Optimization and Machine Learning SI151

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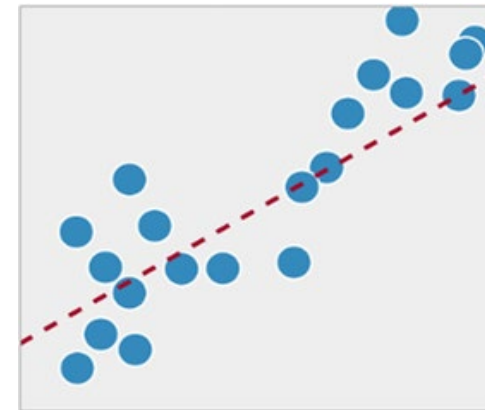
March 16, 2021

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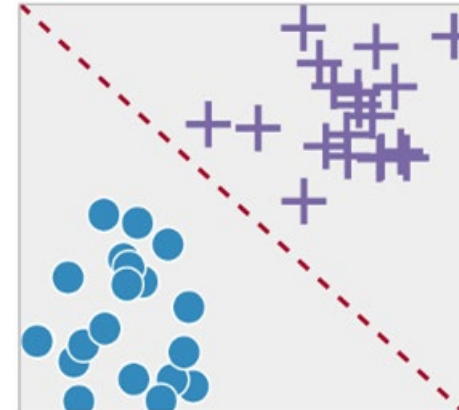 - Linear discriminant analysis

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

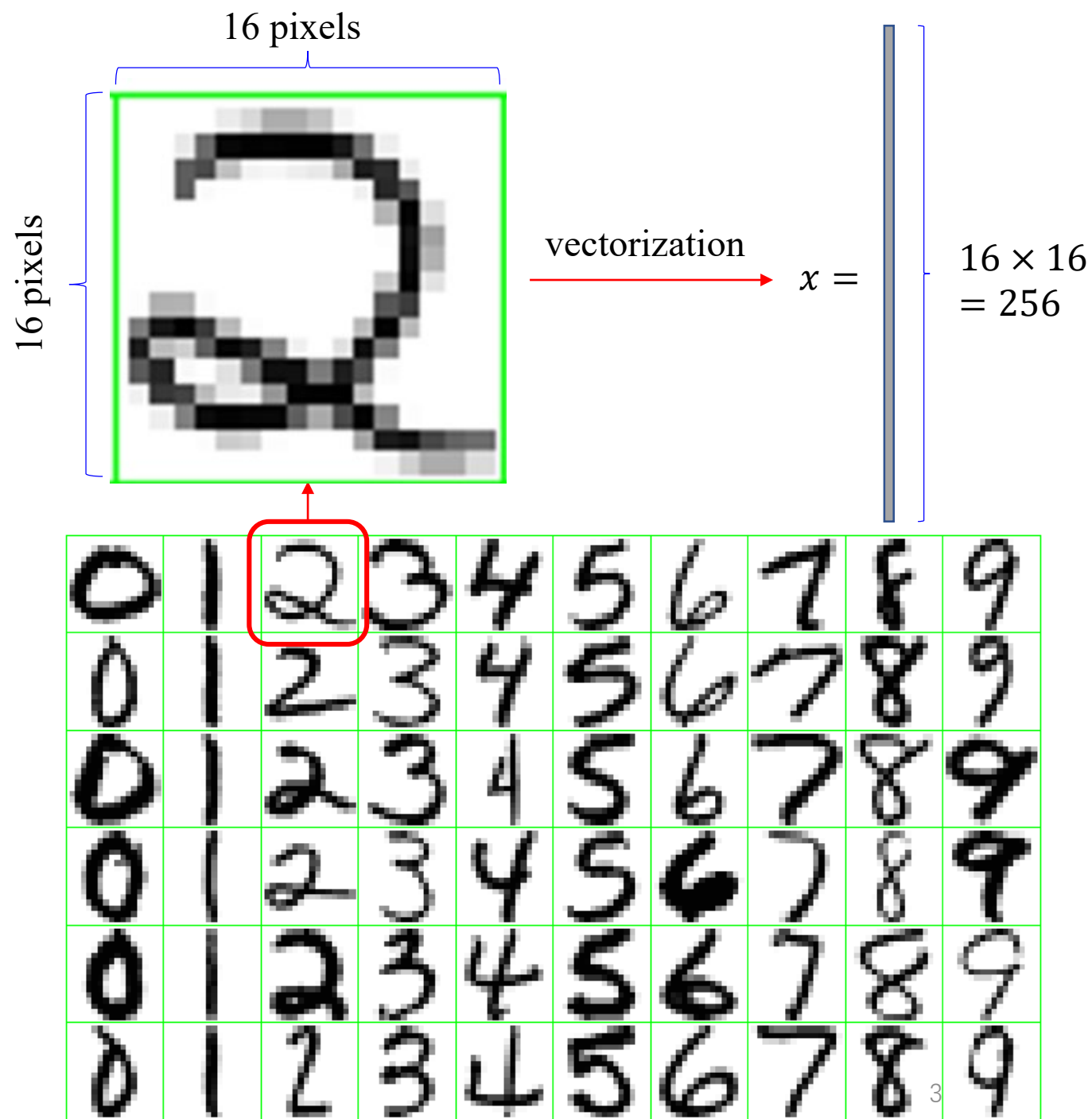**Example**

Handwritten digits recognition

Input variables
$$X = (X_0, X_1, X_2, \ldots, X_{256})^T$$
Categorical output variable G with
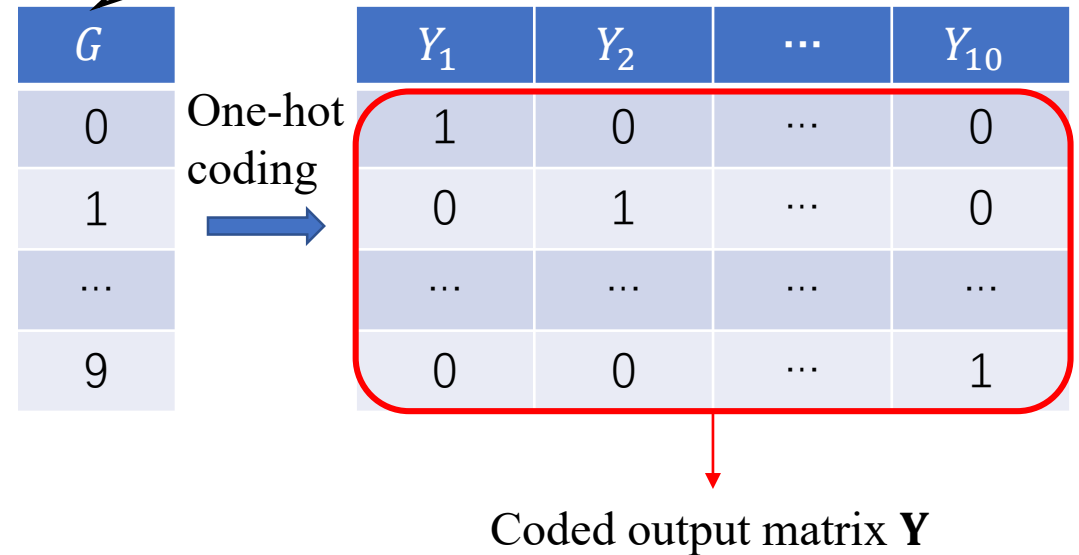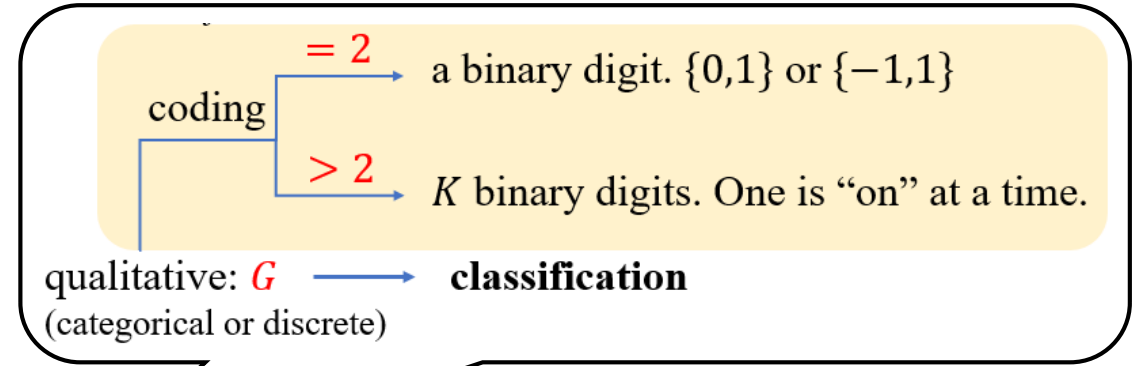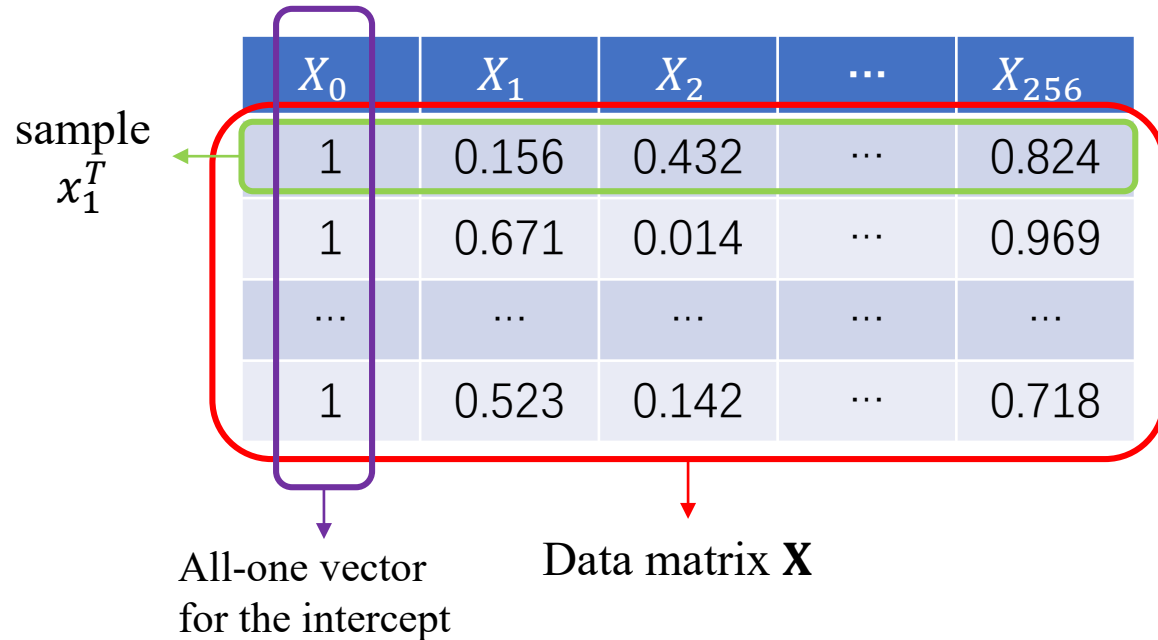values from
$$\mathcal{G} = \{0, 1, 2 \ldots, 9\}$$

Non-binary (multi-class) classification

16 pixels

16 pixels

vectorization

$$x =$$

$16 \times 16 = 256$

Introduction

Example

Handwritten digits recognition

coding		
	= 2	a binary digit. {0,1} or {−1,1}
	> 2	K binary digits. One is "on" at a time.

qualitative: G ⟶ **classification**
(categorical or discrete)

	X_0	X_1	X_2	...	X_{256}
sample x_1^T	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 **X**

G
0
1
...
9

One-hot coding ⟶

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

Coded output matrix **Y**

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

1. Any problems?
2. Other methods?

Introduction

Binary classification

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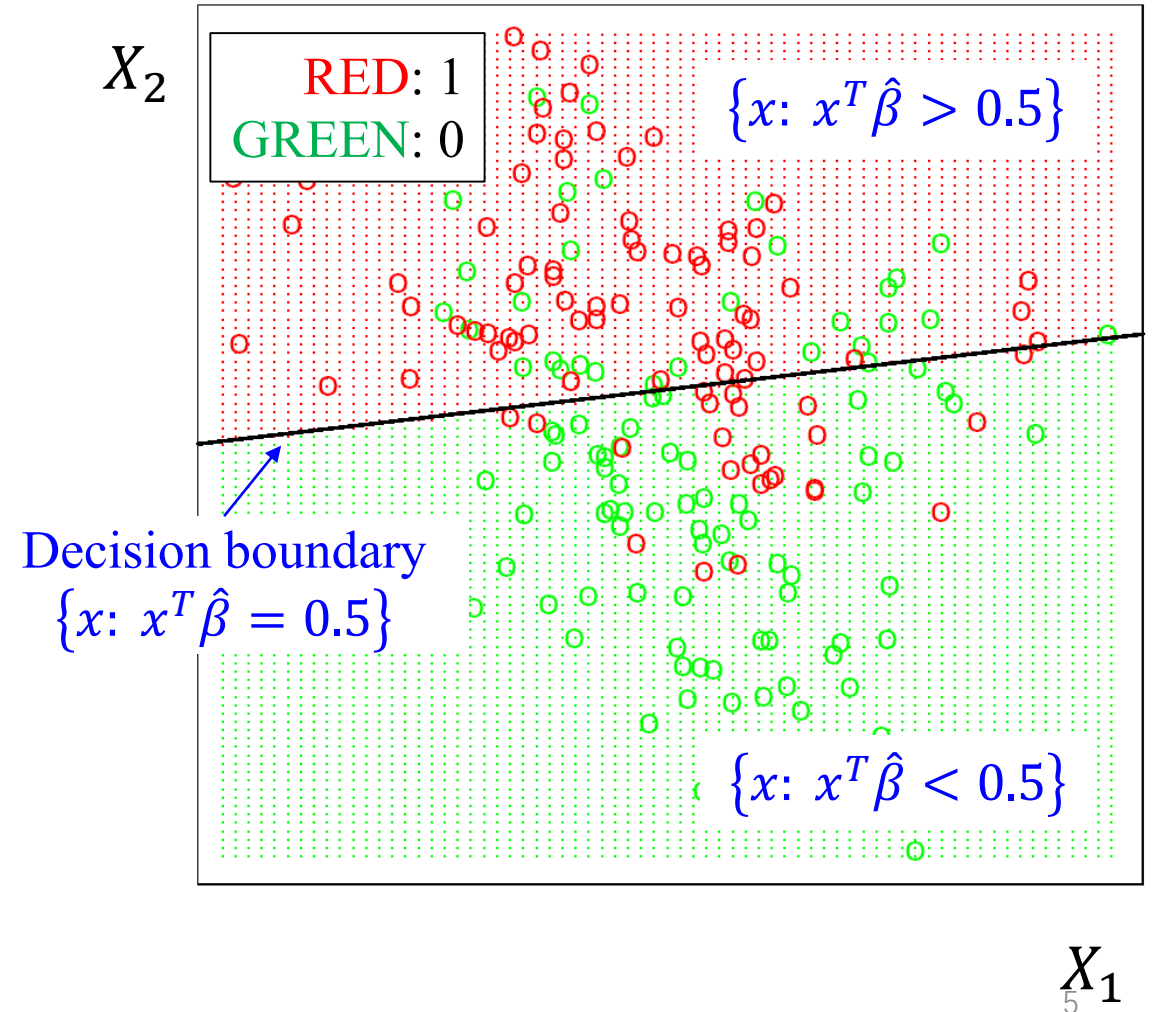
$$f(x) = \beta_0 + x^T \beta$$

- Least squares solution

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

- Decision boundary

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

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

X_2

RED: 1
GREEN: 0

$\{x : x^T \hat{\beta} > 0.5\}$

Decision boundary
$\{x : x^T \hat{\beta} = 0.5\}$

$\{x : x^T \hat{\beta} < 0.5\}$

X_1

Introduction

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 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

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

G
0
1
...
9

coding →

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

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

- Our problem:

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

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

- The fitted values on $\mathbf{X}$:

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

Linear Regression of an Indicator Matrix

A new observation x is classified by

- Compute the fitted output

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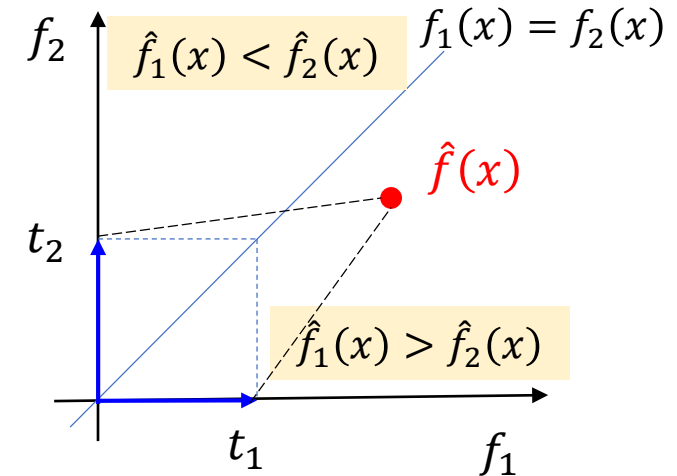
- Classify x according to

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

- Or equivalently,

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

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

Linear Regression of an Indicator Matrix

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

- 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. $\Pr(G, X)$

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

- Pointwise minimization leads to

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

$$= \underset{k \in \mathcal{G}}{\text{argmax}} \; \boxed{\Pr(G = k | X = x)} \longleftarrow \text{posterior}$$

Linear Regression of an Indicator Matrix

A new observation x is classified by

- Compute the fitted output

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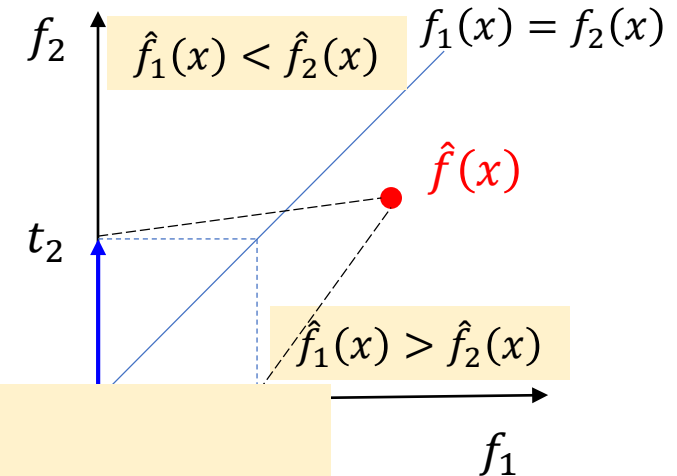
- Classify x according to

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

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

$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\mathrm{argmax}}\, \Pr(\, G = k | X = x)$$

- Our question: ment

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

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

$\hat{f}(x)$

t_2

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

f_1

Linear Regression of an Indicator Matrix

?

Linear classification:
$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\mathrm{argmax}}\, \boxed{\hat{f}_k(x)}$$

Minimizing EPE:
$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\mathrm{argmax}}\, \boxed{\Pr(\,G = k | X = x)}$$

Two defining properties of probability
1. $\sum P = 1$
2. $0 < P < 1$

- It can be verified that $\boxed{\sum_{k \in \mathcal{G}} \hat{f}_k(x) = 1}$
- 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
$$\widehat{\mathbf{Y}} = \hat{f}(\mathbf{X}) = \mathbf{X}\widehat{\mathbf{B}} = \left(\hat{f}_1(\mathbf{X}), \dots, \hat{f}_K(\mathbf{X})\right)$$
We have the followings

Indicator matrix

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

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

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

Minimizing EPE:

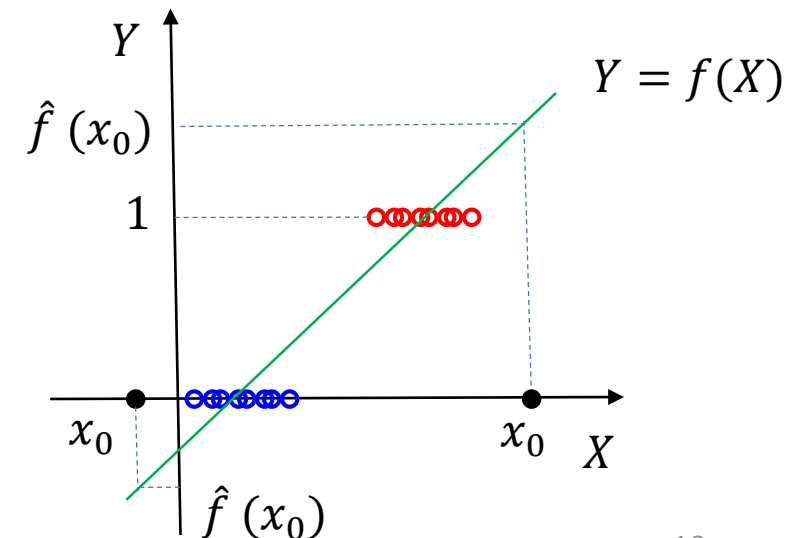$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\mathrm{argmax}}\, \Pr(G = k | X = x)$$

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

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

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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

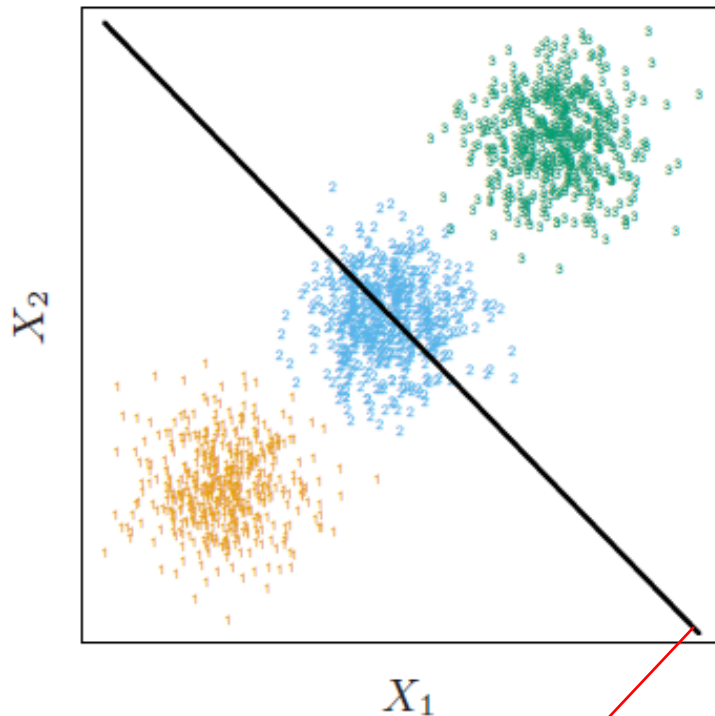Feature region of class 1

Feature region of class 0

Feature region of class 0
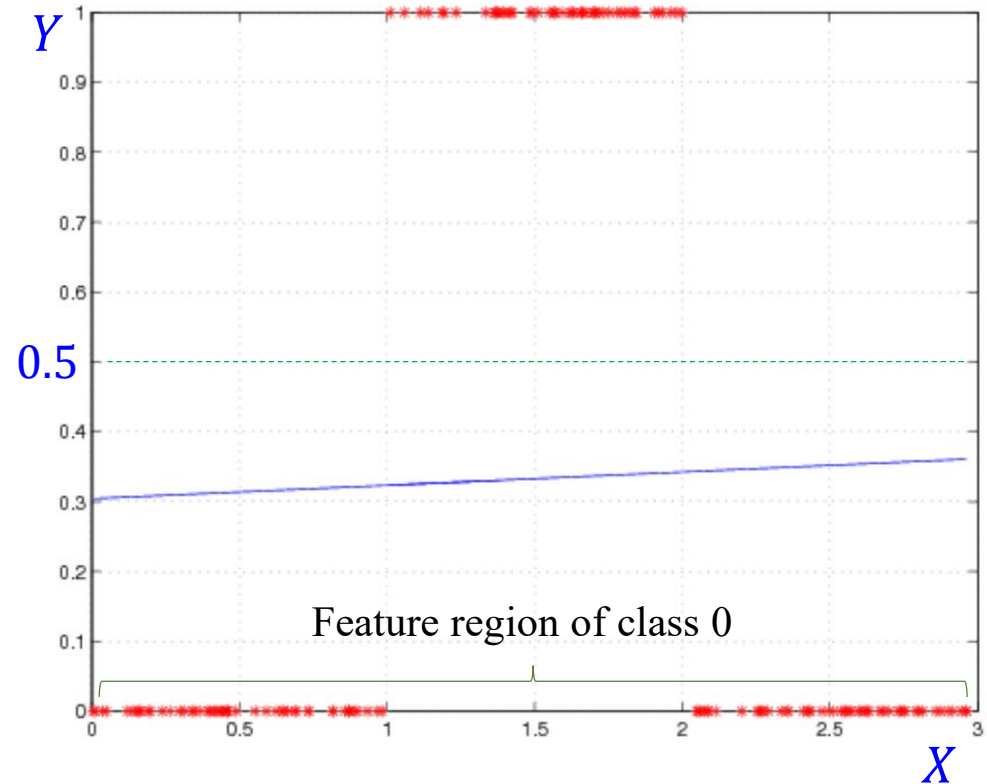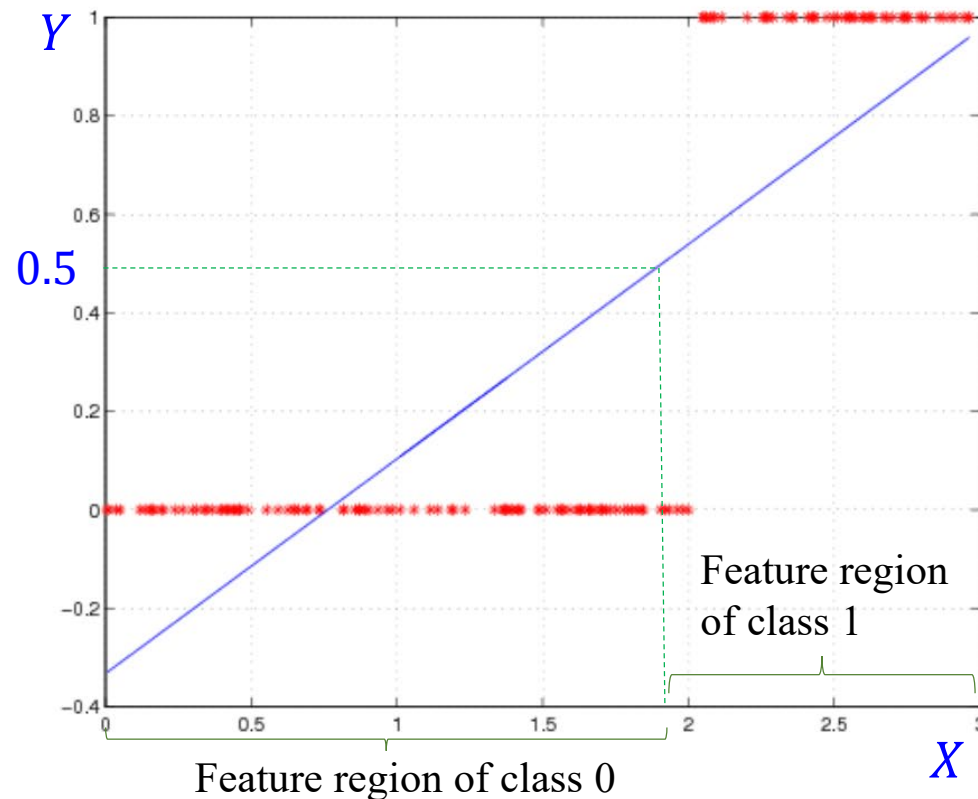
The Phenomenon of Masking

- 3-class classification

Linear Regression

Linear Discriminant Analysis ← Ideal result

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

X_2

X_1

X_2

X_1

Decision boundary between classes 2 and 3

Decision boundary between classes 1 and 2

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

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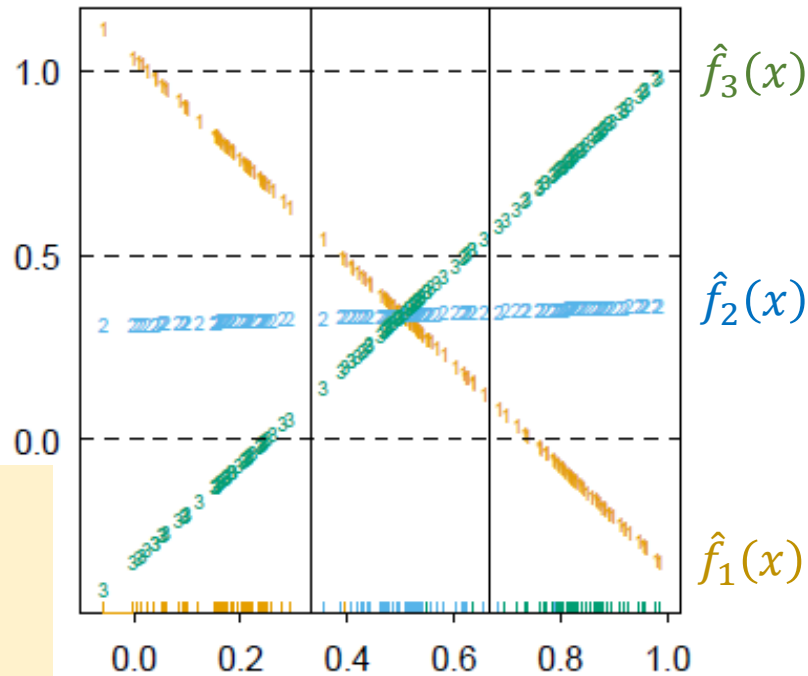
- 3-class classification

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

$$\widehat{\mathbf{B}} = \underset{\mathbf{B}}{\mathrm{argmin}} \|\mathbf{Y} - \mathbf{XB}\|_F^2,$$
$$\text{where } \mathbf{X} = (\mathbf{1}_N, \mathbf{x})$$

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

Degree = 1; Error = 0.33
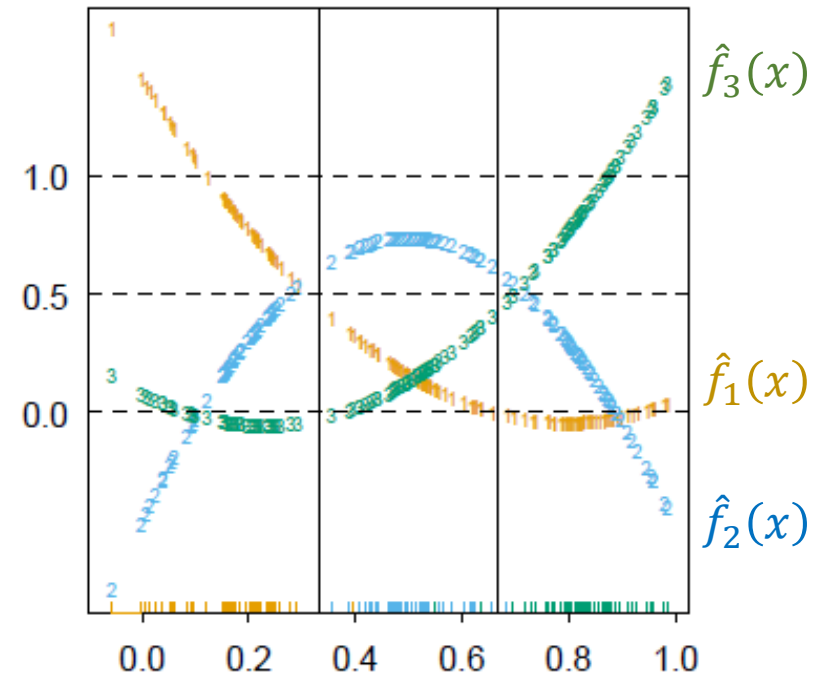
Linear regression
$Y = \beta_0 + \beta X$

Degree = 2; Error = 0.04

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

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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:

$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\arg\max} \; \boxed{\hat{f}_k(x)}$$

Minimizing EPE:

$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\arg\max} \; \boxed{\Pr(G = k | X = x)}$$

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

- Solution: make some monotone transformation of the posterior be linear in X
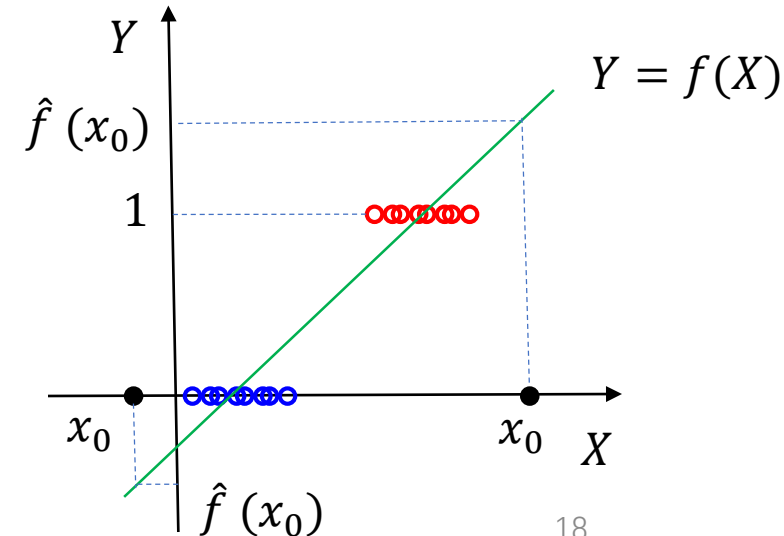
Linear decision boundary

Linear Discriminant Analysis

- Logit transform

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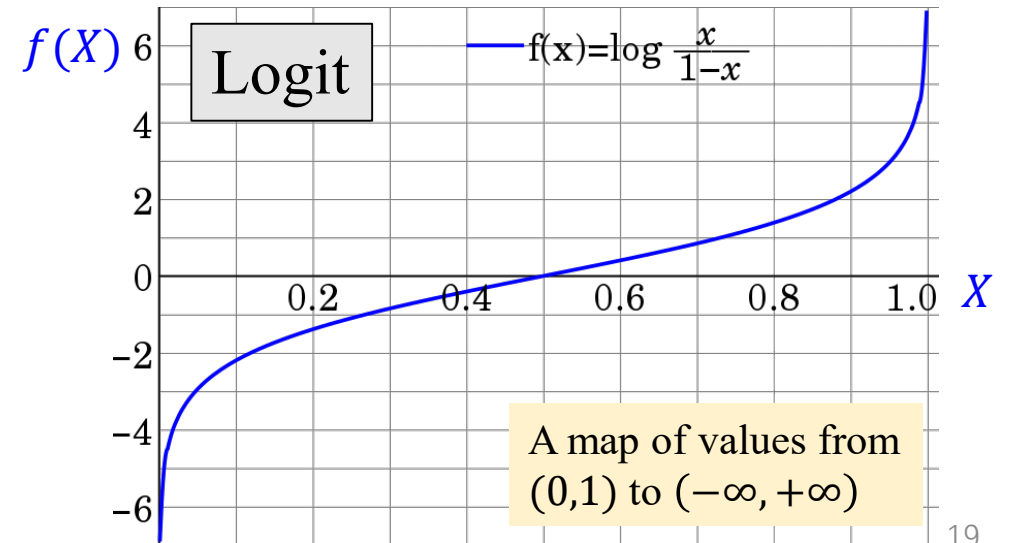
$$\text{logit}(\Pr(x)) = \log\left(\frac{\Pr(x)}{1 - \Pr(x)}\right)$$

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

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

Logit

$f(X)$

$f(x) = \log\frac{x}{1-x}$

X

A map of values from $(0,1)$ to $(-\infty, +\infty)$

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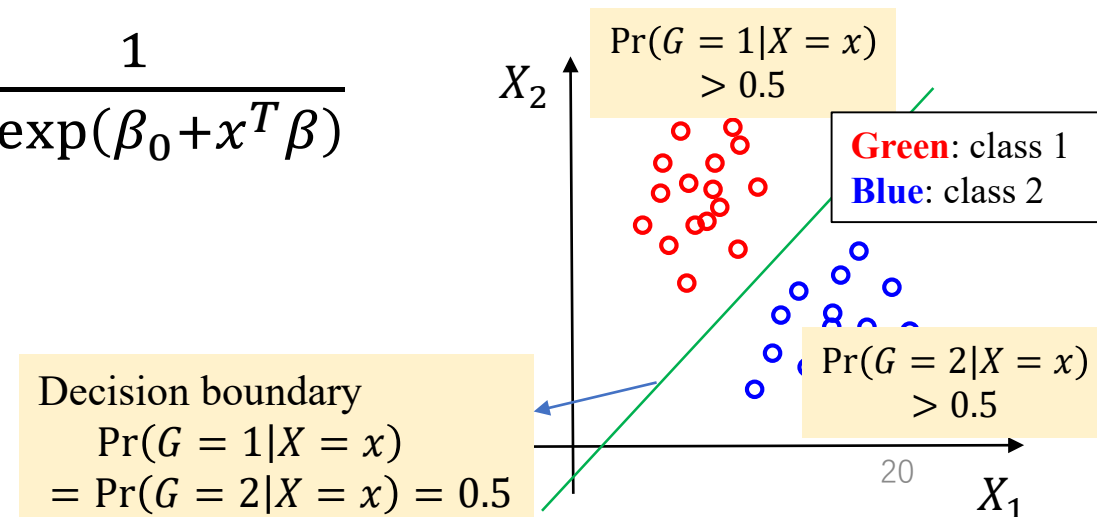
$$\Pr(G = 1|X = x) = \frac{\boxed{\exp(\beta_0 + x^T\beta)}}{1 + \exp(\beta_0 + x^T\beta)},$$

$\exp(x) = e^x$

Q

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

- Decision boundary

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

$\Pr(G = 1|X = x) > 0.5$

Green: class 1
Blue: class 2

$\Pr(G = 2|X = x) > 0.5$

Decision boundary
$\Pr(G = 1|X = x)$
$= \Pr(G = 2|X = x) = 0.5$

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Linear Discriminant Analysis

- Idea:

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

- Posterior

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

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

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

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

X_1	X_2
0.2	0.3
0.8	0.7
0.4	0.6
0.6	0.4
0.3	0.2
0.7	0.8

Row labels: x_1^T, x_2^T, x_3^T, x_4^T, x_5^T, x_6^T

Class

G
1
3
2
2
1
3

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

- Class prior

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

- Class-specific sample mean

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

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

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

- Common covariance

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

$$\frac{\begin{pmatrix} 0.05 & -0.05 \\ -0.05 & 0.05 \end{pmatrix} + \begin{pmatrix} 0.02 & -0.02 \\ -0.02 & 0.02 \end{pmatrix} + \begin{pmatrix} 0.05 & -0.05 \\ -0.05 & 0.05 \end{pmatrix}}{6-3} = \begin{pmatrix} 0.04 & -0.04 \\ -0.04 & 0.04 \end{pmatrix}$$
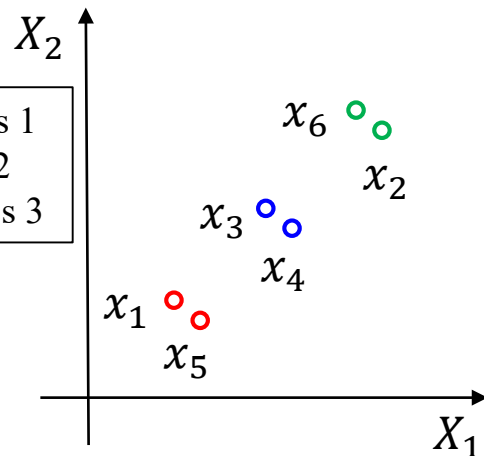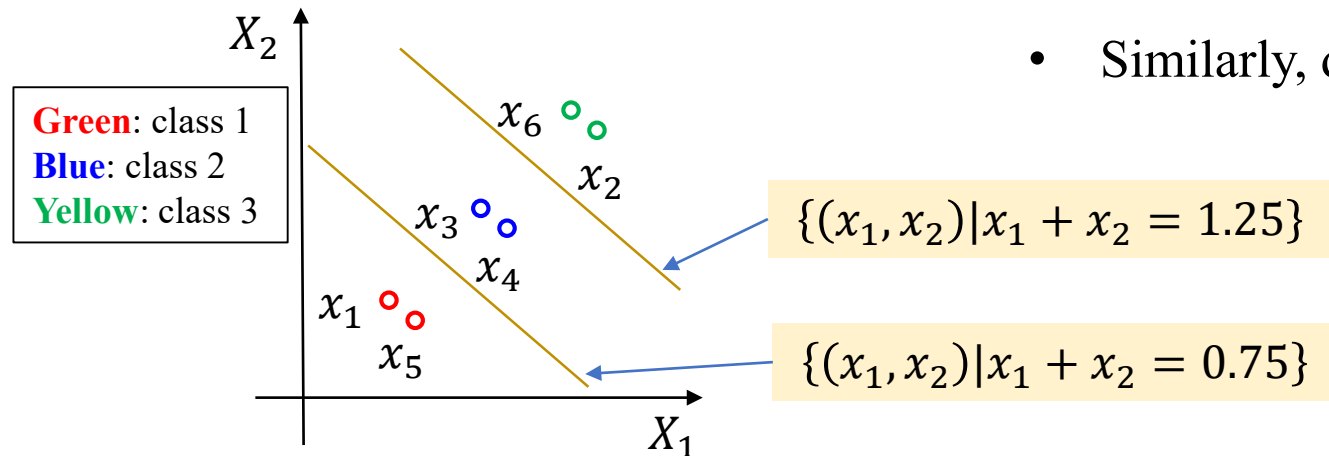
Linear Discriminant Analysis

Data | | Class
|||

X_1	X_2		G
0.2	0.3		1
0.8	0.7		3
0.4	0.6		2
0.6	0.4		2
0.3	0.2		1
0.7	0.8		3

x_1^T, x_2^T, x_3^T, x_4^T, x_5^T, x_6^T

- For classes 1 and 2

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

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

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

$$= \frac{1}{2}(0.75, 0.75)\begin{pmatrix} 0.963 & 0.037 \\ 0.037 & 0.963 \end{pmatrix}\begin{pmatrix} 0.25 \\ 0.25 \end{pmatrix} - (x_1, x_2)\begin{pmatrix} 0.963 & 0.037 \\ 0.037 & 0.963 \end{pmatrix}\begin{pmatrix} 0.25 \\ 0.25 \end{pmatrix}$$

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

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

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

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

$\{(x_1, x_2) | x_1 + x_2 = 1.25\}$

$\{(x_1, x_2) | x_1 + x_2 = 0.75\}$

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

$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\text{argmax}}\, \delta_k(x)$$

Any difference?

Linear classification:
$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\text{argmax}}\, \hat{f}_k(x)$$

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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

Degree = 1; Error = 0.33

Yellow: class 1
Blue: class 2
Green: class 3
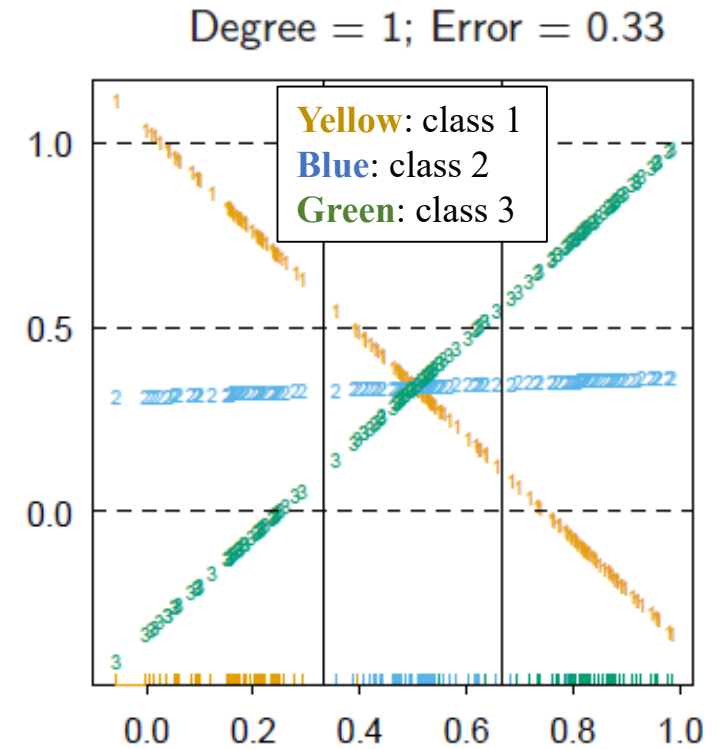
Class 2 is masked by classes 1 and 3

Linear Discriminant Analysis

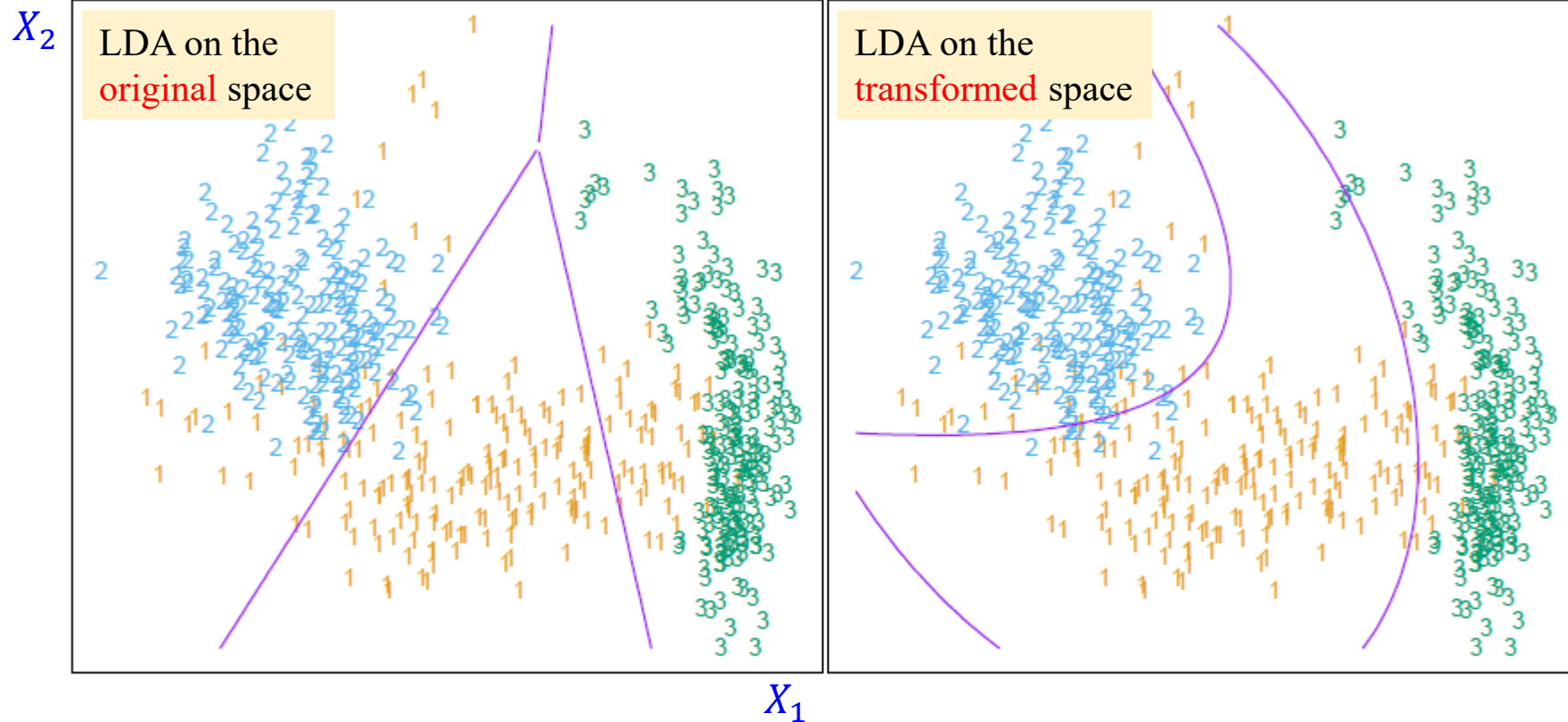FIGURE 4.1. *The left plot shows some data from three classes, with linear decision boundaries found by linear discriminant analysis. The right plot shows quadratic decision boundaries. These were obtained by finding linear boundaries in the five-dimensional space* $X_1, X_2, X_1 X_2, X_1^2, X_2^2.$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

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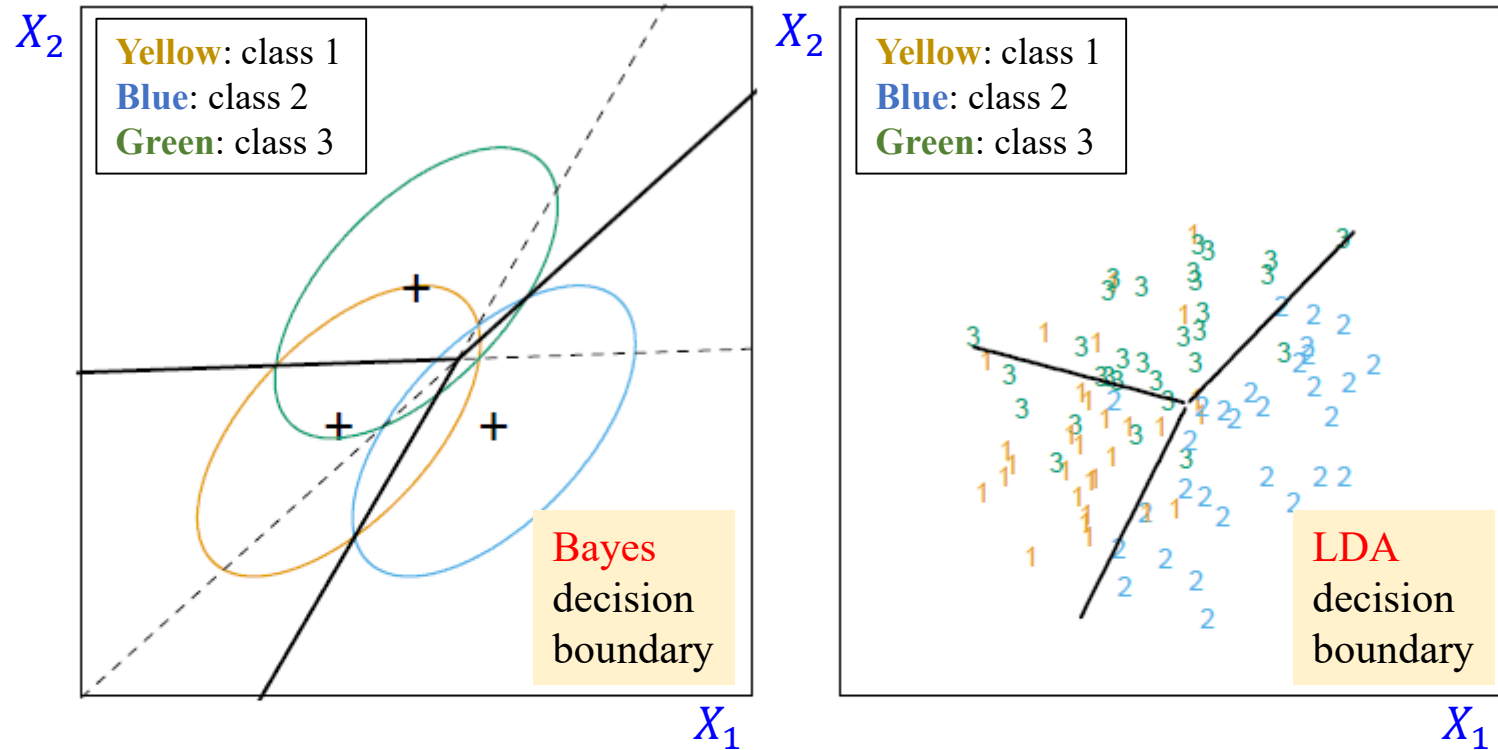
FIGURE 4.5. *The left panel shows three Gaussian distributions, with the same covariance and different means. Included are the contours of constant density enclosing 95% of the probability in each case. The Bayes decision boundaries between each pair of classes are shown (broken straight lines), and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

- Assumption: Each class has a specific covariance Σ_k

- Quadratic discriminant functions

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

- 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

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

30

Quadratic Discriminant Analysis

LDA on the transformed space

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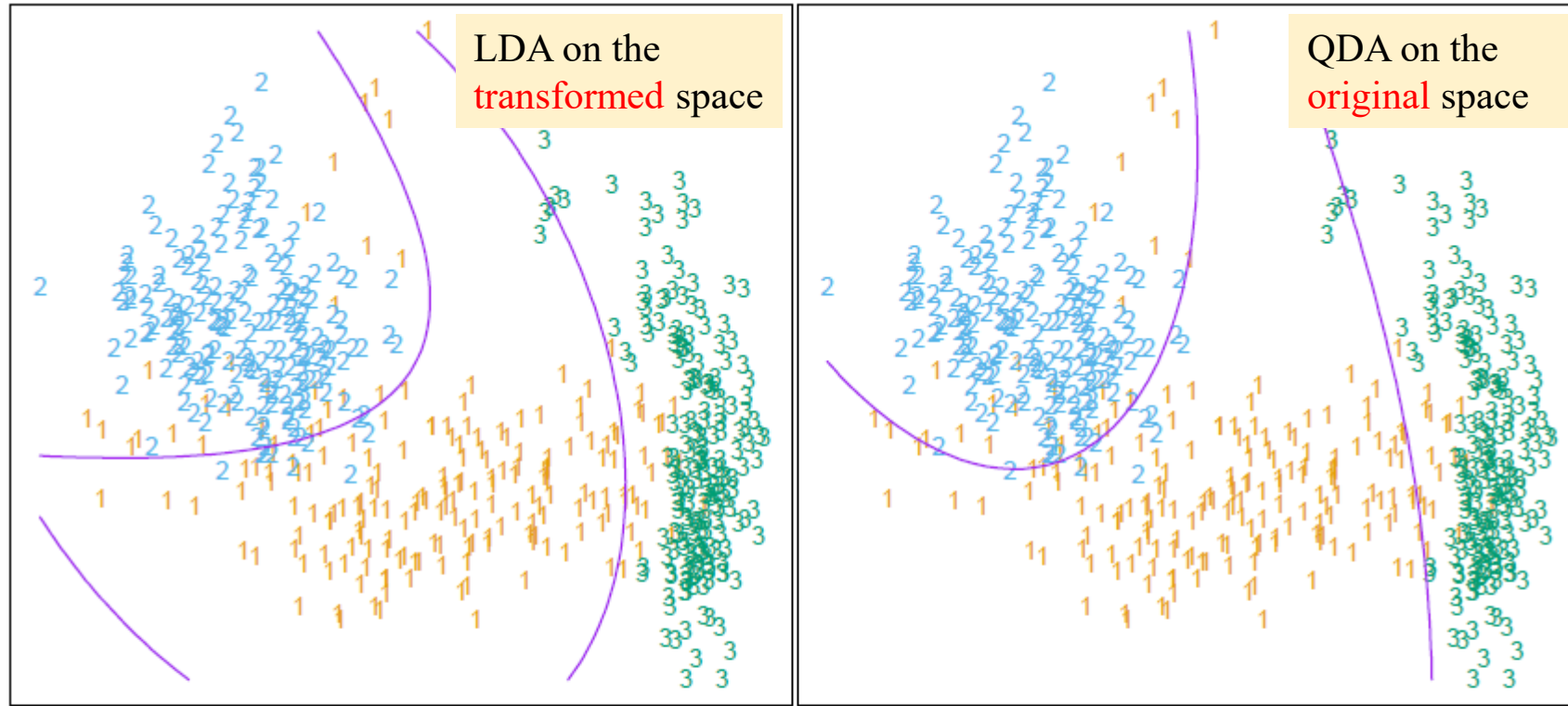
FIGURE 4.6. *Two methods for fitting quadratic boundaries. The left plot shows the quadratic decision boundaries for the data in Figure 4.1 (obtained using LDA in the five-dimensional space* $X_1, X_2, X_1X_2, X_1^2, X_2^2$*). The right plot shows the quadratic decision boundaries found by QDA. The differences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

Summary

- Linear regression of an indicator matrix
  - The indicator matrix
  - Prediction is conducted by $\hat{G}(x) = \text{argmax}_k \hat{f}_k(x)$
  - Suffer from the masking problem

- Linear discriminant analysis
  - Logit transformation: $\text{logit}(\Pr(x)) = \log\left(\frac{\Pr(x)}{1-\Pr(x)}\right)$
  - 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

Simple and straightforward → **Linear regression**

Theoretical → $\min_f \text{EPE}$

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

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

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

$$\hat{G}(x) = \underset{k \in \mathcal{G}}{\arg\max}\, \hat{f}_k(x)$$

Limitation

The masking problem $(K \geq 3)$

Squared error loss → **Regression function** $f(x) = \text{E}(Y|X = x)$

Zero-one loss → **Bayes classifier** $\hat{G}(x) = \underset{k \in \mathcal{G}}{\arg\max}\, \text{Pr}(G = k|X = x)$

Linear → **Least squares**

Nonlinear → **Nearest neighbors**

Regression

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

Logit transformation $\text{logit}(x) = \log\left(\dfrac{x}{1-x}\right)$

Pairwise odds = 1

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

Bayes theorem → **LDA, QDA, RDA**

Linear boundary → **Logistic regression**