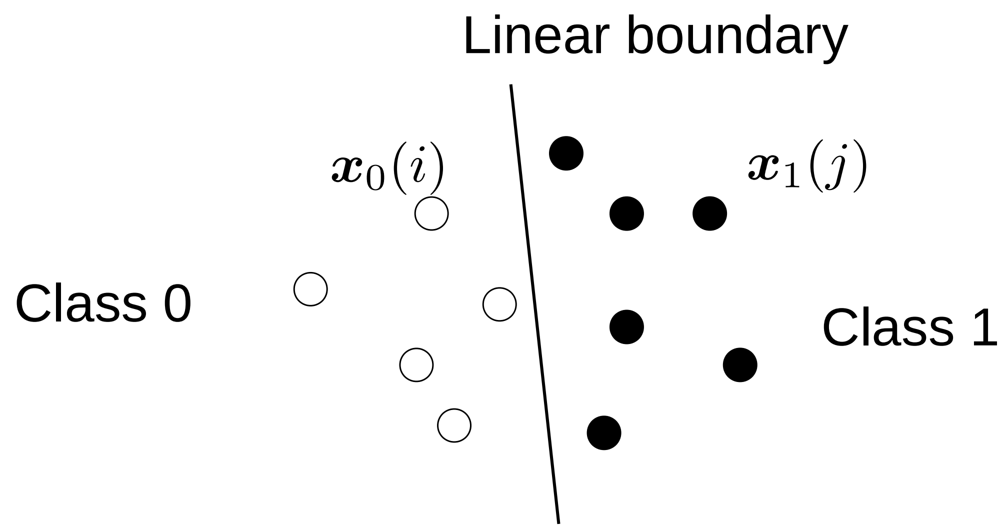
19. Discriminant function analysis

- Discriminant function analysis（判別分析）classifies data into classes
  - Suppose that we have two classes, class 0 and class 1.
    - For example, class 0 may correspond to a normal class while class 1 may correspond to an abnormal (failure, disease, etc) class
  - The problem is to find the best boundary between the two classes
  - Data
    - Data vectors $\boldsymbol{x}_0(1), \ldots, \boldsymbol{x}_0(n_0)$ belong to class 0
    - Data vectors $\boldsymbol{x}_1(1), \ldots, \boldsymbol{x}_1(n_1)$ belong to class 1

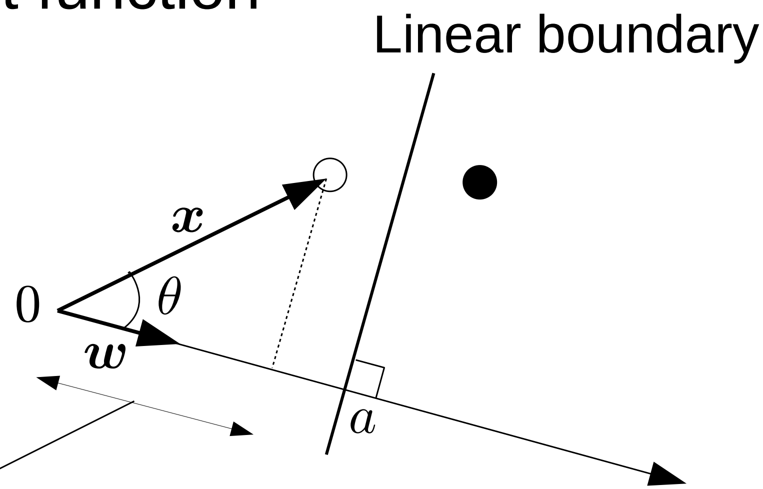
19. Discriminant function analysis

- Linear discriminant function（線形判別関数）
  - The linear function that determines the boundary between the classes. The boundary is linear (a line, a plane or a hyper-plane)



19. Discriminant function analysis

- Linear discriminant function



The length = $\|\boldsymbol{x}\|\cos\theta = \dfrac{\boldsymbol{x}^T\boldsymbol{w}}{\|\boldsymbol{w}\|}\begin{cases} < a & \text{… } \boldsymbol{x} \text{ belongs to class 0} \\ > a & \text{… } \boldsymbol{x} \text{ belongs to class 1} \end{cases}$

$\Updownarrow$

$z = \boldsymbol{w}^T\boldsymbol{x}\begin{cases} < b & \text{… } \boldsymbol{x} \text{ belongs to class 0} \\ > b & \text{… } \boldsymbol{x} \text{ belongs to class 1} \end{cases}$

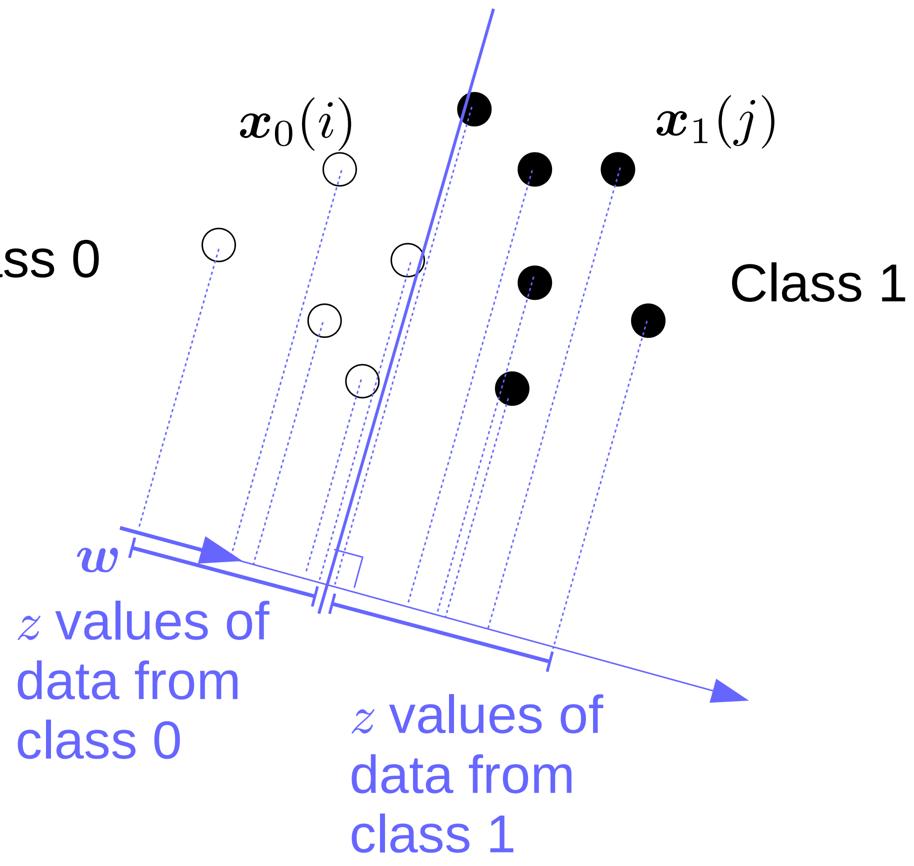
Here $b = a\|\boldsymbol{w}\|$.

Note that the inequality signs can be the other way round depending on the direction of $\boldsymbol{w}$ relative to the positions of the classes

We want to find the best $\boldsymbol{w}$.

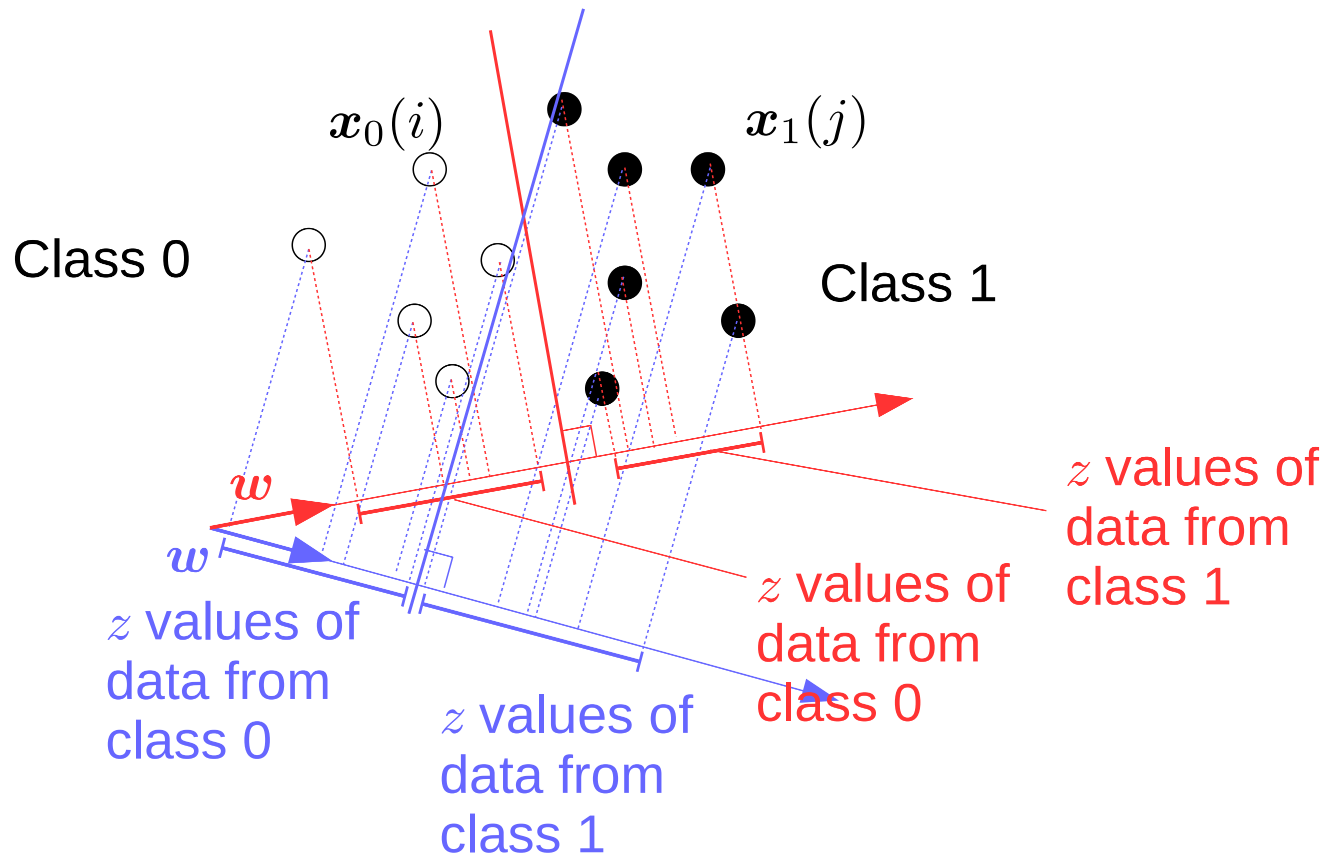
19. Discriminant function analysis

- The best $\boldsymbol{w}$



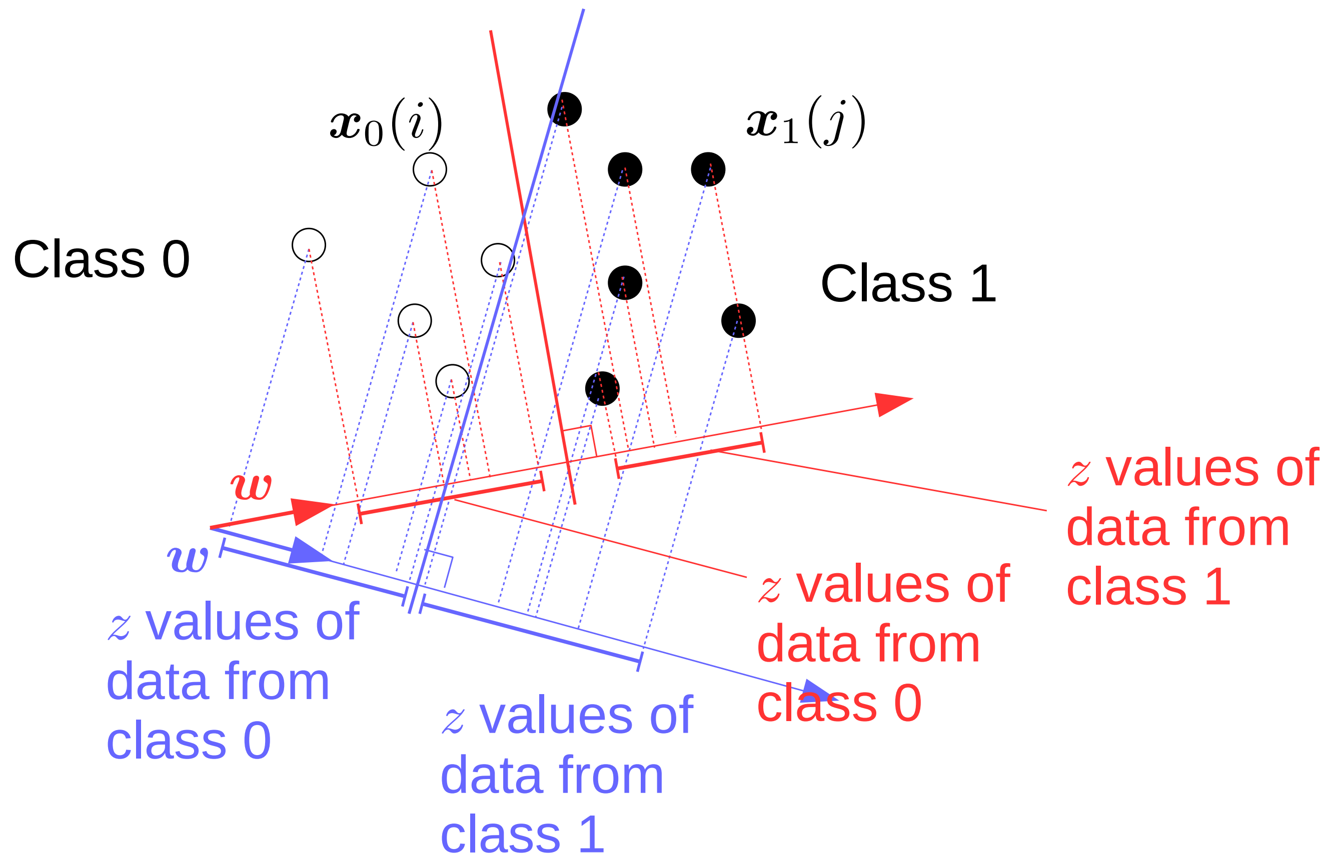
19. Discriminant function analysis

- The best $\boldsymbol{w}$



19. Discriminant function analysis

- The best $\boldsymbol{w}$



Good $\boldsymbol{w}$ ⇨

The values of z from different classes are well separated, while the z values within the same class are close to each other.

19. Discriminant function analysis

- Evaluation of closeness (or dispersity) of z values
  - Averages of $\boldsymbol{x}$
    - $\bar{\boldsymbol{x}}_0 = \dfrac{1}{n_0}\sum_{i=1}^{n_0} \boldsymbol{x}_0(i)$: the average of $\boldsymbol{x}$ from class 0.
    - $\bar{\boldsymbol{x}}_1 = \dfrac{1}{n_1}\sum_{j=1}^{n_1} \boldsymbol{x}_1(j)$: the average of $\boldsymbol{x}$ from class 1.

19. Discriminant function analysis

– Averages of z

- Let us define $z_0(i) = \boldsymbol{w}^T \boldsymbol{x}_0(i)$ and $z_1(j) = \boldsymbol{w}^T \boldsymbol{x}_1(j)$.
- The average of z from class 0

$$\bar{z}_0 = \frac{1}{n_0} \sum_{i=1}^{n_0} z_0(i) = \frac{1}{n_0} \sum_{i=1}^{n_0} \boldsymbol{w}^T \boldsymbol{x}_0(i) = \boldsymbol{w}^T \frac{1}{n_0} \sum_{i=1}^{n_0} \boldsymbol{x}_0(i) = \boldsymbol{w}^T \bar{\boldsymbol{x}}_0.$$

- The average of z from class 1

$$\bar{z}_1 = \frac{1}{n_1} \sum_{j=1}^{n_1} z_1(j) = \boldsymbol{w}^T \bar{\boldsymbol{x}}_1.$$

- Average of all z from either class

$$\bar{z} = \frac{1}{n_0 + n_1} \left(\sum_{i=1}^{n_0} z_0(i) + \sum_{j=1}^{n_1} z_1(j) \right) = \frac{n_o \bar{z}_0 + n_1 \bar{z}_1}{n_0 + n_1}.$$

19. Discriminant function analysis

- Sum of squares of deviations (sum of squares of differences from the average)

$$V = \underbrace{\sum_{i=1}^{n_0} (z_0(i) - \bar{z})^2}_{\|} + \sum_{j=1}^{n_1} (z_1(j) - \bar{z})^2$$

$$\sum_{i=1}^{n_0} (z_0(i) - \bar{z}_0 + \bar{z}_0 - \bar{z})^2$$

$$= \sum_{i=1}^{n_0} \left[(z_0(i) - \bar{z}_0)^2 + 2(z_0(i) - \bar{z}_0)(\bar{z}_0 - \bar{z}) + (\bar{z}_0 - \bar{z})^2 \right]$$

$$= \sum_{i=1}^{n_0} (z_0(i) - \bar{z}_0)^2 + 2(\bar{z}_0 - \bar{z}) \underbrace{\sum_{i=1}^{n_0} (z_0(i) - \bar{z}_0)}_{\substack{\| \\ 0}} + n_0(\bar{z}_0 - \bar{z})^2$$

$$= \sum_{i=1}^{n_0} (z_0(i) - \bar{z}_0)^2 + n_0(\bar{z}_0 - \bar{z})^2$$

19. Discriminant function analysis

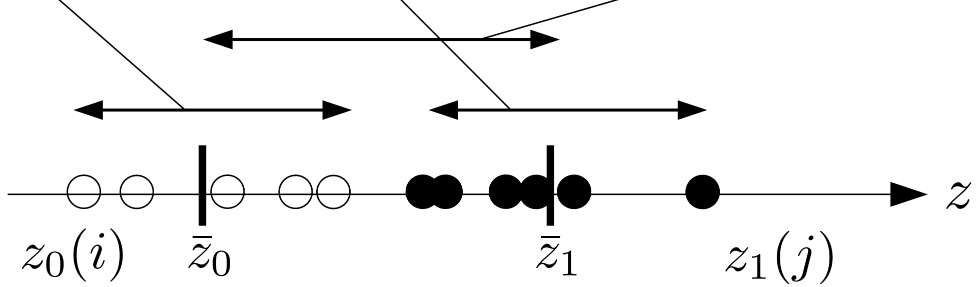
$$V = \sum_{i=1}^{n_0} (z_0(i) - \bar{z}_0)^2 + n_0(\bar{z}_0 - \bar{z})^2 + \sum_{j=1}^{n_1} (z_1(j) - \bar{z}_1)^2 + n_1(\bar{z}_1 - \bar{z})^2$$

$$= \sum_{i=1}^{n_0} (z_0(i) - \bar{z}_0)^2 + \sum_{j=1}^{n_1} (z_1(j) - \bar{z}_1)^2 + n_0(\bar{z}_0 - \bar{z})^2 + n_1(\bar{z}_1 - \bar{z})^2$$

Dispersion or variation（ばらつき, 変動）within class 0

Dispersion or variation（ばらつき, 変動）within class 1

Spread（広がり）of averages of class 0 and class 1 around the average of all the data



Class 0 Class 1

19. Discriminant function analysis

– Intra-class dispersity

$$\begin{aligned}
V_W &= \sum_{i=1}^{n_0} \left(z_0(i) - \bar{z}_0\right)^2 + \sum_{j=1}^{n_1} \left(z_1(j) - \bar{z}_1\right)^2 \\
&= \sum_{i=1}^{n_0} (\boldsymbol{w}^T \boldsymbol{x}_0(i) - \boldsymbol{w}^T \bar{\boldsymbol{x}}_0)^2 + \sum_{j=1}^{n_1} (\boldsymbol{w}^T \boldsymbol{x}_1(j) - \boldsymbol{w}^T \bar{\boldsymbol{x}}_1)^2 \\
&= \sum_{i=1}^{n_0} \boldsymbol{w}^T (\boldsymbol{x}_0(i) - \bar{\boldsymbol{x}}_0)(\boldsymbol{x}_0(i) - \bar{\boldsymbol{x}}_0)^T \boldsymbol{w} \\
&\qquad + \sum_{j=1}^{n_1} \boldsymbol{w}^T (\boldsymbol{x}_1(j) - \bar{\boldsymbol{x}}_1)(\boldsymbol{x}_1(j) - \bar{\boldsymbol{x}}_1)^T \boldsymbol{w} \\
&= \boldsymbol{w}^T W \boldsymbol{w},
\end{aligned}$$

where

$$W = \sum_{i=1}^{n_0} (\boldsymbol{x}_0(i) - \bar{\boldsymbol{x}}_0)(\boldsymbol{x}_0(i) - \bar{\boldsymbol{x}}_0)^T + \sum_{j=1}^{n_1} (\boldsymbol{x}_1(j) - \bar{\boldsymbol{x}}_1)(\boldsymbol{x}_1(j) - \bar{\boldsymbol{x}}_1)^T$$

19. Discriminant function analysis

– Inter-class dispersity

$$
\begin{aligned}
V_B &= n_0(\bar{z}_0 - \bar{z})^2 + n_1(\bar{z}_1 - \bar{z})^2 \\
&= n_0\left(\bar{z}_0 - \frac{n_0\bar{z}_0 + n_1\bar{z}_1}{n_0+n_1}\right)^2 + n_1\left(\bar{z}_1 - \frac{n_0\bar{z}_0 + n_1\bar{z}_1}{n_0+n_1}\right)^2 \\
&= n_0\left(\frac{n_1\bar{z}_0 - n_1\bar{z}_1}{n_0+n_1}\right)^2 + n_1\left(\frac{n_0\bar{z}_1 - n_0\bar{z}_0}{n_0+n_1}\right)^2 \\
&= \frac{n_0{n_1}^2 + n_1{n_0}^2}{(n_0+n_1)^2}(\bar{z}_0 - \bar{z}_1)^2 = \frac{n_0 n_1}{n_0+n_1}(\bar{z}_0 - \bar{z}_1)^2 \\
&= \frac{n_0 n_1}{n_0+n_1}(\boldsymbol{w}^T\bar{\boldsymbol{x}}_0 - \boldsymbol{w}^T\bar{\boldsymbol{x}}_1)^2 \\
&= \frac{n_0 n_1}{n_0+n_1}\boldsymbol{w}^T(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)^T\boldsymbol{w} \\
&= \boldsymbol{w}^T B \boldsymbol{w},
\end{aligned}
$$

where

$$
B = \frac{n_0 n_1}{n_0+n_1}(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)^T
$$

19. Discriminant function analysis

- Good $\boldsymbol{w}$
  - Small V_W, i.e., z values from each class gather closely, and large V_B, i.e., z values from the two classes are well separated.
  - The best $\boldsymbol{w}$ is derived by maximizing V_B while keeping V_W constant, say 1, which is formulated as

$$\text{maximize } \boldsymbol{w}^T B \boldsymbol{w} \text{ subject to } \boldsymbol{w}^T W \boldsymbol{w} - 1 = 0.$$

  - By using a Lagrange multiplier (page 186), the condition for the best $\boldsymbol{w}$ is derived as

$$\frac{\partial}{\partial \boldsymbol{w}}(\boldsymbol{w}^T B \boldsymbol{w}) - v \cdot \frac{\partial}{\partial \boldsymbol{w}}(\boldsymbol{w}^T W \boldsymbol{w} - 1) = \boldsymbol{0}.$$

(Recall the condition $\nabla f(\boldsymbol{x}_0) + \sum_{i=1}^{m} v_i \nabla h_i(\boldsymbol{x}_0) = 0$ derived on page 186.)

19. Discriminant function analysis

$$\frac{\partial}{\partial \boldsymbol{w}}(\boldsymbol{w}^T B \boldsymbol{w}) - v \cdot \frac{\partial}{\partial \boldsymbol{w}}(\boldsymbol{w}^T W \boldsymbol{w} - 1) = \mathbf{0}$$

$$B\boldsymbol{w} + B^T\boldsymbol{w} - v \cdot (W\boldsymbol{w} + W^T\boldsymbol{w}) = \mathbf{0}$$

Here

$$B^T = \left\{ \frac{n_0 n_1}{n_0 + n_1}(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)^T \right\}^T = \frac{n_0 n_1}{n_0 + n_1}(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)^T = B,$$

$$W^T = \left\{ \sum_{i=1}^{n_0}(\boldsymbol{x}_0(i) - \bar{\boldsymbol{x}}_0)(\boldsymbol{x}_0(i) - \bar{\boldsymbol{x}}_0)^T + \sum_{j=1}^{n_1}(\boldsymbol{x}_1(j) - \bar{\boldsymbol{x}}_1)(\boldsymbol{x}_1(j) - \bar{\boldsymbol{x}}_1)^T \right\}^T = W,$$

and therefore

$$2B\boldsymbol{w} - 2vW\boldsymbol{w} = \mathbf{0}$$

$$B\boldsymbol{w} = vW\boldsymbol{w}$$

Notice that if n_0 and n_1 are sufficiently large, the matrix W has its inverse matrix W^{-1}.

19. Discriminant function analysis

Substituting $B = \frac{n_0 n_1}{n_0 + n_1}(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)^T$ into $B\boldsymbol{w} = vW\boldsymbol{w}$, we derive

$$\underbrace{\frac{n_0 n_1}{n_0 + n_1}}_{\text{A scalar}}(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)\underbrace{(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)^T \boldsymbol{w}}_{\text{A scalar}} = \underbrace{v}_{\text{A scalar}} W\boldsymbol{w}.$$

Therefore the vector $\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1$ and the vector $W\boldsymbol{w}$ have the same direction.

In other words, the vector $\boldsymbol{w}$ and the vector $W^{-1}(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)$ have the same direction.

Since only the direction of $\boldsymbol{w}$ matters (its length does not matter), we set

$$\boldsymbol{w} = W^{-1}(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1).$$

Then we define

$$z = \boldsymbol{w}^T \boldsymbol{x} = (\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)^T W^{-1} \boldsymbol{x}.$$

19. Discriminant function analysis

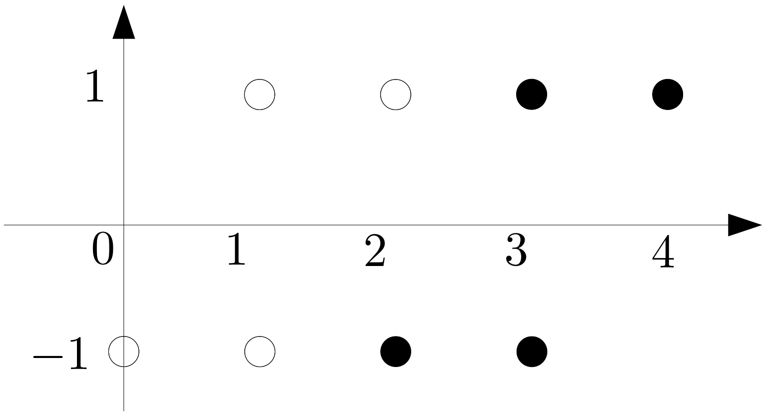
- The value of b
  - The class is determined depending on whether $z = \boldsymbol{w}^T \boldsymbol{x} > b$ or not.

    The value of b is set to the value corresponding to the midpoint between $\bar{\boldsymbol{x}}_0$ and $\bar{\boldsymbol{x}}_1$.

$$
\begin{aligned}
b &= \boldsymbol{w}^T \frac{\bar{\boldsymbol{x}}_0 + \bar{\boldsymbol{x}}_1}{2} = \{W^{-1}(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)\}^T \frac{\bar{\boldsymbol{x}}_0 + \bar{\boldsymbol{x}}_1}{2} \\
&= \frac{1}{2}(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)^T W^{-1}(\bar{\boldsymbol{x}}_0 + \bar{\boldsymbol{x}}_1)
\end{aligned}
$$

19. Discriminant function analysis

- Example
  - Data



$$\boldsymbol{x}_0(1) = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, \boldsymbol{x}_0(2) = \begin{bmatrix} 1 \\ -1 \end{bmatrix},$$

$$\boldsymbol{x}_0(3) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \boldsymbol{x}_0(4) = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

$$\boldsymbol{x}_1(1) = \begin{bmatrix} 2 \\ -1 \end{bmatrix}, \boldsymbol{x}_1(2) = \begin{bmatrix} 3 \\ -1 \end{bmatrix}, \boldsymbol{x}_1(3) = \begin{bmatrix} 3 \\ 1 \end{bmatrix}, \boldsymbol{x}_1(4) = \begin{bmatrix} 4 \\ 1 \end{bmatrix}$$

  - Solution

$$\bar{\boldsymbol{x}}_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \bar{\boldsymbol{x}}_1 = \begin{bmatrix} 3 \\ 0 \end{bmatrix}$$

19. Discriminant function analysis

$$\boldsymbol{x}_0(1) = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, \boldsymbol{x}_0(2) = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \ \boldsymbol{x}_0(3) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \boldsymbol{x}_0(4) = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \qquad \bar{\boldsymbol{x}}_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\boldsymbol{x}_1(1) = \begin{bmatrix} 2 \\ -1 \end{bmatrix}, \boldsymbol{x}_1(2) = \begin{bmatrix} 3 \\ -1 \end{bmatrix}, \boldsymbol{x}_1(3) = \begin{bmatrix} 3 \\ 1 \end{bmatrix}, \boldsymbol{x}_1(4) = \begin{bmatrix} 4 \\ 1 \end{bmatrix} \qquad \bar{\boldsymbol{x}}_1 = \begin{bmatrix} 3 \\ 0 \end{bmatrix}$$

$$W = \sum_{i=1}^{4} (\boldsymbol{x}_0(i) - \bar{\boldsymbol{x}}_0)(\boldsymbol{x}_0(i) - \bar{\boldsymbol{x}}_0)^T + \sum_{j=1}^{4} (\boldsymbol{x}_1(j) - \bar{\boldsymbol{x}}_1)(\boldsymbol{x}_1(j) - \bar{\boldsymbol{x}}_1)^T$$

$$= \begin{bmatrix} -1 \\ -1 \end{bmatrix} \begin{bmatrix} -1 & -1 \end{bmatrix} + \begin{bmatrix} 0 \\ -1 \end{bmatrix} \begin{bmatrix} 0 & -1 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \end{bmatrix}$$

$$+ \begin{bmatrix} -1 \\ -1 \end{bmatrix} \begin{bmatrix} -1 & -1 \end{bmatrix} + \begin{bmatrix} 0 \\ -1 \end{bmatrix} \begin{bmatrix} 0 & -1 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \end{bmatrix}$$

$$= 2 \left(\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \right) = \begin{bmatrix} 4 & 4 \\ 4 & 8 \end{bmatrix}$$

$$W^{-1} = \frac{1}{32 - 16} \begin{bmatrix} 8 & -4 \\ -4 & 4 \end{bmatrix} = \begin{bmatrix} 0.5 & -0.25 \\ -0.25 & 0.25 \end{bmatrix}$$

$$\boldsymbol{w} = W^{-1}(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1) = \begin{bmatrix} 0.5 & -0.25 \\ -0.25 & 0.25 \end{bmatrix} \begin{bmatrix} -2 \\ 0 \end{bmatrix} = \begin{bmatrix} -1 \\ 0.5 \end{bmatrix}$$

19. Discriminant function analysis

$$\boldsymbol{b} = \frac{1}{2}(\bar{\boldsymbol{x}}_0 - \bar{\boldsymbol{x}}_1)^T W^{-1}(\bar{\boldsymbol{x}}_0 + \bar{\boldsymbol{x}}_1) = \frac{1}{2}\begin{bmatrix}-2 & 0\end{bmatrix}\begin{bmatrix}0.5 & -0.25\\ -0.25 & 0.25\end{bmatrix}\begin{bmatrix}4\\ 0\end{bmatrix}$$

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