# Introduction to Machine Learning CS182

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March 3, 2022

#### Today:

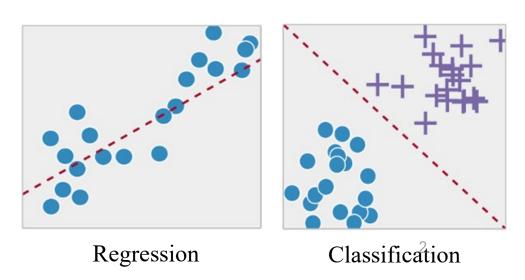
- Linear Methods for Classification I
  - Introduction
  - Linear regression of an indicator matrix
  - Linear discriminant analysis

#### Readings:

• The Elements of Statistical Learning (ESL), Chapters 4.1, 4.2 and 4.3

#### Linear Methods for Classification I

- Introduction
- Linear regression of an indicator matrix
- Linear discriminant analysis



#### Example

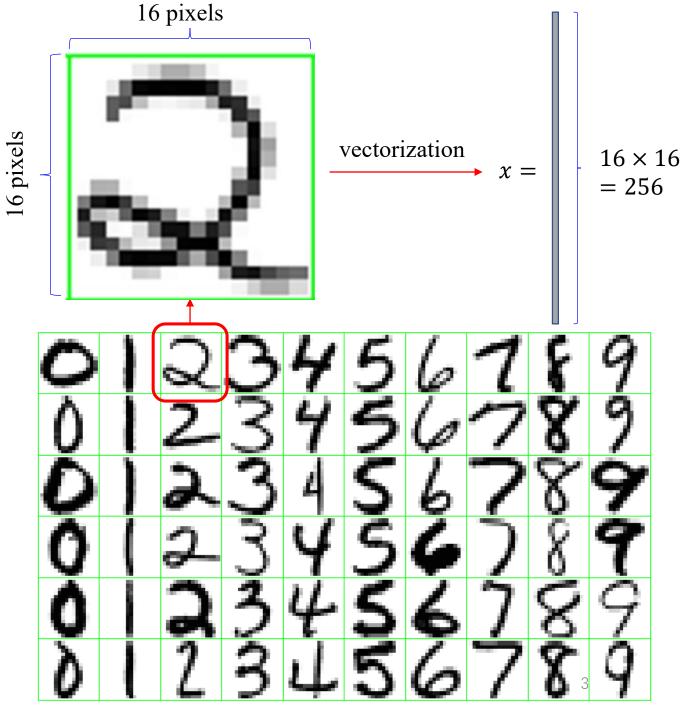
Handwritten digits recognition

Input variables

$$X = (X_0, X_1, X_2, ..., X_{256})^T$$

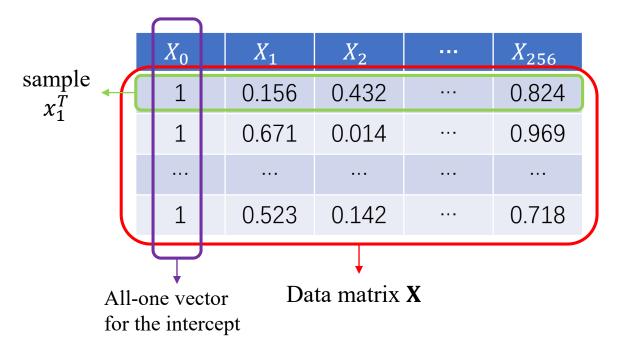
Categorical output variable G with

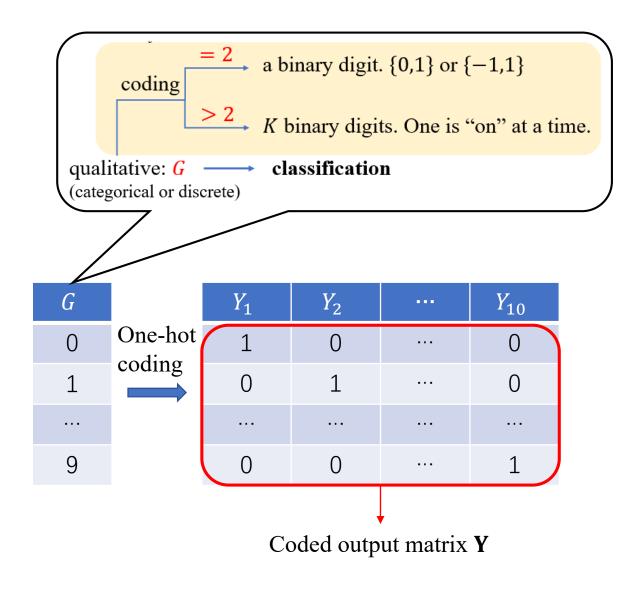
values from  $G = \{0,1,2...,9\}$ Non-binary (multi-class) classification



#### Example

Handwritten digits recognition





$$\min_{\mathbf{B}} \|\mathbf{Y} - \mathbf{X}\mathbf{B}\|_F^2 \longrightarrow \widehat{\mathbf{B}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}$$

$$\hat{\mathbf{B}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}$$

- 1. Any problems?
- Other methods?

#### Binary classification

• Linear regression

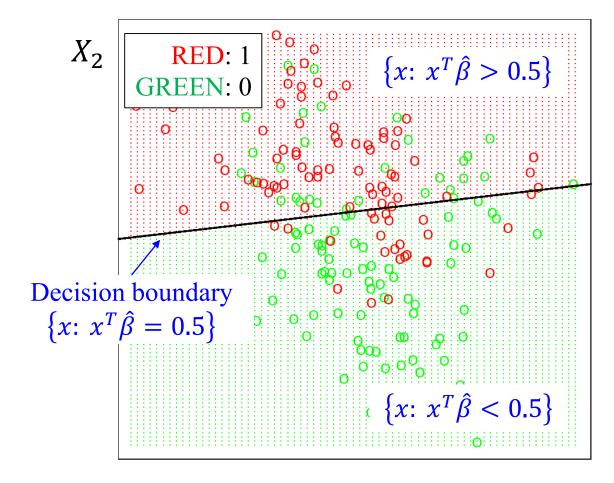
$$f(x) = \beta_0 + x^T \beta$$

• Least squares solution

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Decision boundary

$$\begin{cases} x: x^T \hat{\beta} = threshold \\ threshold = 0, & \text{if } y \in \{-1,1\} \\ threshold = 0.5, & \text{if } y \in \{0,1\} \end{cases}$$



#### Multi-class classification

• Linear regressions for *K* classes

$$f_k(x) = \beta_{k0} + x^T \beta_k, \qquad k = 1, \dots, K$$

• Decision boundary between classes k and  $\ell$ :

$$\left\{x: \hat{f}_k(x) = \hat{f}_\ell(x)\right\}$$

For *K* classes, there are  $\binom{K}{2} = \frac{K(K-1)}{2}$  decision boundaries

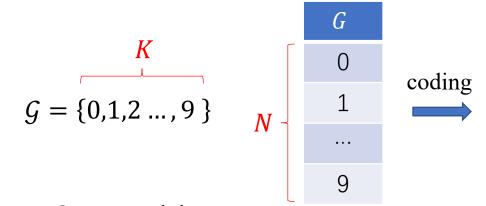
• That is an affine set or hyperplane:

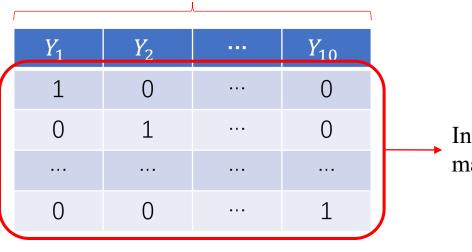
$$\{x: (\hat{\beta}_{k0} - \hat{\beta}_{\ell 0}) + x^T (\hat{\beta}_k - \hat{\beta}_{\ell}) = 0\}$$

#### Linear Methods for Classification I

- Introduction
- Linear regression of an indicator matrix
- Linear discriminant analysis

• Indicator response matrix





Indicator response matrix  $\mathbf{Y} \in \mathbb{R}^{N \times K}$ 

• Our problem:

$$\widehat{\mathbf{B}} = \underset{\mathbf{B}}{\operatorname{argmin}} \|\mathbf{Y} - \mathbf{X}\mathbf{B}\|_F^2$$

$$\mathbf{B} = (\beta_1, \beta_2, \dots, \beta_{10}) \in \mathbb{R}^{(p+1) \times K}$$

• The fitted values on **X**:

$$\widehat{\mathbf{Y}} = \mathbf{X}\widehat{\mathbf{B}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} = \mathbf{H}\mathbf{Y}$$

A new observation x is classified by

• Compute the fitted output

$$\hat{f}(x) = \hat{\mathbf{B}}^T \begin{pmatrix} 1 \\ \chi \end{pmatrix} = \begin{pmatrix} \hat{f}_1(x) \\ \hat{f}_2(x) \\ \vdots \\ \hat{f}_K(x) \end{pmatrix} \in \mathbb{R}^K$$

$$f_2 \uparrow \hat{f}_1(x) < \hat{f}_2(x) \qquad \hat{f}_1(x) = f_2(x)$$

$$\hat{f}_2(x) \uparrow \hat{f}_2(x) \qquad \hat{f}_2(x) \uparrow$$

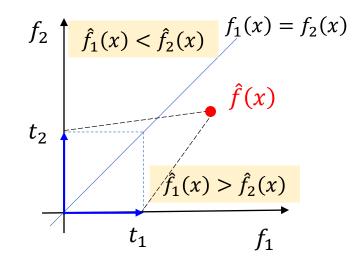
• Classify *x* according to

$$\widehat{G}(x) = \operatorname*{argmax}_{k \in \mathcal{G}} \widehat{f}_k(x)$$

• Or equivalently,

$$\hat{G}(x) = \operatorname{argmin}_{k \in \mathcal{G}} \|\hat{f}(x) - t_k\|_2^2$$

where  $t_k = (0, ..., 0, 1, 0, ..., 0)^T \in \mathbb{R}^K$  is a target with 1 being the k-th element



Categorical output variable G with values from  $G = \{1, ..., K\}$ .

• The zero-one loss function

$$L(k,\ell) = \begin{cases} 1, & k \neq \ell \\ 0, & k = \ell \end{cases}$$

• Expected prediction error (EPE) w.r.t. Pr(G, X)

$$EPE = E\left[L\left(G, \widehat{G}(X)\right)\right]$$

Pointwise minimization leads to

$$\widehat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmin}} \sum_{\ell=1}^{K} L(k, \ell) \Pr(G = \ell | X = x)$$

$$= \underset{k \in \mathcal{G}}{\operatorname{argmax}} \Pr(G = k | X = x) \longrightarrow \text{posterior}$$

A new observation x is classified by

• Compute the fitted output

$$\hat{f}(x) = \hat{B}^T \begin{pmatrix} 1 \\ x \end{pmatrix} = \begin{pmatrix} \hat{f}_1(x) \\ \hat{f}_2(x) \\ \vdots \\ \hat{f}_K(x) \end{pmatrix} \in \mathbb{R}^K$$

$$f_2 \uparrow \hat{f}_1(x) < \hat{f}_2(x) \qquad f_1(x) = f_2(x)$$

• Classify x according to

$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \hat{f}_k(x)$$

 $\hat{f}(x)$   $\hat{f}_1(x) > \hat{f}_2(x)$ 

• Minimizing EPE w.r.t. the 0-1 loss gives rise to

$$\widehat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \Pr(G = k | X = x)$$

• Our question:

Are the  $\hat{f}_k(x)$  reasonable estimates of the posterior  $\Pr(G = k | X = x)$ ?

ment

Linear classification:

$$\widehat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \widehat{f}_k(x)$$

Minimizing EPE:

$$\widehat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \Pr(G = k | X = x)$$

Two defining properties of probability

- 1.  $\sum P = 1$
- 2. 0 < P < 1
- It can be verified that  $\sum_{k \in \mathcal{G}} \hat{f}_k(x) = 1$
- However, it is possible that  $\hat{f}_k(x) < 0$  or  $\hat{f}_k(x) > 1$

Suppose that  $X \leftarrow (\mathbf{1}_N, X)$  and

$$\widehat{\mathbf{Y}} = \widehat{f}(\mathbf{X}) = \mathbf{X}\widehat{\mathbf{B}} = (\widehat{f}_1(\mathbf{X}), ..., \widehat{f}_K(\mathbf{X}))$$

We have the followings

$$\sum_{k=1}^{K} \hat{f}_{K}(\mathbf{X}) = \widehat{\mathbf{Y}} \cdot \mathbf{1}_{K}$$
 Indicator matrix
$$= \mathbf{X} \widehat{\mathbf{B}} \cdot \mathbf{1}_{K}$$

$$= \mathbf{X} (\mathbf{X}^{T} \mathbf{X})^{-1} \mathbf{X}^{T} \mathbf{Y} \cdot \mathbf{1}_{K}$$

$$= \mathbf{X} (\mathbf{X}^{T} \mathbf{X})^{-1} \mathbf{X}^{T} \cdot \mathbf{1}_{N}$$

$$= \mathbf{H} \cdot \mathbf{1}_{N}$$

 $\mathbf{H} \cdot \mathbf{1}_N$  is a projection of  $\mathbf{1}_N$  onto the column space of  $\mathbf{X}$ , thus  $\mathbf{H} \cdot \mathbf{1}_N = \mathbf{1}_{N-12}$ 

Linear classification:

$$\widehat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \widehat{f}_k(x)$$

Minimizing EPE:  

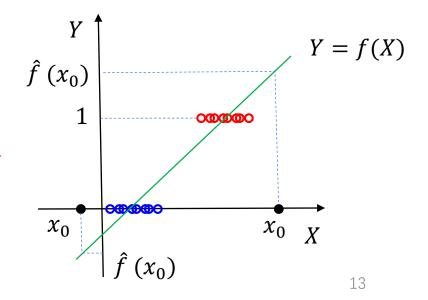
$$\widehat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \Pr(G = k | X = x)$$

Two defining properties of probability

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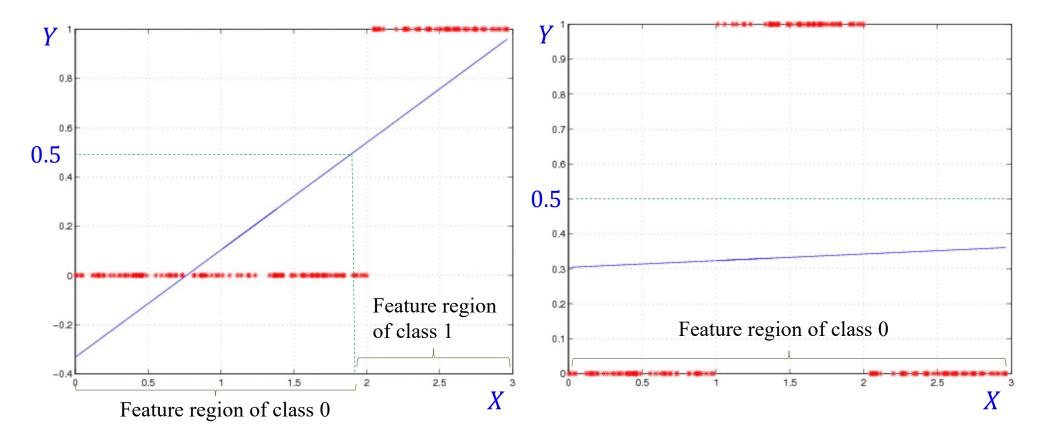
It possibly suffers from the problem of masking

a class may be masked by others, i.e., there is no region in the feature space that is labeled as this class



# The Phenomenon of Masking

- A class may be masked by others, i.e., there is no region in the feature space that is labeled as this class
- The linear regression model is too rigid



# The Phenomenon of Masking

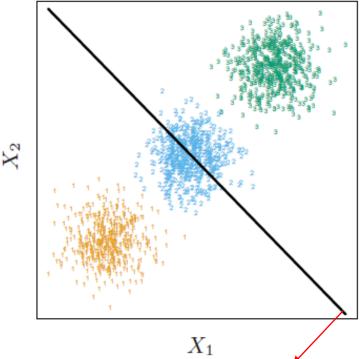
• 3-class classification

#### Linear Regression

Yellow: class 1

Blue: class 2

Green: class 3



Decision boundary between classes 2 and 3

Decision boundary

between classes 1 and 2

 $X_1$ 

Linear Discriminant Analysis ← Ideal result

The decision boundaries between 1 and 2 and between 2 and 3 are the same, so we would never predict class 2.

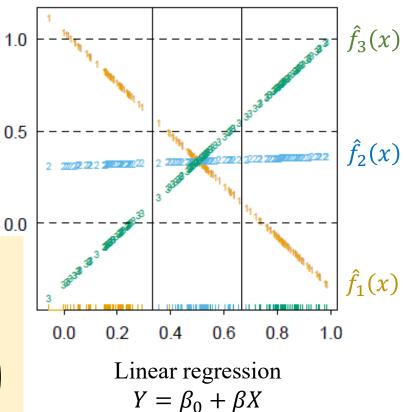
## The Phenomenon of Masking

3-class classification

The indicator matrix  $g = \begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix} \rightarrow \mathbf{Y} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ 

Yellow: class 1 Blue: class 2

Green: class 3



Degree = 1; Error = 0.33

Degree = 2; Error = 0.04 $\hat{f}_3(x)$ 1.0 0.5  $\hat{f}_1(x)$ 0.0  $\hat{f}_2(x)$ 0.2 0.4 0.6 1.0 0.0 0.8 Quadratic regression

 $\widehat{f}(x) = \widehat{\mathbf{B}}^T \begin{pmatrix} 1 \\ \chi \end{pmatrix} = \begin{pmatrix} \widehat{f}_1(x) \\ \widehat{f}_2(x) \end{pmatrix}$ 

 $\widehat{\mathbf{B}} = \underset{\mathbf{B}}{\operatorname{argmin}} \|\mathbf{Y} - \mathbf{X}\mathbf{B}\|_F^2$ ,

where  $\mathbf{X} = (\mathbf{1}_N, \mathbf{x})$ 

Quadratic regression 
$$Y = \beta_0 + \beta_1 X + \beta_2 X^2$$

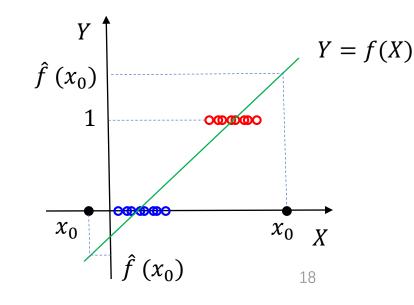
#### Linear Methods for Classification I

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• Recall our discussion on linear regression of an indicator matrix

Linear classification: Minimizing EPE: 
$$\widehat{G}(x) = \operatorname*{argmax}_{k \in \mathcal{G}} \widehat{f}_k(x)$$
 
$$\widehat{G}(x) = \operatorname*{argmax}_{k \in \mathcal{G}} \Pr(G = k | X = x)$$

- It is inappropriate to represent a posterior directly by a linear function.
- Solution: make some monotone transformation of the posterior be linear in *X*



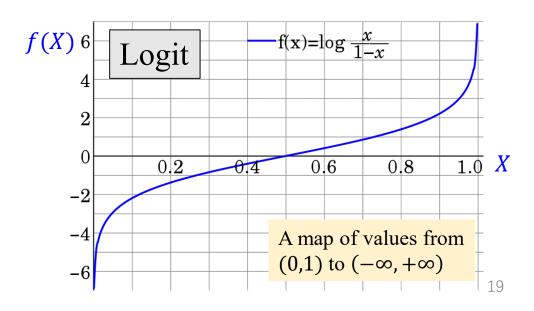
Linear decision boundary

• Logit transform

$$logit(Pr(x)) = log\left(\frac{Pr(x)}{1 - Pr(x)}\right)$$

It maps  $Pr(x) \in (0,1)$  to  $logit(Pr(x)) \in (-\infty, +\infty)$ 

- Decision boundary
  - Odds equals to 1
  - Or, logit equals to 0



Odds (发生比)

• Example: binary (two class) classification

Logit: 
$$\log \frac{\Pr(G=1|X=x)}{1-\Pr(G=1|X=x)} = \log \frac{\Pr(G=1|X=x)}{\Pr(G=2|X=x)} = \beta_0 + x^T \beta$$

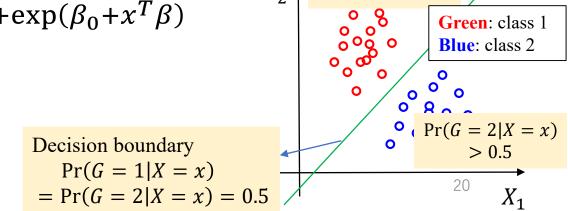
• The posterior probability

$$Pr(G = 1|X = x) = \frac{\exp(\beta_0 + x^T \beta)}{1 + \exp(\beta_0 + x^T \beta)}, \exp(x) = e^x$$

$$Pr(G = 2|X = x) = \frac{1}{1 + \exp(\beta_0 + x^T \beta)}, X_2 \uparrow \begin{cases} \Pr(G = 1|X = x) \\ > 0.5 \end{cases}$$

Decision boundary

$$\{x|\beta_0 + x^T\beta = 0\}$$



The Bayes theorem
$$Pr(A|B) = \frac{Pr(B|A) Pr(A)}{Pr(B)}$$

#### • Idea:

model the posterior Pr(G = k | X = x) based on the Bayes theorem

Posterior

$$\Pr(G = k | X = x) = \frac{\Pr(X = x | G = k) \Pr(G = k)}{\Pr(X = x)} = \frac{\Pr(X = x | G = k) \Pr(G = k)}{\sum_{\ell=1}^{K} \Pr(X = x | G = \ell) \Pr(G = \ell)}$$

 $\Box$  Density of *X* in class G = k:

$$f_k(x) = \Pr(X = x | G = k)$$

Class prior:

$$\pi_k = \Pr(G = k)$$

$$\Pr(G = k | X = x) = \frac{f_k(x)\pi_k}{\sum_{\ell=1}^{K} f_{\ell}(x)\pi_{\ell}}$$

• It produces LDA, QDA (quadratic DA), MDA (mixture DA), kernel DA and naïve Bayes, under various assumptions on  $f_k(x)$ 

$$\Pr(G = k | X = x) = \frac{f_k(x)\pi_k}{\sum_{\ell=1}^{K} f_{\ell}(x)\pi_{\ell}}$$

- Assumptions in LDA
  - 1. Model each class density as multivariate Gaussian

$$f_k(x) = \frac{1}{(2\pi)^{p/2} |\Sigma_k|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k)\right)$$

- 2. Assume that classes share a common covariance  $\Sigma_k = \Sigma$ ,  $\forall k$
- Compare two classes k and  $\ell$

#### Parameter estimation

 $\hat{\pi}_k = N_k/N$ , where  $N_k$  is the number of class-k observations;

$$\hat{\mu}_k = \sum_{g_i = k} x_i / N_k;$$

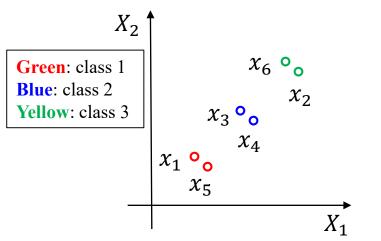
$$\hat{\Sigma} = \sum_{k=1}^{K} \sum_{g_i = k} (x_i - \hat{\mu}_k) (x_i - \hat{\mu}_k)^T / (N - K).$$

Pooled covariance (合并方差)

$$\widehat{\Sigma} = \frac{(N_1 - 1)\widehat{\Sigma}_1 + (N_2 - 1)\widehat{\Sigma}_2 + \dots + (N_K - 1)\widehat{\Sigma}_K}{(N_1 - 1) + (N_2 - 1) + \dots + (N_K - 1)}, \text{ where } \widehat{\Sigma}_k = \frac{\sum_{g_i = k} (x_i - \widehat{\mu}_k)(x_i - \widehat{\mu}_k)^T}{N_k - 1}$$

Weighted average

	Data		Class
	$X_1$	$X_2$	G
$x_1^T$	0.2	0.3	1
$x_2^T$	8.0	0.7	3
$x_3^T$	0.4	0.6	2
$x_4^T$	0.6	0.4	2
$x_5^T$	0.3	0.2	1
$x_6^T$	0.7	8.0	3



• Class prior 
$$\hat{\pi}_1 = \hat{\pi}_2 = \hat{\pi}_3 = \frac{1}{3}$$

Class-specific sample mean

$$\hat{\mu}_1 = \frac{1}{2}(x_1 + x_5) = \frac{1}{2} {0.2 \choose 0.3} + \frac{1}{2} {0.3 \choose 0.2} = {0.25 \choose 0.25}$$

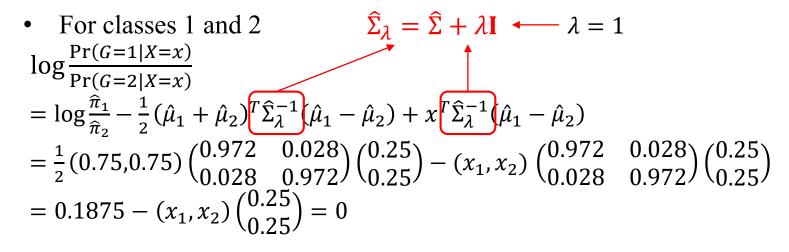
$$\hat{\mu}_2 = \frac{1}{2}(x_3 + x_4) = \frac{1}{2} {0.4 \choose 0.6} + \frac{1}{2} {0.6 \choose 0.4} = {0.5 \choose 0.5}$$

$$\hat{\mu}_3 = \frac{1}{2}(x_2 + x_6) = \frac{1}{2} {0.8 \choose 0.7} + \frac{1}{2} {0.75 \choose 0.8} = {0.75 \choose 0.75}$$

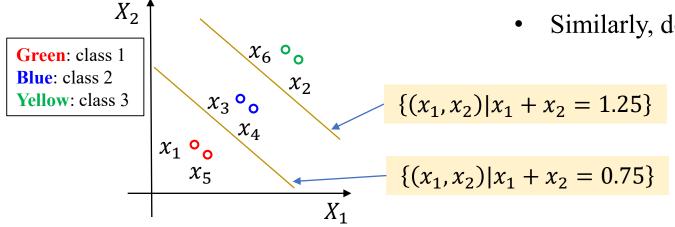
Common covariance

$$\widehat{\Sigma} = \frac{\sum_{k=1}^{K} \sum_{g_{i=k}} (x_i - \widehat{\mu}_i)(x_i - \widehat{\mu}_i)^T}{N - K} = \frac{\binom{0.005}{-0.005} - 0.005}{6 - 3} + \binom{0.005}{-0.005} + \binom{0.002}{-0.005} - 0.005}{0.005} = \binom{0.03}{-0.03} - 0.03$$

	Data		Class	
	$X_1$	$X_2$	G	
$x_1^T$	0.2	0.3	1	
$x_2^T$	8.0	0.7	3	
$x_3^T$	0.4	0.6	2	
$x_4^T$	0.6	0.4	2	
$x_5^T$	0.3	0.2	1	
$x_6^T$	0.7	0.8	3	



- Decision boundary 1-2:  $\{(x_1, x_2) | x_1 + x_2 = 0.75\}$ 
  - Similarly, decision boundary 2-3:  $\{(x_1, x_2) | x_1 + x_2 = 1.25\}$



• Suppose that 
$$\log \frac{\Pr(G=k|X=x)}{\Pr(G=\ell|X=x)} = \delta_k(x) - \delta_\ell(x)$$

- $\delta_k(x) > \delta_\ell(x)$ , class k
- $\delta_k(x) < \delta_\ell(x)$ , class  $\ell$
- $\delta_k(x) = \delta_\ell(x)$ , decision boundary
- Linear discriminant functions

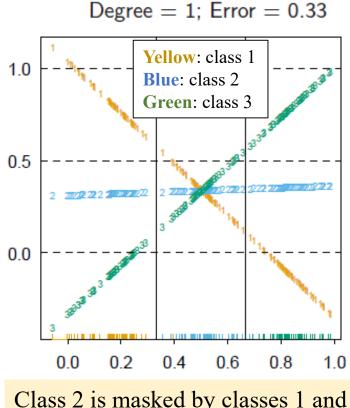
$$\delta_k(x) = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + \log \pi_k$$

Classify to class k that maximizes the discriminant function

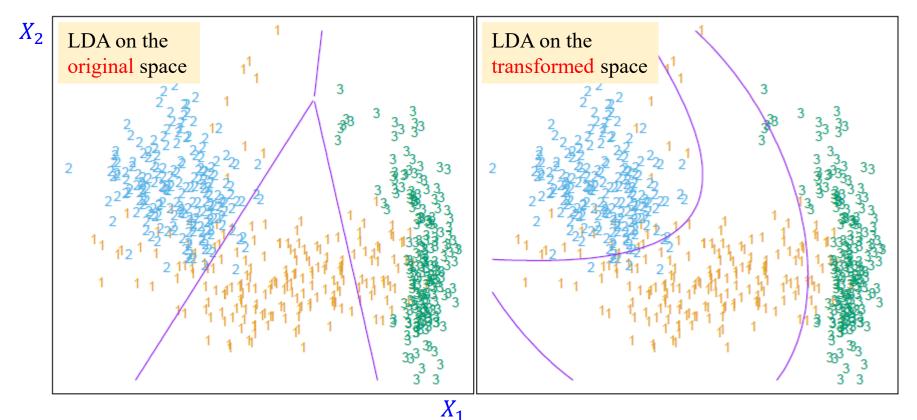
$$\widehat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \, \delta_k(x)$$
 Any difference? Linear classification: 
$$\widehat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \, \widehat{f}_k(x)$$

- Binary classification (K = 2)
  - Correspondence between LDA and linear classification

- Multi-class classification  $(K \ge 3)$ 
  - □ LDA is different with linear classification
  - Avoid the masking problem



Class 2 is masked by classes 1 and 3



**FIGURE 4.1.** The left plot shows some data from three classes, with linear decision boundaries found by linear discriminant analysis. The right plot shows quadratic decision boundaries. These were obtained by finding linear boundaries in the five-dimensional space  $X_1, X_2, X_1X_2, X_1^2, X_2^2$ . Linear inequalities in this space are quadratic inequalities in the original space.

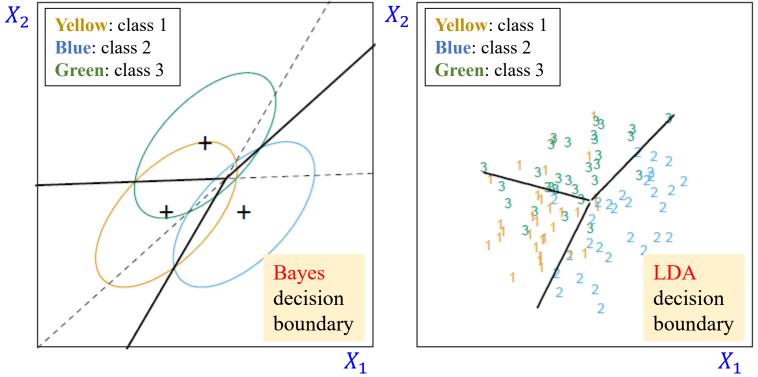


FIGURE 4.5. The left panel shows three Gaussian distributions, with the same covariance and different means. Included are the contours of constant density enclosing 95% of the probability in each case. The Bayes decision boundaries between each pair of classes are shown (broken straight lines), and the Bayes decision boundaries separating all three classes are the thicker solid lines (a subset of the former). On the right we see a sample of 30 drawn from each Gaussian distribution, and the fitted LDA decision boundaries.

# **Quadratic Discriminant Analysis**

#### Assumptions in LDA

1. Model each class density as multivariate Gaussian

$$f_k(x) = \frac{1}{(2\pi)^{p/2} |\Sigma_k|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k)\right)$$

- 2. Assume that classes share a common covariance  $\Sigma_k = \Sigma, \forall k$
- Assumption: Each class has a specific covariance  $\Sigma_k$
- Quadratic discriminant functions

$$\delta_k(x) = -\frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k) + \log \pi_k.$$

• The quadratic decision boundary between two classes k and  $\ell$ 

$$\{x: \delta_k(x) = \delta_\ell(x)\}\$$

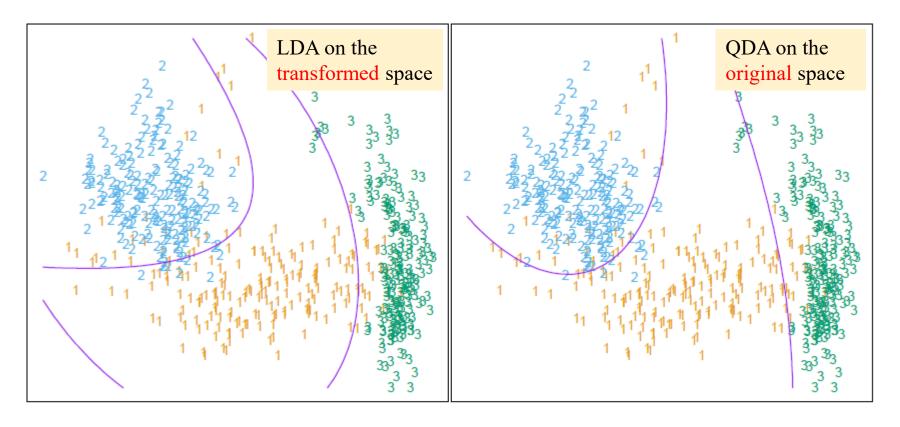
• Difference with LDA

$$\mu_k$$
,  $k = 1, ..., K$ 

- Difference with LDA  $\mu_k, k = 1, ..., K$   $\Sigma_k$  has to be estimated for each class

  LDA need to estimate  $K \times p + p \times p$  parameters  $\Sigma_k, k = 1, ..., K$ QDA need to estimate  $K \times p + p \times p$  parameters

# Quadratic Discriminant Analysis



**FIGURE 4.6.** Two methods for fitting quadratic boundaries. The left plot shows the quadratic decision boundaries for the data in Figure 4.1 (obtained using LDA in the five-dimensional space  $X_1, X_2, X_1X_2, X_1^2, X_2^2$ ). The right plot shows the quadratic decision boundaries found by QDA. The differences are small, as is usually the case.

# Summary

- Linear regression of an indicator matrix
  - The indicator matrix
  - Prediction is conducted by  $\hat{G}(x) = \operatorname{argmax}_k \hat{f}_k(x)$
  - Suffer from the masking problem
- Linear discriminant analysis
  - Logit transformation:  $logit(Pr(x)) = log(\frac{Pr(x)}{1-Pr(x)})$
  - $\square$  Model the posterior Pr(G = k | X = x)
  - □ Assumptions on Pr(X = x | G = k)
  - $_{\circ}$  Discriminant functions  $\delta_k(x)$
- Quadratic discriminant analysis
  - Difference with LDA

#### Classification



Linear regression

$$\mathcal{G} = \{1, 2 \dots, K\}$$

Indicator matrix 
$$\mathbf{Y} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

#### Multi-output regression

Prediction
$$\hat{f}(x) = \hat{\mathbf{B}}^T \begin{pmatrix} 1 \\ x \end{pmatrix} = \begin{pmatrix} \hat{f}_1(x) \\ \hat{f}_2(x) \\ \vdots \\ \hat{f}_K(x) \end{pmatrix}$$

$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \hat{f}_k(x)$$

#### Limitation

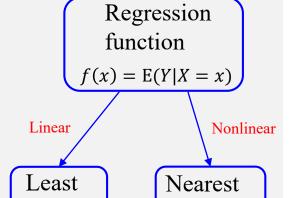
The masking problem  $(K \ge 3)$ 



neighbors

**Theoretical** 

#### Squared error loss



#### Regression

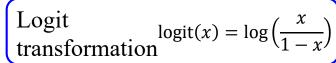
squares

#### Bayes classifier

Zero-one loss

$$\widehat{G}(x) = \underset{k \in \mathcal{G}}{\operatorname{argmax}} \Pr(G = k | X = x)$$

$$(0,1) \rightarrow (-\infty, +\infty)$$



Pairwise odds = 1

Decision boundary 
$$\log \frac{\Pr(G = k|X = x)}{\Pr(G = \ell|X = x)} = 0$$

Bayes theorem

LDA, QDA, RDA Linear boundary

Logistic regression