

Introduction to Machine Learning CS182

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Today:

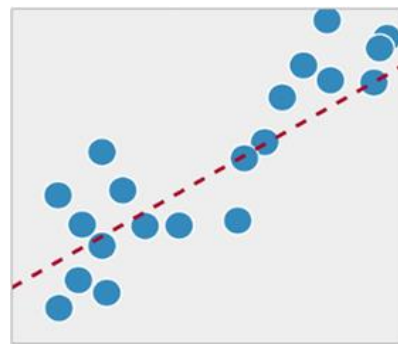
- Linear Methods for Classification I
 - Introduction
 - Linear regression of an indicator matrix
 - Linear discriminant analysis

Readings:

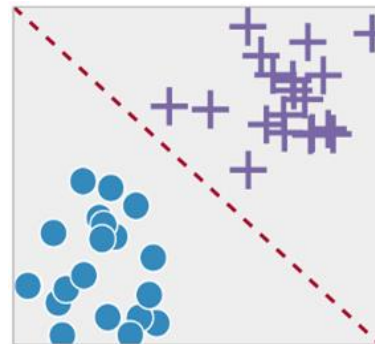
- The Elements of Statistical Learning (ESL), Chapters 4.1, 4.2 and 4.3

Linear Methods for Classification I

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



Regression



Classification

Introduction

Example

Handwritten digits recognition

Input variables

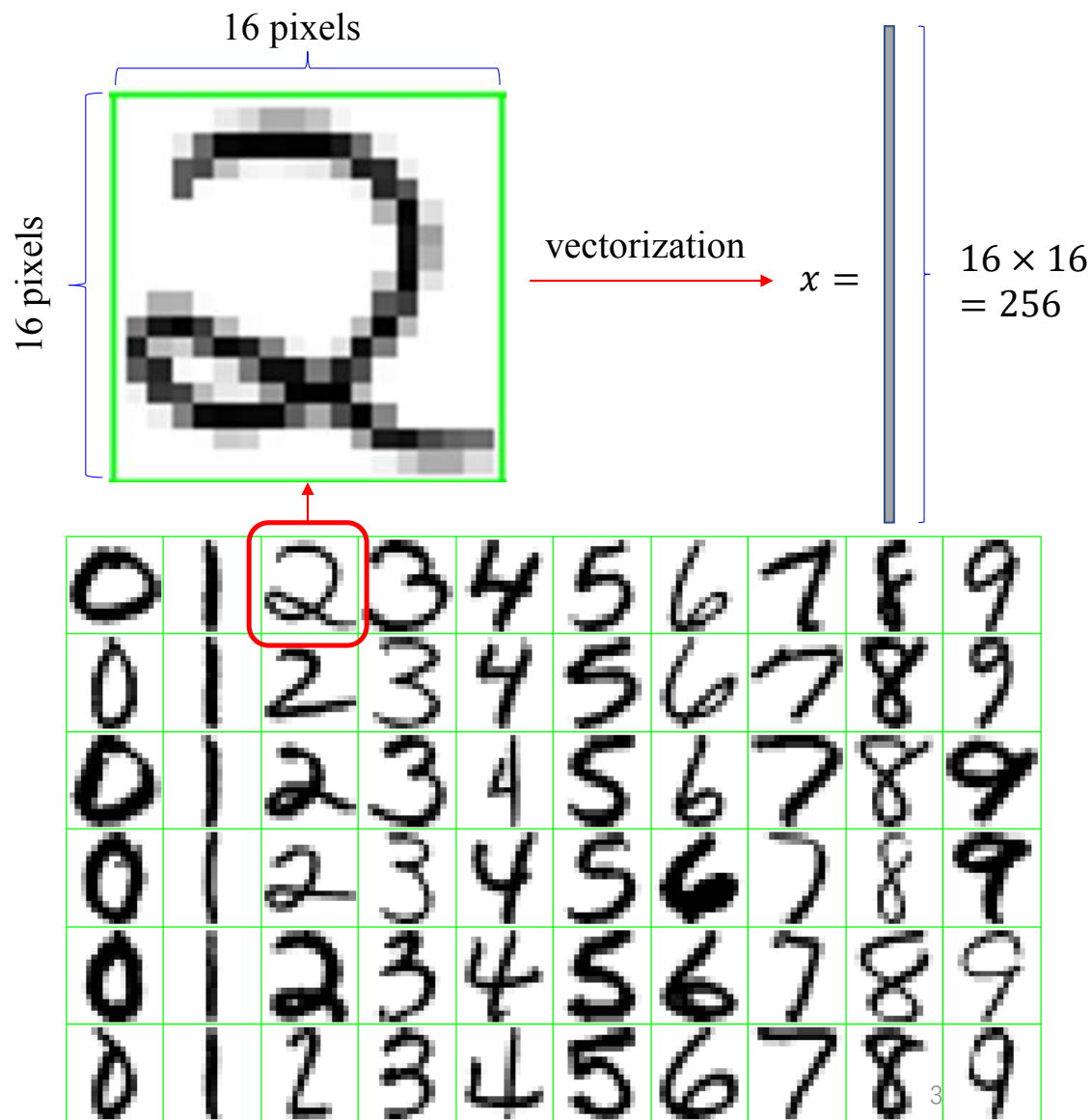
$$X = (X_0, X_1, X_2, \dots, X_{256})^T$$

Categorical output variable G with values from

$$G = \{0, 1, 2, \dots, 9\}$$

Handwritten digits

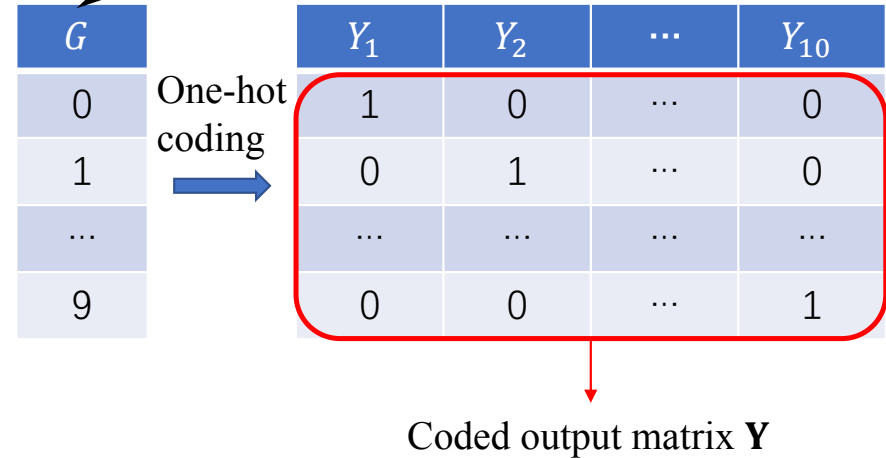
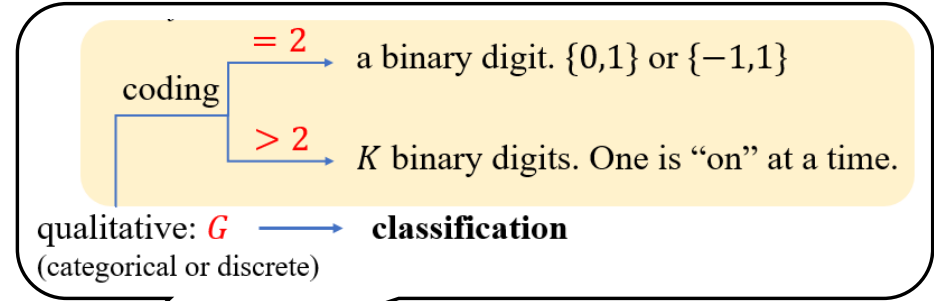
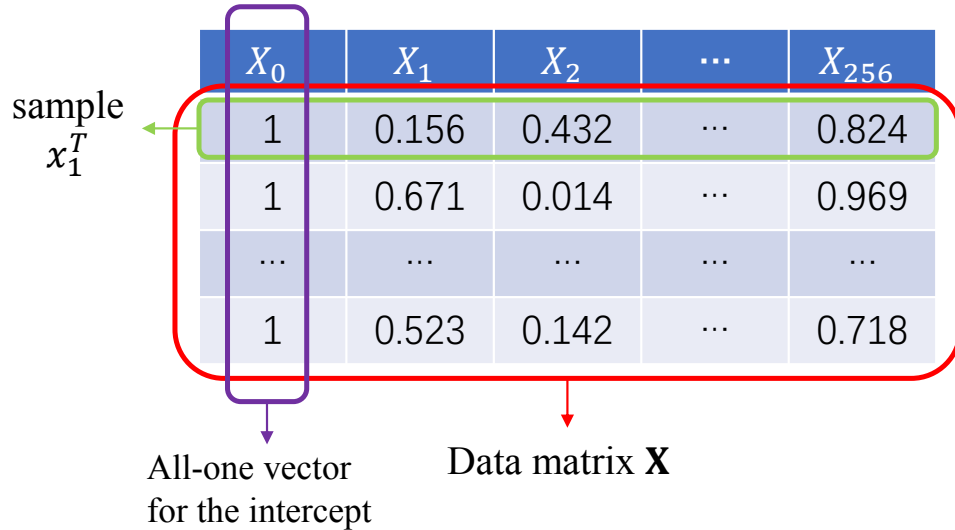
Non-binary (multi-class) classification



Introduction

Example

Handwritten digits recognition



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

1. Any problems?
2. Other methods?

Introduction

Binary classification

- Linear regression

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

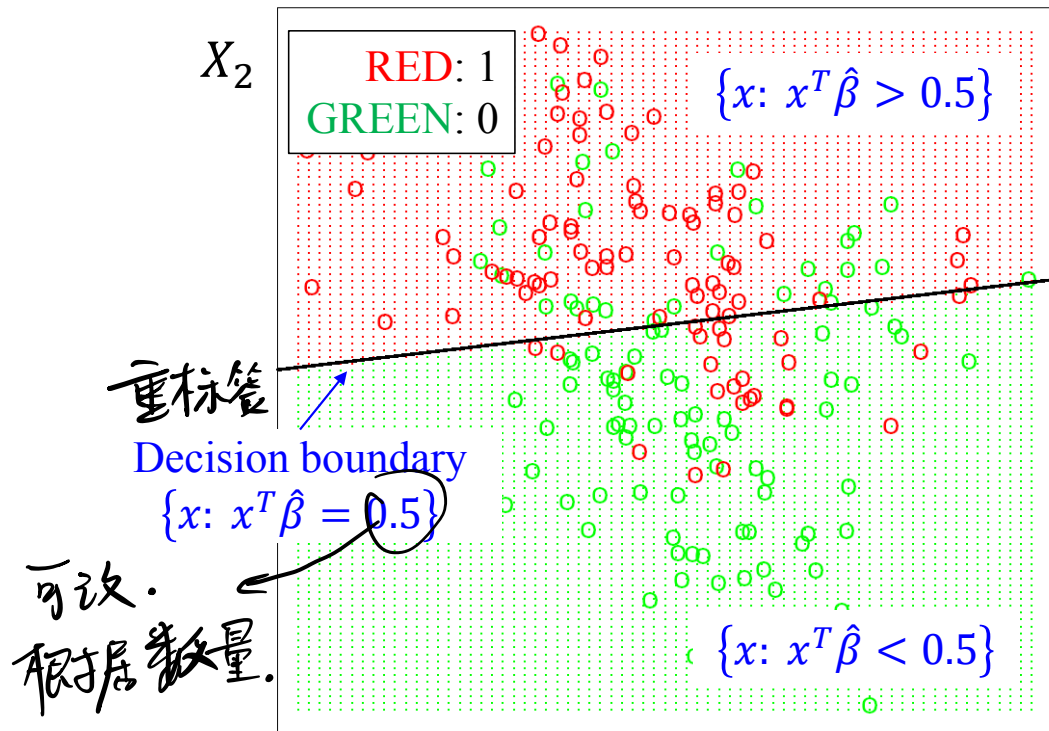
- Least squares solution

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

- Decision boundary

$$\{x : x^T \hat{\beta} = \text{threshold}\}$$

- \square $\text{threshold} = 0$, if $y \in \{-1, 1\}$
- \square $\text{threshold} = 0.5$, if $y \in \{0, 1\}$



Introduction

Multi-class classification

- Linear regressions for K classes

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

- Decision boundary** between classes k and ℓ :

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

有很多种情况 (n^2 级)

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

- That is an **affine set** or **hyperplane**:

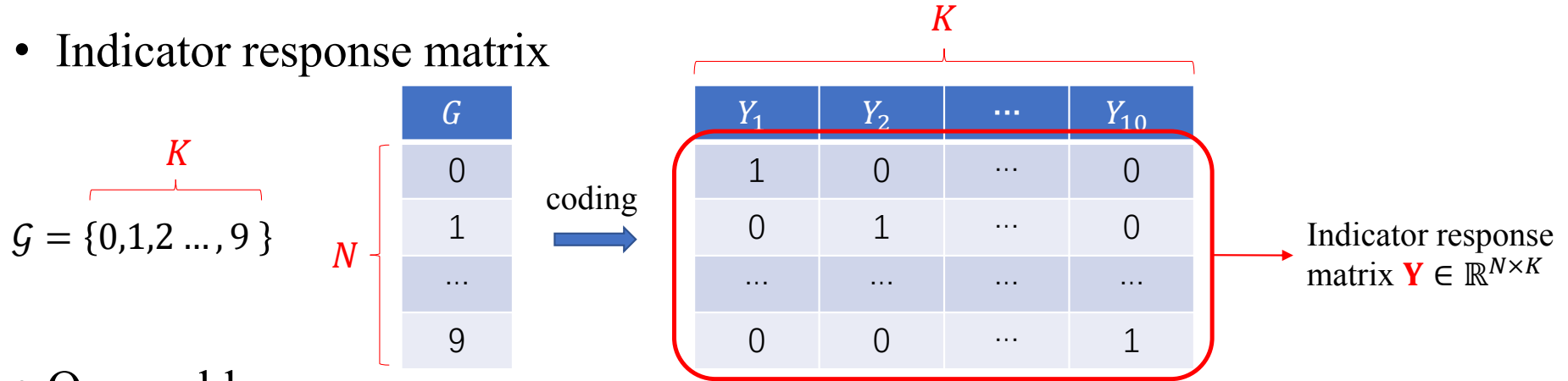
$$\{x: (\hat{\beta}_{k0} - \hat{\beta}_{\ell0}) + x^T (\hat{\beta}_k - \hat{\beta}_\ell) = 0\}$$

Linear Methods for Classification I

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

Linear Regression of an Indicator Matrix

- Indicator response matrix



- Our problem:

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

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

- The fitted values on \mathbf{X} :

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

Linear Regression of an Indicator Matrix

A new observation x is classified by

- Compute the fitted output

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

向量 \Rightarrow 对每个类别输出
 \Rightarrow 找最大值对应的类别

- Classify x according to

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

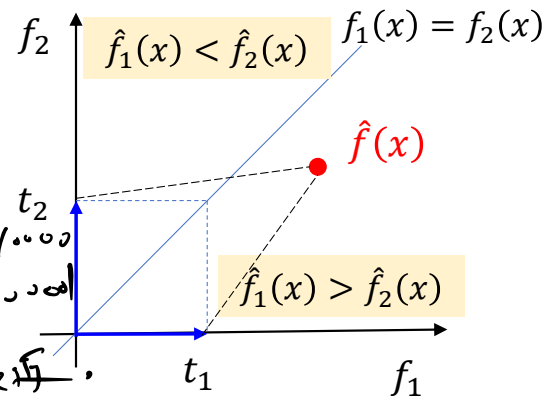
定义编码为 $\begin{cases} t_1 = 1, \dots, 0 \\ \vdots \\ t_k = 0, \dots, 1 \end{cases}$

- Or equivalently,

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

找最近

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



Linear Regression of an Indicator Matrix

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

- 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. $\Pr(G, X)$

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

- Pointwise** minimization leads to

$$\begin{aligned} \hat{G}(x) &= \operatorname{argmin}_{k \in \mathcal{G}} \sum_{\ell=1}^K L(k, \ell) \Pr(G = \ell | X = x) \\ &= \operatorname{argmax}_{k \in \mathcal{G}} \boxed{\Pr(G = k | X = x)} \leftarrow \text{posterior} \end{aligned}$$

Linear Regression of an Indicator Matrix

A new observation x is classified by

- Compute the fitted output

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

- Classify x according to

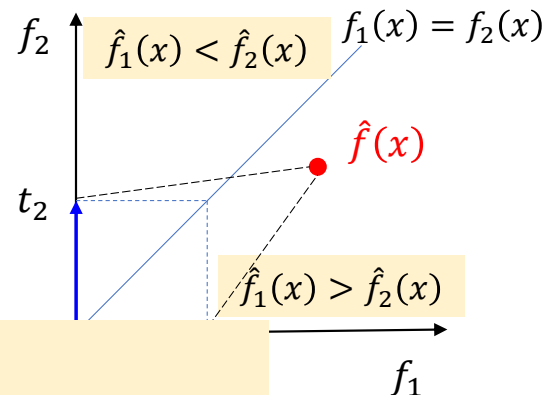
$$\hat{G}(x) = \operatorname{argmax}_{k \in \mathcal{G}} \hat{f}_k(x)$$

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

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

- Our question:

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



ment

Linear Regression of an Indicator Matrix

?

Linear classification:

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

Minimizing EPE:

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

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 $\hat{f}_k(x) > 1$

可取负或+1

$\operatorname{span}(\operatorname{col}(\mathbf{X}))$

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

$$\hat{\mathbf{Y}} = \hat{\mathbf{f}}(\mathbf{X}) = \mathbf{X}\hat{\mathbf{B}} = (\hat{f}_1(\mathbf{X}), \dots, \hat{f}_K(\mathbf{X}))$$

We have the followings \rightarrow 维度为1的列向量

$$\begin{aligned} \sum_{k=1}^K \hat{f}_k(\mathbf{X}) &= \hat{\mathbf{Y}} \cdot \mathbf{1}_K \\ &= \mathbf{X}\hat{\mathbf{B}} \cdot \mathbf{1}_K \\ &= \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y} \cdot \mathbf{1}_K \\ &= \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \cdot \mathbf{1}_N \\ &= \mathbf{H} \cdot \mathbf{1}_N \end{aligned}$$

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

Linear Regression of an Indicator Matrix

?

Linear classification:

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

Minimizing EPE:

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

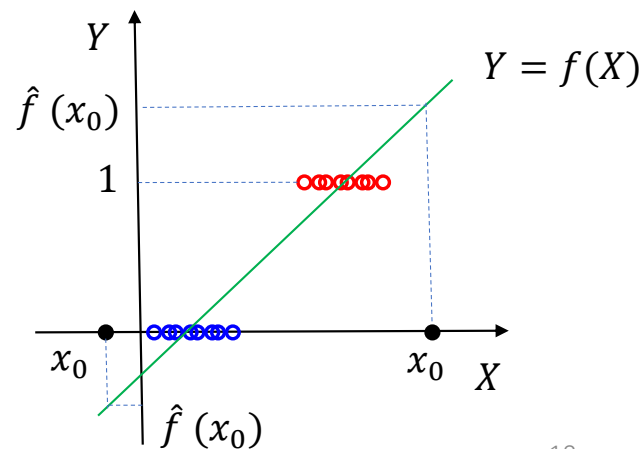
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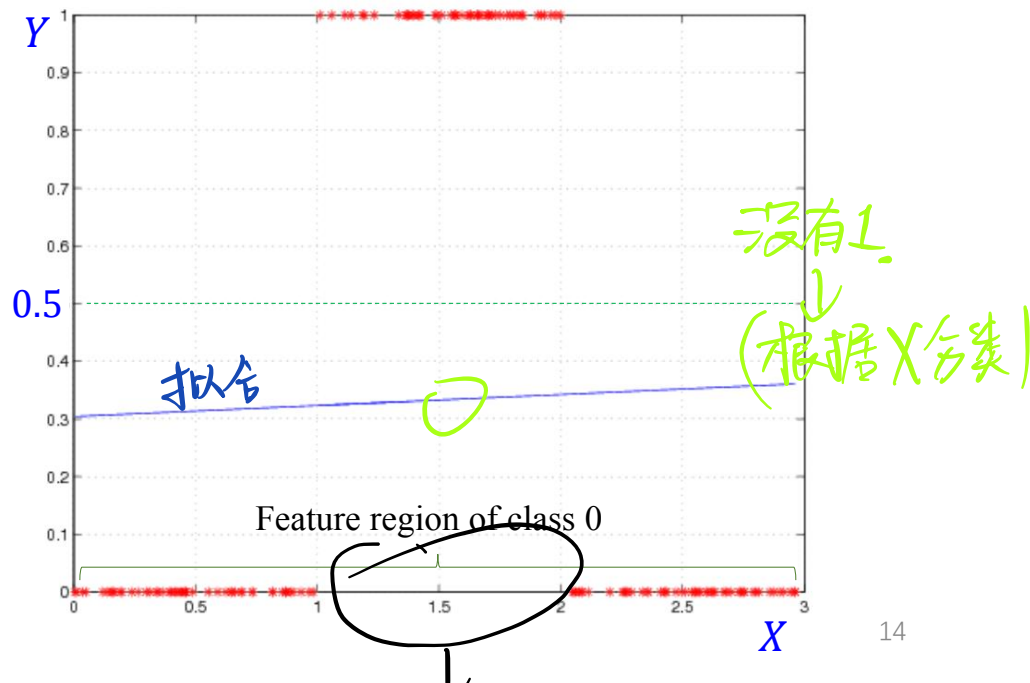
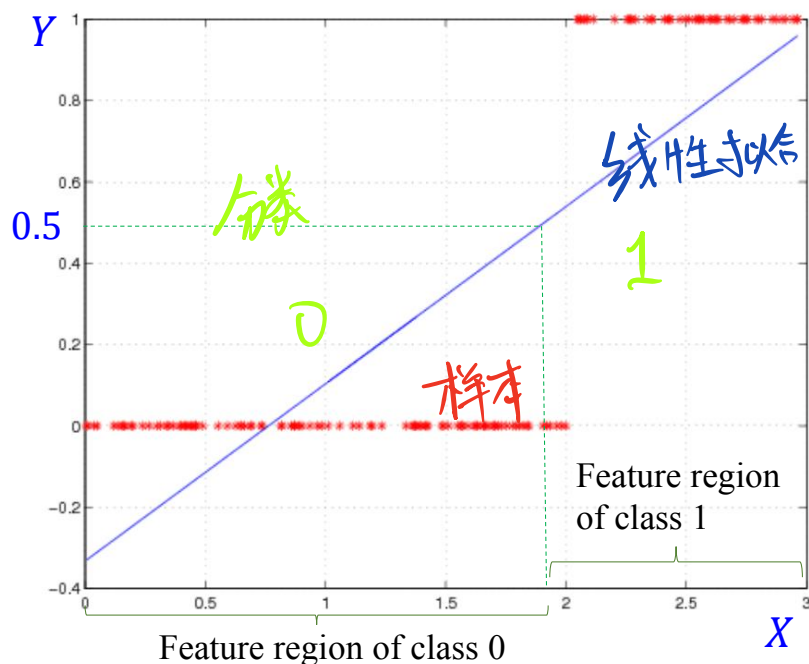
It possibly suffers from **the problem of masking**

- 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**



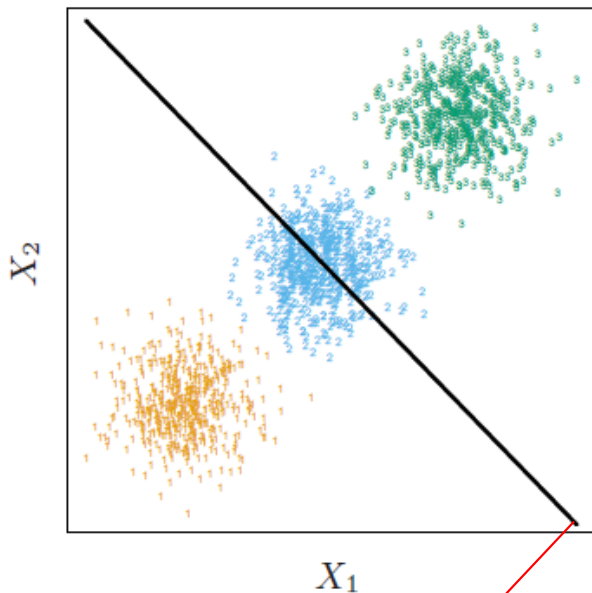
The Phenomenon of Masking

这里会被遮住。
变成全为0的集合。

- 3-class classification

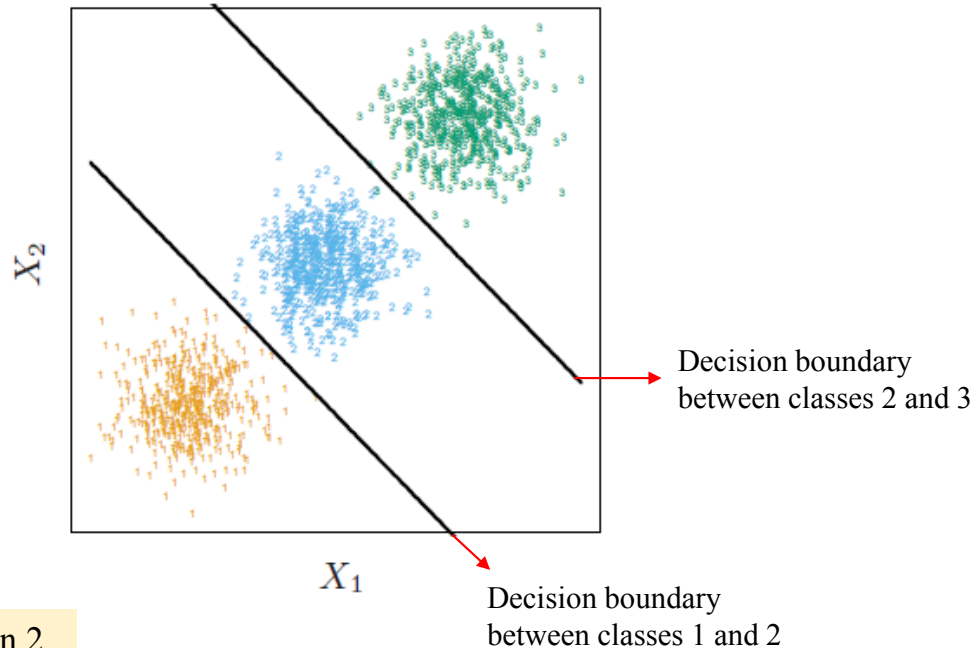
Linear Regression

Yellow: class 1
Blue: class 2
Green: class 3



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

Linear Discriminant Analysis ← Ideal result



The Phenomenon of Masking

- 3-class classification \rightarrow 我哪个值大就是哪一类 \Rightarrow 不会有蓝色类.

The indicator matrix

$$g = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \rightarrow \mathbf{Y} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

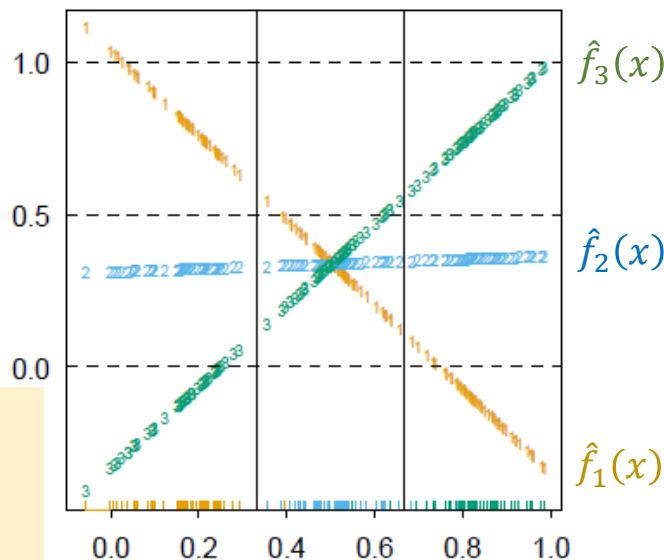
Yellow: class 1
Blue: class 2
Green: class 3

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

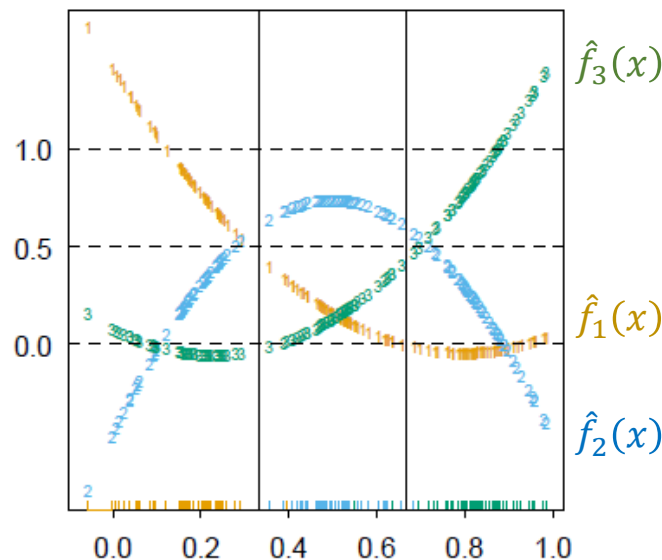
where $\mathbf{X} = (\mathbf{1}_N, \mathbf{x})$

$$\hat{f}(x) = \hat{\mathbf{B}}^T \begin{pmatrix} 1 \\ x \end{pmatrix} = \begin{pmatrix} \hat{f}_1(x) \\ \hat{f}_2(x) \\ \hat{f}_3(x) \end{pmatrix}$$

Degree = 1; Error = 0.33



Degree = 2; Error = 0.04



\Rightarrow 拓展到非线性空间

Linear Methods for Classification I

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

Linear Discriminant Analysis

- Recall our discussion on linear regression of an indicator matrix

×

Linear classification:

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

Minimizing EPE:

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

- It is inappropriate to represent a posterior directly by a linear function.

Linear Discriminant Analysis

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

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

↑ 用 gaussian 模型

↪ 常数, 可约

□ Density of X in class $G = k$:

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

□ Class prior:

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

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

伯努利 Bernoulli: $\pi^x(1-\pi)^{1-x}$

类别 Categorical: $\prod_{k=1}^K \pi_k^{\mathbb{I}_{x=k}}$

$$\mathbb{I}_{x=k} = \begin{cases} 1 & x=k \\ 0 & x \neq k \end{cases}$$

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

朴素贝叶斯

$$\{x | \Pr(G=k|X=x) = \Pr(G=l|X=x)\} \Rightarrow \Pr(k|x) = \Pr(l|x) \Leftrightarrow \Pr(x|k)\Pr(k) = \Pr(x|l)\Pr(l)$$

贝叶斯

$\Leftrightarrow \ln \frac{P(x|k)P(k)}{P(x|l)P(l)} = 0 \Leftrightarrow \text{LDA: } \beta^T X + \beta_0 = 0$

Linear Discriminant Analysis

$p \in (0, 1) \rightarrow \text{LDA} \in (-10, +10)$

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

Assumptions in LDA

1. Model each class density as **multivariate Gaussian**

高维 Gaussian

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

→ 多维向量

2. Assume that classes share a **common covariance** $\Sigma_k = \Sigma, \forall k$

- Compare two classes **k** and **l**

假设: 任意 k, Σ_k 相互相等.

Logit:

$$\log \frac{\Pr(G = k | X = x)}{\Pr(G = \ell | X = x)} = \log \frac{f_k(x)}{f_{\ell}(x)} + \log \frac{\pi_k}{\pi_{\ell}}$$

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

→ 代入 $f_k(x)$

Quadratic term **vanished** due to the common covariance

只有一个, 是关于 x 的线性

Decision boundary is **linear** w.r.t. X

原有二次项, 但因为为有假设故去掉

Linear Discriminant Analysis

- 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)

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

Weighted average

不是 N_k , 保证
无偏估计.

Linear Discriminant Analysis

	Data		Class
	X_1	X_2	G
x_1^T	0.2	0.3	1
x_2^T	0.8	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

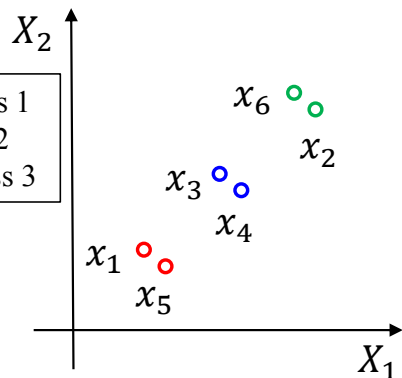
- Class **prior**
 $\hat{\pi}_1 = \hat{\pi}_2 = \hat{\pi}_3 = \frac{1}{3} = \frac{N_k}{N}$

- Class-specific **sample mean** ↗ = 多维空间
⇒ = 多维向量
 $\hat{\mu}_1 = \frac{1}{2}(x_1 + x_5) = \frac{1}{2} \begin{pmatrix} 0.2 \\ 0.3 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 0.3 \\ 0.2 \end{pmatrix} = \begin{pmatrix} 0.25 \\ 0.25 \end{pmatrix}$
 $\hat{\mu}_2 = \frac{1}{2}(x_3 + x_4) = \frac{1}{2} \begin{pmatrix} 0.4 \\ 0.6 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 0.6 \\ 0.4 \end{pmatrix} = \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix}$
 $\hat{\mu}_3 = \frac{1}{2}(x_2 + x_6) = \frac{1}{2} \begin{pmatrix} 0.8 \\ 0.7 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 0.7 \\ 0.8 \end{pmatrix} = \begin{pmatrix} 0.75 \\ 0.75 \end{pmatrix}$

- Common **covariance**

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

$$\frac{\begin{pmatrix} 0.005 & -0.005 \\ -0.005 & 0.005 \end{pmatrix} + \begin{pmatrix} 0.02 & -0.02 \\ -0.02 & 0.02 \end{pmatrix} + \begin{pmatrix} 0.005 & -0.005 \\ -0.005 & 0.005 \end{pmatrix}}{6-3} = \begin{pmatrix} 0.03 & -0.03 \\ -0.03 & 0.03 \end{pmatrix}$$



Linear Discriminant Analysis

	Data		Class
	X_1	X_2	G
x_1^T	0.2	0.3	1
x_2^T	0.8	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

- For classes 1 and 2

$$\log \frac{\Pr(G=1|X=x)}{\Pr(G=2|X=x)}$$

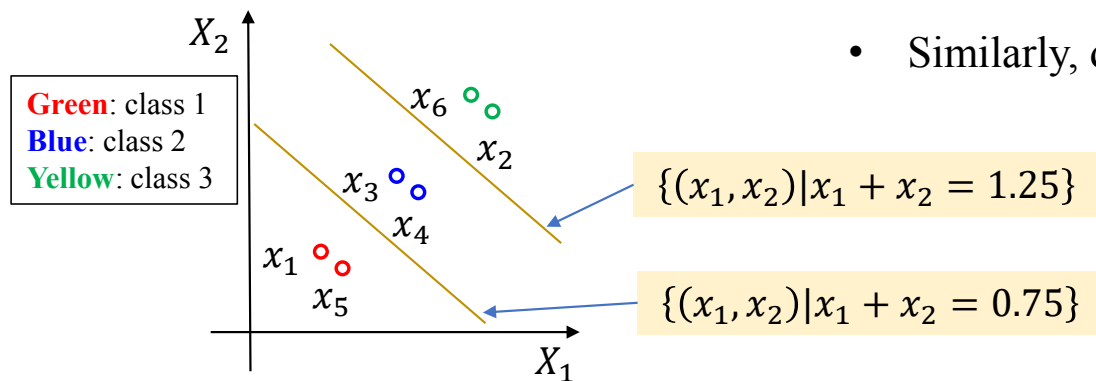
$$= \log \frac{\hat{\pi}_1}{\hat{\pi}_2} - \frac{1}{2}(\hat{\mu}_1 + \hat{\mu}_2)^T \hat{\Sigma}_\lambda^{-1}(\hat{\mu}_1 - \hat{\mu}_2) + x^T \hat{\Sigma}_\lambda^{-1}(\hat{\mu}_1 - \hat{\mu}_2)$$

$$= \frac{1}{2}(0.75, 0.75) \begin{pmatrix} 0.972 & 0.028 \\ 0.028 & 0.972 \end{pmatrix} \begin{pmatrix} 0.25 \\ 0.25 \end{pmatrix} - (x_1, x_2) \begin{pmatrix} 0.972 & 0.028 \\ 0.028 & 0.972 \end{pmatrix} \begin{pmatrix} 0.25 \\ 0.25 \end{pmatrix}$$

$$= 0.1875 - (x_1, x_2) \begin{pmatrix} 0.25 \\ 0.25 \end{pmatrix} = 0$$

$$\hat{\Sigma}_\lambda = \hat{\Sigma} + \lambda \mathbf{I} \leftarrow \lambda = 1$$

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



Linear Discriminant Analysis

• 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 ℓ
- $\delta_k(x) = \delta_\ell(x)$, decision boundary

线性判别函数：算每个类别的 δ_k 看哪个最大。

• Linear discriminant functions

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

Classify to class k that **maximizes** the discriminant function

$$\hat{G}(x) = \operatorname{argmax}_{k \in \mathcal{G}} \delta_k(x)$$

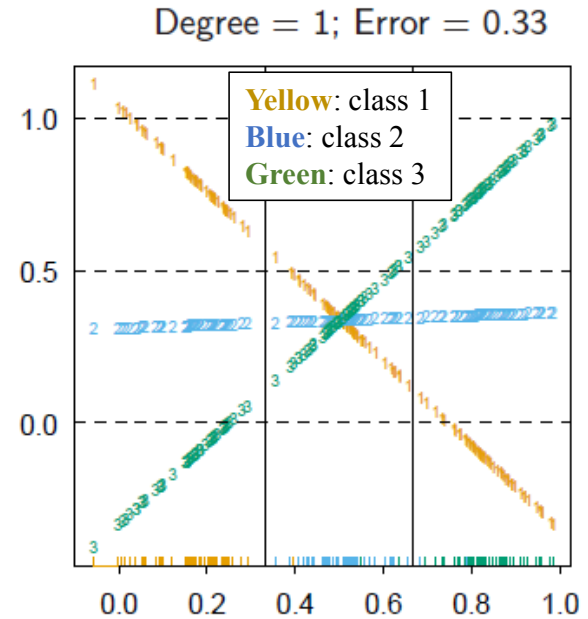
Any difference?

Linear classification:

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

Linear Discriminant Analysis

- **Binary** classification ($K = 2$)
 - Correspondence between LDA and linear classification
- **Multi-class** classification ($K \geq 3$)
 - LDA is different with linear classification
 - Avoid the masking problem



Class 2 is masked by classes 1 and 3²⁵

Linear Discriminant Analysis

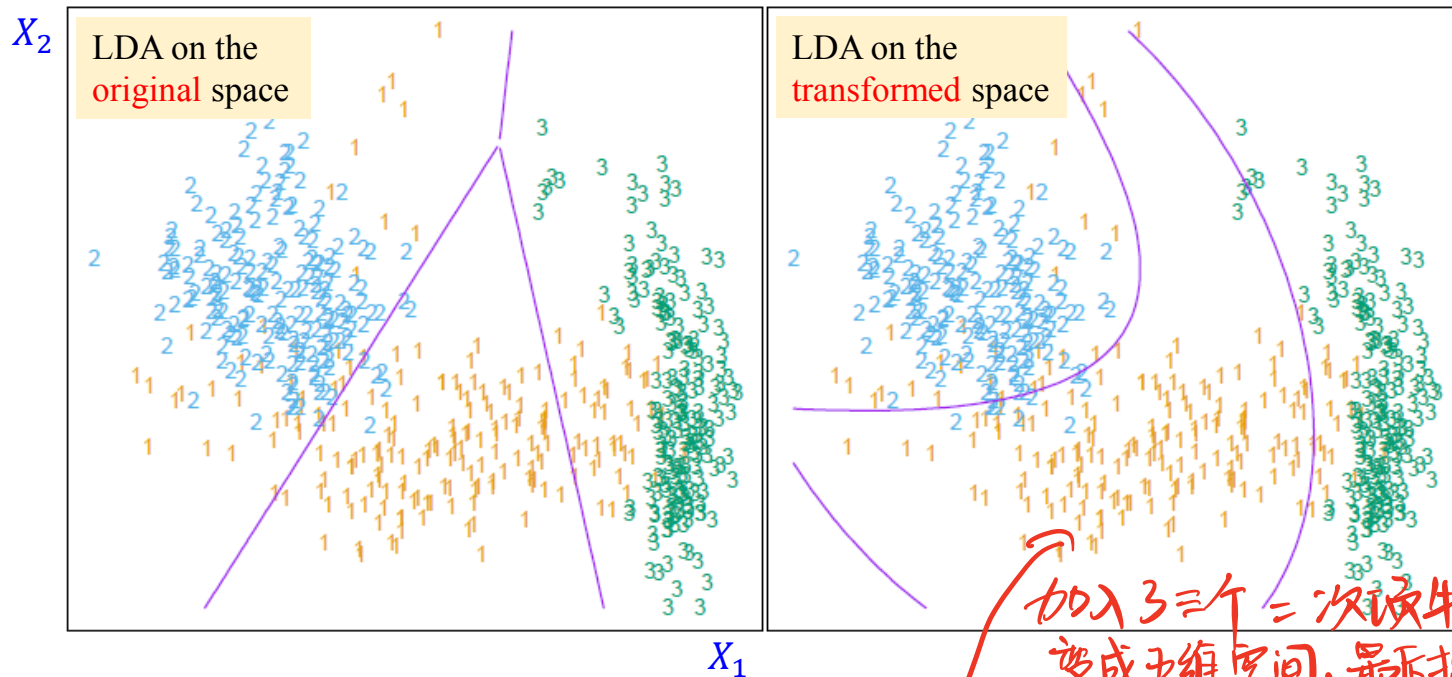


FIGURE 4.1. The left plot shows some data from three classes, with linear decision boundaries found by linear discriminant analysis. The right plot shows quadratic decision boundaries. These were obtained by finding linear boundaries in the five-dimensional space $X_1, X_2, X_1X_2, X_1^2, X_2^2$. Linear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

取哪些二次项是一个超参数。

Linear Discriminant Analysis

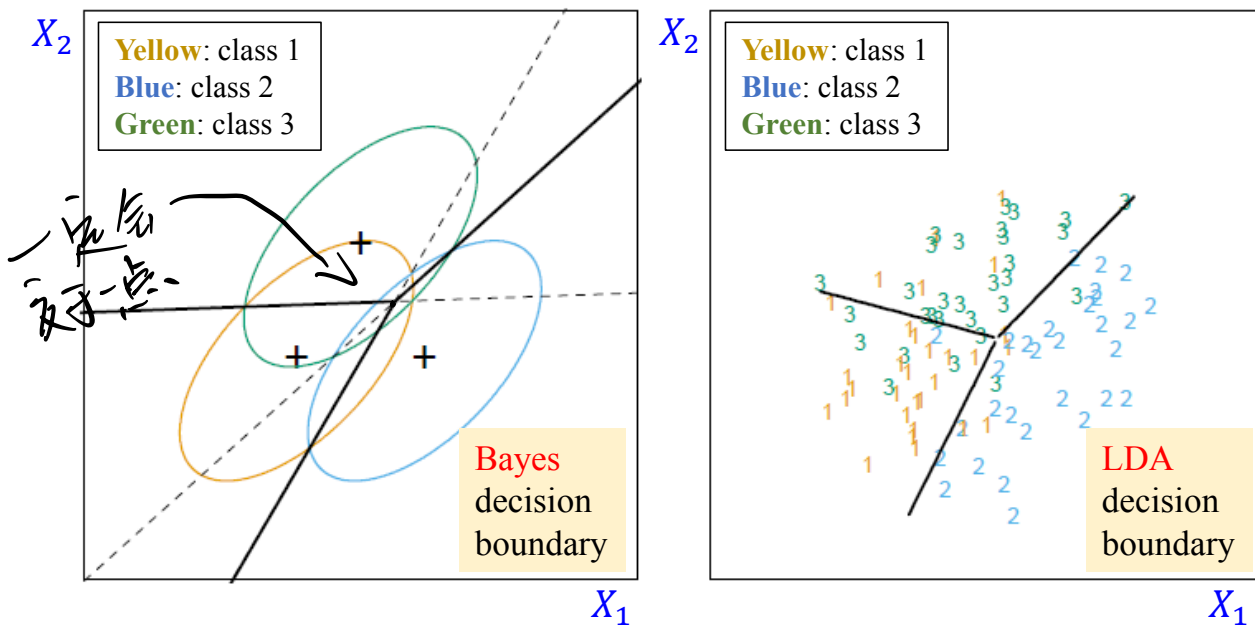


FIGURE 4.5. The left panel shows three Gaussian distributions, with the same covariance and different means. Included are the contours of constant density enclosing 95% of the probability in each case. The Bayes decision boundaries between each pair of classes are shown (broken straight lines), and the 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.

→ 特征表达更好但需要计算的更多。(相对LDA)

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

Difference with LDA

- Σ_k has to be estimated for each class
- LDA need to estimate $K \times p + p \times p$ parameters
- QDA need to estimate $K \times p + K \times p \times p$ parameters

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

Σ

$\Sigma_k, k = 1, \dots, K$

只估计 π, μ, Σ

需要 K 个 Σ

Quadratic Discriminant Analysis

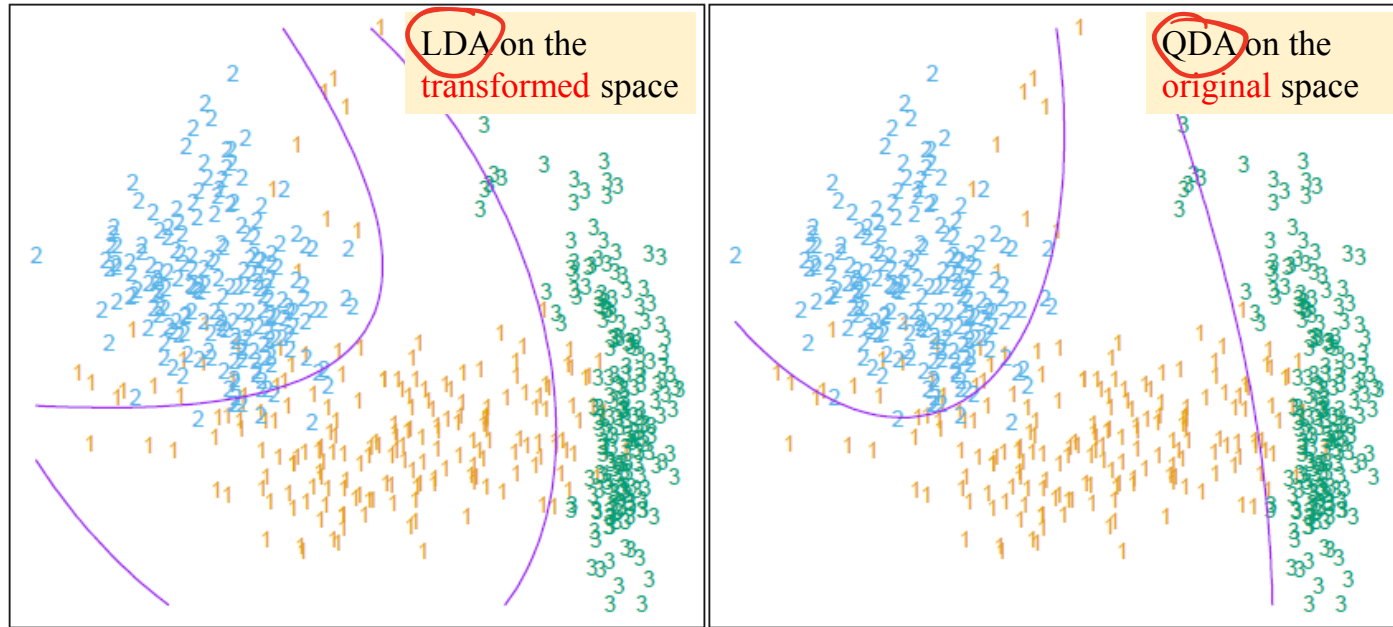


FIGURE 4.6. Two methods for fitting quadratic boundaries. The left plot shows the quadratic decision boundaries for the data in Figure 4.1 (obtained using LDA in the five-dimensional space $X_1, X_2, X_1X_2, X_1^2, X_2^2$). The right plot shows the quadratic decision boundaries found by QDA. The differences 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: $\operatorname{logit}(\operatorname{Pr}(x)) = \log\left(\frac{\operatorname{Pr}(x)}{1-\operatorname{Pr}(x)}\right)$
 - Model the posterior $\operatorname{Pr}(G = k|X = x)$
 - Assumptions on $\operatorname{Pr}(X = x|G = k)$
 - Discriminant functions $\delta_k(x)$
- Quadratic discriminant analysis
 - Difference with LDA

Classification

