Machine Learning Basics
Multiclass Classification

HKUST MSBD 6000B

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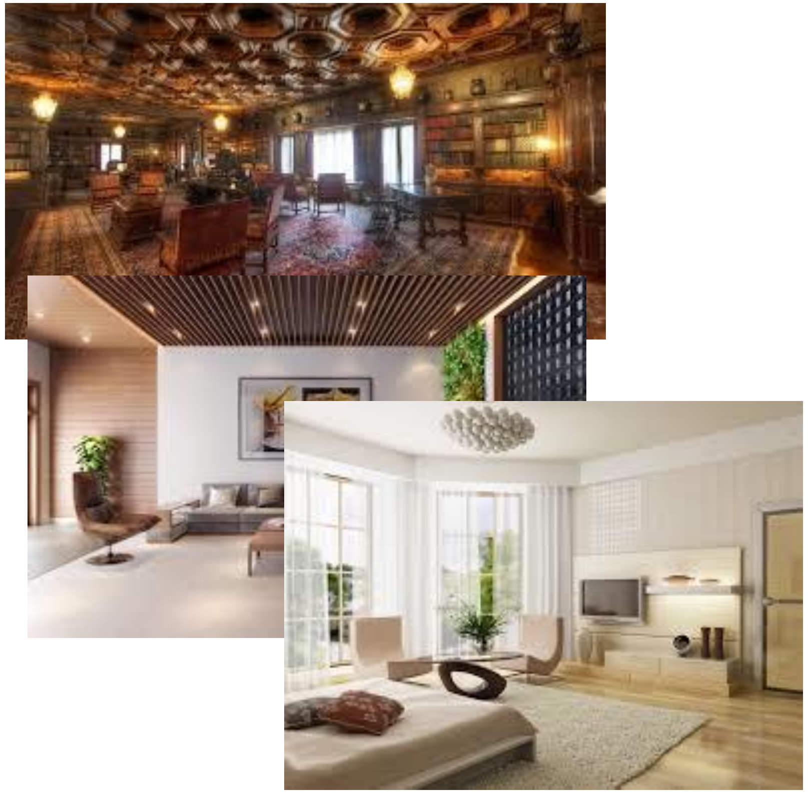
Example: image classification



Indoor

outdoor

Example: image classification (multiclass)

ImageNet figure borrowed from vision.standford.edu

Multiclass classification

- Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
  - $x_i \in R^d$, $y_i \in \{1,2, \dots, K\}$
- Find $f(x): R^d \to \{1,2, \dots, K\}$ that outputs correct labels

- What kind of f?

Approaches for multiclass classification

Approach 1: reduce to regression

- Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
- Find $f_w(x) = w^T x$ that minimizes $\hat{L}(f_w) = \frac{1}{n}\sum_{i=1}^{n}(w^T x_i - y_i)^2$

- Bad idea even for binary classification

Reduce to linear regression;
ignore the fact $y \in \{1, 2 \ldots, K\}$

Approach 1: reduce to regression

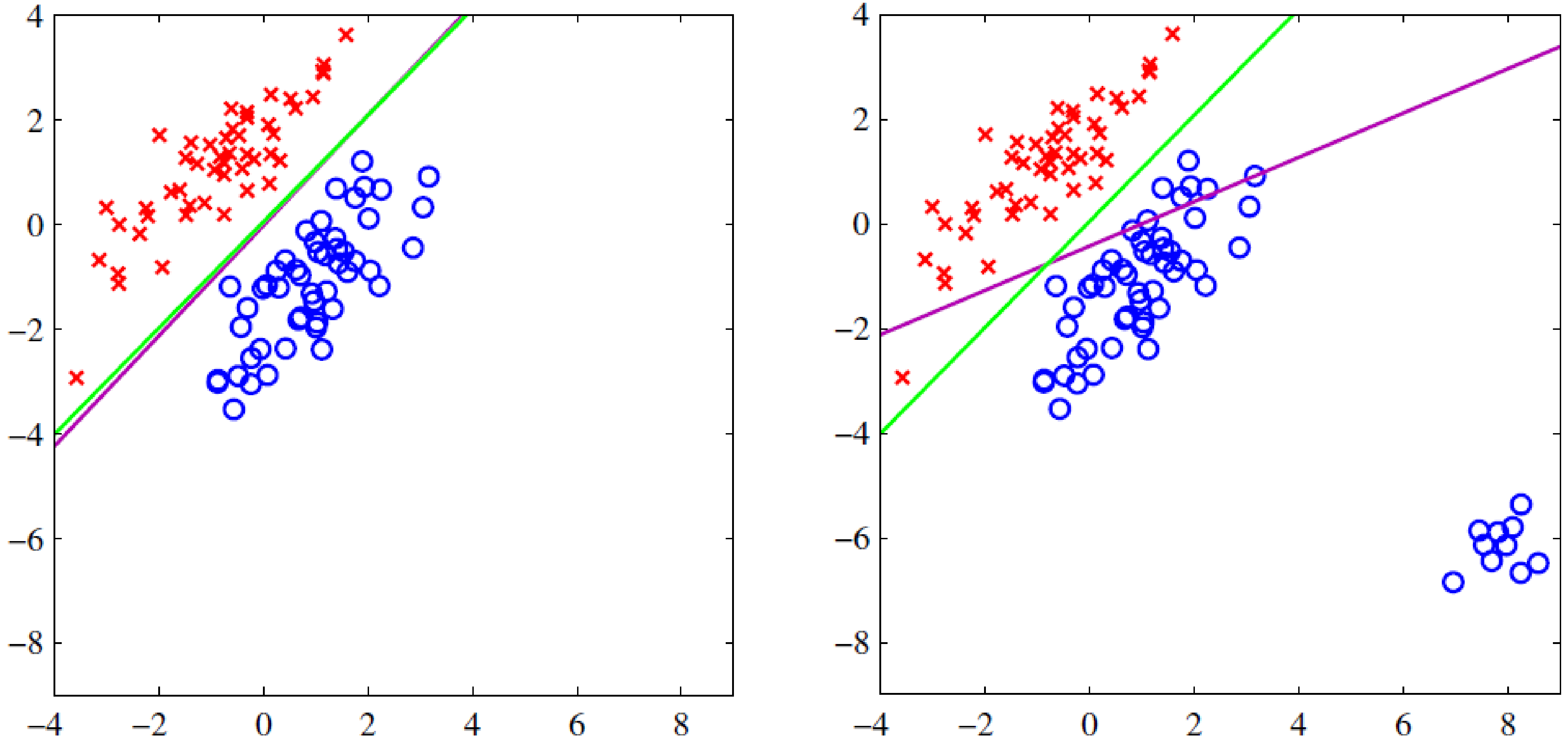


Figure 4.4 The left plot shows data from two classes, denoted by red crosses and blue circles, together with the decision boundary found by least squares (magenta curve) and also by the logistic regression model (green curve), which is discussed later in Section 4.3.2. The right-hand plot shows the corresponding results obtained when extra data points are added at the bottom left of the diagram, showing that least squares is highly sensitive to outliers, unlike logistic regression.

Bad idea even for binary classification

Figure from *Pattern Recognition and Machine Learning*, Bishop

Approach 2: one-versus-the-rest

- Find $K-1$ classifiers $f_1, f_2, \dots, f_{K-1}$
  - f_1 classifies $1\ vs\ \{2,3,\dots,K\}$
  - f_2 classifies $2\ vs\ \{1,3,\dots,K\}$
  - …
  - f_{K-1} classifies $K-1\ vs\ \{1,2,\dots,K-2\}$
  - Points not classified to classes $\{1,2,\dots,K-1\}$ are put to class K

- Problem of ambiguous region: some points may be classified to more than one classes

Approach 2: one-versus-the-rest

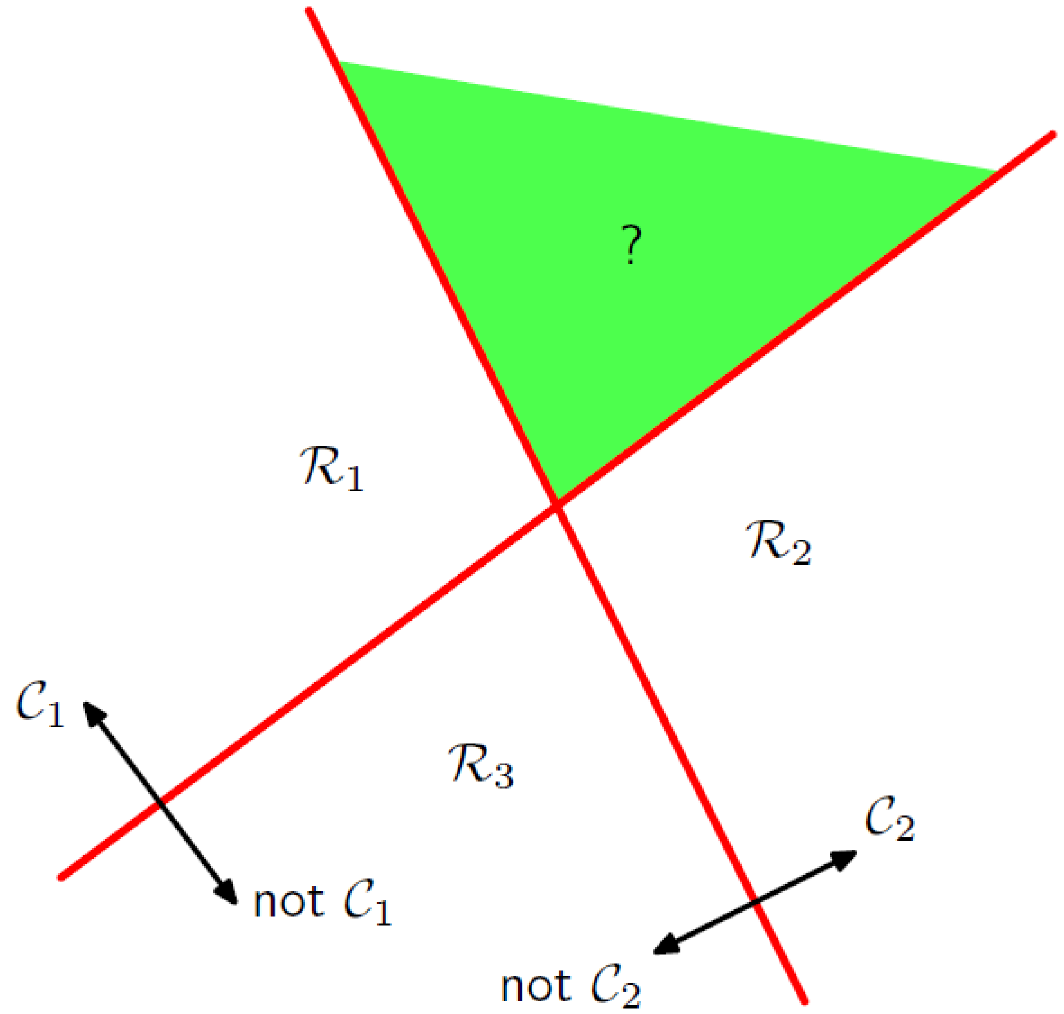


Figure from
Pattern Recognition and Machine Learning, Bishop

Approach 3: one-versus-one

- Find $(K-1)K/2$ classifiers $f_{(1,2)}, f_{(1,3)}, \dots, f_{(K-1,K)}$
  - $f_{(1,2)}$ classifies $1\ vs\ 2$
  - $f_{(1,3)}$ classifies $1\ vs\ 3$
  - …
  - $f_{(K-1,K)}$ classifies $K-1\ vs\ K$

- Computationally expensive: think of $K = 1000$
- Problem of ambiguous region

Approach 3: one-versus-one

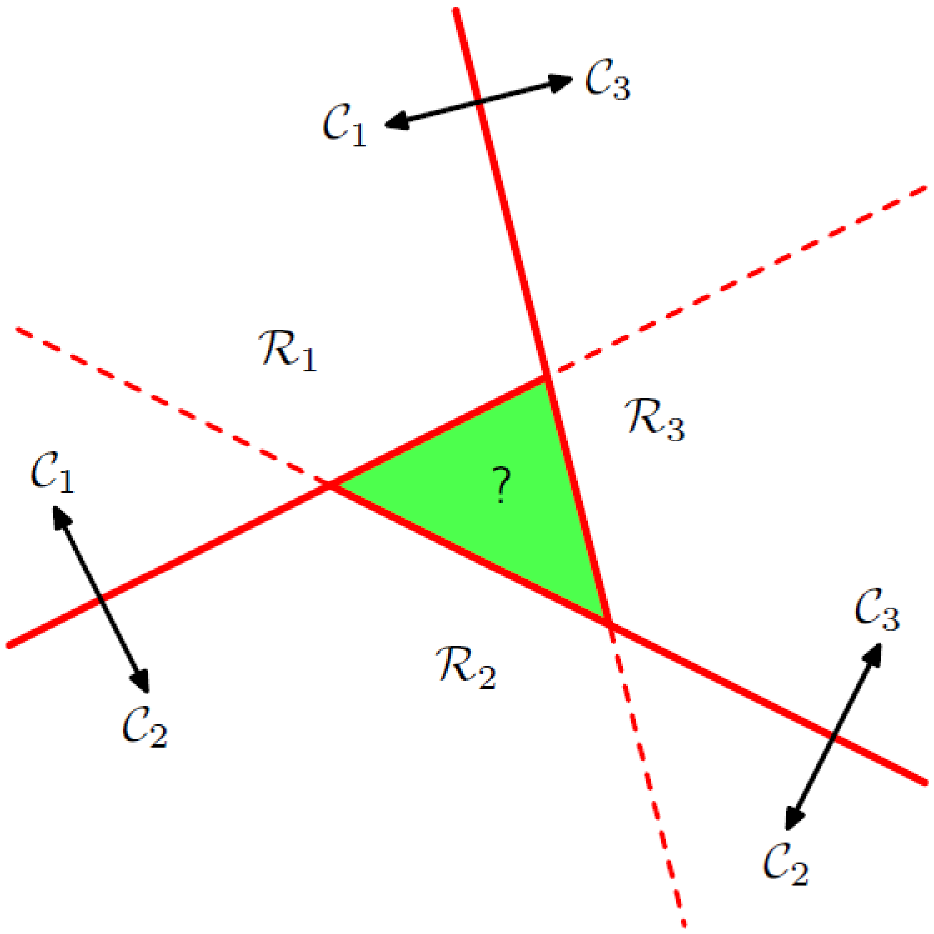


Figure from
Pattern Recognition and Machine Learning, Bishop

Approach 4: discriminant functions

- Find K scoring functions $s_1, s_2, \dots, s_K$
- Classify x to class $y = \text{argmax}_i \, s_i(x)$

- Computationally cheap
- No ambiguous regions

Linear discriminant functions

- Find K discriminant functions $s_1, s_2, \ldots, s_K$
- Classify x to class $y = \mathrm{argmax}_i \, s_i(x)$

- Linear discriminant: $s_i(x) = \left(w^i\right)^T x$, with $w^i \in R^d$

Linear discriminant functions

- Linear discriminant: $s_i(x) = \left(w^i\right)^T x$, with $w^i \in R^d$
- Lead to convex region for each class: by $y = \mathrm{argmax}_i \left(w^i\right)^T x$

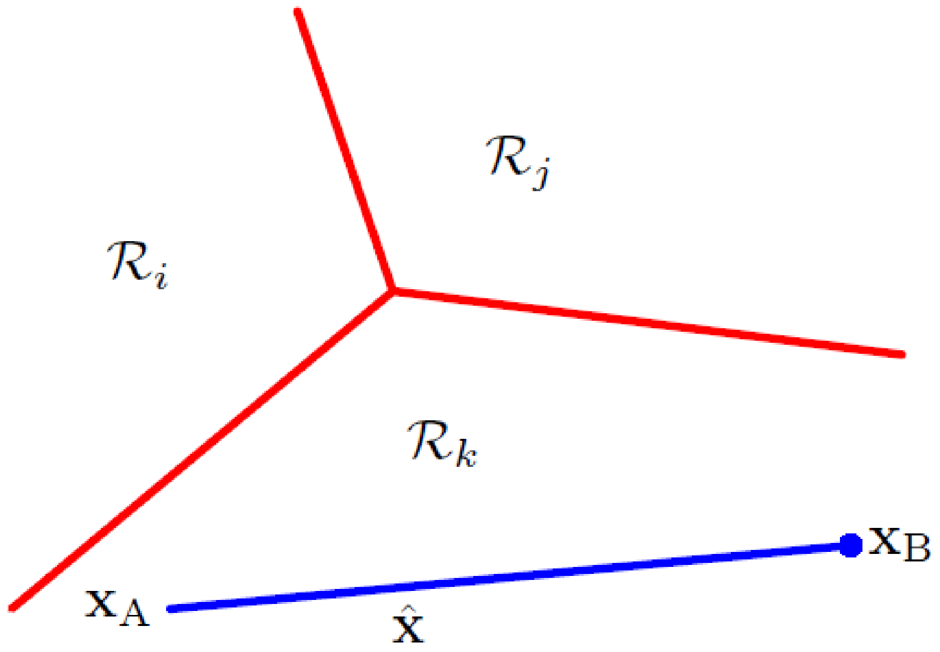


Figure from *Pattern Recognition and Machine Learning*, Bishop

Conditional distribution as discriminant

- Find K discriminant functions $s_1, s_2, \dots, s_K$
- Classify x to class $y = \mathrm{argmax}_i\, s_i(x)$

- Conditional distributions: $s_i(x) = p(y = i|x)$
- Parametrize by w^i: $s_i(x) = p_{w^i}(y = i|x)$

Multiclass logistic regression

Review: binary logistic regression

- Sigmoid

$$\sigma(w^T x + b) = \frac{1}{1 + \exp(-(w^T x + b))}$$

- Interpret as conditional probability

$$p_w(y = 1|x) = \sigma(w^T x + b)$$

$$p_w(y = 0|x) = 1 - p_w(y = 1|x) = 1 - \sigma(w^T x + b)$$

- How to extend to multiclass?

Review: binary logistic regression

- Suppose we model the class-conditional densities $p(x|y=i)$ and class probabilities $p(y=i)$
- Conditional probability by Bayesian rule:

$$p(y=1|x) = \frac{p(x|y=1)p(y=1)}{p(x|y=1)p(y=1) + p(x|y=2)p(y=2)} = \frac{1}{1+\exp(-a)} = \sigma(a)$$

where we define

$$a \coloneqq \ln \frac{p(x|y=1)p(y=1)}{p(x|y=2)p(y=2)} = \ln \frac{p(y=1|x)}{p(y=2|x)}$$

Review: binary logistic regression

- Suppose we model the class-conditional densities $p(x|y=i)$ and class probabilities $p(y=i)$
- $p(y=1|x) = \sigma(a) = \sigma(w^T x + b)$ is equivalent to setting log odds

$$a = \ln \frac{p(y=1|x)}{p(y=2|x)} = w^T x + b$$

- Why linear log odds?

Review: binary logistic regression

- Suppose the class-conditional densities $p(x|y=i)$ is normal

$$p(x|y=i) = N(x|\mu_i, I) = \frac{1}{(2\pi)^{d/2}} \exp\{-\frac{1}{2}||x-\mu_i||^2\}$$

- log odd is

$$a = \ln \frac{p(x|y=1)p(y=1)}{p(x|y=2)p(y=2)} = w^T x + b$$

where

$$w = \mu_1 - \mu_2, \qquad b = -\frac{1}{2}\mu_1^T \mu_1 + \frac{1}{2}\mu_2^T \mu_2 + \ln \frac{p(y=1)}{p(y=2)}$$

Multiclass logistic regression

- Suppose we model the class-conditional densities $p(x|y=i)$ and class probabilities $p(y=i)$
- Conditional probability by Bayesian rule:

$$p(y=i|x) = \frac{p(x|y=i)p(y=i)}{\sum_j p(x|y=j)p(y=j)} = \frac{\exp(a_i)}{\sum_j \exp(a_j)}$$

where we define

$$a_i \coloneqq \ln\left[p(x|y=i)p(y=i)\right]$$

Multiclass logistic regression

- Suppose the class-conditional densities $p(x|y=i)$ is normal

$$p(x|y=i) = N(x|\mu_i, I) = \frac{1}{(2\pi)^{d/2}} \exp\{-\frac{1}{2}||x-\mu_i||^2\}$$

- Then

$$a_i \coloneqq \ln\left[p(x|y=i)p(y=i)\right] = -\frac{1}{2}x^T x + \left(w^i\right)^T x + b^i$$

where

$$w^i = \mu_i, \qquad b^i = -\frac{1}{2}\mu_i^T \mu_i + \ln p(y=i) + \ln \frac{1}{(2\pi)^{d/2}}$$

Multiclass logistic regression

- Suppose the class-conditional densities $p(x|y=i)$ is normal

$$p(x|y=i) = N(x|\mu_i, I) = \frac{1}{(2\pi)^{d/2}} \exp\{-\frac{1}{2}||x-\mu_i||^2\}$$

- Cancel out $-\frac{1}{2}x^T x$, we have

$$p(y=i|x) = \frac{\exp(a_i)}{\sum_j \exp(a_j)}, \qquad a_i := (w^i)^T x + b^i$$

where

$$w^i = \mu_i, \qquad b^i = -\frac{1}{2}\mu_i^T \mu_i + \ln p(y=i) + \ln \frac{1}{(2\pi)^{d/2}}$$

Multiclass logistic regression: conclusion

- Suppose the class-conditional densities $p(x|y=i)$ is normal

$$p(x|y=i) = N(x|\mu_i, I) = \frac{1}{(2\pi)^{d/2}} \exp\{-\frac{1}{2}||x-\mu_i||^2\}$$

- Then

$$p(y=i|x) = \frac{\exp(\left(w^i\right)^T x + b^i)}{\sum_j \exp(\left(w^j\right)^T x + b^j)}$$

which is the hypothesis class for multiclass logistic regression

- It is softmax on linear transformation; it can be used to derive the negative log-likelihood loss (cross entropy)

Softmax

- A way to squash $a = (a_1, a_2, \dots, a_i, \dots)$ into probability vector p

$$\mathrm{softmax}(a) = \left(\frac{\exp(a_1)}{\sum_j \exp(a_j)}, \frac{\exp(a_2)}{\sum_j \exp(a_j)}, \dots, \frac{\exp(a_i)}{\sum_j \exp(a_j)}, \dots \right)$$

- Behave like max: when $a_i \gg a_j (\forall j \neq i)$, $p_i \cong 1, p_j \cong 0$

Cross entropy for conditional distribution

- Let $p_{\text{data}}(y|x)$ denote the empirical distribution of the data
- Negative log-likelihood

$$-\frac{1}{n}\sum_{i=1}^{n} \log p(y = y_i|x_i) = -\mathrm{E}_{p_{\text{data}}(y|x)} \log p(y|x)$$

is the cross entropy between p_{data} and the model output p

- Information theory viewpoint: KL divergence

$$D(p_{\text{data}}||p) = \mathrm{E}_{p_{\text{data}}}[\log \frac{p_{\text{data}}}{p}] = \underbrace{\mathrm{E}_{p_{\text{data}}}[\log p_{\text{data}}]}_{\text{Entropy; constant}} - \underbrace{\mathrm{E}_{p_{\text{data}}}[\log p]}_{\text{Cross entropy}}$$

Cross entropy for full distribution

- Let $p_{\text{data}}(x, y)$ denote the empirical distribution of the data
- Negative log-likelihood

$$-\frac{1}{n}\sum_{i=1}^{n} \log p(x_i, y_i) = -\mathrm{E}_{p_{\text{data}}(x,y)} \log p(x, y)$$

  is the cross entropy between p_{data} and the model output p

Multiclass logistic regression: summary