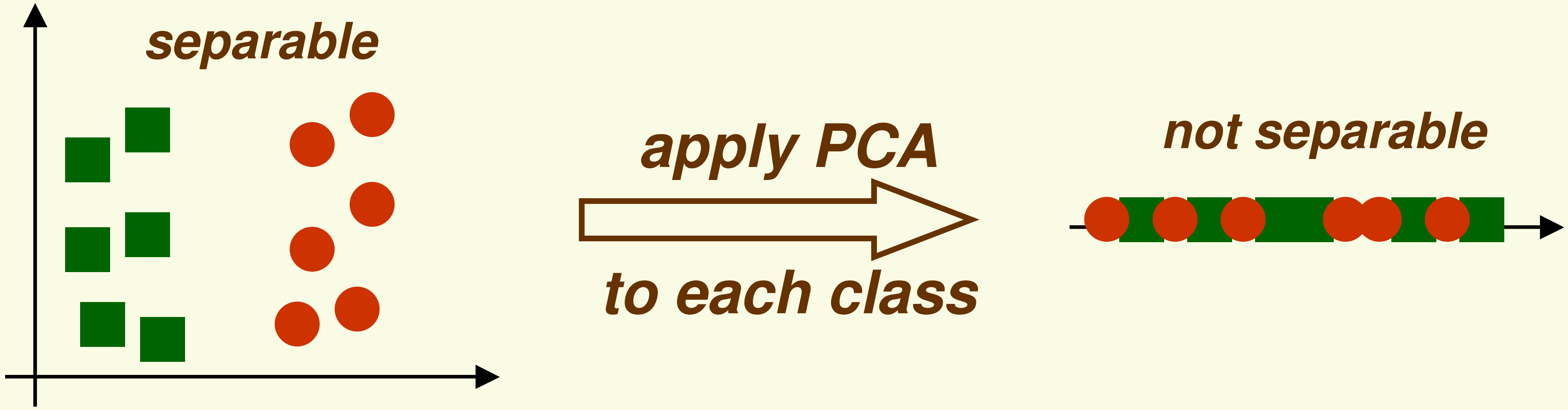
Data Representation vs. Data Classification

- PCA finds the most accurate *data representation* in a lower dimensional space
  - Project data in the directions of maximum variance
- However the directions of maximum variance may be useless for classification

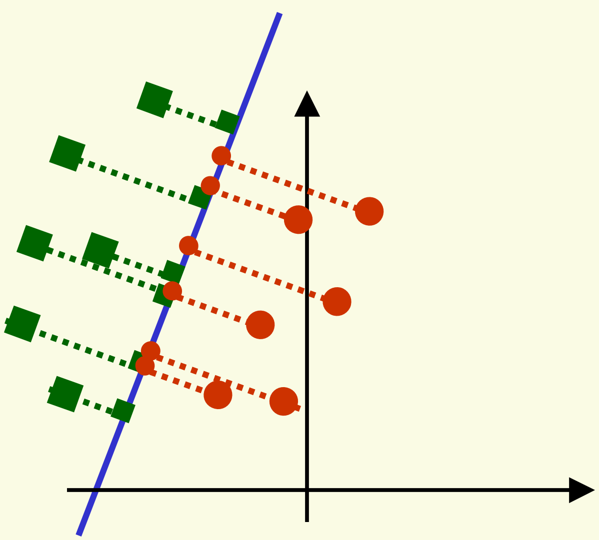


- Fisher Linear Discriminant project to a line which preserves direction useful for *data classification*

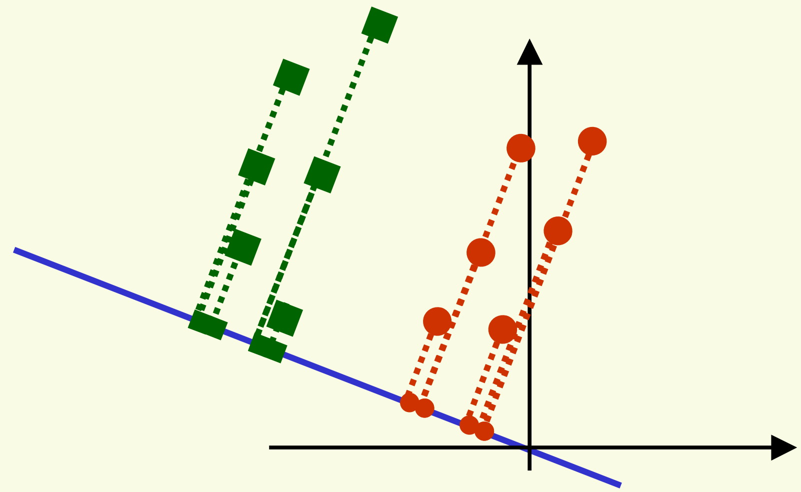
Fisher Linear Discriminant

- Main idea: find projection to a line s.t. samples from different classes are well separated

Example in 2D



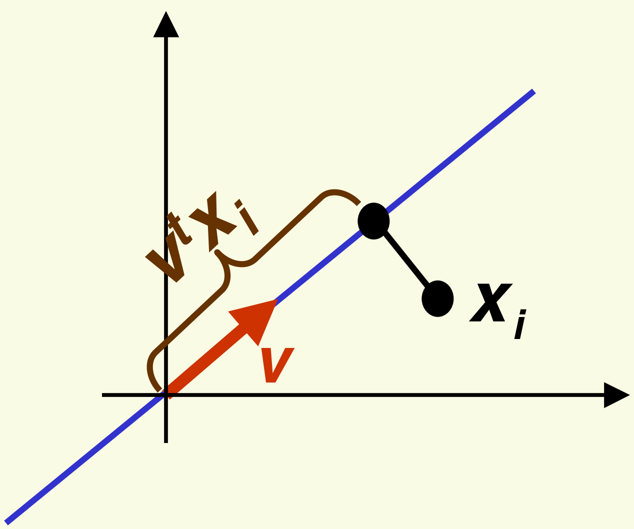
bad line to project to, classes are mixed up



good line to project to, classes are well separated

Fisher Linear Discriminant

- Suppose we have 2 classes and $\boldsymbol{d}$-dimensional samples $\boldsymbol{x_1},\ldots,\boldsymbol{x_n}$ where
  - $\boldsymbol{n_1}$ samples come from the first class
  - $\boldsymbol{n_2}$ samples come from the second class
- consider projection on a line
- Let the line direction be given by unit vector $\boldsymbol{v}$



- Scalar $\boldsymbol{v^t x_i}$ is the distance of projection of $\boldsymbol{x_i}$ from the origin
- Thus it $\boldsymbol{v^t x_i}$ is the projection of $\boldsymbol{x_i}$ into a one dimensional subspace

Fisher Linear Discriminant

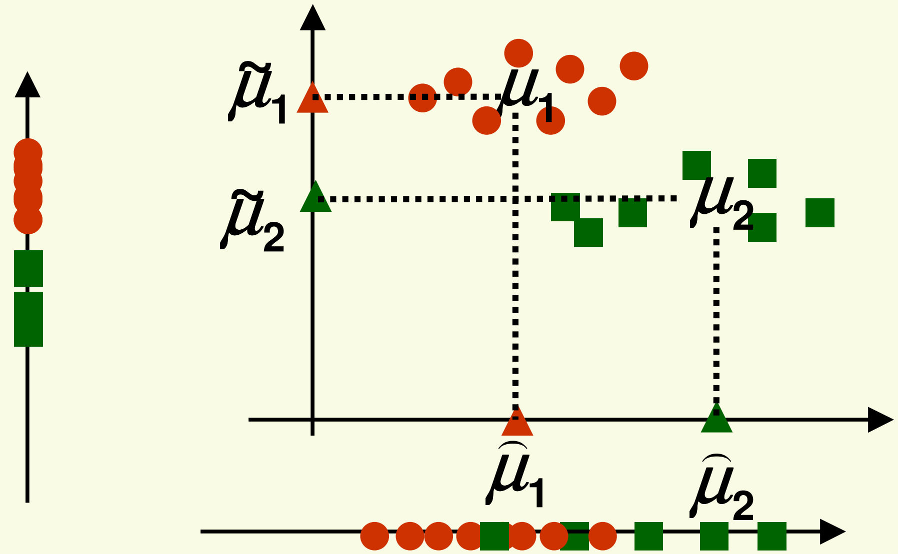
- Thus the projection of sample $\boldsymbol{x_i}$ onto a line in direction $\boldsymbol{v}$ is given by $\boldsymbol{v^t x_i}$
- How to measure separation between projections of different classes?
- Let $\tilde{\mu}_1$ and $\tilde{\mu}_2$ be the means of projections of classes 1 and 2
- Let μ_1 and μ_2 be the means of classes 1 and 2
- $|\tilde{\mu}_1 - \tilde{\mu}_2|$ seems like a good measure

$$\tilde{\mu}_1 = \frac{1}{n_1} \sum_{x_i \in C1}^{n_1} \boldsymbol{v}^t \boldsymbol{x}_i = \boldsymbol{v}^t \left(\frac{1}{n_1} \sum_{x_i \in C1}^{n_1} \boldsymbol{x}_i \right) = \boldsymbol{v}^t \mu_1$$

similarly, $\quad \tilde{\mu}_2 = \boldsymbol{v}^t \mu_2$

Fisher Linear Discriminant

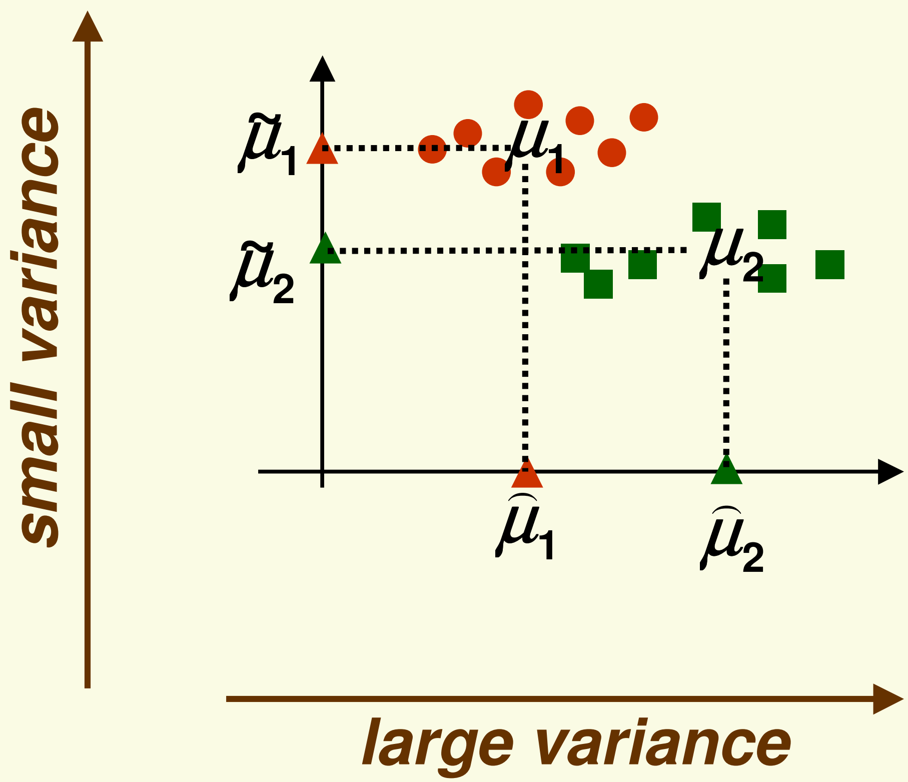
- How good is $|\tilde{\mu}_1 - \tilde{\mu}_2|$ as a measure of separation?
  - The larger $|\tilde{\mu}_1 - \tilde{\mu}_2|$, the better is the expected separation



- the vertical axes is a better line than the horizontal axes to project to for class separability
- however $|\hat{\mu}_1 - \hat{\mu}_2| > |\tilde{\mu}_1 - \tilde{\mu}_2|$

Fisher Linear Discriminant

- The problem with $|\tilde{\mu}_1 - \tilde{\mu}_2|$ is that it does not consider the variance of the classes



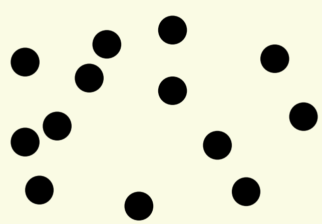
Fisher Linear Discriminant

- We need to normalize $|\tilde{\mu}_1 - \tilde{\mu}_2|$ by a factor which is proportional to variance
- Have samples $z_1, \ldots, z_n$. Sample mean is $\mu_z = \frac{1}{n}\sum_{i=1}^{n} z_i$
- Define their ***scatter*** as

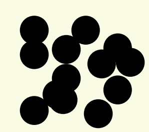
$$s = \sum_{i=1}^{n} (z_i - \mu_z)^2$$

- Thus scatter is just sample variance multiplied by ***n***
  - scatter measures the same thing as variance, the spread of data around the mean
  - scatter is just on different scale than variance

larger scatter:



smaller scatter:



Fisher Linear Discriminant

- Fisher Solution: normalize $|\tilde{\mu}_1 - \tilde{\mu}_2|$ by scatter
- Let $\boldsymbol{y_i} = \boldsymbol{v^t x_i}$, i.e. $\boldsymbol{y_i}$ ‘s are the projected samples
- Scatter for projected samples of class 1 is

$$\tilde{s}_1^2 = \sum_{y_i \in Class\ 1} (y_i - \tilde{\mu}_1)^2$$

- Scatter for projected samples of class 2 is

$$\tilde{s}_2^2 = \sum_{y_i \in Class\ 2} (y_i - \tilde{\mu}_2)^2$$

Fisher Linear Discriminant

- We need to normalize by both scatter of class 1 and scatter of class 2
- Thus Fisher linear discriminant is to project on line in the direction ***v*** which maximizes

$$J(v) = \frac{\overbrace{(\tilde{\mu}_1 - \tilde{\mu}_2)^2}^{\textit{want projected means are far from each other}}}{\tilde{s}_1^2 + \tilde{s}_2^2}$$

want scatter in class 1 is as small as possible, i.e. samples of class 1 cluster around the projected mean $\tilde{\mu}_1$

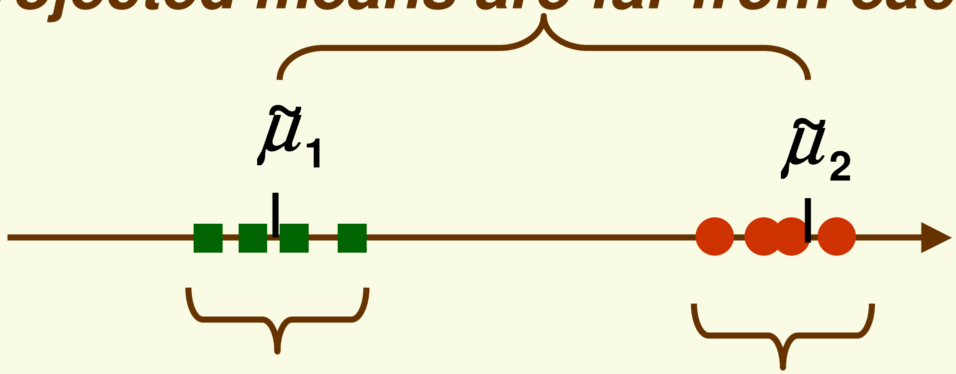
want scatter in class 2 is as small as possible, i.e. samples of class 2 cluster around the projected mean $\tilde{\mu}_2$

Fisher Linear Discriminant

$$J(\mathbf{v}) = \frac{(\tilde{\mu}_1 - \tilde{\mu}_2)^2}{\tilde{s}_1^2 + \tilde{s}_2^2}$$

- If we find $\mathbf{v}$ which makes $J(\mathbf{v})$ large, we are guaranteed that the classes are well separated

projected means are far from each other



small $\tilde{s}_1$ implies that projected samples of class 1 are clustered around projected mean

small $\tilde{s}_2$ implies that projected samples of class 2 are clustered around projected mean

Fisher Linear Discriminant Derivation

$$J(v) = \frac{(\tilde{\mu}_1 - \tilde{\mu}_2)^2}{\tilde{s}_1^2 + \tilde{s}_2^2}$$

- All we need to do now is to express ***J*** explicitly as a function of ***v*** and maximize it
  - straightforward but need linear algebra and Calculus
- Define the separate class scatter matrices S_1 and S_2 for classes 1 and 2. These measure the scatter of original samples x_i (before projection)

$$S_1 = \sum_{x_i \in Class\ 1} (x_i - \mu_1)(x_i - \mu_1)^t$$

$$S_2 = \sum_{x_i \in Class\ 2} (x_i - \mu_2)(x_i - \mu_2)^t$$

Fisher Linear Discriminant Derivation

- Now define the ***within*** the class scatter matrix

$$\boldsymbol{S}_W = \boldsymbol{S}_1 + \boldsymbol{S}_2$$

- Recall that $\tilde{\boldsymbol{s}}_1^2 = \sum_{y_i \in Class\ 1} (\boldsymbol{y}_i - \tilde{\mu}_1)^2$

- Using $\boldsymbol{y_i} = \boldsymbol{v^t x_i}$ and $\tilde{\mu}_1 = \boldsymbol{v}^t \mu_1$

$$\begin{aligned}
\tilde{\boldsymbol{s}}_1^2 &= \sum_{y_i \in Class\ 1} \left(\boldsymbol{v}^t \boldsymbol{x}_i - \boldsymbol{v}^t \mu_1\right)^2 \\
&= \sum_{y_i \in Class\ 1} \left(\boldsymbol{v}^t (\boldsymbol{x}_i - \mu_1)\right)^t \left(\boldsymbol{v}^t (\boldsymbol{x}_i - \mu_1)\right) \\
&= \sum_{y_i \in Class\ 1} \left((\boldsymbol{x}_i - \mu_1)^t \boldsymbol{v}\right)^t \left((\boldsymbol{x}_i - \mu_1)^t \boldsymbol{v}\right) \\
&= \sum_{y_i \in Class\ 1} \boldsymbol{v}^t (\boldsymbol{x}_i - \mu_1)(\boldsymbol{x}_i - \mu_1)^t \boldsymbol{v} = \boldsymbol{v}^t \boldsymbol{S}_1 \boldsymbol{v}
\end{aligned}$$

Fisher Linear Discriminant Derivation

- Similarly $\tilde{s}_2^2 = \boldsymbol{v}^t \boldsymbol{S}_2 \boldsymbol{v}$
- Therefore $\tilde{s}_1^2 + \tilde{s}_2^2 = \boldsymbol{v}^t \boldsymbol{S}_1 \boldsymbol{v} + \boldsymbol{v}^t \boldsymbol{S}_2 \boldsymbol{v} = \boldsymbol{v}^t \boldsymbol{S}_W \boldsymbol{v}$
- Define between the class scatter matrix

$$\boldsymbol{S}_B = (\mu_1 - \mu_2)(\mu_1 - \mu_2)^t$$

- $\boldsymbol{S}_B$ measures separation between the means of two classes (before projection)
- Let's rewrite the separations of the projected means

$$\begin{aligned}
(\tilde{\mu}_1 - \tilde{\mu}_2)^2 &= \left(\boldsymbol{v}^t \mu_1 - \boldsymbol{v}^t \mu_2\right)^2 \\
&= \boldsymbol{v}^t (\mu_1 - \mu_2)(\mu_1 - \mu_2)^t \boldsymbol{v} \\
&= \boldsymbol{v}^t \boldsymbol{S}_B \boldsymbol{v}
\end{aligned}$$

Fisher Linear Discriminant Derivation

- Thus our objective function can be written:

$$J(v) = \frac{(\tilde{\mu}_1 - \tilde{\mu}_2)^2}{\tilde{s}_1^2 + \tilde{s}_2^2} = \frac{v^t S_B v}{v^t S_W v}$$

- Minimize $J(v)$ by taking the derivative w.r.t. v and setting it to 0

$$\frac{d}{dv} J(v) = \frac{\left(\frac{d}{dv} v^t S_B v\right) v^t S_W v - \left(\frac{d}{dv} v^t S_W v\right) v^t S_B v}{\left(v^t S_W v\right)^2}$$

$$= \frac{(2 S_B v) v^t S_W v - (2 S_W v) v^t S_B v}{\left(v^t S_W v\right)^2} = 0$$

Fisher Linear Discriminant Derivation

- Need to solve $\quad v^t S_W v (S_B v) - v^t S_B v (S_W v) = 0$

$$\Rightarrow \frac{v^t S_W v (S_B v)}{v^t S_W v} - \frac{v^t S_B v (S_W v)}{v^t S_W v} = 0$$

$$\Rightarrow S_B v - \underbrace{\frac{v^t S_B v (S_W v)}{v^t S_W v}}_{= \lambda} = 0$$

$$\Rightarrow \underbrace{S_B v = \lambda S_W v}_{\text{generalized eigenvalue problem}}$$

Fisher Linear Discriminant Derivation

$$\mathbf{S}_B \mathbf{v} = \lambda \mathbf{S}_W \mathbf{v}$$

- If $\mathbf{S}_W$ has full rank (the inverse exists), can convert this to a standard eigenvalue problem

$$\mathbf{S}_W^{-1} \mathbf{S}_B \mathbf{v} = \lambda \mathbf{v}$$

- But $\mathbf{S}_B \mathbf{x}$ for any vector $\mathbf{x}$, points in the same direction as $\mu_1 - \mu_2$

$$\mathbf{S}_B \mathbf{x} = (\mu_1 - \mu_2)(\mu_1 - \mu_2)^t \mathbf{x} = (\mu_1 - \mu_2)\overbrace{\left((\mu_1 - \mu_2)^t \mathbf{x}\right)}^{\alpha} = \alpha(\mu_1 - \mu_2)$$

- Thus can solve the eigenvalue problem immediately

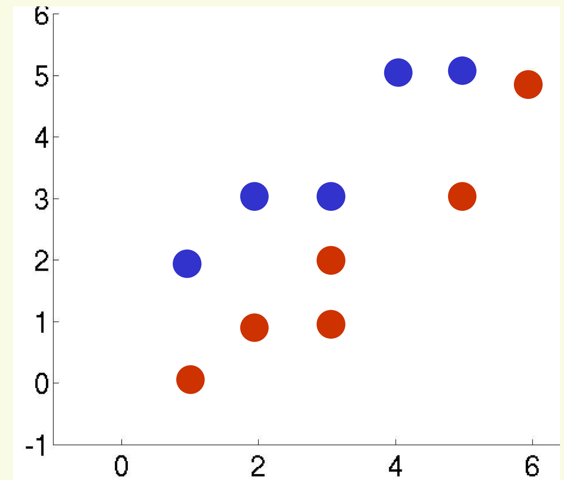
$$\boxed{\mathbf{v} = \mathbf{S}_W^{-1}(\mu_1 - \mu_2)}$$

$$\mathbf{S}_W^{-1} \mathbf{S}_B \underbrace{\left[\mathbf{S}_W^{-1}(\mu_1 - \mu_2)\right]}_{\mathbf{v}} = \mathbf{S}_W^{-1}\left[\alpha(\mu_1 - \mu_2)\right] = \underbrace{\alpha}_{\lambda} \underbrace{\left[\mathbf{S}_W^{-1}(\mu_1 - \mu_2)\right]}_{\mathbf{v}}$$

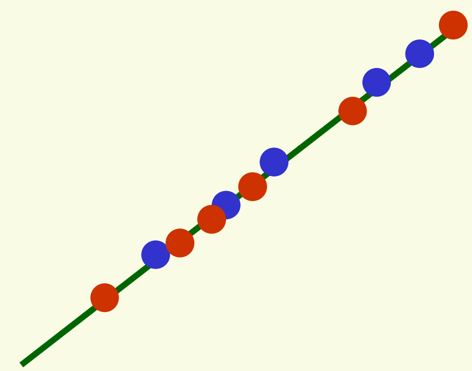
Fisher Linear Discriminant Example

- Data
  - Class 1 has 5 samples c_1=[(1,2),(2,3),(3,3),(4,5),(5,5)]
  - Class 2 has 6 samples c_2=[(1,0),(2,1),(3,1),(3,2),(5,3),(6,5)]
- Arrange data in 2 separate matrices

$$c_1 = \begin{bmatrix} 1 & 2 \\ \vdots & \vdots \\ 5 & 5 \end{bmatrix} \qquad c_2 = \begin{bmatrix} 1 & 0 \\ \vdots & \vdots \\ 6 & 5 \end{bmatrix}$$



- Notice that PCA performs very poorly on this data because the direction of largest variance is not helpful for classification



Fisher Linear Discriminant Example

- First compute the mean for each class

$$\mu_1 = mean(c_1) = [3 \quad 3.6] \qquad \mu_2 = mean(c_2) = [3.3 \quad 2]$$

- Compute scatter matrices S_1 and S_2 for each class

$$S_1 = 4 * cov(c_1) = \begin{bmatrix} 10 & 8.0 \\ 8.0 & 7.2 \end{bmatrix} \qquad S_2 = 5 * cov(c_2) = \begin{bmatrix} 17.3 & 16 \\ 16 & 16 \end{bmatrix}$$

- Within the class scatter:

$$S_W = S_1 + S_2 = \begin{bmatrix} 27.3 & 24 \\ 24 & 23.2 \end{bmatrix}$$

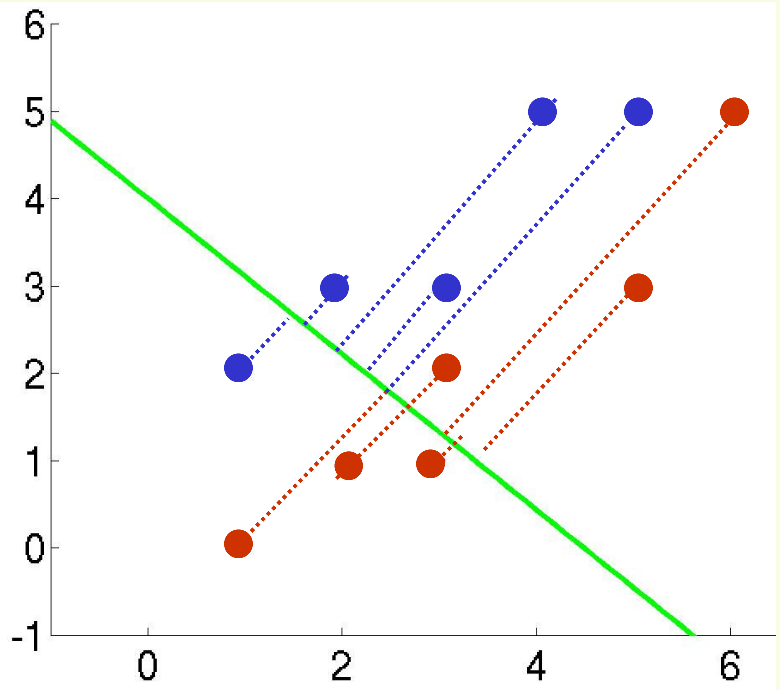
  - it has full rank, don't have to solve for eigenvalues

- The inverse of S_W is $S_W^{-1} = inv(S_W) = \begin{bmatrix} 0.39 & -0.41 \\ -0.41 & 0.47 \end{bmatrix}$
- Finally, the optimal line direction v

$$v = S_W^{-1}(\mu_1 - \mu_2) = \begin{bmatrix} -0.79 \\ 0.89 \end{bmatrix}$$

Fisher Linear Discriminant Example

- Notice, as long as the line has the right direction, its exact position does not matter



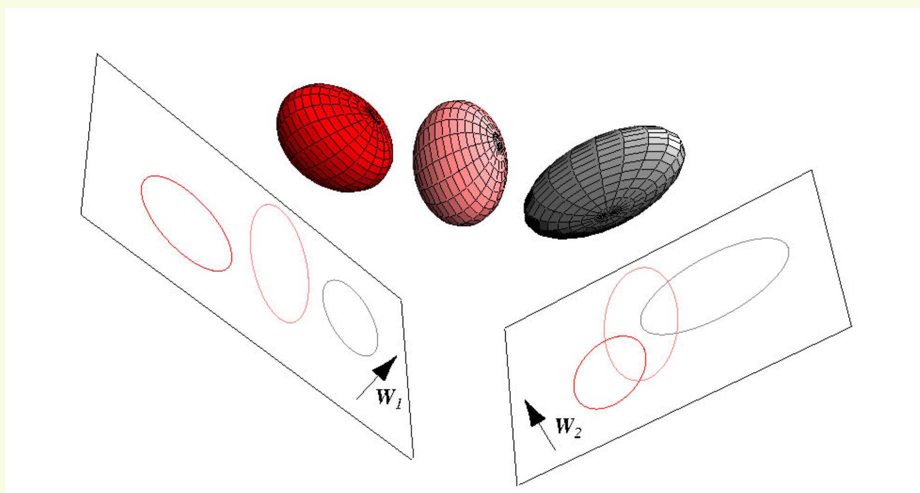
- Last step is to compute the actual ***1D*** vector ***y***. Let's do it separately for each class

$$Y_1 = v^t c_1^t = \begin{bmatrix} -0.65 & 0.73 \end{bmatrix} \begin{bmatrix} 1 & \cdots & 5 \\ 2 & \cdots & 5 \end{bmatrix} = \begin{bmatrix} 0.81 & \cdots & 0.4 \end{bmatrix}$$

$$Y_2 = v^t c_2^t = \begin{bmatrix} -0.65 & 0.73 \end{bmatrix} \begin{bmatrix} 1 & \cdots & 6 \\ 0 & \cdots & 5 \end{bmatrix} = \begin{bmatrix} -0.65 & \cdots & -0.25 \end{bmatrix}$$

Multiple Discriminant Analysis (MDA)

- Can generalize FLD to multiple classes
- In case of ***c*** classes, can reduce dimensionality to 1, 2, 3,…, ***c***-1 dimensions
- Project sample $\boldsymbol{x_i}$ to a linear subspace $\boldsymbol{y_i = V^t x_i}$
  - $\boldsymbol{V}$ is called projection matrix



Multiple Discriminant Analysis (MDA)

- Let
  - n_i by the number of samples of class i
  - and μ_i be the sample mean of class i
  - μ be the total mean of all samples

$$\mu_i = \frac{1}{n_i} \sum_{x \in class\ i} x \qquad \mu = \frac{1}{n} \sum_{x_i} x_i$$

- Objective function: $J(V) = \dfrac{\det\left(V^t S_B V\right)}{\det\left(V^t S_W V\right)}$
- within the class scatter matrix S_W is

$$S_W = \sum_{i=1}^{c} S_i = \sum_{i=1}^{c} \sum_{x_k \in class\ i} (x_k - \mu_i)(x_k - \mu_i)^t$$

- between the class scatter matrix S_B is

$$S_B = \sum_{i=1}^{c} n_i (\mu_i - \mu)(\mu_i - \mu)^t$$

maximum rank is c -1

Multiple Discriminant Analysis (MDA)

$$J(V) = \frac{\det\left(V^t S_B V\right)}{\det\left(V^t S_W V\right)}$$

- First solve the ***generalized eigenvalue*** problem:

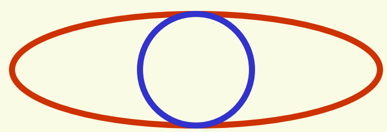
$$S_B v = \lambda S_W v$$

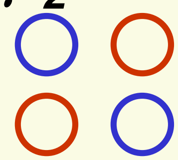
- At most $c-1$ distinct solution eigenvalues
- Let $v_1, v_2, \ldots, v_{c-1}$ be the corresponding eigenvectors
- The optimal projection matrix V to a subspace of dimension k is given by the eigenvectors corresponding to the largest k eigenvalues
- Thus can project to a subspace of dimension at most $c-1$

FDA and MDA Drawbacks

- Reduces dimension only to ***k*** = ***c*-*1*** (unlike PCA)
  - For complex data, projection to even the best line may result in unseparable projected samples
- Will fail:

1. ***J***(***v***) is always 0: happens if $\mu_1 = \mu_2$





PCA performs reasonably well here:

PCA also fails:

2. If ***J***(***v***) is always large: classes have large overlap when projected to any line (PCA will also fail)