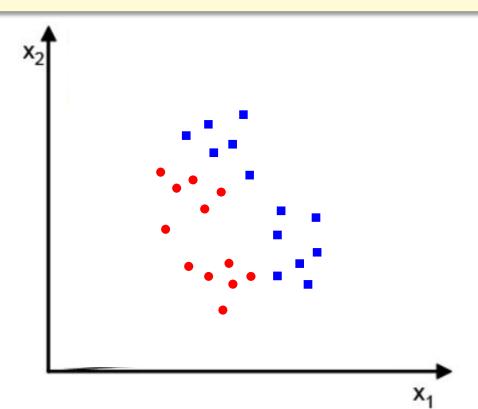
# Machine Learning & Pattern Recognition

**SONG Xuemeng** 

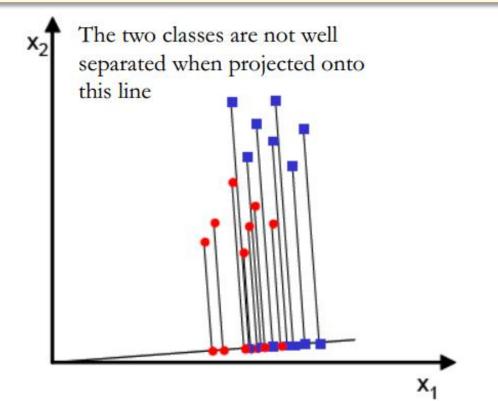
sxmustc@gmail.com

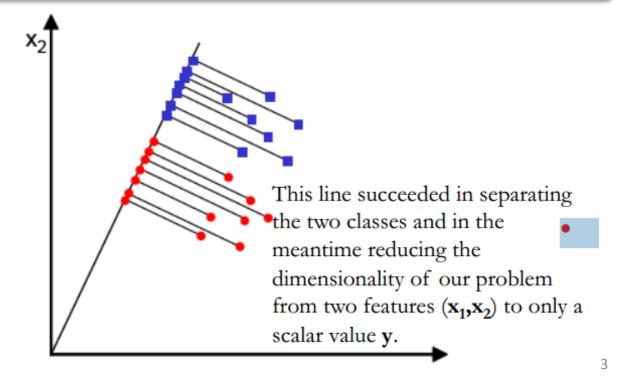
http://xuemeng.bitcron.com/

- Given a set of points (2-d) from two classes, we want to project them to a line that can well separate them.
- What is a good criterion?

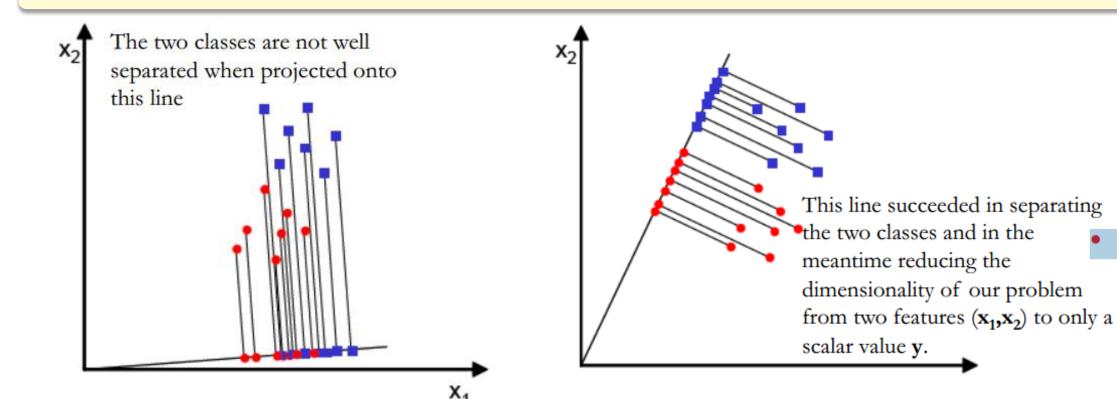


- What is a good criterion?
  - Separating different classes





- What is a good criterion?
  - Separating different classes
  - Maximize the between-class distance (means)

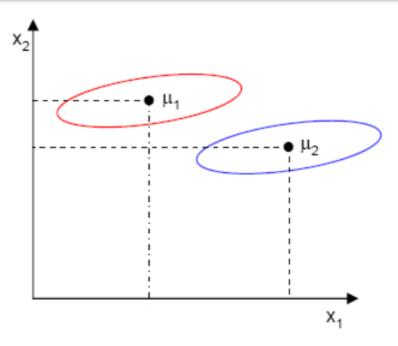


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Is it enough?

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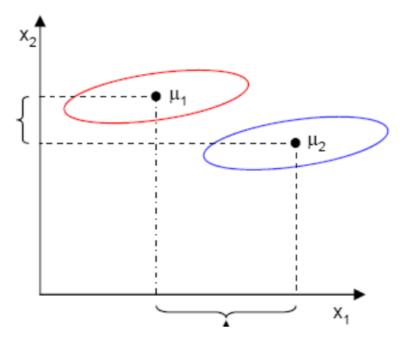
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Is it enough?

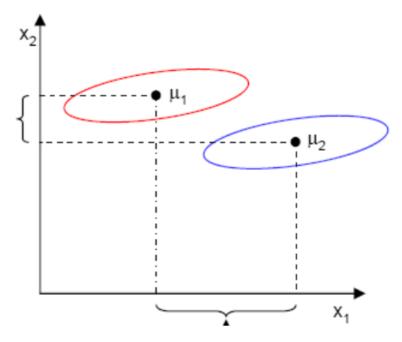
This axis yields better class separability



This axis has a larger distance between means

- What is a good criterion?
  - Separating different classes
  - Maximize the between-class distance (means)
  - Minimize the within-class variability (scatter)

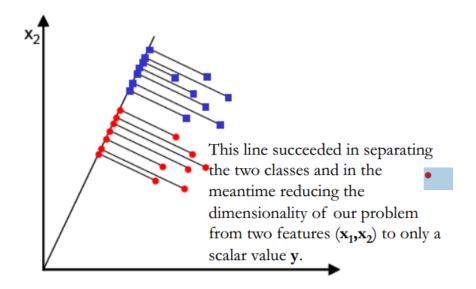
This axis yields better class separability



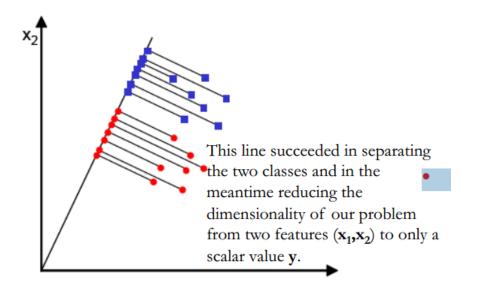
This axis has a larger distance between means

- We have N d-dimensional samples from C classes, e.g., seabass, tuna, ...
- Each class has  $n_i$  samples, where i = 1, 2, ..., C
- Stacking these samples from different classes into one big fat matrix  $X \in \mathbb{R}^{d \times N}$  such that each column represents one sample  $x \in \mathbb{R}^{d \times 1}$ .
- We seek to obtain a transformation to project the d-dimensional samples in X onto a p-dimensional subspace (p < d), such that after the projection we have:

class means to be as <b>far</b> apart from each other as possible	<b></b>	the <b>between-class</b> scatter to be <b>large</b>
samples from the same class to be as <b>close</b> to their mean as possible	<b></b>	the within-class scatter to be small

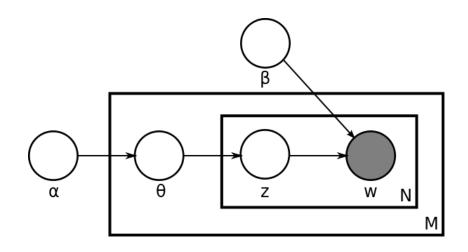


Linear Discriminant Analysis, a method to find a linear combination of features that separates two or more classes of objects.

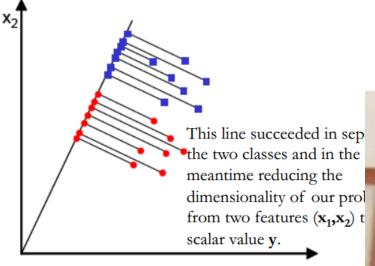


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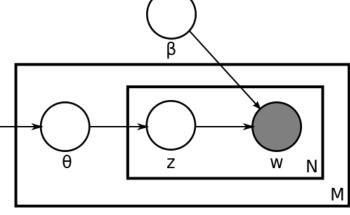
#### Latent Dirichlet Allocation



In natural language processing, latent Dirichlet allocation (LDA) is an example of a topic model. <a href="https://en.wikipedia.org/wiki/Latent Dirichlet allocation">https://en.wikipedia.org/wiki/Latent Dirichlet allocation</a>



irichlet Allocation



Linear Discriminant Analysis, find a linear combination of features that separates two or more classes of objects.

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- Linear Discriminant Analysis—Two Classes
- Linear Discriminant Analysis—C Classes

- Assume we have d-dimensional samples  $\{x_1, x_2, ..., x_N\}, n_1$  of which belong to  $C_1$  and  $n_2$  belong to  $C_2$ .
- We seek to obtain a transformation  $\theta \in \mathbb{R}^{d \times 1}$  that projects the samples x onto a line (p = 1).

• 
$$y_i = \boldsymbol{\theta}^T \boldsymbol{x}_i$$
, where  $\boldsymbol{x}_i = \begin{bmatrix} x_{i1} \\ \vdots \\ x_{id} \end{bmatrix}$  and  $\boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}$ 

• where  $\theta$  is the projection vectors used to project x to y.

#### **Statistical Facts**

Within-class scatter:

$$S_w = \sum_{x \in C_1} (x - \mu_1)(x - \mu_1)^T + \sum_{x \in C_2} (x - \mu_2)(x - \mu_2)^T$$
  $S_w \in \mathbb{R}^{d \times d}$ 

Between-class scatter:

$$S_b = (\mu_1 - \mu_2)(\mu_1 - \mu_2)^T$$

$$\mathbf{S}_b \in \mathbb{R}^{d \times d}$$

Class mean vector (sample):

$$\mu_i = \frac{1}{n_i} \sum_{x \in C_i} x$$
,  $\mu_i \in \mathbb{R}^{d \times 1}$ 

• The mean vector of each class in x and y feature space is:

$$\mu_i = \frac{1}{n_i} \sum_{x \in C_i} x \qquad \qquad \widetilde{\mu}_i = \frac{1}{n_i} \sum_{y \in C_i} y = \frac{1}{n_i} \sum_{x \in C_i} \theta^T x = \theta^T \mu_i$$

• Projecting x to y will lead to projecting the mean of x to the mean of y.

- The within-class scatter:  $\widetilde{S}_w = \sum_{y \in C_1} (y \widetilde{\mu}_1)^2 + \sum_{y \in C_2} (y \widetilde{\mu}_1)^2 = \theta^T S_w \theta$
- The between-class scatter:  $\tilde{S}_b = (\tilde{\mu}_1 \tilde{\mu}_2)^2 = \theta^T S_b \theta$

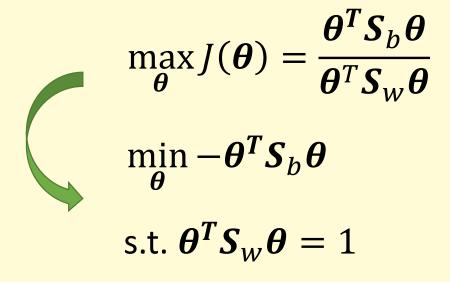
 On one hand, we want maximize the distance between the projected means:

$$J_{1}(\theta) = (\tilde{\mu}_{1} - \tilde{\mu}_{2})^{2} = (\theta^{T} \mu_{1} - \theta^{T} \mu_{2})^{2}$$
$$= \theta^{T} (\mu_{1} - \mu_{2})(\mu_{1} - \mu_{2})^{T} \theta = \theta^{T} S_{b} \theta = \tilde{S}_{b}$$

• On the other hand, we want minimize the within-class scatter:

$$J_2(\boldsymbol{\theta}) = \tilde{\boldsymbol{S}}_{w1} + \tilde{\boldsymbol{S}}_{w2} = \tilde{\boldsymbol{S}}_w = \boldsymbol{\theta}^T \boldsymbol{S}_w \boldsymbol{\theta}$$

• We can finally express the Fisher criterion in terms of  $S_w$  and  $S_b$ :



$$\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = -\boldsymbol{\theta}^T \boldsymbol{S}_b \boldsymbol{\theta} + \lambda (\boldsymbol{\theta}^T \boldsymbol{S}_w \boldsymbol{\theta} - 1)$$

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$$\frac{\partial J(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = 2$$

$$\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = -\boldsymbol{\theta}^T \boldsymbol{S}_b \boldsymbol{\theta} + \lambda (\boldsymbol{\theta}^T \boldsymbol{S}_w \boldsymbol{\theta} - 1)$$

$$\frac{\partial J(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = -2\boldsymbol{S}_b \boldsymbol{\theta} + 2\lambda \boldsymbol{S}_w \boldsymbol{\theta} = 0 \qquad \Longrightarrow \qquad \boldsymbol{S}_b \boldsymbol{\theta} = \lambda \boldsymbol{S}_w \boldsymbol{\theta}$$

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- $\theta$ : the eigenvectors of  $S_w^{-1}S_b$ , and  $\lambda$  is the corresponding eigenvalue.
- How to choose  $\theta$ ?

• Let  $\lambda$  be a Lagrange multiplier

$$\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = -\boldsymbol{\theta}^T \boldsymbol{S}_b \boldsymbol{\theta} + \lambda (\boldsymbol{\theta}^T \boldsymbol{S}_w \boldsymbol{\theta} - 1)$$

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Remember the objective function

$$\begin{cases} \min_{\boldsymbol{\theta}} -\boldsymbol{\theta}^T \boldsymbol{S}_b \boldsymbol{\theta} \\ \text{s.t. } \boldsymbol{\theta}^T \boldsymbol{S}_w \boldsymbol{\theta} = 1 \end{cases}$$

• Let  $\lambda$  be a Lagrange multiplier

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Remember the objective function

$$\begin{cases} \min_{\boldsymbol{\theta}} -\boldsymbol{\theta}^T \boldsymbol{S}_b \boldsymbol{\theta} & \boldsymbol{S}_b \boldsymbol{\theta}^* = \lambda \boldsymbol{S}_w \boldsymbol{\theta}^* \\ \text{s.t. } \boldsymbol{\theta}^T \boldsymbol{S}_w \boldsymbol{\theta} = 1 \end{cases} \Longrightarrow -\boldsymbol{\theta}^{*T} \boldsymbol{S}_b \boldsymbol{\theta}^* = -\lambda \boldsymbol{\theta}^{*T} \boldsymbol{S}_w \boldsymbol{\theta}^* = -\lambda$$

How to choose? The eigenvector corresponds to the largest eigenvalue.

• Let  $\lambda$  be a Lagrange multiplier

$$\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = -\boldsymbol{\theta}^T \boldsymbol{S}_b \boldsymbol{\theta} + \lambda (\boldsymbol{\theta}^T \boldsymbol{S}_w \boldsymbol{\theta} - 1)$$

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• Alternatively, as  $S_b=(\mu_1-\mu_2)(\mu_1-\mu_2)^T$ ,  $S_b\theta=(\mu_1-\mu_2)(\mu_1-\mu_2)^T heta$ 

$$\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = -\boldsymbol{\theta}^T \boldsymbol{S}_b \boldsymbol{\theta} + \lambda (\boldsymbol{\theta}^T \boldsymbol{S}_w \boldsymbol{\theta} - 1)$$

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- As  $S_b = (\mu_1 \mu_2)(\mu_1 \mu_2)^T$ ,  $S_b \theta = (\mu_1 \mu_2)(\mu_1 \mu_2)^T \theta$
- Let  $S_b\theta = \lambda_{\theta}(\mu_1 \mu_2)$  then  $\lambda S_w\theta = \lambda_{\theta}(\mu_1 \mu_2)$
- The scale of  $oldsymbol{ heta}^*$  does not matter, only direction matters.

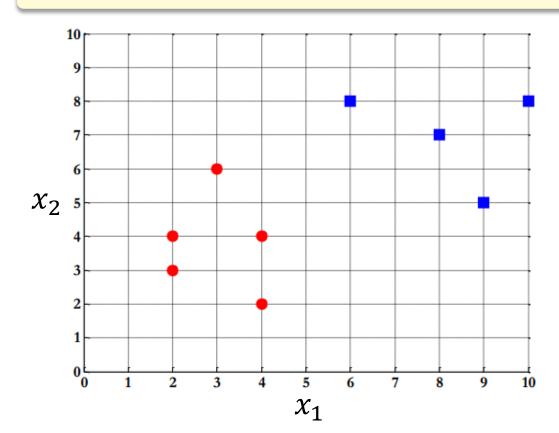
$$\boldsymbol{\theta}^* = \boldsymbol{S}_w^{-1} \left( \boldsymbol{\mu}_1 - \boldsymbol{\mu}_2 \right)$$

#### Workflow of LDA for the binary classification

- 1. Build  $X_1$  and  $X_2$  from the training set
- 2. Compute  $\mu_1$  and  $\mu_2$
- 3. Compute  $S_w$
- 4. Compute  $S_w^{-1}$
- 5. Compute  $\theta^* = S_w^{-1} (\mu_1 \mu_2)$
- 6. Given a testing sample,  $y = \theta^{*T} x$
- 7. Set the threshold  $\gamma = \frac{n_1 \theta^{*T} \mu_1 + n_2 \theta^{*T} \mu_2}{n_1 + n_2}$ .
- 8. Compare y with  $\gamma$  to determine the class.

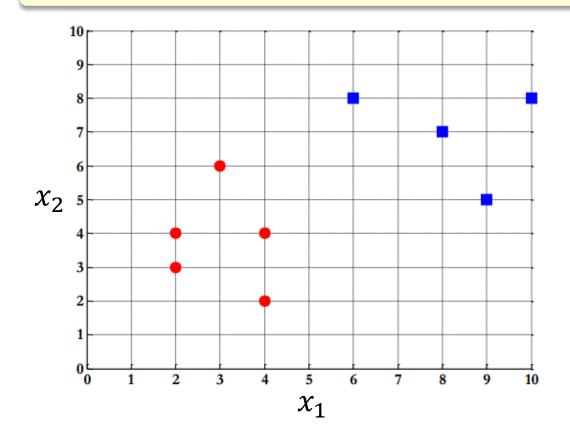
Compute the Linear Discriminant projection for the following two dimensional dataset.

- Samples for class  $\omega_1$ :  $X_1 = (x_1, x_2) = \{(4,2), (2,4), (2,3), (3,6), (4,4)\}$
- Sample for class  $\omega_2$ :  $X_2 = (x_1, x_2) = \{(9,10), (6,8), (9,5), (8,7), (10,8)\}$



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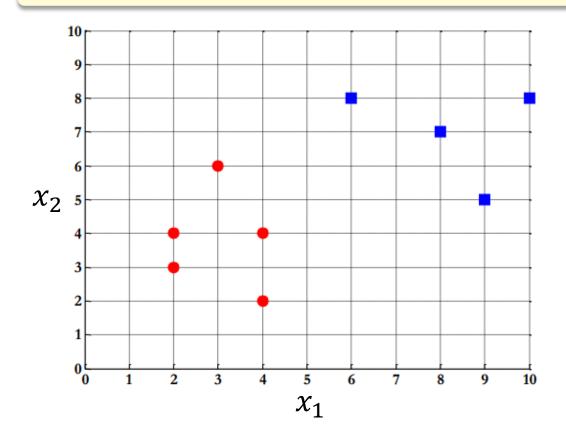
Mean of each class:

$$\mu_{1} = \frac{1}{N_{1}} \sum_{x \in \omega_{1}} x = \frac{1}{5} \left[ \binom{4}{2} + \binom{2}{4} + \binom{2}{3} + \binom{3}{6} + \binom{4}{4} \right] = \binom{3}{3.8}$$

$$\mu_{2} = \frac{1}{N_{2}} \sum_{x \in \omega_{2}} x = \frac{1}{5} \left[ \binom{9}{10} + \binom{6}{8} + \binom{9}{5} + \binom{8}{7} + \binom{10}{8} \right] = \binom{8.4}{7.6}$$

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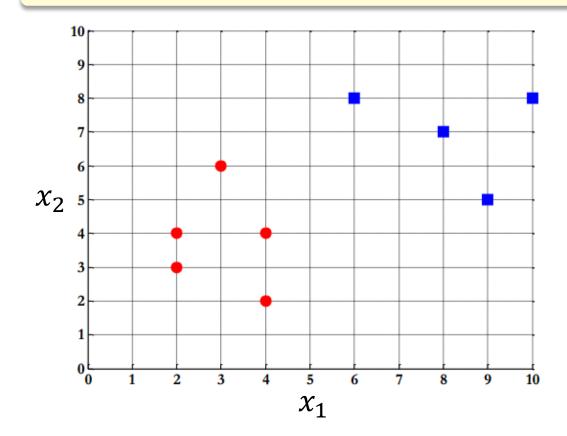


Covariance matrix of the first class:

$$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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \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} + \left[ \begin{pmatrix} 4 \\ 4 \end{pmatrix} - \begin{pmatrix} 4 \\ 4 \end{pmatrix}$$

Compute the Linear Discriminant projection for the following two dimensional dataset.

- Samples for class  $\omega_1$ :  $X_1 = (x_1, x_2) = \{(4,2), (2,4), (2,3), (3,6), (4,4)\}$
- Sample for class  $\boldsymbol{\omega}_2$ :  $\boldsymbol{X}_2 = (x_1, x_2) = \{(9,10), (6,8), (9,5), (8,7), (10,8)\}$

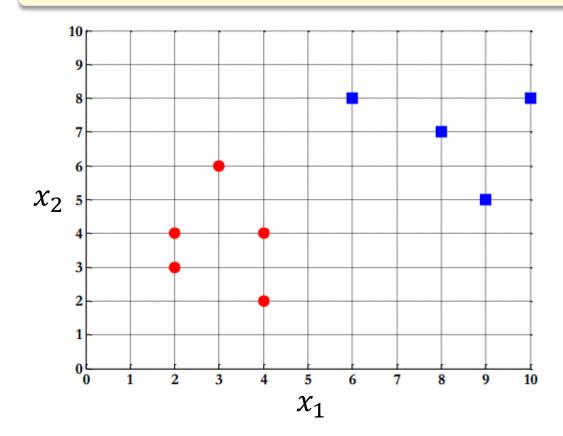


Covariance matrix of the second class:

$$S_{2} = \sum_{x \in \omega_{2}} (x - \mu_{2})(x - \mu_{2})^{T} = \begin{bmatrix} 9 \\ 10 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}^{2} + \begin{bmatrix} 6 \\ 8 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}^{2} + \begin{bmatrix} 9 \\ 5 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}^{2} + \begin{bmatrix} 8 \\ 7 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}^{2} + \begin{bmatrix} 10 \\ 8 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}^{2} + \begin{bmatrix} 2.3 & -0.05 \\ -0.05 & 3.3 \end{bmatrix}$$

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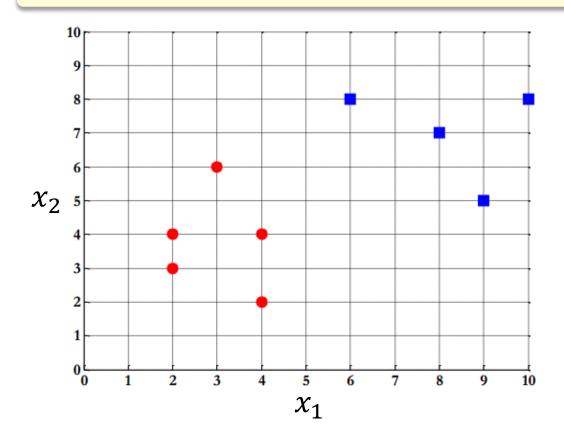


Within-class scatter matrix:

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

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Between-class scatter matrix:

$$S_{B} = (\mu_{1} - \mu_{2})(\mu_{1} - \mu_{2})^{T}$$

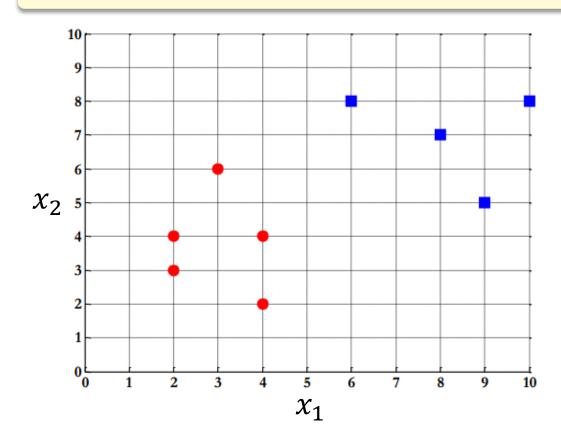
$$= \begin{bmatrix} 3 \\ 3.8 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix} \begin{bmatrix} 3 \\ 3.8 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}^{T}$$

$$= \begin{bmatrix} -5.4 \\ -3.8 \end{bmatrix} (-5.4 - 3.8)$$

$$= \begin{bmatrix} 29.16 & 20.52 \\ 20.52 & 14.44 \end{bmatrix}$$

Compute the Linear Discriminant projection for the following two dimensional dataset.

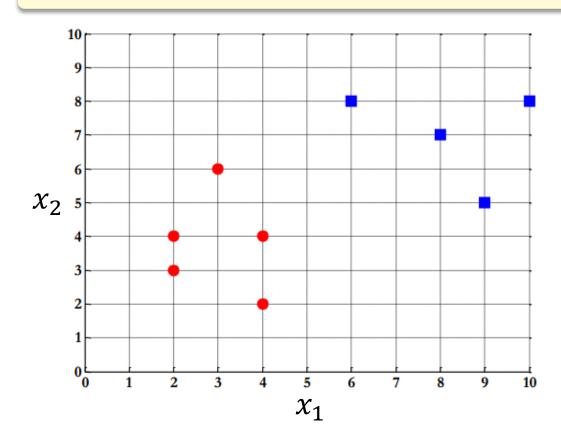
- Samples for class  $\omega_1$ :  $X_1 = (x_1, x_2) = \{(4,2), (2,4), (2,3), (3,6), (4,4)\}$
- Sample for class  $\omega_2$ :  $X_2 = (x_1, x_2) = \{(9,10), (6,8), (9,5), (8,7), (10,8)\}$



$$\begin{split} S_W^{-1} S_B w &= \lambda w \\ \Rightarrow \left| S_W^{-1} S_B - \lambda I \right| = 0 \\ \Rightarrow \left| \begin{pmatrix} 3.3 & -0.3 \\ -0.3 & 5.5 \end{pmatrix}^{-1} \begin{pmatrix} 29.16 & 20.52 \\ 20.52 & 14.44 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right| = 0 \\ \Rightarrow \left| \begin{pmatrix} 0.3045 & 0.0166 \\ 0.0166 & 0.1827 \end{pmatrix} \begin{pmatrix} 29.16 & 20.52 \\ 20.52 & 14.44 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right| = 0 \\ \Rightarrow \left| \begin{pmatrix} 9.2213 - \lambda & 6.489 \\ 4.2339 & 2.9794 - \lambda \end{pmatrix} \right| \\ &= (9.2213 - \lambda)(2.9794 - \lambda) - 6.489 \times 4.2339 = 0 \\ \Rightarrow \lambda^2 - 12.2007\lambda = 0 \Rightarrow \lambda(\lambda - 12.2007) = 0 \\ \Rightarrow \lambda_1 = 0, \lambda_2 = 12.2007 \end{split}$$

Compute the Linear Discriminant projection for the following two dimensional dataset.

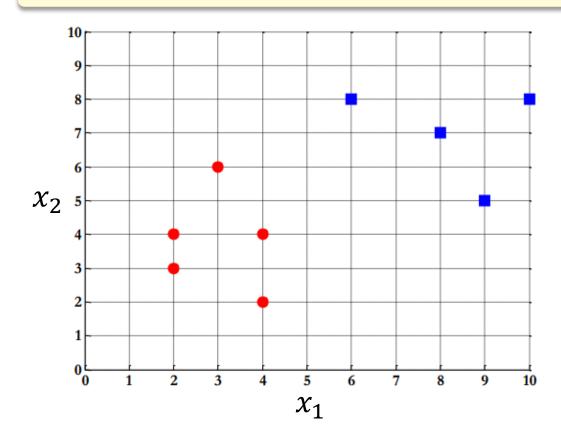
- Samples for class  $\omega_1$ :  $X_1 = (x_1, x_2) = \{(4,2), (2,4), (2,3), (3,6), (4,4)\}$
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$$\begin{split} S_W^{-1} S_B w &= \lambda w \\ \Rightarrow \left| S_W^{-1} S_B - \lambda I \right| = 0 \\ \Rightarrow \left| \begin{pmatrix} 3.3 & -0.3 \\ -0.3 & 5.5 \end{pmatrix}^{-1} \begin{pmatrix} 29.16 & 20.52 \\ 20.52 & 14.44 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right| = 0 \\ \Rightarrow \left| \begin{pmatrix} 0.3045 & 0.0166 \\ 0.0166 & 0.1827 \end{pmatrix} \begin{pmatrix} 29.16 & 20.52 \\ 20.52 & 14.44 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right| = 0 \\ \Rightarrow \left| \begin{pmatrix} 9.2213 - \lambda & 6.489 \\ 4.2339 & 2.9794 - \lambda \end{pmatrix} \right| \\ &= (9.2213 - \lambda)(2.9794 - \lambda) - 6.489 \times 4.2339 = 0 \\ \Rightarrow \lambda^2 - 12.2007\lambda = 0 \Rightarrow \lambda(\lambda - 12.2007) = 0 \\ \Rightarrow \lambda_1 = 0, \lambda_2 = 12.2007 \end{split}$$

Compute the Linear Discriminant projection for the following two dimensional dataset.

- Samples for class  $\omega_1$ :  $X_1 = (x_1, x_2) = \{(4,2), (2,4), (2,3), (3,6), (4,4)\}$
- Sample for class  $\boldsymbol{\omega}_2$ :  $\boldsymbol{X}_2 = (x_1, x_2) = \{(9,10), (6,8), (9,5), (8,7), (10,8)\}$



• The optimal projection is the one that given maximum  $\boldsymbol{J} = -\boldsymbol{\theta}^T \boldsymbol{S}_b \boldsymbol{\theta} = -\lambda$ 

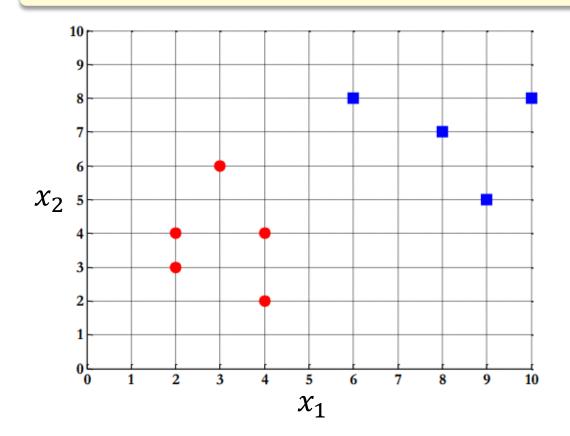
$$\begin{pmatrix} 9.2213 & 6.489 \\ 4.2339 & 2.9794 \end{pmatrix} w_1 = \underbrace{0}_{\lambda_1} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$$
and
$$\begin{pmatrix} 9.2213 & 6.489 \\ 4.2339 & 2.9794 \end{pmatrix} w_2 = \underbrace{12.2007}_{\lambda_2} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$$

Thus;

$$w_1 = \begin{pmatrix} -0.5755 \\ 0.8178 \end{pmatrix}$$
 and  $w_2 = \begin{pmatrix} 0.9088 \\ 0.4173 \end{pmatrix}$ 

Compute the Linear Discriminant projection for the following two dimensional dataset.

- Samples for class  $\omega_1$ :  $X_1 = (x_1, x_2) = \{(4,2), (2,4), (2,3), (3,6), (4,4)\}$
- Sample for class  $\boldsymbol{\omega}_2$ :  $\boldsymbol{X}_2 = (x_1, x_2) = \{(9,10), (6,8), (9,5), (8,7), (10,8)\}$

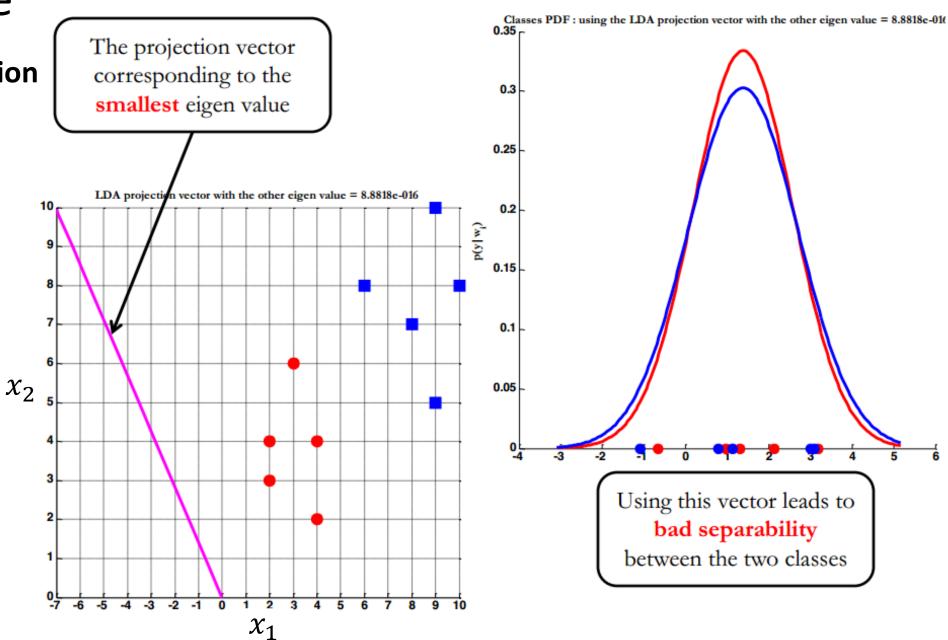


Or directly,

$$w^* = S_W^{-1}(\mu_1 - \mu_2) = \begin{pmatrix} 3.3 & -0.3 \\ -0.3 & 5.5 \end{pmatrix}^{-1} \begin{bmatrix} 3 \\ 3.8 \end{pmatrix} - \begin{pmatrix} 8.4 \\ 7.6 \end{pmatrix} \end{bmatrix}$$
$$= \begin{pmatrix} 0.3045 & 0.0166 \\ 0.0166 & 0.1827 \end{pmatrix} \begin{pmatrix} -5.4 \\ -3.8 \end{pmatrix}$$
$$= \begin{pmatrix} 0.9088 \\ 0.4173 \end{pmatrix}$$

Example

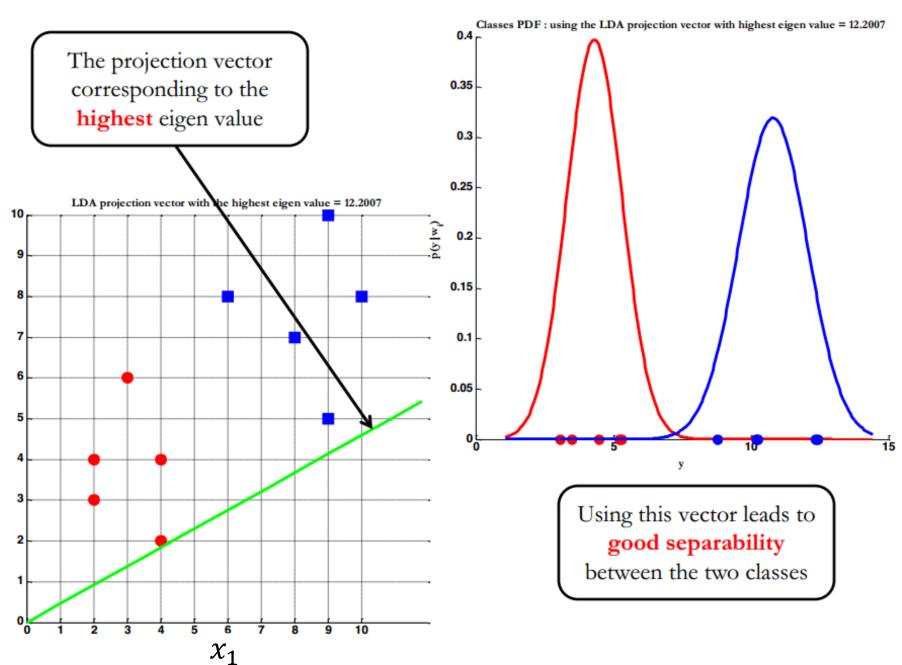
**LDA--Projection** 



# Example

**LDA--Projection** 

 $\chi_2$ 



- Assume we have C classes, each class has  $n_i$  d-dimensional samples, where  $i=1,2,\ldots,C$
- A transformation  $\mathbf{\Theta} \in \mathbb{R}^{d \times p}$ : project the samples in X onto Y ( $p \ll d$ ). In fact,  $p \leq C+1$ , we will see later.

$$egin{aligned} oldsymbol{y}_i &= oldsymbol{\Theta}^T oldsymbol{x}_i \ oldsymbol{x}_i &= egin{bmatrix} oldsymbol{x}_{i1} \ oldsymbol{x}_{i2} \ dots \ oldsymbol{x}_{id} \end{bmatrix} & oldsymbol{y}_i &= egin{bmatrix} oldsymbol{y}_{i1} \ oldsymbol{y}_{i2} \ dots \ oldsymbol{y}_{in} \end{bmatrix} & oldsymbol{\Theta} &= egin{bmatrix} oldsymbol{ heta}_1, oldsymbol{ heta}_2, \dots, oldsymbol{ heta}_p \end{bmatrix} \in \mathbb{R}^{d imes p} \end{aligned}$$

Class mean vector (sample):

$$\mu_i = \frac{1}{n_i} \sum_{x \in C_i} x, \mu_i \in \mathbb{R}^{d \times 1}$$

Within-class scatter:

$$S_w = \sum_{i=1}^C S_{wi}$$
  $S_{wi} = \sum_{x \in C_i} (x - \mu_i)(x - \mu_i)^T$ 

$$\mathbf{S}_w \in \mathbb{R}^{d \times d}$$

Between-class scatter:

$$S_b = \sum_{i=1}^{C} n_i (\mu_i - \mu) (\mu_i - \mu)^T = \frac{1}{2N} \sum_{i,j=1}^{C} n_i n_j (\mu_i - \mu_j) (\mu_i - \mu_j)^T$$
  $S_b \in \mathbb{R}^{d \times d}$ 

Total covariance (sample):

$$S_t = \sum_x (x - \mu)(x - \mu)^T = S_w + S_b$$

$$S_{t} = \sum_{x} (x - \mu)(x - \mu)^{T} = \sum_{i=1}^{C} \sum_{j=1}^{n_{i}} (x_{ij} - \mu)(x_{ij} - \mu)^{T} \qquad x_{ij} \in C_{i}$$

$$= \sum_{i=1}^{C} \sum_{j=1}^{n_{i}} [(x_{ij} - \mu_{i}) + (\mu_{i} - \mu)][(x_{ij} - \mu_{i}) + (\mu_{i} - \mu)]^{T}$$

$$= \sum_{i=1}^{C} \sum_{j=1}^{n_{i}} [(x_{ij} - \mu_{i})(x_{ij} - \mu_{i})^{T} + (\mu_{i} - \mu)(x_{ij} - \mu_{i})^{T} + (x_{ij} - \mu_{i})(\mu_{i} - \mu)^{T} + (\mu_{i} - \mu)(\mu_{i} - \mu)^{T}]$$

$$= \sum_{i=1}^{C} \sum_{j=1}^{n_{i}} [(x_{ij} - \mu_{i})(x_{ij} - \mu_{i})^{T} + (\mu_{i} - \mu)(\mu_{i} - \mu)^{T}] = S_{w} + S_{b}$$

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$$= \sum_{i=1}^{C} \sum_{j=1}^{n_{i}} [(x_{ij} - \mu_{i}) + (\mu_{i} - \mu)][(x_{ij} - \mu_{i}) + (\mu_{i} - \mu)]^{T}$$

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$$\sum_{i=1}^{C} \sum_{j=1}^{n_i} (\mu_i - \mu) (x_{ij} - \mu_i)^T = \sum_{i=1}^{C} (\mu_i - \mu) (\sum_{j=1}^{n_i} x_{ij} - \sum_{j=1}^{n_i} \mu_i)^T = 0$$

- Assume we have C classes, each class has  $n_i$  d-dimensional samples, where  $i=1,2,\ldots,C$
- A transformation  $\mathbf{\Theta} \in \mathbb{R}^{d \times p}$ : project the samples in X onto Y ( $p \ll d$ ). In fact,  $p \leq C + 1$ , we will see later.

$$\mathbf{y}_i = \mathbf{\Theta}^T \mathbf{x}_i$$

$$[y_{i1}]$$

$$\boldsymbol{x}_{i} = \begin{bmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{id} \end{bmatrix} \qquad \boldsymbol{y}_{i} = \begin{bmatrix} y_{i1} \\ y_{i2} \\ \vdots \\ y_{in} \end{bmatrix} \qquad \boldsymbol{\Theta} = [\boldsymbol{\theta}_{1}, \boldsymbol{\theta}_{2}, \dots, \boldsymbol{\theta}_{p}] \in \mathbb{R}^{d \times p}$$

$$\tilde{S}_w = \boldsymbol{\Theta}^T S_w \boldsymbol{\Theta} \qquad \tilde{S}_b = \boldsymbol{\Theta}^T S_b \boldsymbol{\Theta} \qquad \tilde{\boldsymbol{\mu}}_i = \boldsymbol{\Theta}^T \boldsymbol{\mu}_i \qquad \tilde{\boldsymbol{\mu}} = \boldsymbol{\Theta}^T \boldsymbol{\mu}_i$$

Popular objective function:

$$J_1(\mathbf{\Theta}) = \max_{\mathbf{\Theta}} \frac{tr(\tilde{\mathbf{S}}_b)}{tr(\tilde{\mathbf{S}}_w)} = \max_{\mathbf{\Theta}} \frac{tr(\mathbf{\Theta}^T \mathbf{S}_b \mathbf{\Theta})}{tr(\mathbf{\Theta}^T \mathbf{S}_w \mathbf{\Theta})}$$

$$J_2(\mathbf{\Theta}) = \max_{\mathbf{\Theta}} tr(\tilde{\mathbf{S}}_w^{-1}\tilde{\mathbf{S}}_b) = \max_{\mathbf{\Theta}} tr((\mathbf{\Theta}^T \mathbf{S}_w \mathbf{\Theta})^{-1} \mathbf{\Theta}^T \mathbf{S}_b \mathbf{\Theta})$$

$$J_3(\mathbf{\Theta}) = \frac{|\tilde{\mathbf{S}}_b|}{|\tilde{\mathbf{S}}_w|}$$

This technique was developed by R. A. Fisher (1936) for **the two-class case** and extended by C. R. Rao (1948) to handle **the multiclass case**.

In  $J_1(\mathbf{\Theta})$ , what is the meaning of "trace"?

$$J_1(\mathbf{\Theta}) = \max_{\mathbf{\Theta}} \frac{tr(\tilde{\mathbf{S}}_b)}{tr(\tilde{\mathbf{S}}_w)} = \max_{\mathbf{\Theta}} \frac{tr(\mathbf{\Theta}^T \mathbf{S}_b \mathbf{\Theta})}{tr(\mathbf{\Theta}^T \mathbf{S}_w \mathbf{\Theta})}$$

$$\mathbf{\Theta}^{T} \mathbf{S}_{b} \mathbf{\Theta} = \begin{bmatrix} \boldsymbol{\theta}_{1}^{T} \\ \vdots \\ \boldsymbol{\theta}_{p}^{T} \end{bmatrix} \mathbf{S}_{b} [\boldsymbol{\theta}_{1}, \boldsymbol{\theta}_{2}, \dots, \boldsymbol{\theta}_{p}] = \begin{bmatrix} \boldsymbol{\theta}_{1}^{T} \\ \vdots \\ \boldsymbol{\theta}_{p}^{T} \end{bmatrix} [\mathbf{S}_{b} \boldsymbol{\theta}_{1}, \mathbf{S}_{b} \boldsymbol{\theta}_{2}, \dots, \mathbf{S}_{b} \boldsymbol{\theta}_{p}]$$

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$$tr(\mathbf{\Theta}^T \mathbf{S}_b \mathbf{\Theta}) = \sum_{i=1}^p \boldsymbol{\theta}_i^T \mathbf{S}_b \boldsymbol{\theta}_i \qquad tr(\mathbf{\Theta}^T \mathbf{S}_w \mathbf{\Theta}) = \sum_{i=1}^p \boldsymbol{\theta}_i^T \mathbf{S}_w \boldsymbol{\theta}_i$$

### Optimization $J_1(\mathbf{\Theta})$ :

Recall in two-classes case, we solved the eigen value problem.

$$\min_{\boldsymbol{\theta}} -\boldsymbol{\theta}^T \boldsymbol{S}_b \boldsymbol{\theta}$$
s.t.  $\boldsymbol{\theta}^T \boldsymbol{S}_w \boldsymbol{\theta} = 1$ 

$$\Rightarrow \boldsymbol{S}_b \boldsymbol{\theta} = \lambda \boldsymbol{S}_w \boldsymbol{\theta}$$

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• For C-classes case, we have p projection vectors,

$$S_w^{-1}S_b\theta_i = \lambda\theta_i, \qquad i = 1, 2, ..., p$$

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Columns of  $\Theta^*$  are eigenvectors corresponding to the largest eigenvalues:

$$\mathbf{S}_{w}^{-1}\mathbf{S}_{b}\mathbf{\Theta}^{*}=\lambda\mathbf{\Theta}^{*}$$
  $\mathbf{\Theta}^{*}=\left[\boldsymbol{\theta}_{1}^{*},\boldsymbol{\theta}_{2}^{*},...,\boldsymbol{\theta}_{p}^{*}\right]$ 

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$$S_w^{-1}S_b\theta_i = \lambda\theta_i, \qquad i = 1, 2, ..., p$$

Columns of  $\Theta^*$  are eigenvectors corresponding to the largest eigenvalues:

$$S_w^{-1}S_b\mathbf{\Theta}^* = \lambda\mathbf{\Theta}^*$$
  $\mathbf{\Theta}^* = [\boldsymbol{\theta}_1^*, \boldsymbol{\theta}_2^*, ..., \boldsymbol{\theta}_p^*]$   $p \leq C + 1$ , why?

## Optimization $J_1(\mathbf{\Theta})$ :

- $S_b$  has a maximum rank of C-1.
- $S_b$  is the sum of C rank = 1 matrices, and because only C 1 of these are independent,

$$S_b = \sum_{i=1}^C \frac{n_i}{N} (\boldsymbol{\mu}_i - \boldsymbol{\mu}) (\boldsymbol{\mu}_i - \boldsymbol{\mu})^T$$

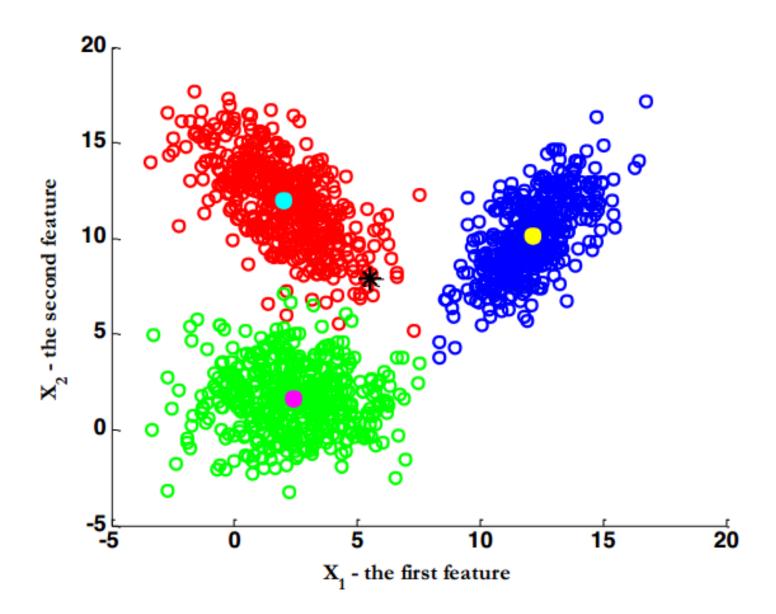
- lacksquare Given a matrix  $m{A}_{m imes n}$  and  $m{B}_{n imes k}$ ,
- $\blacksquare$   $rank(A + B) \le rank(A) + rank(B)$

$$rank\left((\boldsymbol{\mu}_i - \boldsymbol{\mu})(\boldsymbol{\mu}_i - \boldsymbol{\mu})^T\right) \le rank(\boldsymbol{\mu}_i - \boldsymbol{\mu}) = 1 \qquad rank(\boldsymbol{S}_w^{-1}\boldsymbol{S}_b) \le rank(\boldsymbol{S}_b) \le C - 1$$

#### Workflow of LDA for the C-classification

- 1. Compute  $\mu_i$
- 2. Compute  $S_b$
- 3. Compute  $S_w^{-1}$
- 4. Compute the largest p eigenvalues of  $S_w^{-1}S_b$  and the corresponding eigenvectors  $\{\theta_1, \theta_2, ..., \theta_p\}$ .
- 5. Let  $\mathbf{\Theta} = [\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, ..., \boldsymbol{\theta}_p]$ , then  $\boldsymbol{y}_i = \mathbf{\Theta}^T \boldsymbol{x}_i$

## Illustration-3 Classes



```
%% computing the LDA
% class means
Mu1 = mean(X1')';
Mu2 = mean(X2')';
Mu3 = mean(X3')';
% overall mean
Mu = (Mu1 + Mu2 + Mu3)./3;
% class covariance matrices
S1 = cov(X1');
S2 = cov(X2');
s3 = cov(X3');
% within-class scatter matrix
Sw = S1 + S2 + S3;
% number of samples of each class
N1 = size(X1,2);
N2 = size(X2,2);
N3 = size(X3,2);
% between-class scatter matrix
SB1 = N1 .* (Mu1-Mu) * (Mu1-Mu) ';
SB2 = N2 .* (Mu2-Mu) * (Mu2-Mu) ';
SB3 = N3 .* (Mu3-Mu) * (Mu3-Mu) ';
SB = SB1 + SB2 + SB3;
% computing the LDA projection
invSw = inv(Sw);
invSw by SB = invSw * SB;
% getting the projection vectors
%[V,D] = EIG(X) produces a diagonal matrix D of eigenvalues and a
%full matrix V whose columns are the corresponding eigenvectors
[V,D] = eig(invSw by SB);
% the projection vectors - we will have at most C-1 projection vectors,
% from which we can choose the most important ones ranked by their
% corresponding eigen values ... lets investigate the two projection
% vectors
W1 = V(:,1);
W2 = V(:,2);
```

#### Recall ...

$$S_{W} = \sum_{i=1}^{C} S_{i}$$
where  $S_{i} = \sum_{x \in \omega_{i}} (x - \mu_{i})(x - \mu_{i})^{T}$ 
and  $\mu_{i} = \frac{1}{N_{i}} \sum_{x \in \omega_{i}} x$ 

$$S_B = \sum_{i=1}^C N_i (\mu_i - \mu)(\mu_i - \mu)^T$$

where 
$$\mu = \frac{1}{N} \sum_{\forall x} x = \frac{1}{N} \sum_{\forall x} N_i \mu_i$$

and 
$$\mu_i = \frac{1}{N_i} \sum_{x \in \omega_i} x$$

```
%% lets visualize them ...
% we will plot the scatter plot to better visualize the features
                                                                             25
hfig = figure;
axes1 = axes('Parent', hfig, 'FontWeight', 'bold', 'FontSize', 12);
hold('all');
                                                                             20
% Create xlabel
xlabel('X 1 - the first feature', 'FontWeight', 'bold', 'FontSize', 12,...
                                                                             15
    'FontName', 'Garamond'):
% Create ylabel
ylabel('X_2 - the second feature', 'FontWeight', 'bold', 'FontSize', 12, ...
                                                                            10
    'FontName', 'Garamond');
% the first class
                                                                       the
scatter(X1(1,:),X1(2,:), 'r','LineWidth',2,'Parent',axes1);
hold on
% class's mean
plot(Mu1 est(1),Mu1 est(2),'co','MarkerSize',8,'MarkerEdgeColor','c',...
    'Color','c','LineWidth',2,'MarkerFaceColor','c','Parent',axes1);
                                                                             -5
hold on
% the second class
                                                                            -10
scatter(X2(1,:),X2(2,:), 'g', 'LineWidth',2, 'Parent', axes1);
                                                                              -15
hold on
% class's mean
plot(Mu2 est(1), Mu2 est(2), 'mo', 'MarkerSize', 8, 'MarkerEdgeColor', 'm',...
    'Color', 'm', 'LineWidth', 2, 'MarkerFaceColor', 'm', 'Parent', axes1);
hold on
% the third class
scatter(X3(1,:),X3(2,:), 'b', 'LineWidth',2, 'Parent', axes1);
hold on
% class's mean
plot(Mu3_est(1),Mu3_est(2),'yo','LineWidth',2,'MarkerSize',8,'MarkerEdgeColor',...
    'y','Color','y','MarkerFaceColor','y','Parent',axes1);
hold on
```

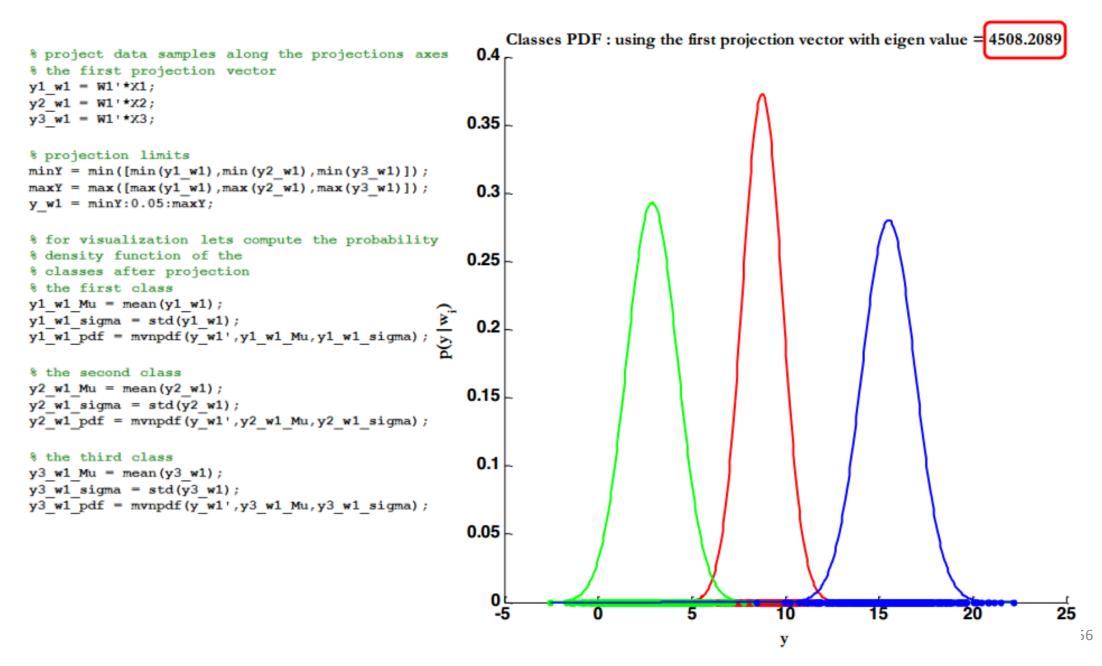
```
-10
         -5
                          5
                                 10
                                         15
                                                 20
                                                          25
                X, - the first feature
```

```
% drawing the projection vectors
% the first vector
t = -10:25;
line x1 = t .* W1(1);
line y1 = t .* W1(2);

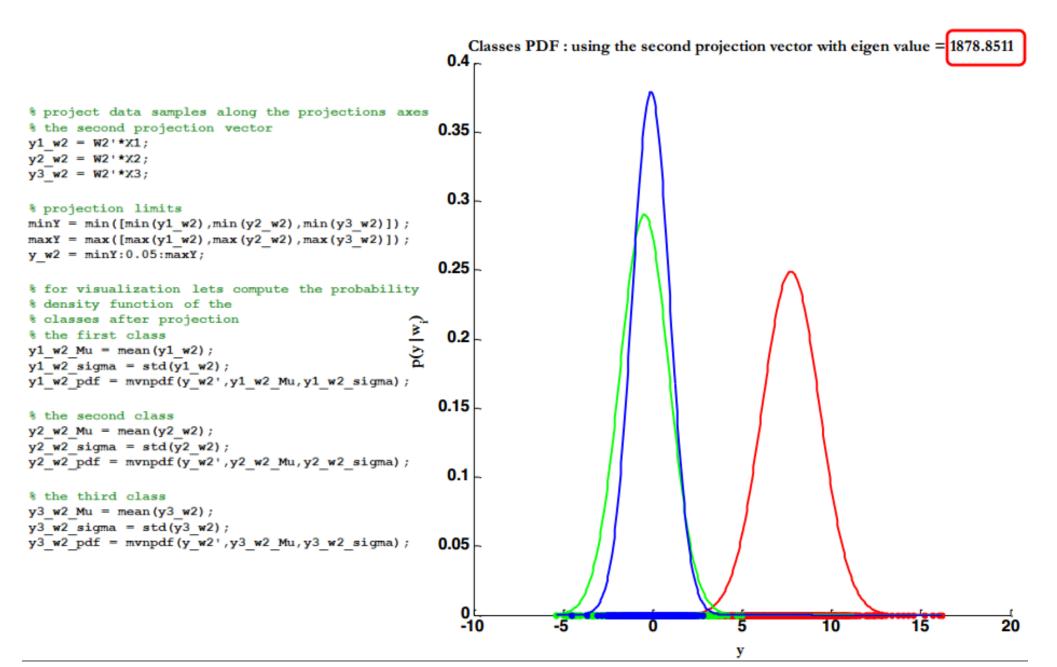
% the second vector
t = -5:20;
line x2 = t .* W2(1);
line y2 = t .* W2(2);

plot(line x1, line y1, 'k-', 'LineWidth', 3);
hold on
plot(line x2, line y2, 'm-', 'LineWidth', 3);
grid on
```

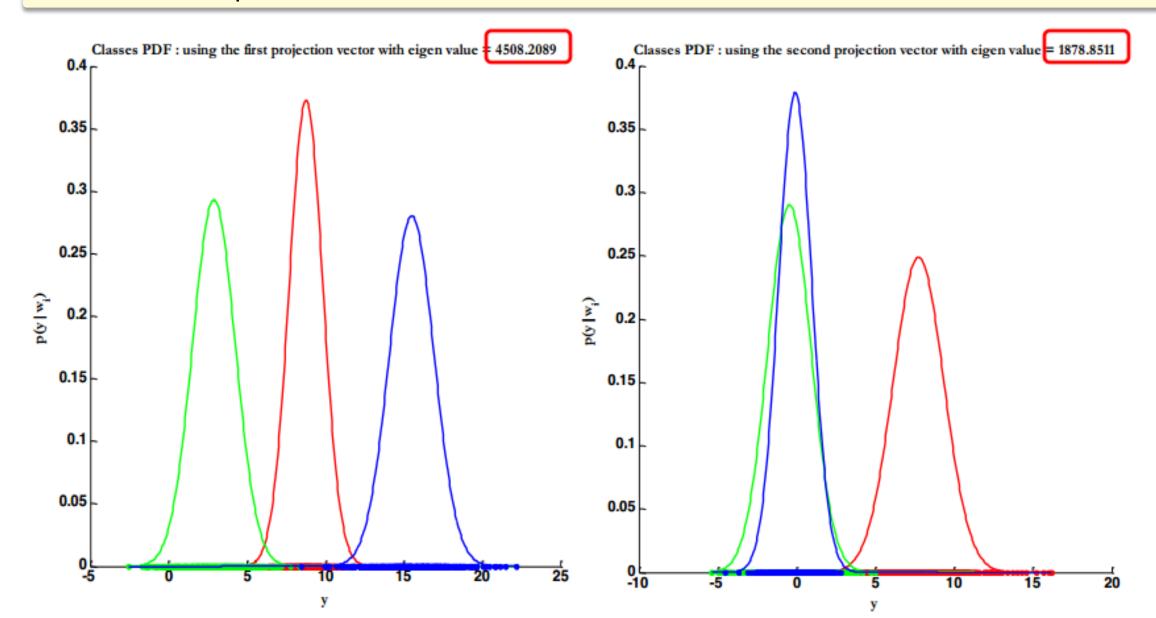
## Along <u>first</u> projection vector $y = w_1^T x$



### Along second projection vector $y = w_2^T x$



Apparently, the projection vector that has the highest eigenvalue provides higher discrimination power between classes.



## Classification with LDA

• First, select the number of feature dimension for the low-dimensional feature space. (In most cases, LDA is used for dimension reduction.)

Nearest Neighbor or other classifiers.

• In practice, mostly PCA shall be performed before LDA to avoid the singularity issue.

## Summary

- Linear Discriminant Analysis—Two Classes
  - Minimize within-class scatter
  - Maximize between-class scatter
  - The eigenvector of the largest eigenvalue of  $S_w^{-1}S_b$  (as  $-\theta^*^TS_b\theta^* = -\lambda\theta^*^TS_w\theta^* = -\lambda$ )
  - Or  $\theta^* = S_w^{-1} (\mu_1 \mu_2)$
- Linear Discriminant Analysis—C Classes
  - Dimension reduction.  $\mathbf{\Theta} \in \mathbb{R}^{d \times p} : \mathbf{X} \to \mathbf{Y} \ (p \ll d)$ . In fact,  $p \leq C + 1$ .
  - Columns of  $\mathbf{\Theta}^*$  are eigenvectors of  $\mathbf{S}_w^{-1}\mathbf{S}_b$  corresponding to the p largest eigenvalues.

Between-class scatter:

$$S_b = \sum_{i=1}^{C} n_i (\mu_i - \mu) (\mu_i - \mu)^T = \frac{1}{2N} \sum_{i,j=1}^{C} n_i n_j (\mu_i - \mu_j) (\mu_i - \mu_j)^T$$

$$\frac{1}{2N} \sum_{i,j=1}^{C} n_i n_j (\mu_i - \mu_j) (\mu_i - \mu_j)^T = \frac{1}{2N} \sum_{i,j=1}^{C} n_i n_j [(\mu_i - \mu) + (\mu - \mu_j)] [(\mu_i - \mu) + (\mu - \mu_j)]^T$$

$$= \frac{1}{2N} \sum_{i,j=1}^{C} n_i n_j [(\mu_i - \mu) (\mu_i - \mu)^T + (\mu - \mu_j) (\mu_i - \mu)^T + (\mu_i - \mu) (\mu - \mu_j)^T + (\mu - \mu_j) (\mu - \mu_j)^T]$$

$$= \frac{1}{2N} \sum_{i,j=1}^{C} n_i n_j [(\mu_i - \mu) (\mu_i - \mu)^T + (\mu - \mu_j) (\mu - \mu_j)^T]$$

$$= \frac{1}{2N} \sum_{i=1}^{C} n_i (\mu_i - \mu) (\mu_i - \mu)^T + \frac{1}{2N} \sum_{i=1}^{C} n_i (\mu - \mu_i) (\mu - \mu_i)^T$$

$$= \sum_{i=1}^{C} n_i (\mu_i - \mu) (\mu_i - \mu)^T = \mathbf{S}_b$$