

Optimization and Machine Learning SI151

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Today:

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

Readings:

- The Element of Statistical Learning, Chapters 4.1, 4.2 and 4.3

Linear Methods for Classification I

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

Introduction

Example

Handwritten digits recognition

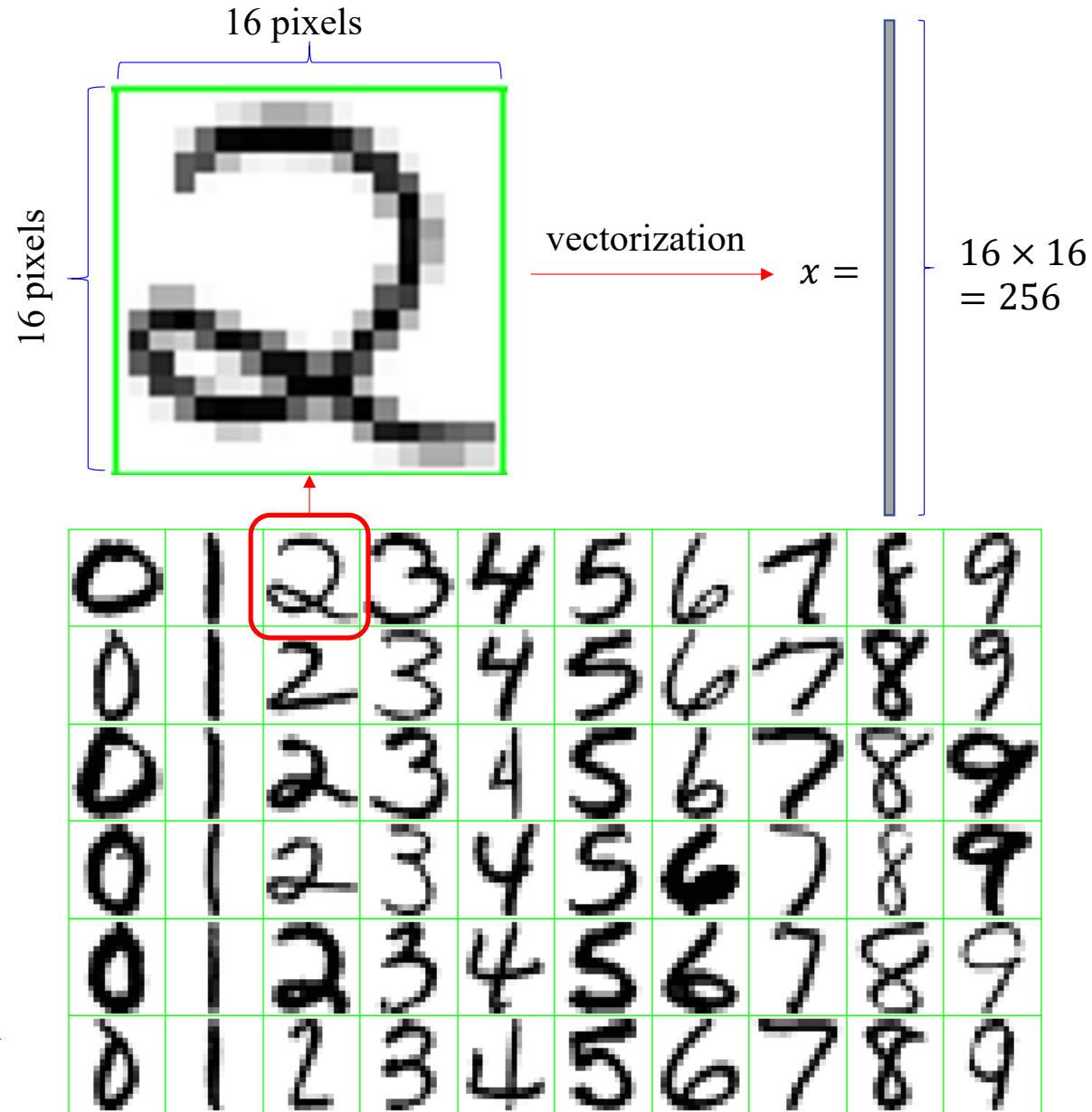
Input variables

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

Categorical output variable G with values from

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

Non-binary (multi-class) classification



Introduction

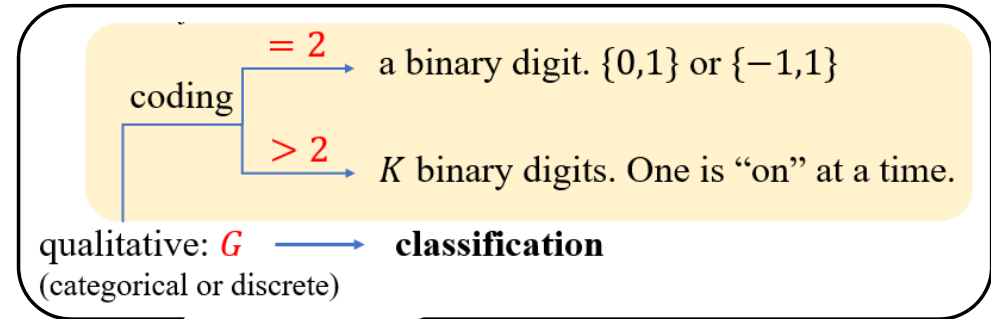
Example

Handwritten digits recognition

sample x_1^T →

X_0	X_1	X_2	...	X_{256}
1	0.156	0.432	...	0.824
1	0.671	0.014	...	0.969
...
1	0.523	0.142	...	0.718

↓ All-one vector for the intercept ↓ Data matrix \mathbf{X}



G				
0				
1				
...				
9				

coding →

Y_1	Y_2	...	Y_{10}
1	0	...	0
0	1	...	0
...
0	0	...	1

↓ Coded output matrix \mathbf{Y}

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

1. Any problems?
2. Other methods?

Introduction

Binary classification

- Linear regression

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

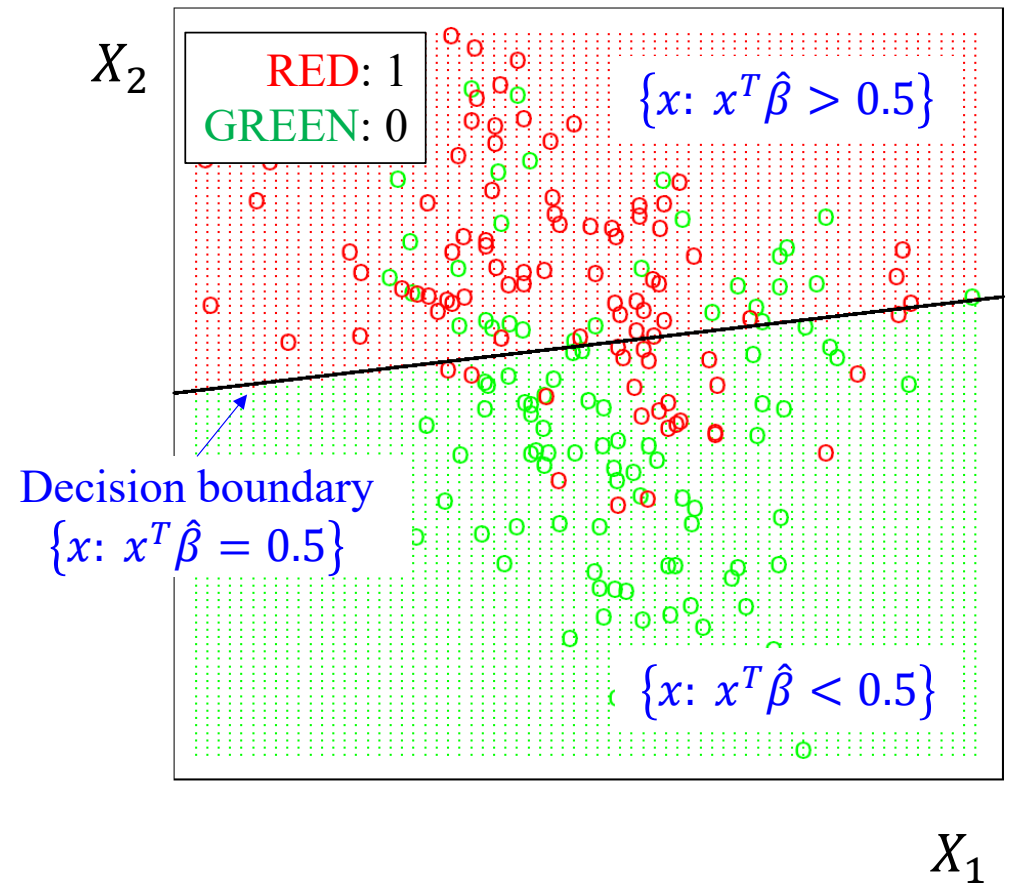
- Least squares solution

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

- Decision boundary

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

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

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

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

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

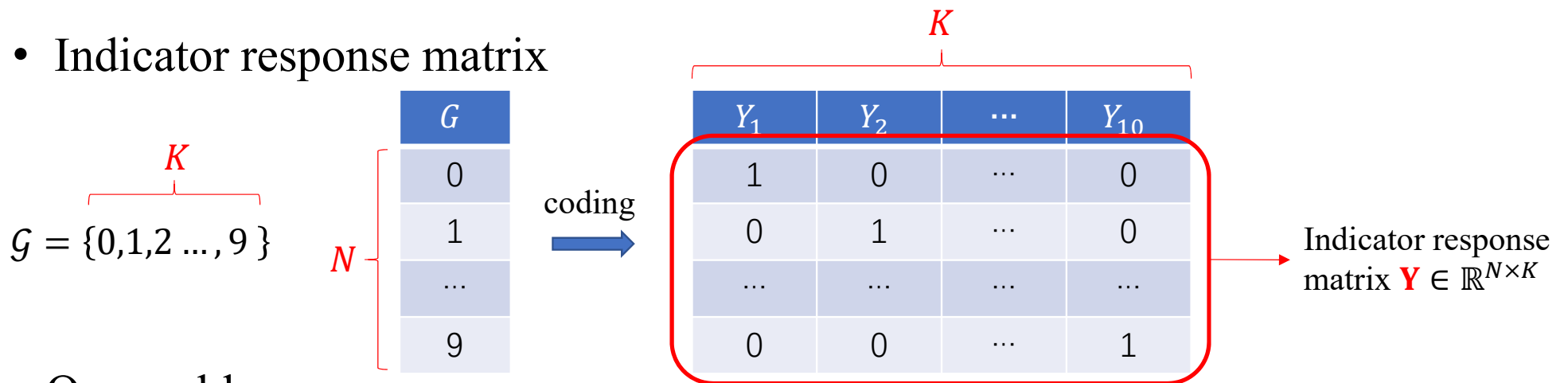
$$\{x: (\hat{\beta}_{k0} - \hat{\beta}_{\ell 0}) + x^T (\hat{\beta}_k - \hat{\beta}_\ell) = 0\}$$

Linear Methods for Classification I

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

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

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

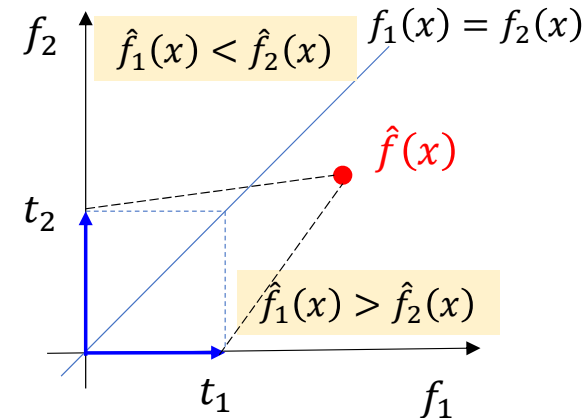
- Classify x according to

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

- Or equivalently,

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

where $t_k = (0, \dots, 0, 1, 0, \dots, 0)^T \in \mathbb{R}^K$ 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

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

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

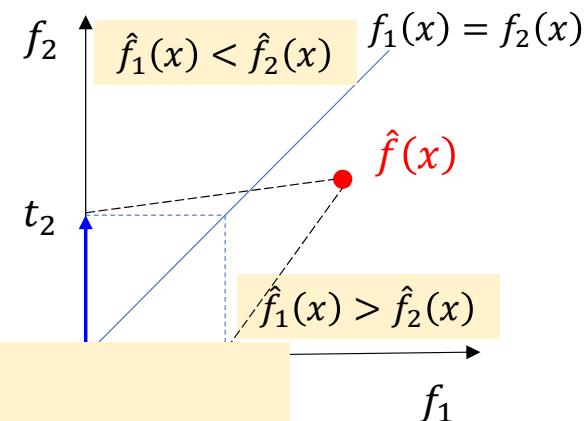
$$\hat{G}(x) = \operatorname{argmax}_{k \in \mathcal{G}} \hat{f}_k(x)$$

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

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

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

We have the followings

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

Indicator matrix

$\mathbf{H} \cdot \mathbf{1}_N$ 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:

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

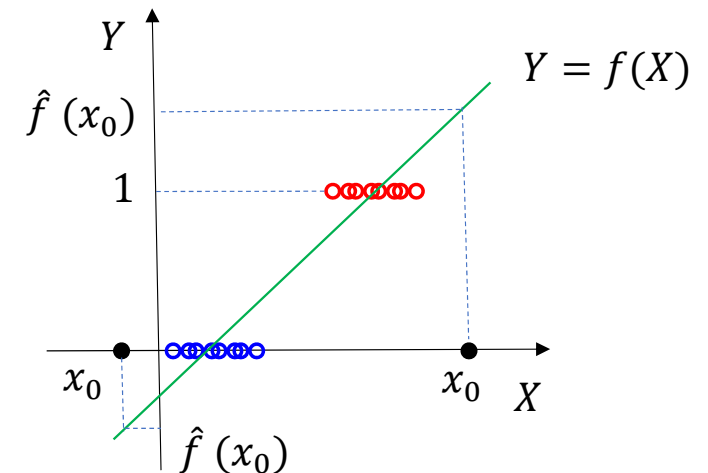
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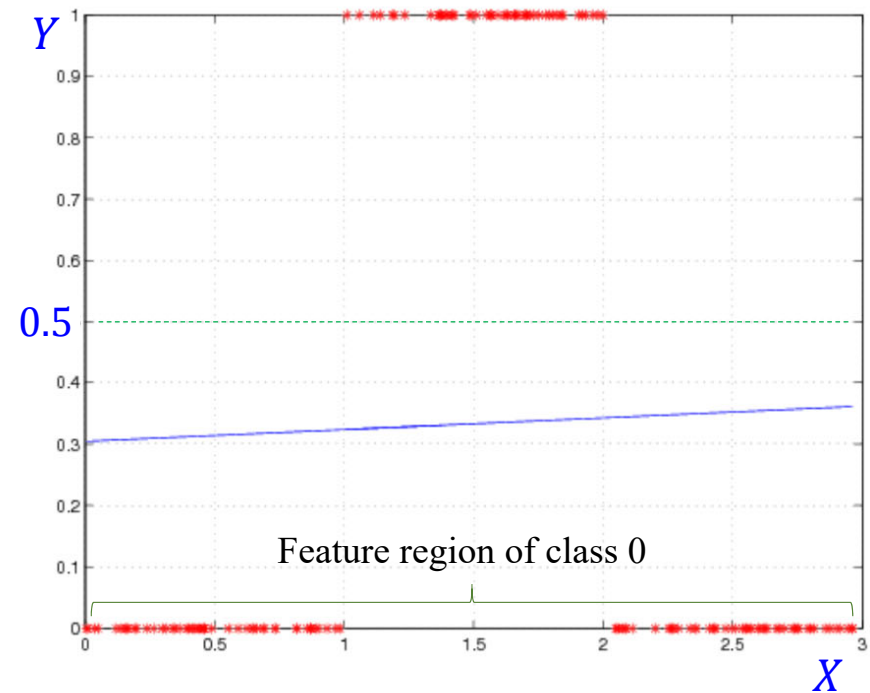
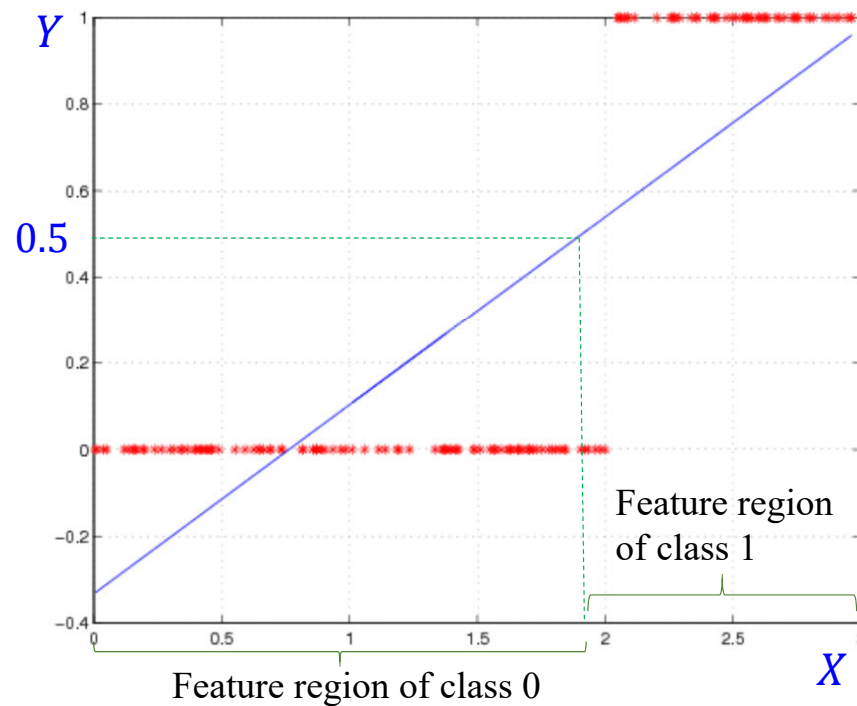
It suffers from **the problem of masking**, if #classes $K \geq 3$

- 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**

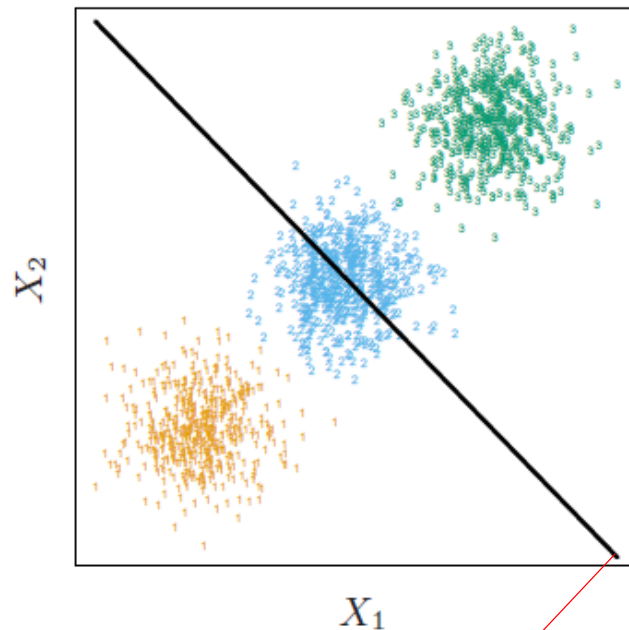


The Phenomenon of Masking

- 3-class classification

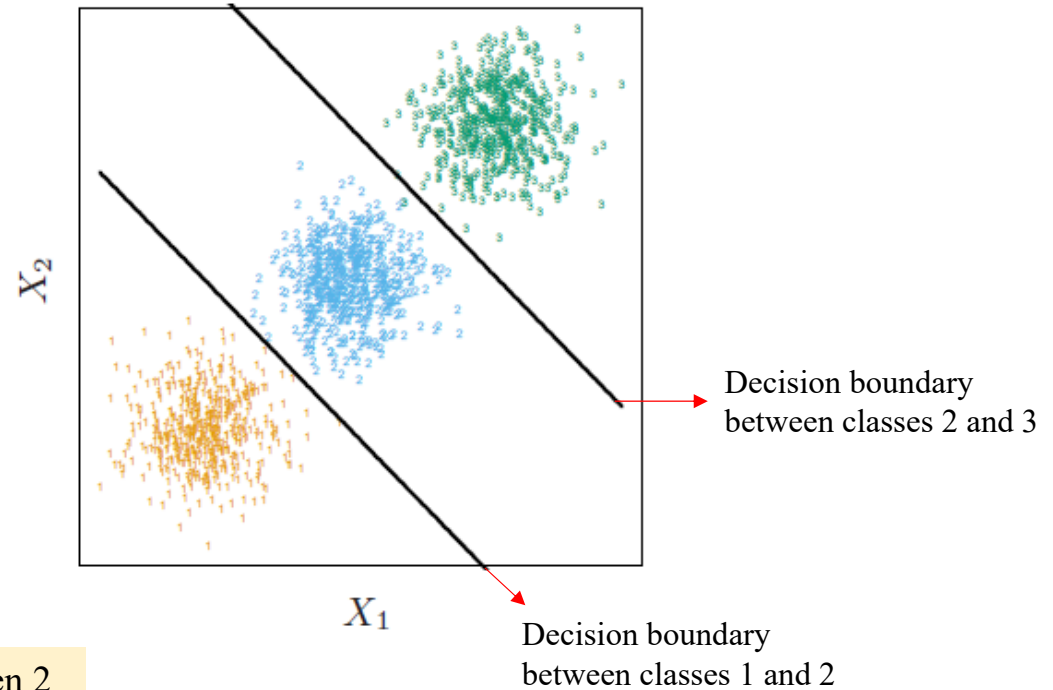
Yellow: class 1
Blue: class 2
Green: class 3

Linear Regression



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

The indicator matrix

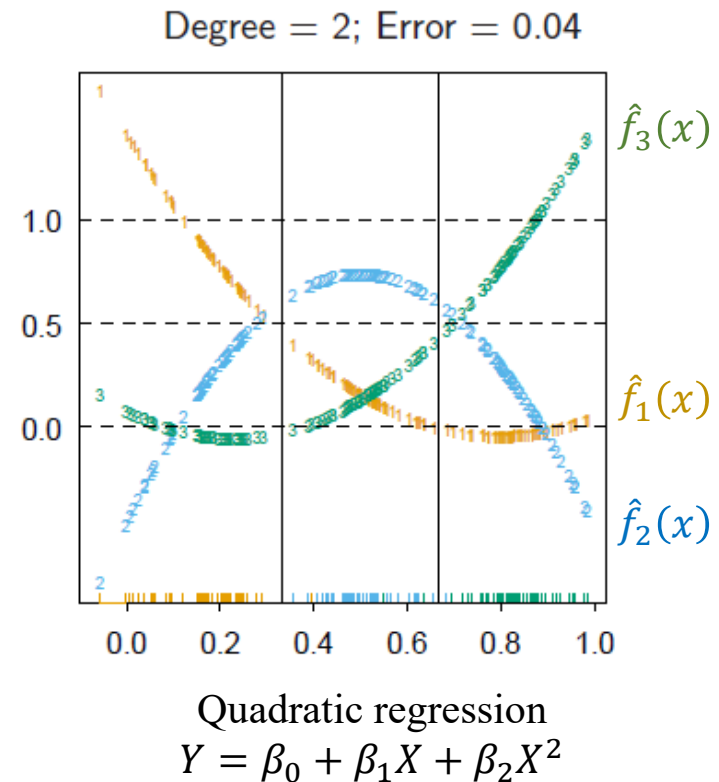
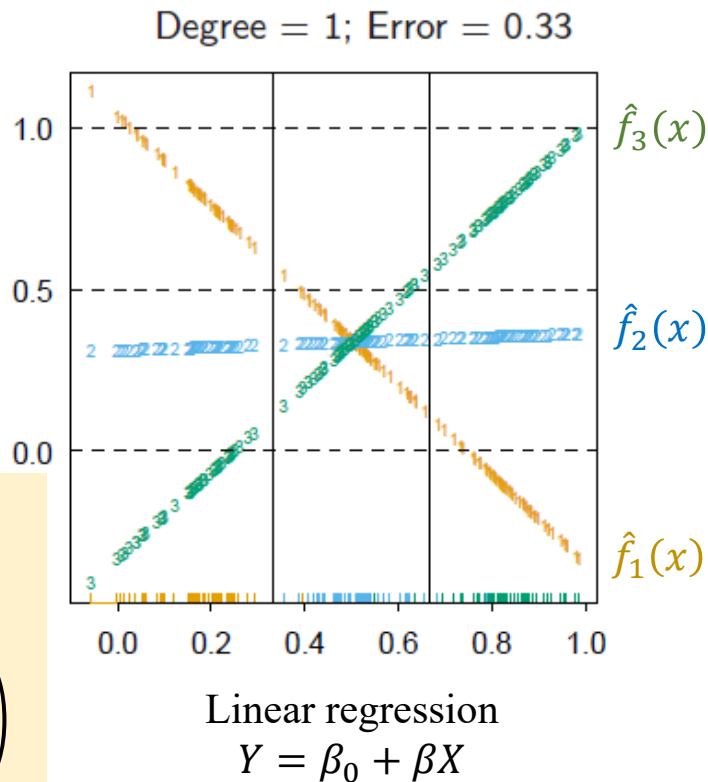
$$g = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \rightarrow \mathbf{Y} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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

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

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

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



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

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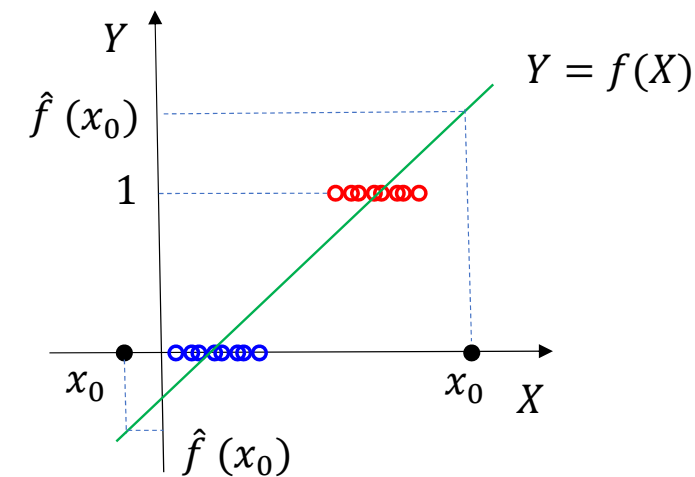
Linear classification:

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

Minimizing EPF:

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

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



Linear decision boundary

Linear Discriminant Analysis

- Logit transform

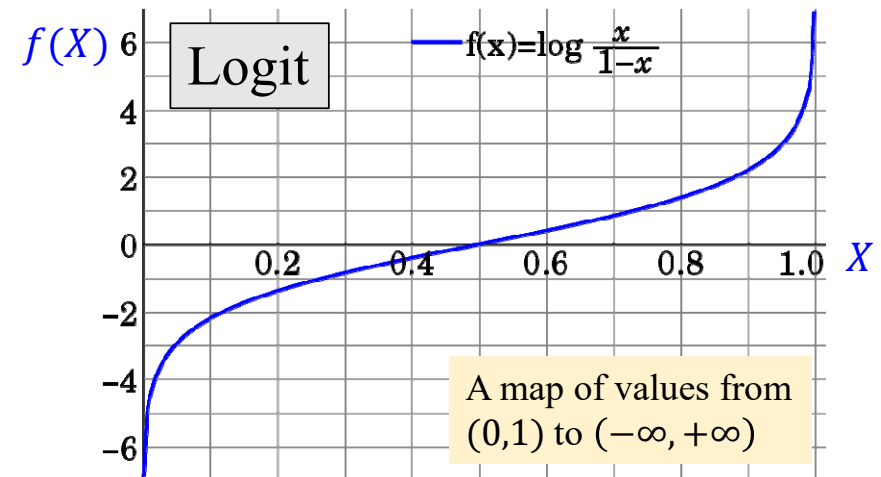
$$\text{logit}(\text{Pr}(x)) = \log \left(\frac{\text{Pr}(x)}{1 - \text{Pr}(x)} \right)$$

Odds (发生比)

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

- Decision boundary

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



Linear Discriminant Analysis

- **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

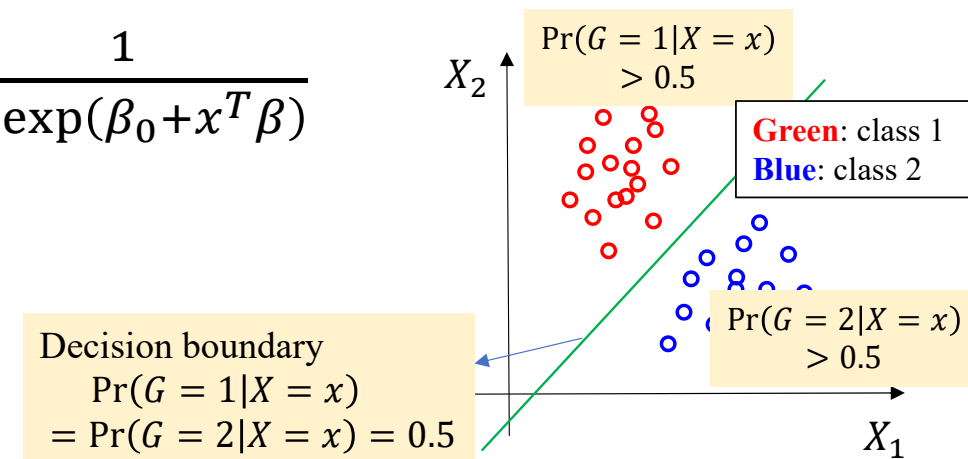
Q

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

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

- Decision boundary

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



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**

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

- 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 $f_k(x)$**

Linear Discriminant Analysis

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

- 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 ***ℓ***

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

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

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

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

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

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**

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

- Class-specific **sample mean**

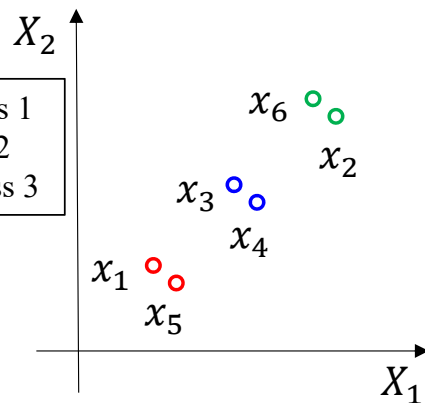
$$\hat{\mu}_1 = \frac{1}{2}(x_1 + x_5) = \frac{1}{2} \begin{pmatrix} 0.2 \\ 0.3 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 0.3 \\ 0.2 \end{pmatrix} = \begin{pmatrix} 0.25 \\ 0.25 \end{pmatrix}$$

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

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

- Common **covariance**

$$\hat{\Sigma} = \frac{\sum_{k=1}^K \sum_{g_i=k} (x_i - \hat{\mu}_i)(x_i - \hat{\mu}_i)^T}{N-K} = \frac{\begin{pmatrix} 0.05 & -0.05 \\ -0.05 & 0.05 \end{pmatrix} + \begin{pmatrix} 0.02 & -0.02 \\ -0.02 & 0.02 \end{pmatrix} + \begin{pmatrix} 0.05 & -0.05 \\ -0.05 & 0.05 \end{pmatrix}}{6-3} = \begin{pmatrix} 0.04 & -0.04 \\ -0.04 & 0.04 \end{pmatrix}$$



Linear Discriminant Analysis

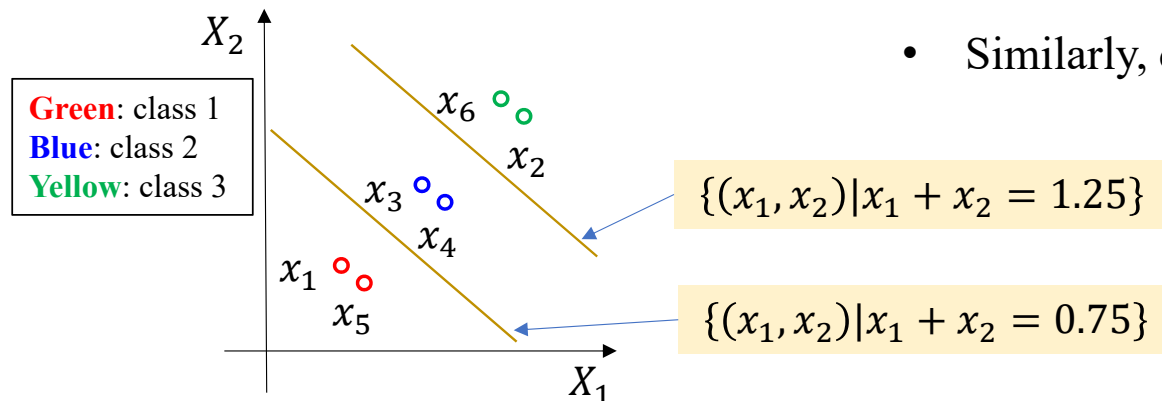
	Data		Class
	X_1	X_2	G
x_1^T	0.2	0.3	1
x_2^T	0.8	0.7	3
x_3^T	0.4	0.6	2
x_4^T	0.6	0.4	2
x_5^T	0.3	0.2	1
x_6^T	0.7	0.8	3

- For classes 1 and 2

$$\begin{aligned}
 & \log \frac{\Pr(G=1|X=x)}{\Pr(G=2|X=x)} \\
 &= \log \frac{\hat{\pi}_1}{\hat{\pi}_2} - \frac{1}{2}(\hat{\mu}_1 + \hat{\mu}_2)^T \hat{\Sigma}_\lambda^{-1} (\hat{\mu}_1 - \hat{\mu}_2) + x^T \hat{\Sigma}_\lambda^{-1} (\hat{\mu}_1 - \hat{\mu}_2) \\
 &= \frac{1}{2}(0.75, 0.75) \begin{pmatrix} 0.963 & 0.037 \\ 0.037 & 0.963 \end{pmatrix} \begin{pmatrix} 0.25 \\ 0.25 \end{pmatrix} - (x_1, x_2) \begin{pmatrix} 0.963 & 0.037 \\ 0.037 & 0.963 \end{pmatrix} \begin{pmatrix} 0.25 \\ 0.25 \end{pmatrix} \\
 &= 0.1875 - (x_1, x_2) \begin{pmatrix} 0.25 \\ 0.25 \end{pmatrix} = 0
 \end{aligned}$$

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

- 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

- 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

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

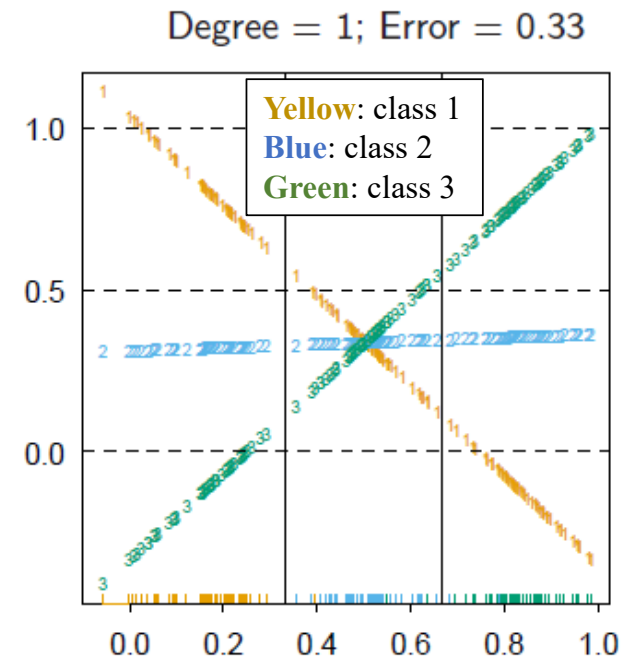
Any difference?

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 3

Linear Discriminant Analysis

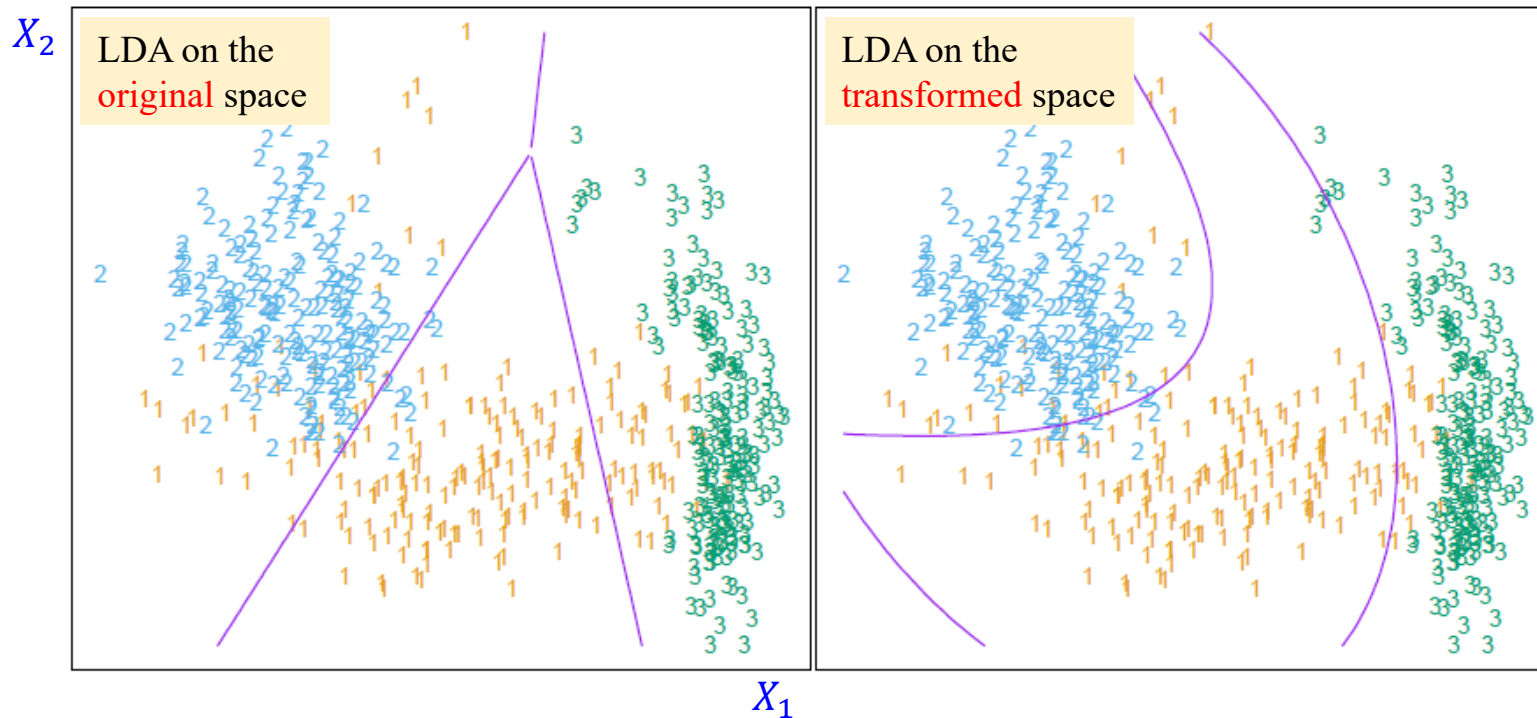


FIGURE 4.1. The left plot shows some data from three classes, with linear decision boundaries found by linear discriminant analysis. The right plot shows quadratic decision boundaries. These were obtained by finding linear boundaries in the five-dimensional space $X_1, X_2, X_1X_2, X_1^2, X_2^2$. Linear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

Linear Discriminant Analysis

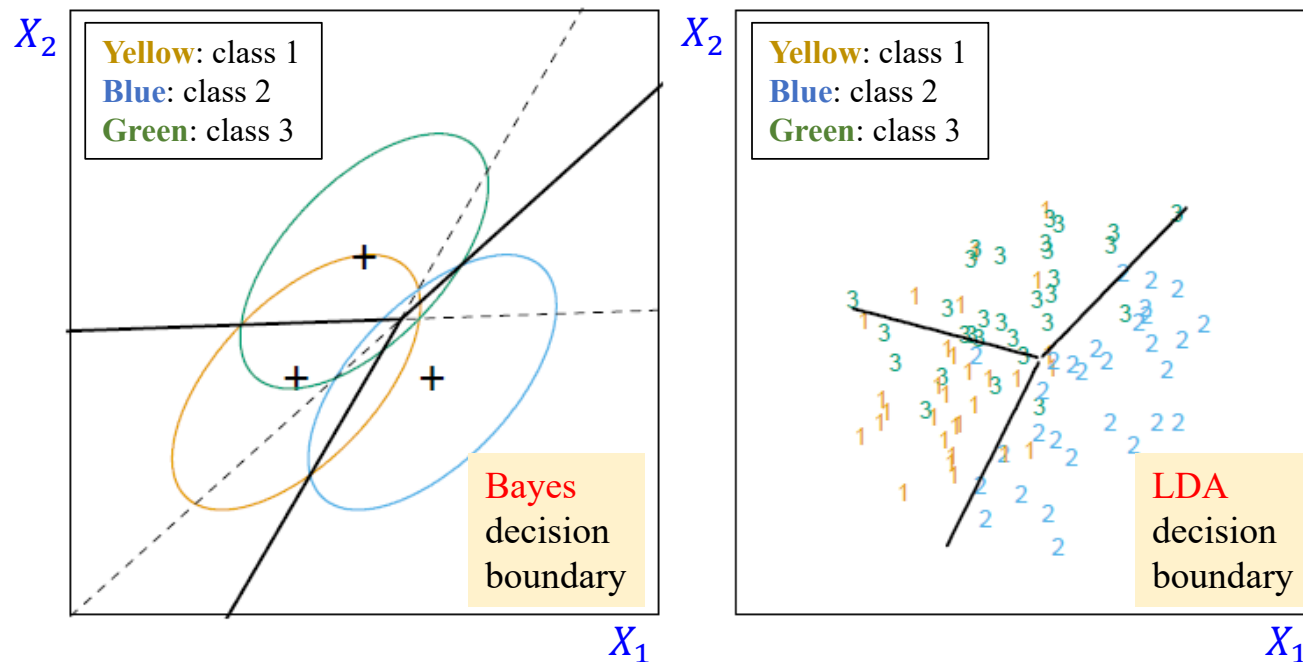


FIGURE 4.5. The left panel shows three Gaussian distributions, with the same covariance and different means. Included are the contours of constant density enclosing 95% of the probability in each case. The Bayes decision boundaries between each pair of classes are shown (broken straight lines), and the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

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

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

Quadratic Discriminant Analysis

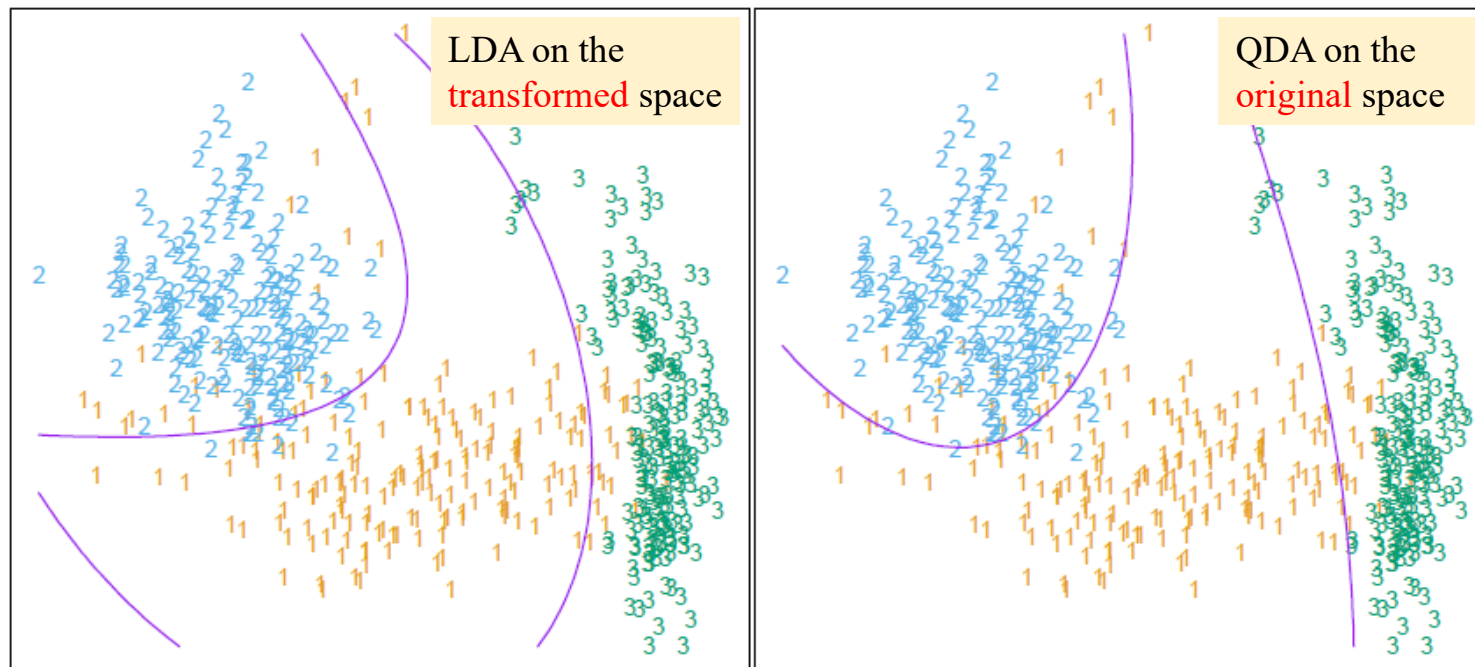


FIGURE 4.6. Two methods for fitting quadratic boundaries. The left plot shows the quadratic decision boundaries for the data in Figure 4.1 (obtained using LDA in the five-dimensional space $X_1, X_2, X_1X_2, X_1^2, X_2^2$). The right plot shows the quadratic decision boundaries found by QDA. The differences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

Classification

