^T \\ r \times n \end{array}$$

# SVD - Properties

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

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

- $\mathbf{U}$  is the  $m \times m$  or  $m \times r$  matrix (**left singular matrix**) whose columns are orthonormal eigenvectors of  $\mathbf{A}^* \mathbf{A}^T$ :  $\mathbf{A} \mathbf{A}^T = \mathbf{U} \Sigma \mathbf{V}^T \mathbf{V} \Sigma \mathbf{U}^T = \mathbf{U} \Sigma^2 \mathbf{U}^T$

# SVD - Properties

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

- $\mathbf{V}$  is the  $n \times n$  or  $n \times r$  matrix (**right singular matrix**) whose columns are orthonormal eigenvectors of  $\mathbf{A}^T \mathbf{A}$ :  $\mathbf{A}^T \mathbf{A} = \mathbf{V} \Sigma \mathbf{U}^T \mathbf{U} \Sigma \mathbf{V}^T = \mathbf{V} \Sigma^2 \mathbf{V}^T$

# SVD - Properties

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

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

- $\Sigma$  is an  $m \times n$  or  $r \times r$  diagonal matrix with non-negative numbers on the diagonal (These non-negative numbers are the square root of eigenvalues shared by  $\mathbf{A}^* \mathbf{A}^T$  and  $\mathbf{A}^T \mathbf{A}$ ) (also call **singular values** of matrix  $\mathbf{A}$ )



# SVD - Properties

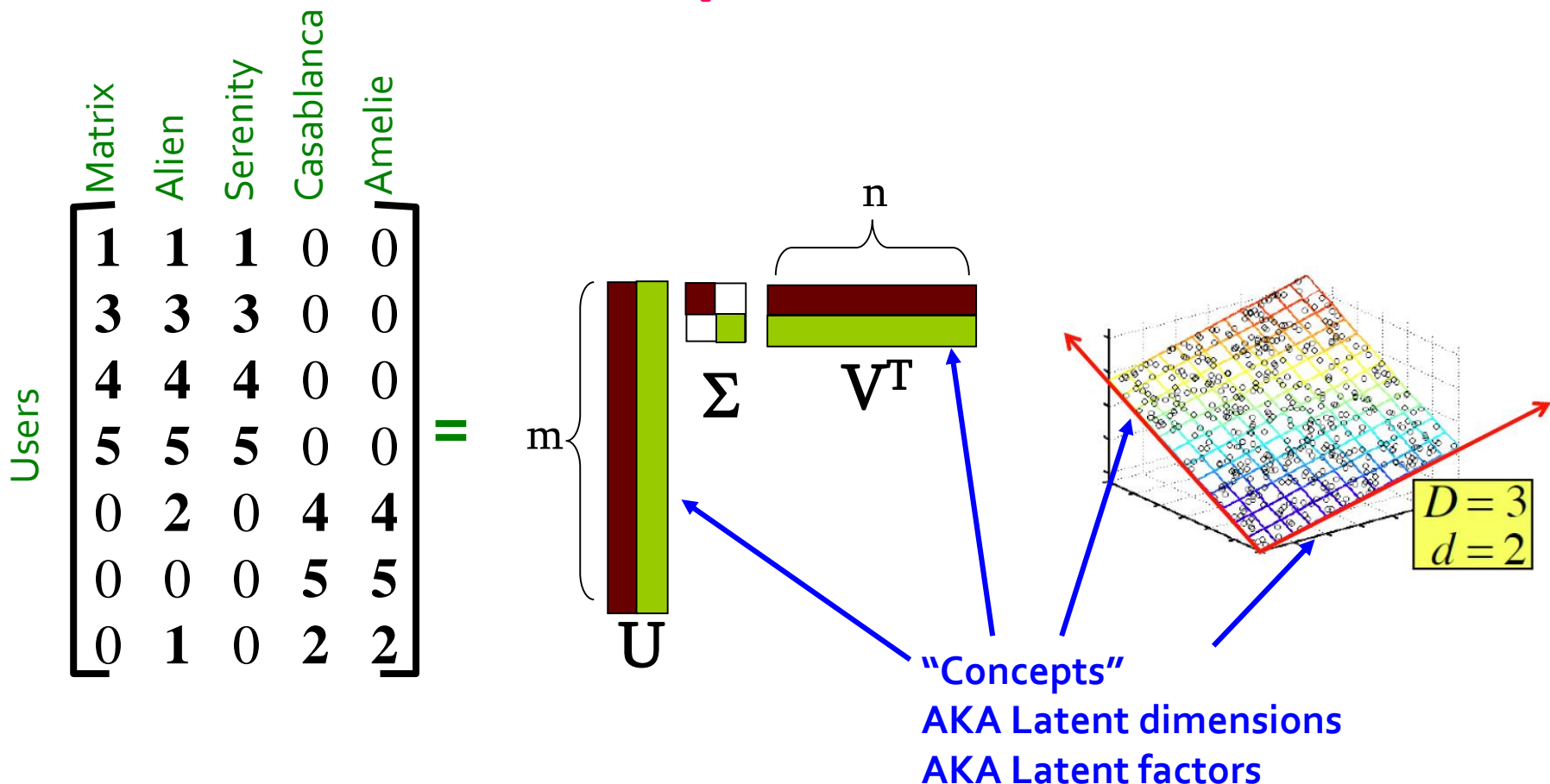
$$\mathbf{A}_{[m \times n]} = \mathbf{U}_{[m \times m]} \mathbf{\Sigma}_{[m \times n]} (\mathbf{V}_{[n \times n]})^T$$

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- $\mathbf{V}$  is the  $n \times n$  or  $n \times r$  matrix (**right singular matrix**) whose columns are orthonormal eigenvectors of  $\mathbf{A}^T \mathbf{A}$ :  $\mathbf{A}^T \mathbf{A} = \mathbf{V} \mathbf{\Sigma} \mathbf{U}^T \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T = \mathbf{V} \mathbf{\Sigma}^2 \mathbf{V}^T$
- $\mathbf{\Sigma}$  is an  $m \times n$  or  $r \times r$  diagonal matrix with non-negative numbers on the diagonal (These non-negative numbers are the square root of eigenvalues shared by  $\mathbf{A}^* \mathbf{A}^T$  and  $\mathbf{A}^T \mathbf{A}$ ) (also call **singular values** of matrix  $\mathbf{A}$ )

# 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

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

# SVD – Example: Users-to-Movies

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

Users

	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

SciFi-concept

Romance-concept

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

# SVD – Example: Users-to-Movies

■  $A = U \Sigma V^T$  - example:

$U$  is “user-to-concept” similarity matrix

$$\begin{array}{c} \text{Users} \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{array}{c} \text{SciFi-concept} \\ \text{Romance-concept} \end{array}
 \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}
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# SVD – Example: Users-to-Movies

## ■ $A = U \Sigma V^T$ - example:

Users

	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

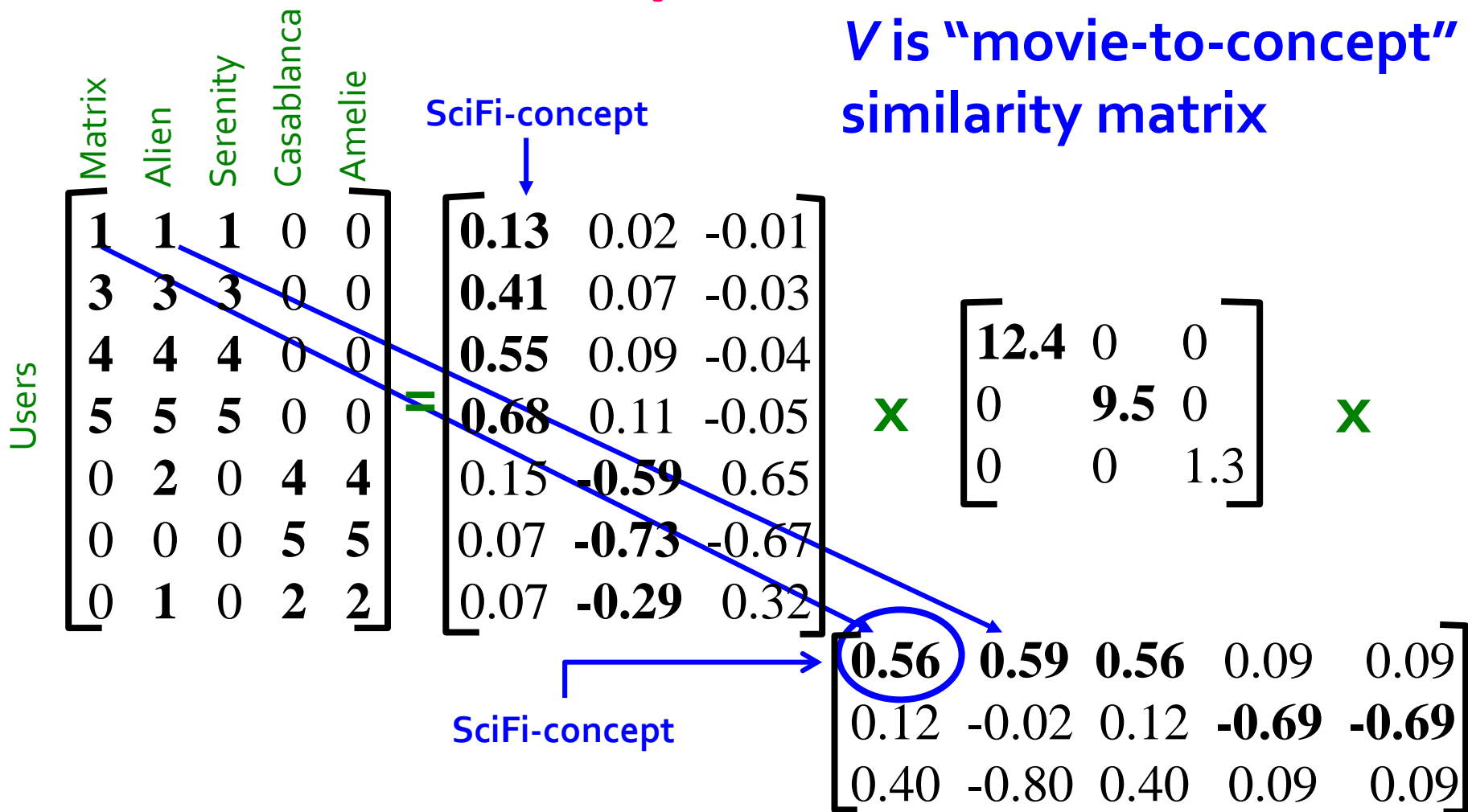
SciFi-concept

"strength" of the SciFi-concept

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

# SVD – Example: Users-to-Movies

## ■ $A = U \Sigma V^T$ - example:



# SVD - Interpretation

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

- $U$ : user-to-concept similarity matrix
- $V$ : movie-to-concept similarity matrix
- $\Sigma$ : its diagonal elements:  
‘strength’ of each concept



# SVD for DR

## More details

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

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

# SVD for DR

## More details

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

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

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The diagram illustrates the SVD decomposition of a matrix. The first matrix is a 7x5 matrix. The second matrix is a 7x3 matrix, with its third column crossed out by a red line. The third matrix is a 3x3 diagonal matrix, with its third row and column crossed out by a red line. The fourth matrix is a 3x5 matrix, with its third row and column crossed out by a red line. The green 'x' symbols indicate the multiplication of the matrices.

# SVD for DR

## More details

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

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

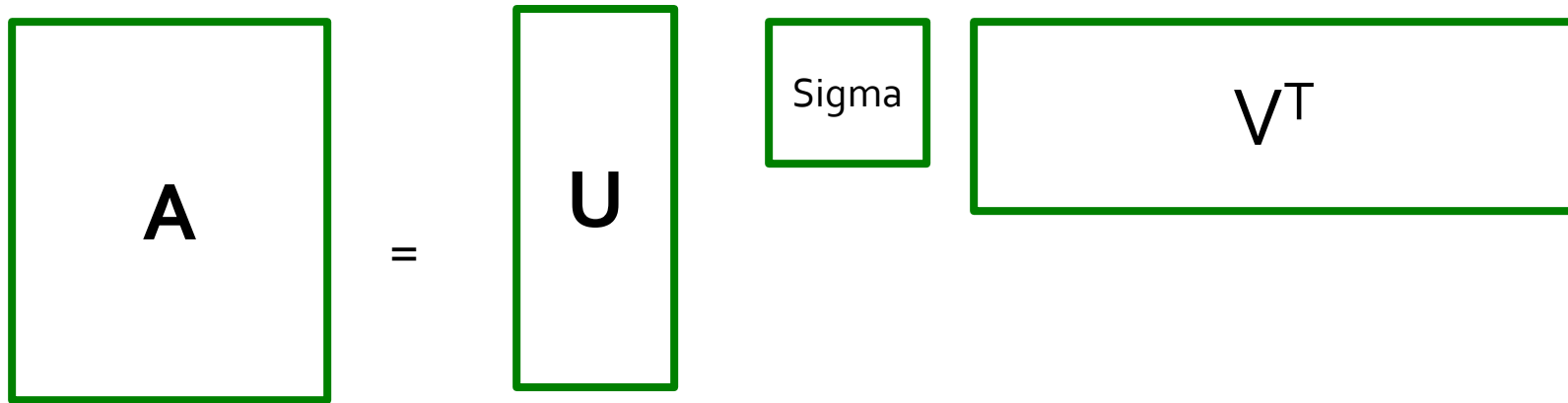
# SVD for DR

## More details

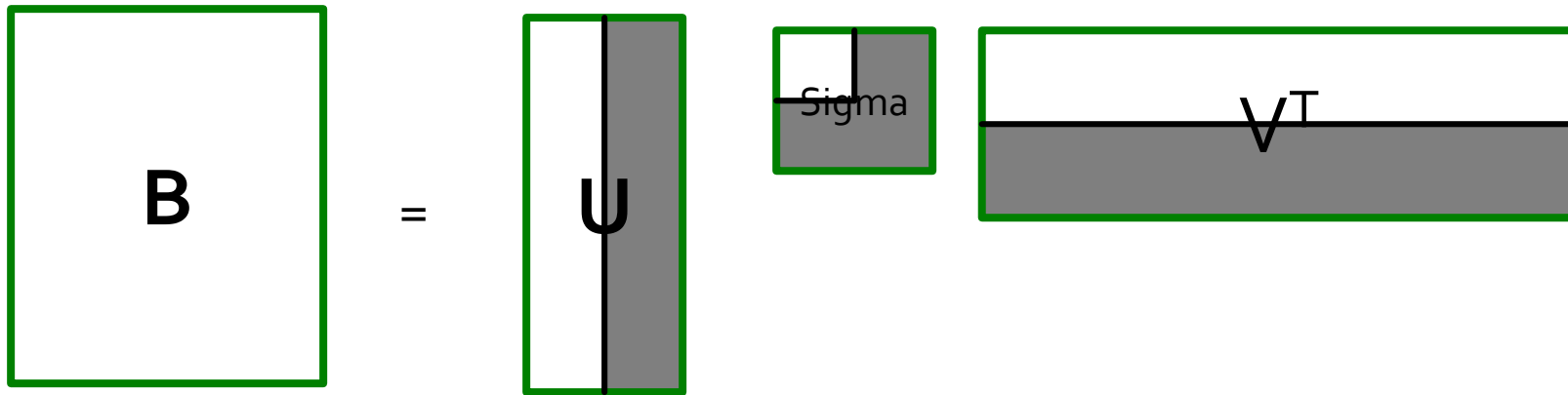
- **Q:** How exactly is dim. reduction done?
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$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix} \approx \begin{bmatrix} 0.92 & 0.95 & 0.92 & 0.01 & 0.01 \\ 2.91 & 3.01 & 2.91 & -0.01 & -0.01 \\ 3.90 & 4.04 & 3.90 & 0.01 & 0.01 \\ 4.82 & 5.00 & 4.82 & 0.03 & 0.03 \\ 0.70 & 0.53 & 0.70 & 4.11 & 4.11 \\ -0.69 & 1.34 & -0.69 & 4.78 & 4.78 \\ 0.32 & 0.23 & 0.32 & 2.01 & 2.01 \end{bmatrix}$$

# SVD – Best Low Rank Approx.



**B is best approximation of A**



# SVD – Best Low Rank Approx.

## ■ Theorem:

Let  $A = U \Sigma V^T$  and  $B = U S V^T$  where  
 $S = \text{diagonal } r \times r \text{ matrix}$  with  $s_i = \sigma_i$  ( $i=1 \dots k$ ) else  $s_i=0$   
 then  $B$  is a **best**  $\text{rank}(B)=k$  approx. to  $A$

What do we mean by “best”:

- $B$  is a solution to  $\min_B \|A - B\|_F$  where  $\text{rank}(B)=k$

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

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



# 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, where rows represent genres (SciFi, Romance) and columns represent movies (Matrix, Alien, Serenity, Casablanca, Amelie). The matrix is:

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

The matrix is multiplied by a 5x3 matrix (Concept Space) to produce a 6x3 matrix (Result):

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

Annotations:

- Green arrows indicate the mapping from the query matrix to the concept space matrix.
- Green 'X' symbols indicate the multiplication operation.
- Green text labels 'SciFi' and 'Romance' are positioned next to the first and last rows of the query matrix, respectively.

# 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?

Compactly, we have:

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

E.g.:

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

# Case study: How to query?

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

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

E.g.:

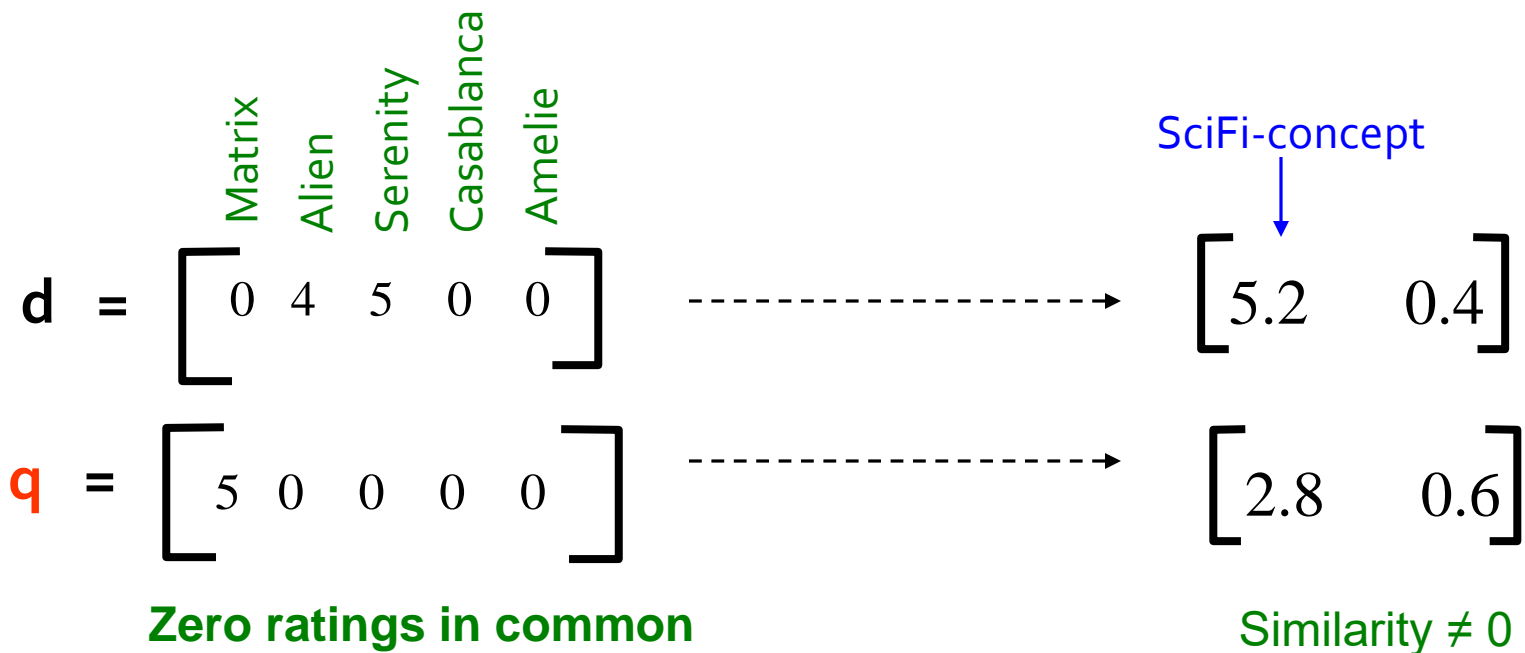
$$\mathbf{d} = \begin{matrix} & \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \\ \begin{bmatrix} 0 & 4 & 5 & 0 & 0 \end{bmatrix} & \mathbf{x} & \begin{bmatrix} 0.56 & 0.12 \\ 0.59 & -0.02 \\ 0.56 & 0.12 \\ 0.09 & -0.69 \\ 0.09 & -0.69 \end{bmatrix} & = & \begin{bmatrix}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

movie-to-concept  
similarities (V)

SciFi-concept  
↓

# Case study: How to query?

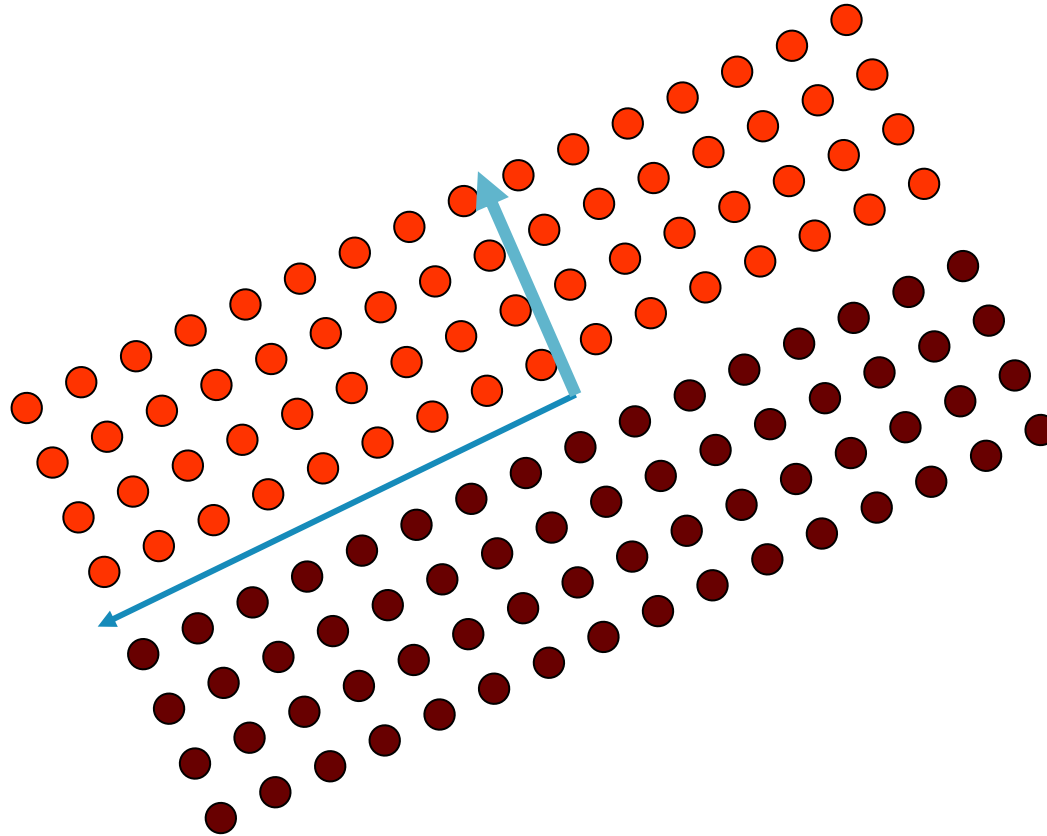
- **Observation:** User  $d$  that rated ('*Alien*', '*Serenity*') will be **similar** to user  $q$  that rated ('*Matrix*'), although  $d$  and  $q$  have **zero ratings in common!**



# Linear Discriminant Analysis (LDA)

# Limitations of PCA

- PCA is **not** always an optimal dimensionality-reduction technique for classification purposes.



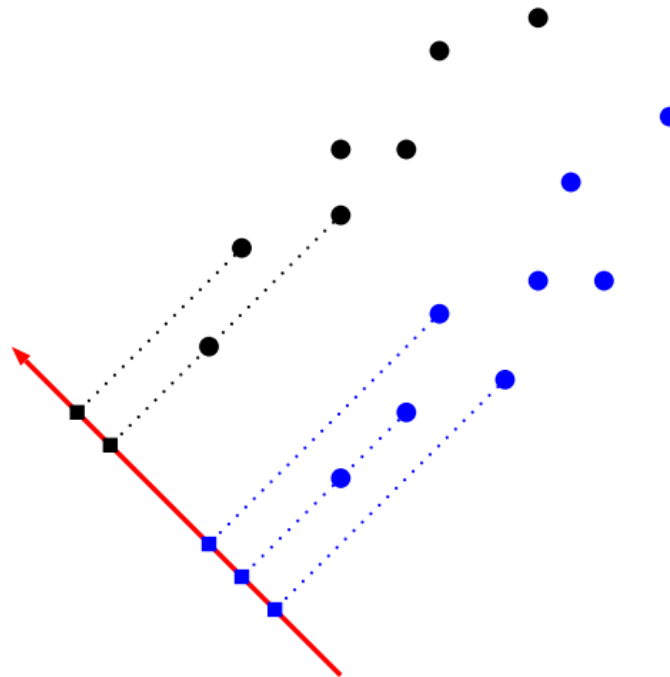
# Objective of LDA

- Perform dimensionality reduction “while preserving as much of the class discriminative information as possible”.
- Seeks to find directions along which the classes are best separated, rather than the directions with the maximum variance.



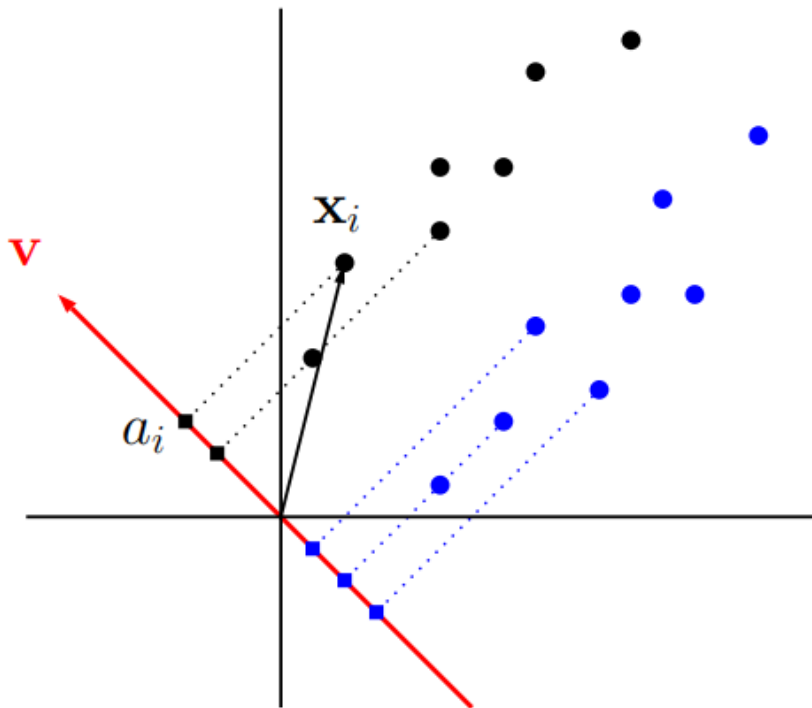
# LDA: Two Classes

Given a training data set  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$  consisting of two classes  $C_1, C_2$ , find a direction that “best” discriminates between the two classes.



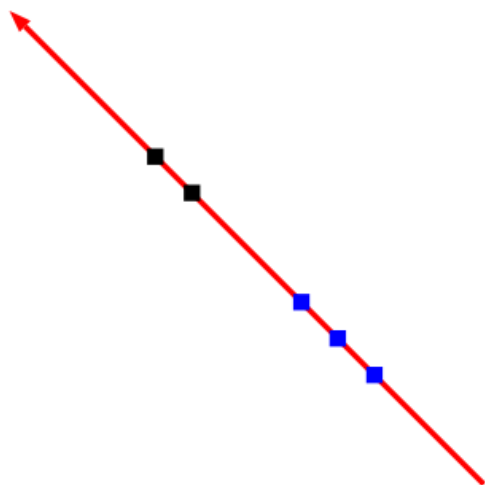
# LDA: 1-D Projection

- Consider any unit vector  $\mathbf{v} \in R^d$  as the projection direction
- The 1D projections of the points are:  
 $a_i = \mathbf{v}^T \mathbf{x}_i$  ( $i = 1, \dots, n$ )



# LDA: Initial Idea

Now the data look like this:



How do we quantify the separation between the two classes (in order to compare different directions  $\mathbf{v}$  and select the best one)?

One (naive) idea is to measure the distance between the two class means in the 1D projection space:  $|\mu_1 - \mu_2|$ , where

$$\begin{aligned}\mu_1 &= \frac{1}{n_1} \sum_{\mathbf{x}_i \in C_1} a_i = \frac{1}{n_1} \sum_{\mathbf{x}_i \in C_1} \mathbf{v}^T \mathbf{x}_i \\ &= \mathbf{v}^T \cdot \frac{1}{n_1} \sum_{\mathbf{x}_i \in C_1} \mathbf{x}_i = \mathbf{v}^T \mathbf{m}_1\end{aligned}$$

and similarly,

$$\mu_2 = \mathbf{v}^T \mathbf{m}_2, \quad \mathbf{m}_2 = \frac{1}{n_2} \sum_{\mathbf{x}_i \in C_2} \mathbf{x}_i.$$

# LDA: Problem of the Initial Idea

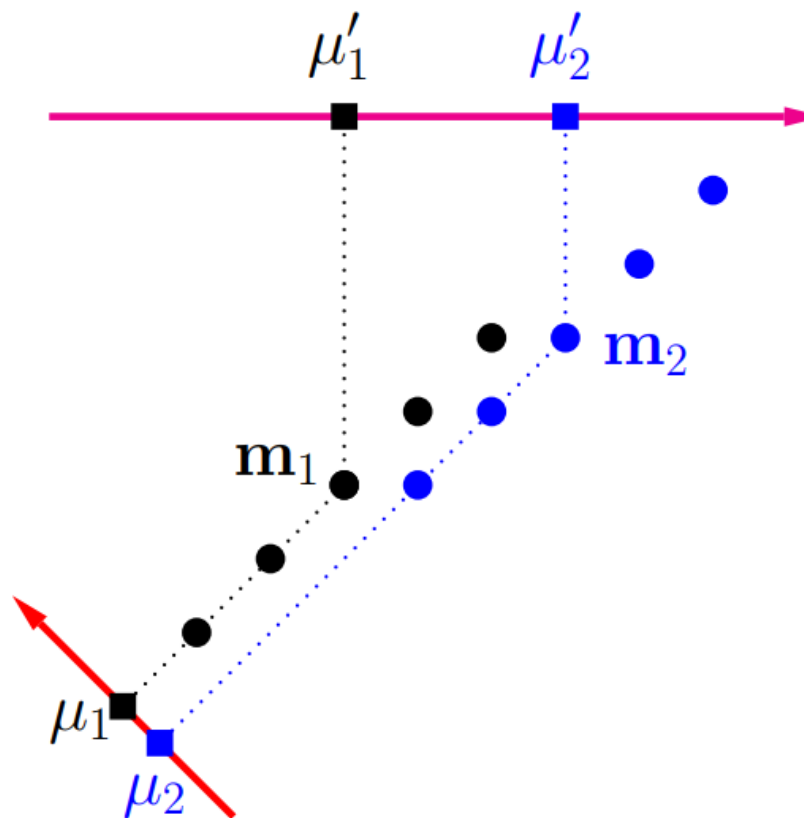
That is, we solve the following problem

$$\max_{\mathbf{v}: \|\mathbf{v}\|=1} |\mu_1 - \mu_2|$$

where

$$\mu_j = \mathbf{v}^T \mathbf{m}_j, \quad j = 1, 2.$$

However, this criterion does not always work (as shown in the right plot).



What else do we need to consider?

# LDA: Further Considerations

We should also consider the **variance** of each projected class:

$$s_1^2 = \sum_{\mathbf{x}_i \in C_1} (a_i - \mu_1)^2, \quad s_2^2 = \sum_{\mathbf{x}_i \in C_2} (a_i - \mu_2)^2$$

Ideally, the projected classes have both **faraway means** and **small variances**.

$$\max_{\mathbf{v}: \|\mathbf{v}\|=1} \frac{(\mu_1 - \mu_2)^2}{s_1^2 + s_2^2}.$$

$$\text{where } \mu_1 = \mathbf{v}^T \mathbf{m}_1, \quad \mu_2 = \mathbf{v}^T \mathbf{m}_2.$$

# LDA: Mathematical Derivation

$$\max_{\mathbf{v}: \|\mathbf{v}\|=1} \frac{(\mu_1 - \mu_2)^2}{s_1^2 + s_2^2}.$$

$$\text{where } \mu_1 = \mathbf{v}^T \mathbf{m}_1, \quad \mu_2 = \mathbf{v}^T \mathbf{m}_2.$$

First, we can rewrite the distance between the two centroids as follows:

$$\begin{aligned} (\mu_1 - \mu_2)^2 &= (\mathbf{v}^T \mathbf{m}_1 - \mathbf{v}^T \mathbf{m}_2)^2 = (\mathbf{v}^T (\mathbf{m}_1 - \mathbf{m}_2))^2 \\ &= \mathbf{v}^T (\mathbf{m}_1 - \mathbf{m}_2) \cdot (\mathbf{m}_1 - \mathbf{m}_2)^T \mathbf{v} \\ &= \mathbf{v}^T \mathbf{S}_b \mathbf{v}, \end{aligned}$$

where

$$\mathbf{S}_b = (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T \in \mathbb{R}^{d \times d}$$

is called the **between-class scatter matrix**.

# LDA: Mathematical Derivation

$$\max_{\mathbf{v}: \|\mathbf{v}\|=1} \frac{(\mu_1 - \mu_2)^2}{s_1^2 + s_2^2}.$$

$$\text{where } \mu_1 = \mathbf{v}^T \mathbf{m}_1, \quad \mu_2 = \mathbf{v}^T \mathbf{m}_2.$$

Next, for each class  $j = 1, 2$ , the variance of the projection (onto  $\mathbf{v}$ ) is

$$\begin{aligned} s_j^2 &= \sum_{\mathbf{x}_i \in C_j} (a_i - \mu_j)^2 = \sum_{\mathbf{x}_i \in C_j} (\mathbf{v}^T \mathbf{x}_i - \mathbf{v}^T \mathbf{m}_j)^2 \\ &= \sum_{\mathbf{x}_i \in C_j} \mathbf{v}^T (\mathbf{x}_i - \mathbf{m}_j) (\mathbf{x}_i - \mathbf{m}_j)^T \mathbf{v} \\ &= \mathbf{v}^T \left[ \sum_{\mathbf{x}_i \in C_j} (\mathbf{x}_i - \mathbf{m}_j) (\mathbf{x}_i - \mathbf{m}_j)^T \right] \mathbf{v} \\ &= \mathbf{v}^T \mathbf{S}_j \mathbf{v}, \end{aligned}$$

where

$$\mathbf{S}_j = \sum_{\mathbf{x}_i \in C_j} (\mathbf{x}_i - \mathbf{m}_j) (\mathbf{x}_i - \mathbf{m}_j)^T \in \mathbb{R}^{d \times d}$$

is called the **within-class scatter matrix** for class  $j$ .

# LDA: Mathematical Derivation

$$\max_{\mathbf{v}: \|\mathbf{v}\|=1} \frac{(\mu_1 - \mu_2)^2}{s_1^2 + s_2^2}.$$

$$\text{where } \mu_1 = \mathbf{v}^T \mathbf{m}_1, \quad \mu_2 = \mathbf{v}^T \mathbf{m}_2.$$

The total within-class scatter of the two classes in the projection space is

$$s_1^2 + s_2^2 = \mathbf{v}^T \mathbf{S}_1 \mathbf{v} + \mathbf{v}^T \mathbf{S}_2 \mathbf{v} = \mathbf{v}^T (\mathbf{S}_1 + \mathbf{S}_2) \mathbf{v} = \mathbf{v}^T \mathbf{S}_w \mathbf{v}$$

where

$$\mathbf{S}_w = \mathbf{S}_1 + \mathbf{S}_2 = \sum_{\mathbf{x}_i \in C_1} (\mathbf{x}_i - \mathbf{m}_1)(\mathbf{x}_i - \mathbf{m}_1)^T + \sum_{\mathbf{x}_i \in C_2} (\mathbf{x}_i - \mathbf{m}_2)(\mathbf{x}_i - \mathbf{m}_2)^T$$

is called the **total within-class scatter matrix** of the (original) training data.

Putting everything together, we have arrived at the following optimization problem:

$$\max_{\mathbf{v}: \|\mathbf{v}\|=1} \frac{\mathbf{v}^T \mathbf{S}_b \mathbf{v}}{\mathbf{v}^T \mathbf{S}_w \mathbf{v}}$$



# LDA: Mathematical Derivation

$$\max_{\mathbf{v}: \|\mathbf{v}\|=1} \frac{\mathbf{v}^T \mathbf{S}_b \mathbf{v}}{\mathbf{v}^T \mathbf{S}_w \mathbf{v}}$$

Let  $J(\mathbf{v}) = \frac{\mathbf{v}^T \mathbf{S}_b \mathbf{v}}{\mathbf{v}^T \mathbf{S}_w \mathbf{v}}$ , then  $\frac{d}{d\mathbf{v}} J(\mathbf{v}) = 0$

$$\Rightarrow (\mathbf{v}^T \mathbf{S}_w \mathbf{v}) \frac{d}{d\mathbf{v}} (\mathbf{v}^T \mathbf{S}_b \mathbf{v}) - (\mathbf{v}^T \mathbf{S}_b \mathbf{v}) \frac{d}{d\mathbf{v}} (\mathbf{v}^T \mathbf{S}_w \mathbf{v}) = 0$$

$$\Rightarrow (\mathbf{v}^T \mathbf{S}_w \mathbf{v}) 2\mathbf{S}_b \mathbf{v} - (\mathbf{v}^T \mathbf{S}_b \mathbf{v}) 2\mathbf{S}_w \mathbf{v} = 0$$

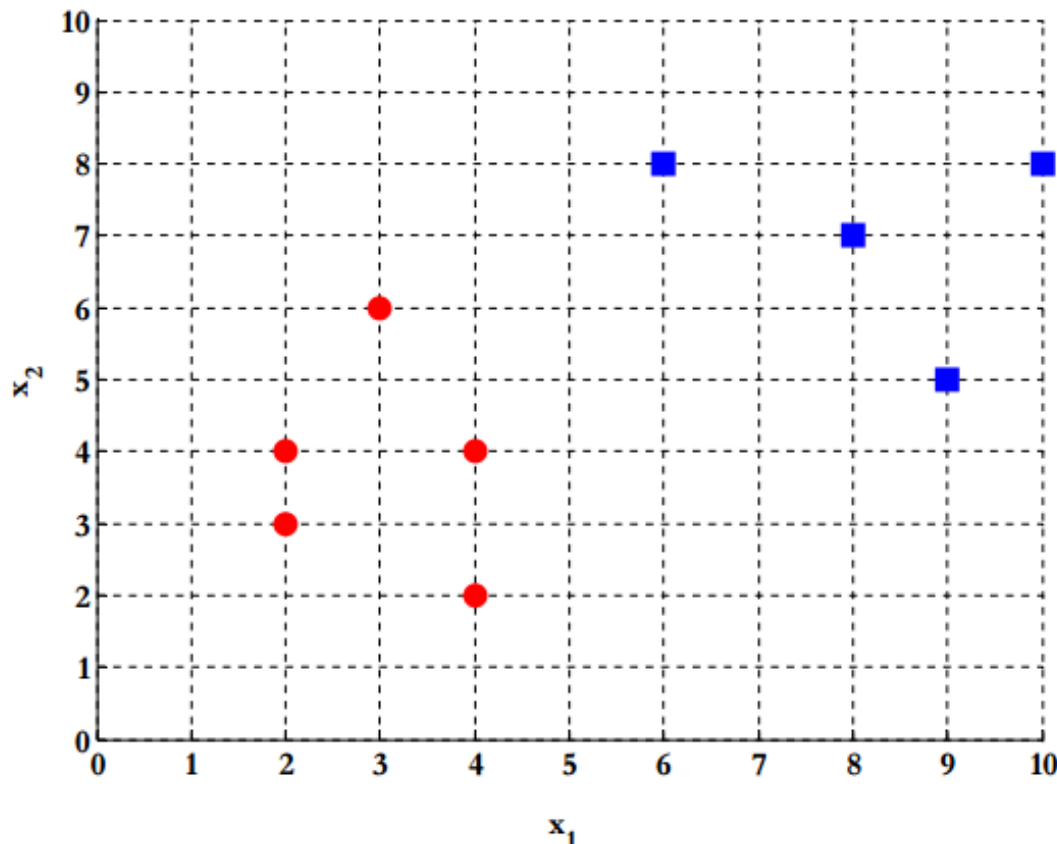
$$\Rightarrow \left( \frac{\mathbf{v}^T \mathbf{S}_w \mathbf{v}}{\mathbf{v}^T \mathbf{S}_w \mathbf{v}} \right) \mathbf{S}_b \mathbf{v} - \left( \frac{\mathbf{v}^T \mathbf{S}_b \mathbf{v}}{\mathbf{v}^T \mathbf{S}_w \mathbf{v}} \right) \mathbf{S}_w \mathbf{v} = 0$$

$$\Rightarrow \mathbf{S}_b \mathbf{v} - J(\mathbf{v}) \mathbf{S}_w \mathbf{v} = 0 \quad \Rightarrow \quad (\mathbf{S}_w^{-1} \mathbf{S}_b) \mathbf{v} = [J(\mathbf{v})] \mathbf{v}$$

$\mathbf{v}$  is the eigenvector corresponding to the largest eigenvalue of  $\mathbf{S}_w^{-1} \mathbf{S}_b$

# LDA: Two Classes - Example

- Compute the Linear Discriminant projection for the following two-dimensional dataset.
  - Samples for class  $\omega_1$  :  $\mathbf{X}_1=(x_1,x_2)=\{(4,2),(2,4),(2,3),(3,6),(4,4)\}$
  - Sample for class  $\omega_2$  :  $\mathbf{X}_2=(x_1,x_2)=\{(9,10),(6,8),(9,5),(8,7),(10,8)\}$



```
% samples for class 1
X1 = [4,2;
      2,4;
      2,3;
      3,6;
      4,4];

% samples for class 2
X2 = [9,10;
      6,8;
      9,5;
      8,7;
      10,8];
```

# LDA: Two Classes - Example

- The classes mean are :

$$\mu_1 = \frac{1}{N_1} \sum_{x \in \omega_1} x = \frac{1}{5} \left[ \begin{pmatrix} 4 \\ 2 \end{pmatrix} + \begin{pmatrix} 2 \\ 4 \end{pmatrix} + \begin{pmatrix} 2 \\ 3 \end{pmatrix} + \begin{pmatrix} 3 \\ 6 \end{pmatrix} + \begin{pmatrix} 4 \\ 4 \end{pmatrix} \right] = \begin{pmatrix} 3 \\ 3.8 \end{pmatrix}$$

$$\mu_2 = \frac{1}{N_2} \sum_{x \in \omega_2} x = \frac{1}{5} \left[ \begin{pmatrix} 9 \\ 10 \end{pmatrix} + \begin{pmatrix} 6 \\ 8 \end{pmatrix} + \begin{pmatrix} 9 \\ 5 \end{pmatrix} + \begin{pmatrix} 8 \\ 7 \end{pmatrix} + \begin{pmatrix} 10 \\ 8 \end{pmatrix} \right] = \begin{pmatrix} 8.4 \\ 7.6 \end{pmatrix}$$

```
% class means  
Mu1 = mean(X1) ' ;  
Mu2 = mean(X2) ' ;
```

# LDA: Two Classes - Example

- Covariance matrix of the first class:

$$\begin{aligned} S_1 &= \sum_{x \in \omega_1} (x - \mu_1)(x - \mu_1)^T = \left[ \begin{pmatrix} 4 \\ 2 \end{pmatrix} - \begin{pmatrix} 3 \\ 3.8 \end{pmatrix} \right]^2 + \left[ \begin{pmatrix} 2 \\ 4 \end{pmatrix} - \begin{pmatrix} 3 \\ 3.8 \end{pmatrix} \right]^2 \\ &\quad + \left[ \begin{pmatrix} 2 \\ 3 \end{pmatrix} - \begin{pmatrix} 3 \\ 3.8 \end{pmatrix} \right]^2 + \left[ \begin{pmatrix} 3 \\ 6 \end{pmatrix} - \begin{pmatrix} 3 \\ 3.8 \end{pmatrix} \right]^2 + \left[ \begin{pmatrix} 4 \\ 4 \end{pmatrix} - \begin{pmatrix} 3 \\ 3.8 \end{pmatrix} \right]^2 \\ &= \begin{pmatrix} 1 & -0.25 \\ -0.25 & 2.2 \end{pmatrix} \end{aligned}$$

```
% covariance matrix of the first class  
S1 = cov(X1);
```

# LDA: Two Classes - Example

- Covariance matrix of the second class:

$$\begin{aligned} S_2 &= \sum_{x \in \omega_2} (x - \mu_2)(x - \mu_2)^T = \left[ \begin{pmatrix} 9 \\ 10 \end{pmatrix} - \begin{pmatrix} 8.4 \\ 7.6 \end{pmatrix} \right]^2 + \left[ \begin{pmatrix} 6 \\ 8 \end{pmatrix} - \begin{pmatrix} 8.4 \\ 7.6 \end{pmatrix} \right]^2 \\ &\quad + \left[ \begin{pmatrix} 9 \\ 5 \end{pmatrix} - \begin{pmatrix} 8.4 \\ 7.6 \end{pmatrix} \right]^2 + \left[ \begin{pmatrix} 8 \\ 7 \end{pmatrix} - \begin{pmatrix} 8.4 \\ 7.6 \end{pmatrix} \right]^2 + \left[ \begin{pmatrix} 10 \\ 8 \end{pmatrix} - \begin{pmatrix} 8.4 \\ 7.6 \end{pmatrix} \right]^2 \\ &= \begin{pmatrix} 2.3 & -0.05 \\ -0.05 & 3.3 \end{pmatrix} \end{aligned}$$

```
% covariance matrix of the first class  
S2 = cov(X2);
```

# LDA: Two Classes - Example

- Within-class scatter matrix:

$$\begin{aligned} S_w = S_1 + S_2 &= \begin{pmatrix} 1 & -0.25 \\ -0.25 & 2.2 \end{pmatrix} + \begin{pmatrix} 2.3 & -0.05 \\ -0.05 & 3.3 \end{pmatrix} \\ &= \begin{pmatrix} 3.3 & -0.3 \\ -0.3 & 5.5 \end{pmatrix} \end{aligned}$$

```
% within-class scatter matrix  
Sw = S1 + S2 ;
```

# LDA: Two Classes - Example

- Between-class scatter matrix:

$$\begin{aligned} S_B &= (\mu_1 - \mu_2)(\mu_1 - \mu_2)^T \\ &= \left[ \begin{pmatrix} 3 \\ 3.8 \end{pmatrix} - \begin{pmatrix} 8.4 \\ 7.6 \end{pmatrix} \right] \left[ \begin{pmatrix} 3 \\ 3.8 \end{pmatrix} - \begin{pmatrix} 8.4 \\ 7.6 \end{pmatrix} \right]^T \\ &= \begin{pmatrix} -5.4 \\ -3.8 \end{pmatrix} \begin{pmatrix} -5.4 & -3.8 \end{pmatrix} \\ &= \begin{pmatrix} 29.16 & 20.52 \\ 20.52 & 14.44 \end{pmatrix} \end{aligned}$$

```
% between-class scatter matrix  
SB = (Mu1-Mu2) * (Mu1-Mu2) ' ;
```

# LDA: Two Classes - Example

- The LDA projection is then obtained as the solution of the generalized eigen value problem

$$S_W^{-1}S_B w = \lambda w$$

$$\Rightarrow |S_W^{-1}S_B - \lambda I| = 0$$

$$\Rightarrow \left| \begin{pmatrix} 3.3 & -0.3 \\ -0.3 & 5.5 \end{pmatrix}^{-1} \begin{pmatrix} 29.16 & 20.52 \\ 20.52 & 14.44 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right| = 0$$

$$\Rightarrow \left| \begin{pmatrix} 0.3045 & 0.0166 \\ 0.0166 & 0.1827 \end{pmatrix} \begin{pmatrix} 29.16 & 20.52 \\ 20.52 & 14.44 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right| = 0$$

$$\Rightarrow \left| \begin{pmatrix} 9.2213 - \lambda & 6.489 \\ 4.2339 & 2.9794 - \lambda \end{pmatrix} \right|$$

$$= (9.2213 - \lambda)(2.9794 - \lambda) - 6.489 \times 4.2339 = 0$$

$$\Rightarrow \lambda^2 - 12.2007\lambda = 0 \Rightarrow \lambda(\lambda - 12.2007) = 0$$



# LDA: Two Classes - Example

- Hence

$$\begin{pmatrix} 9.2213 & 6.489 \\ 4.2339 & 2.9794 \end{pmatrix} w_1 = \underbrace{0}_{\lambda_1} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$$

and

$$\begin{pmatrix} 9.2213 & 6.489 \\ 4.2339 & 2.9794 \end{pmatrix} w_2 = \underbrace{12.2007}_{\lambda_2} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$$

Thus;

$$w_1 = \begin{pmatrix} -0.5755 \\ 0.8178 \end{pmatrix} \quad \text{and} \quad w_2 = \begin{pmatrix} 0.9088 \\ 0.4173 \end{pmatrix} = w^*$$

```
% computing the LDA projection
invSw = inv(Sw);

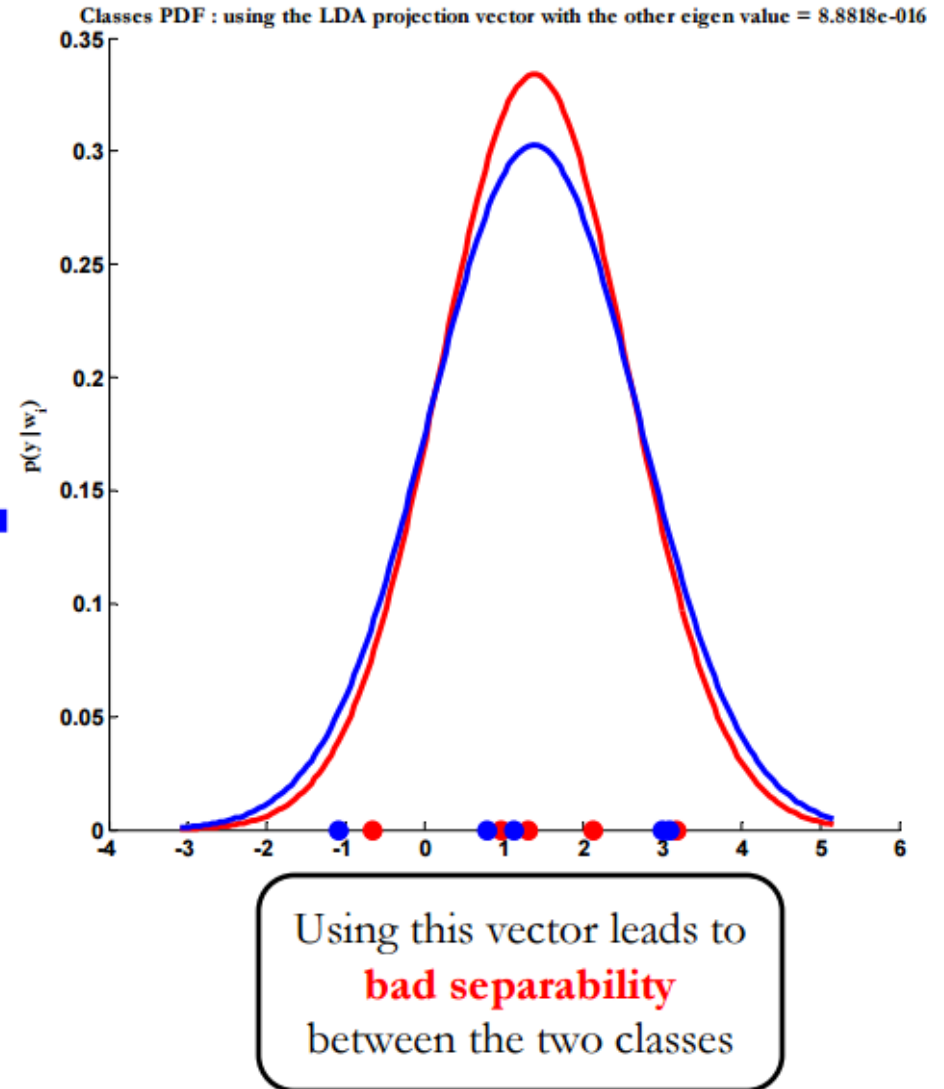
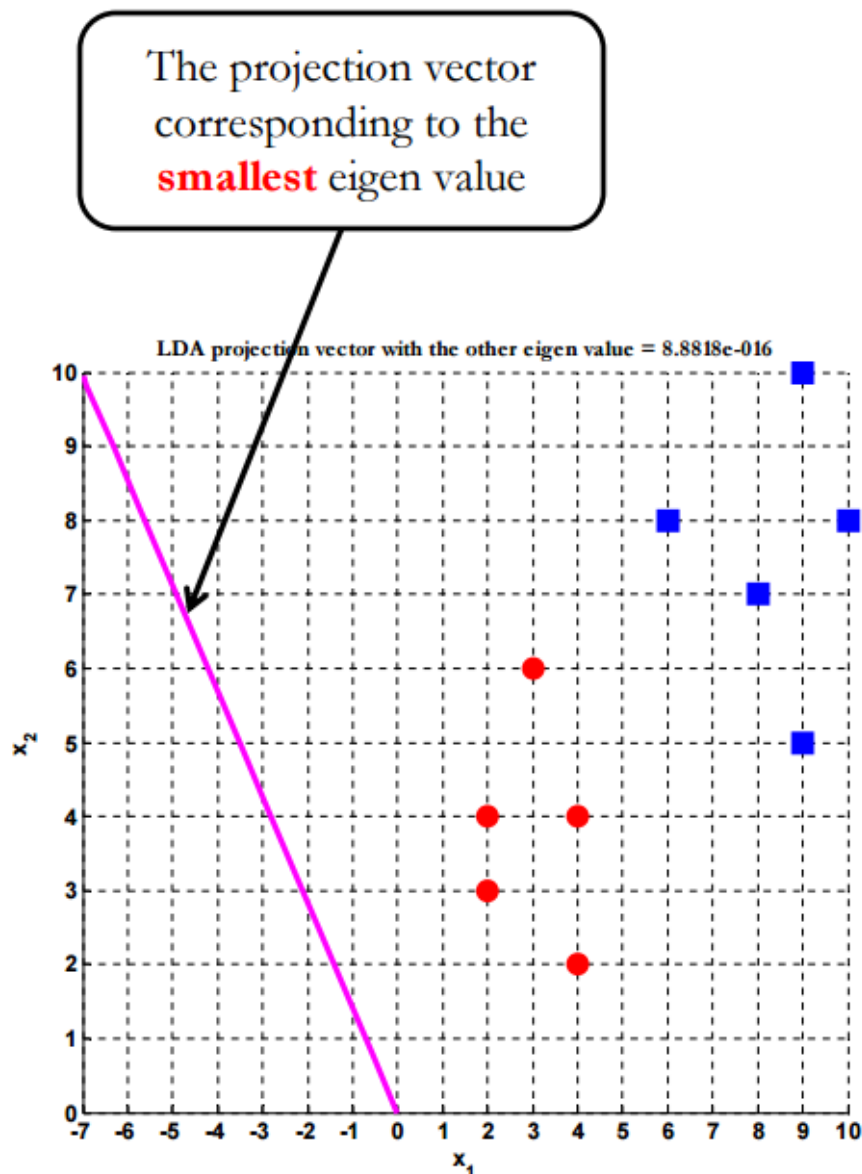
invSw_by_SB = invSw * SB;

% getting the projection vector
[V,D] = eig(invSw_by_SB)

% the projection vector
W = V(:,1);
```

- The optimal projection is the one that given maximum  $\lambda = J(w)$

# LDA: Two Classes - Example



# LDA: Two Classes - Example

