KUBIG
Data Science and Machine Learning

Week 2.
Regression and Classification

Announcements

Announcements

- 월요일은 선택, 목요일은 필수 참석
- 목요일 지각 및 결석은 쿠빅 내부 규정에 따른다.

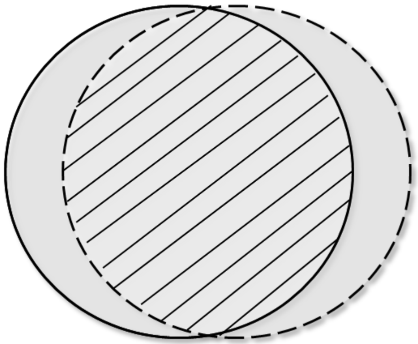
Statistics vs Machine Learning

전통적인 통계학

- 규칙의 통계적 추론에 중점 (전문적인 통계적, 수학적 지식)
- 자료의 특성(다변량, 시계열, 범주형 등)에 따라 분석.

통계적 머신러닝

- 규칙의 일반화에 중점
- 목적변수의 관측여부에 따라 지도학습, 비지도학습으로 분석



——— 통계학

– – – 통계적 머신러닝

Corrections

- Assumptions about the Errors: Normality Assumption
  - 적률가정은 정규성을 요구하지 않는다.
  - Gauss-Markov 정리는 적률가정만 요구하며 정규성을 요구하지 않는다.
  - Normality Assumption은 MLE 증명과 Error Analysis, 가설검정 및 신뢰구간 에 중요하다.

Corrections

Plots of the standardized residuals

- Plot (a) suggests a quadratic term in X.
- Plot (b) shows non-constant error.

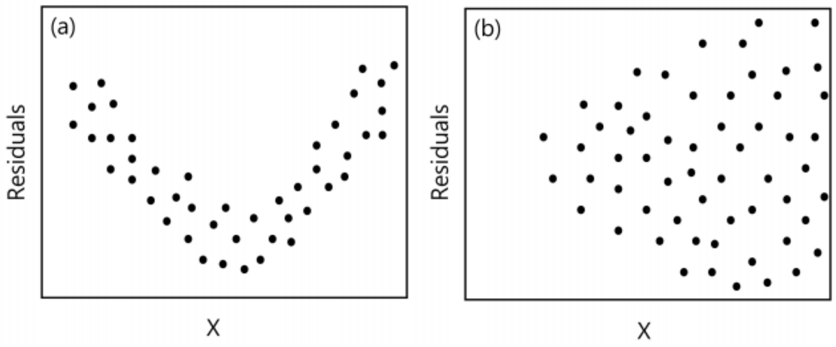


Figure: Two scatter plots of residuals versus X illustrating violations of model assumptions.

Learning Objectives

Learning Objectives

Review

- Risk Function

$$R(\theta, T(X)) = E[L(\tau(\theta), T(X))] \approx \frac{1}{n} L(\tau(\theta), T(X))$$

- Loss Function

$$L[\tau(\theta), T(X)] = \sum (Y_i - \hat{Y}_i)^2 \qquad \Rightarrow SSE\ (MSE)$$

$$= \sum |Y_i - \hat{Y}_i| \qquad \Rightarrow SAE\ (MAE)$$

Review

- Regression

$$Y_i \overset{ind}{\sim} \mathrm{N}(\mu_i(\mathbf{X}_i),\ \sigma) \qquad \text{where} \quad E[Y_i] = \mu_i(\mathbf{X}_i)$$

$$\mu_i(\mathbf{X}_i) = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_p X_{pi} = \boldsymbol{\beta}^T \mathbf{X}_i$$

$$\boldsymbol{\mu}(\mathbf{X}) = \mathbf{X}\ \boldsymbol{\beta}$$

Review

- Likelihood

$$\mathbf{Y} \sim N_n(\boldsymbol{\mu}(\mathbf{X}),\ \sigma\mathbf{I}) \quad \text{where} \quad E[\mathbf{Y}] = \boldsymbol{\mu}(\mathbf{X}) = \mathbf{X}\,\boldsymbol{\beta}$$

$$L(\boldsymbol{\mu}, \Sigma) = \frac{1}{(2\pi)^{\frac{n}{2}}|\det\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{Y}-\boldsymbol{\mu})^T\Sigma^{-1}(\mathbf{Y}-\boldsymbol{\mu})\right)$$

$$\Rightarrow \quad L(\boldsymbol{\beta}, \sigma) = \frac{1}{(2\pi)^{\frac{n}{2}}|\det\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2\sigma}(\mathbf{Y}-\mathbf{X}\boldsymbol{\beta})^T(\mathbf{Y}-\mathbf{X}\boldsymbol{\beta})\right)$$

Review

- Likelihood

$$l(\boldsymbol{\beta},\sigma) = \log L(\boldsymbol{\beta},\sigma) = -\frac{n}{2}\log(2\pi) - \frac{1}{2}\log|\det\Sigma| - \frac{1}{2\sigma}(\mathbf{Y}-\mathbf{X}\boldsymbol{\beta})^T(\mathbf{Y}-\mathbf{X}\boldsymbol{\beta})$$

$$\frac{\partial}{\partial\boldsymbol{\beta}} l(\boldsymbol{\beta},\sigma) = \mathbf{X}^T(\mathbf{Y}-\mathbf{X}\boldsymbol{\beta}) \overset{set}{=} 0$$

$$\text{Normal equation : } (\mathbf{X}^T\mathbf{X})\boldsymbol{\beta} = \mathbf{X}^T\mathbf{Y}$$

Review

- Estimation

$$\underset{\boldsymbol{\beta}}{argmin} \sum (Y_i - \hat{Y}_i)^2 \iff \underset{\boldsymbol{\beta}}{argmax}\, L(\boldsymbol{\beta}, \sigma)$$

$$\text{Normal equation :}\quad (\mathbf{X}^T\mathbf{X})\boldsymbol{\beta} = \mathbf{X}^T\mathbf{Y}$$

$$\widehat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

Logistic Regression

$$Y_i \overset{ind}{\sim} \text{Bernoulli}(\pi_i(\mathbf{X}_i)) \quad \text{where} \quad E[Y_i] = \pi_i(\mathbf{X}_i)$$

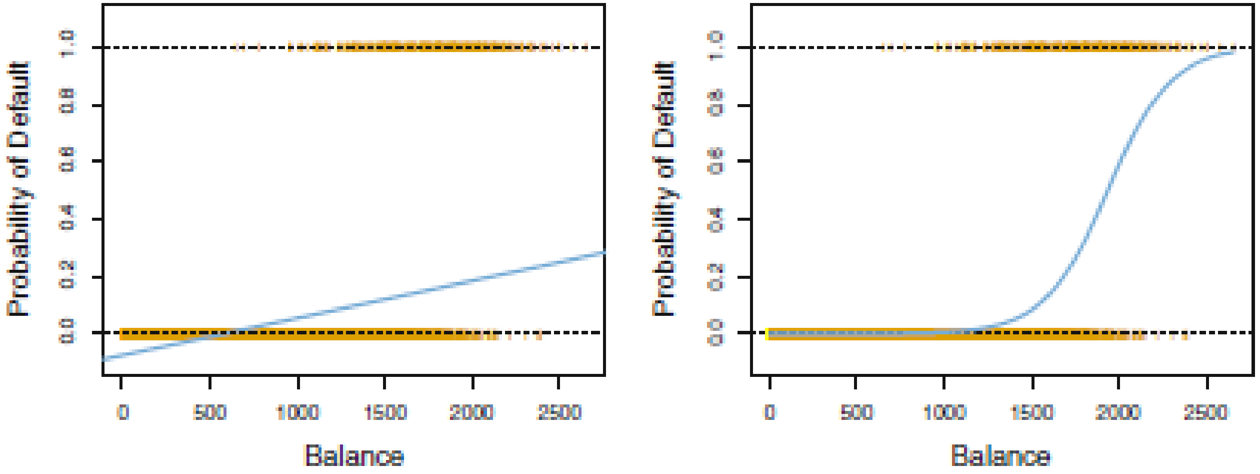
$$\log\left(\frac{\pi_i(\mathbf{X}_i)}{1-\pi_i(\mathbf{X}_i)}\right) = \beta_0 + \beta_1 X_{1\mathrm{i}} + \beta_2 X_{2\mathrm{i}} + \cdots + \beta_p X_{p\mathrm{i}}$$

Logistic Regression

$$\mathrm{P}(Y_i = 1|\mathbf{X}_i) = \pi_i(\mathbf{X}_i) = \frac{e^{\beta_0+\beta_1 X_{1i}+\beta_2 X_{2\mathrm{i}}+\cdots+\beta_p X_{p\mathrm{i}}}}{1+e^{\beta_0+\beta_1 X_{1i}+\beta_2 X_{2\mathrm{i}}+\cdots+\beta_p X_{p\mathrm{i}}}}$$

$$= \frac{e^{\boldsymbol{\beta}^T \mathbf{x}_i}}{1+e^{\boldsymbol{\beta}^T \mathbf{x}_i}} = \frac{1}{1+e^{-\boldsymbol{\beta}^T \mathbf{x}_i}}$$ (sigmoid function)

Logistic Regression



Logistic Regression

- How to Estimate? $\underset{\boldsymbol{\beta}}{argmax}\ L(\boldsymbol{\beta})$

$$L(\boldsymbol{\pi};\mathbf{X}) = \prod_{i=1}^{n} \pi_i^{y_i}\,(1-\pi_i)^{1-y_i}$$

$$l(\boldsymbol{\pi};\mathbf{X}) = \sum_{i=1}^{n} [\,y_i \log \pi_i + (1-y_i)\log(1-\pi_i)]$$

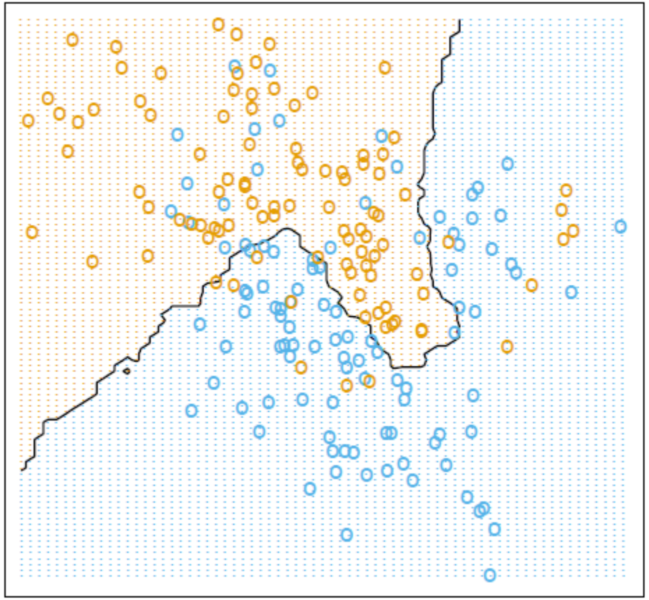
Logistic Regression

- How to Estimate?

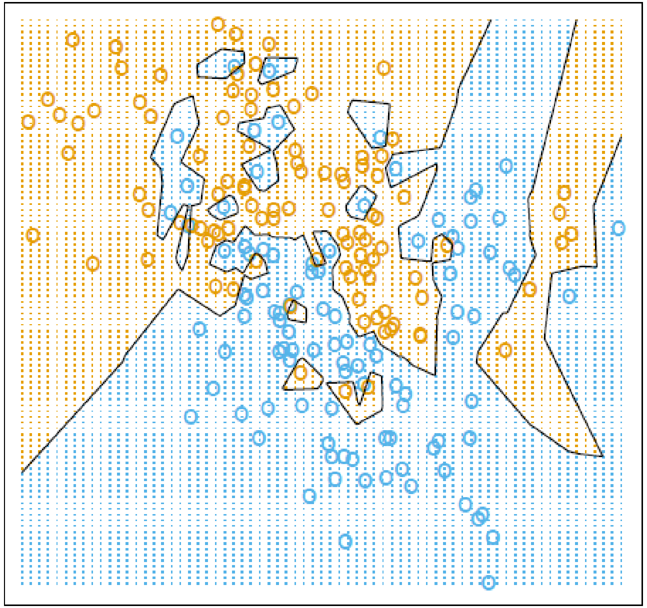
```
> fit.indep = glm(count ~ G + I + H, family=poisson(link=log), data=data2)
> summary(fit.indep) # loglinear model (G, I, H)

Call:
glm(formula = count ~ G + I + H, family = poisson(link = log),
    data = data2)

Deviance Residuals:
       1         2         3         4         5         6         7
-0.01163   0.62672  -2.14775  -0.15776   1.27750  -1.49031  -1.57956
       8
 2.22245

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)  3.53231    0.11459  30.826  < 2e-16 ***
Gmale       -0.28205    0.08106  -3.480 0.000502 ***
Isupport     1.77495    0.11399  15.571  < 2e-16 ***
Hsupport    -0.69315    0.08513  -8.143 3.87e-16 ***
---
```

KNN Classifier

15-Nearest Neighbor Classifier



1−Nearest Neighbor Classifier

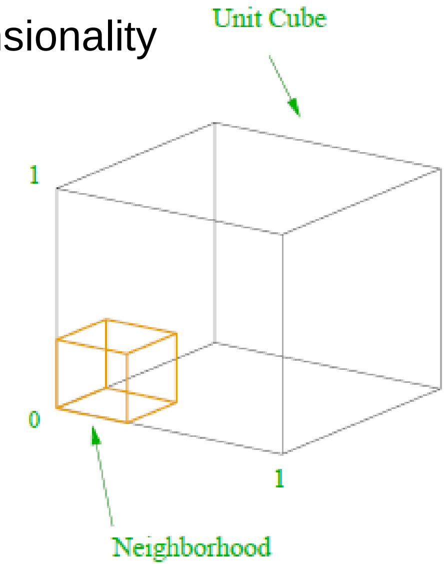


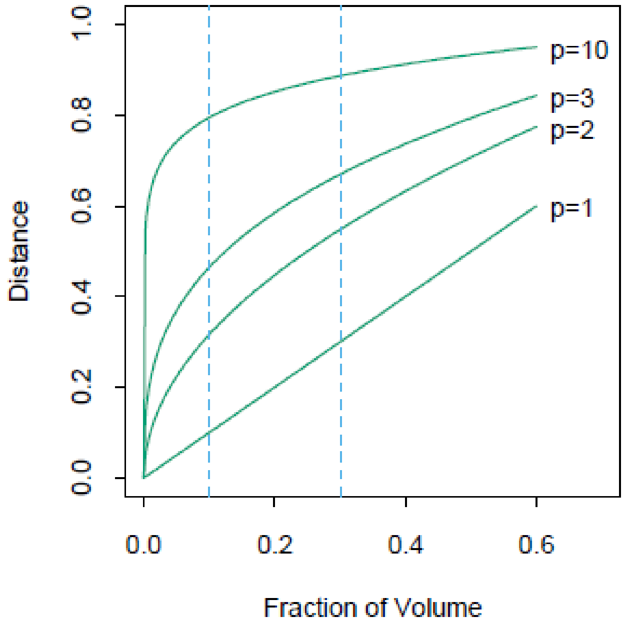
KNN Classifier

- Scenario 1
  - The training data in each class were generated from bivariate Gaussian distributions with uncorrelated components and different means.
- Scenario 2
  - The training data in each class came from a mixture of 10 low-variance Gaussian distributions, with individual means themselves distributed as Gaussian.

KNN Classifier

- Curse of dimensionality





KNN Classifier

- Distance measure

$$d(\mathbf{u},\mathbf{v}) = \left(\sum |u_i - v_i|^2\right)^{\frac{1}{2}} = ||\mathbf{u}-\mathbf{v}||_2 \qquad \textit{Euclidean (L2 norm)}$$

$$d(\mathbf{u},\mathbf{v}) = \sum |u_i - v_i| = ||\mathbf{u}-\mathbf{v}||_1 \qquad \textit{Manhattan (L1 norm)}$$

$$d(\mathbf{u},\mathbf{v}) = \left(\sum |u_i - v_i|^p\right)^{\frac{1}{p}} = ||\mathbf{u}-\mathbf{v}||_p \qquad \textit{Minkowski (Lp norm)}$$

$$d(\mathbf{u},\mathbf{v}) = \sqrt{(\mathbf{x}-\boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x}-\boldsymbol{\mu})} \qquad \textit{Mahalanobis Distance}$$

Kernel Density Estimation

- Kernel function

$$K(\mathbf{x}_i, \mathbf{x}_j) = \text{exp}(-\gamma(\mathbf{x}_i - \mathbf{x}_j)^T(\mathbf{x}_i - \mathbf{x}_j))$$

Gaussian Kernel (Radial Basis function)

$$K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^p$$

polynomial Kernel

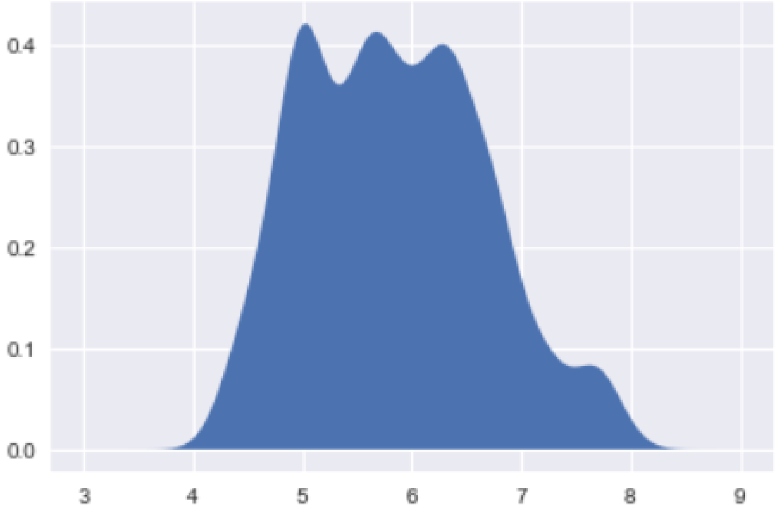
$$K(\mathbf{x}_i, \mathbf{x}_j) = \text{tanh}(k_1 \mathbf{x}_i^T \mathbf{x}_j + k_2)$$

Sigmoid Kernel

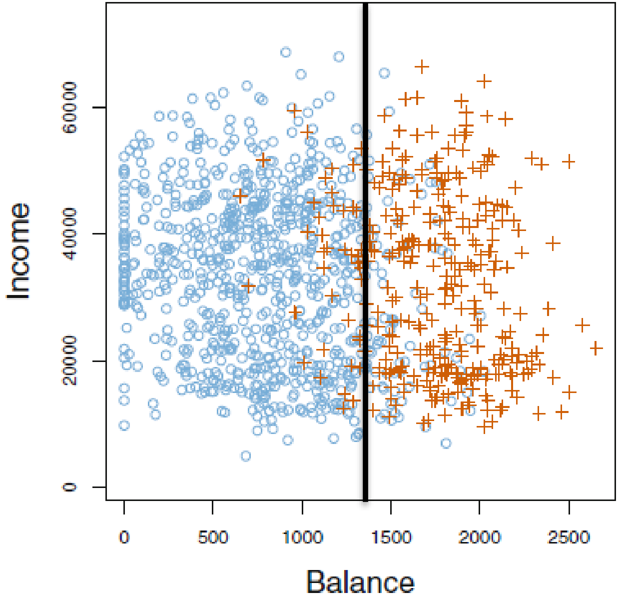
Kernel Density Estimation

- Density estimation at $x = x_0$

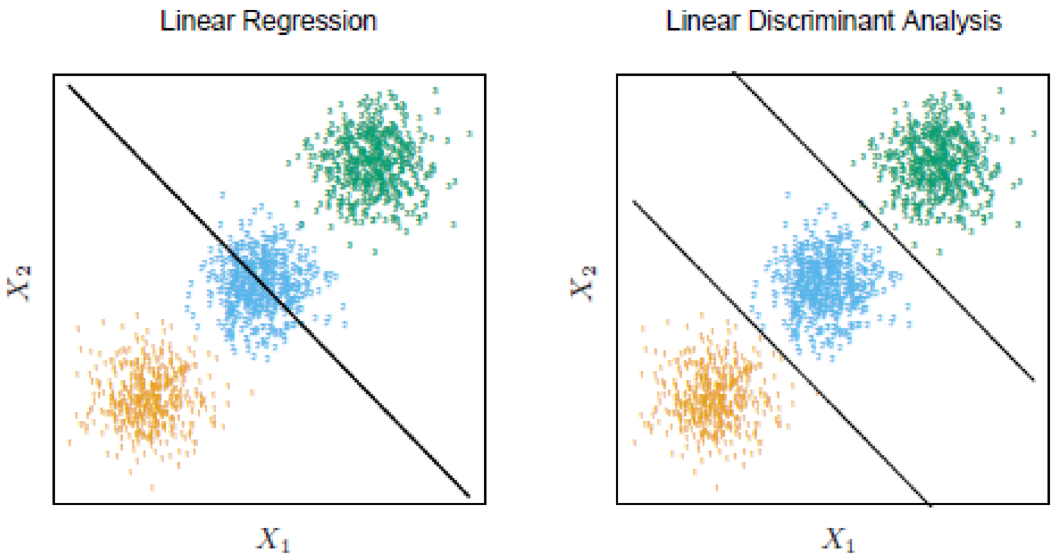
$$\widehat{f_X}(x_0) = \frac{1}{n}\sum K(x_0, x_i)$$



Classification with regression



Discriminant Analysis



Naïve Bayes Classifier

$$P(Y_i = k|\mathbf{X}_i) = \frac{P(\mathbf{X}_i|k)P(k)}{\sum_k P\,(\mathbf{X}_i|k)P(k)} \qquad Bayes'\ Theorem$$

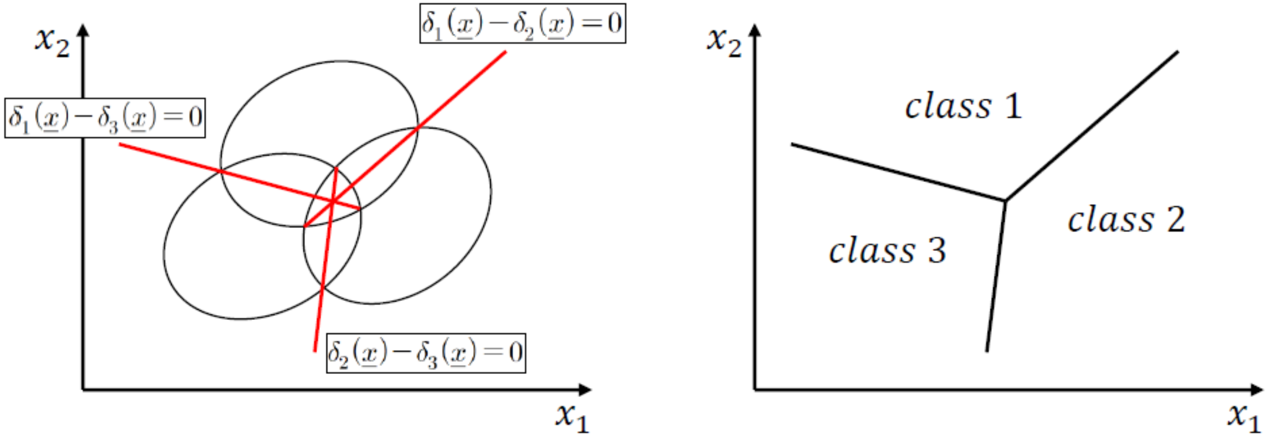
$$\text{where}\quad P(\mathbf{X}_i|k) = \prod_j^p P\,(X_{ij}|k)$$

Linear Discriminant Analysis

$$P(Y_i = k|\mathbf{X}_i) = \frac{P(\mathbf{X}_i|k)P(k)}{\sum_k P\,(\mathbf{X}_i|k)P(k)} \qquad Bayes'\ Theorem$$

$$\text{where}\quad P(\mathbf{X}_i|k) \sim N_p(\boldsymbol{\mu}_k, \Sigma)$$

Linear Discriminant Analysis



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Linear Discriminant Analysis

$$\text{IF } P(Y_i = k|\mathbf{X}_i) > P(Y_i = l|\mathbf{X}_i) \rightarrow \textit{estimate class of } Y_i \textit{ to } k$$

$$\log \frac{P(Y_i = k|\mathbf{X}_i)}{P(Y_i = l|\mathbf{X}_i)} = \delta_k(\mathbf{X}_i) - \delta_l(\mathbf{X}_i)$$

$$\textit{where} \quad \delta_k(\mathbf{X}_i) = \mathbf{X}_i^T \Sigma^{-1} \boldsymbol{\mu}_k - \frac{1}{2} \boldsymbol{\mu}_k^T \Sigma^{-1} \boldsymbol{\mu}_k + \log P(k)$$

Quadratic Discriminant Analysis

$$P(Y_i = k|\mathbf{X}_i) = \frac{P(\mathbf{X}_i|k)P(k)}{\sum_k P\,(\mathbf{X}_i|k)P(k)} \qquad Bayes'\ Theorem$$

$$\text{where} \quad P(\mathbf{X}_i|k) \sim N_p(\boldsymbol{\mu}_k, \Sigma_k)$$

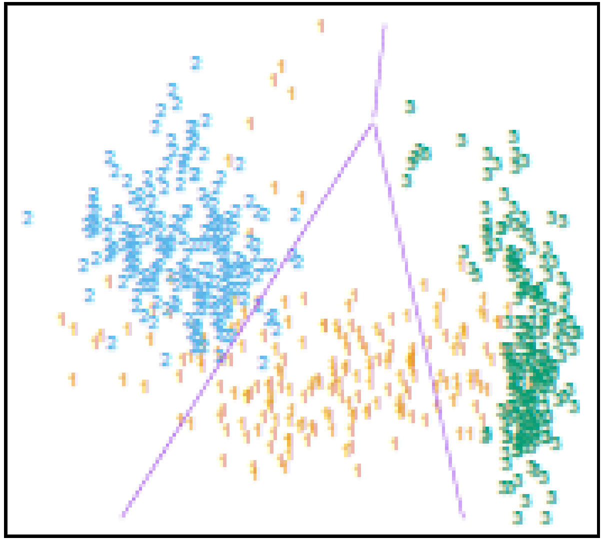
Quadratic Discriminant Analysis

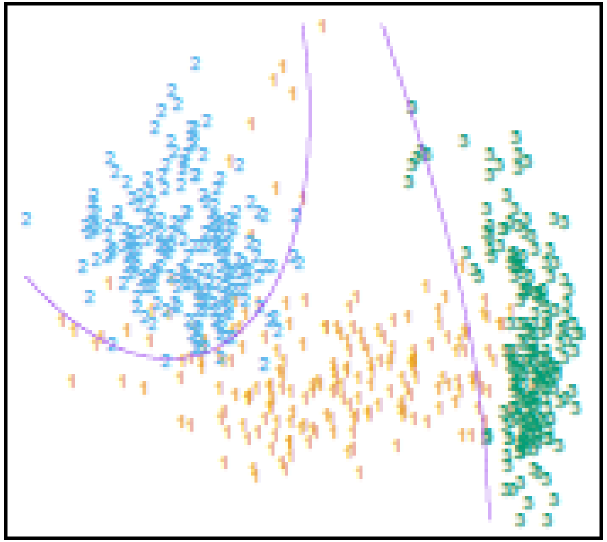
$$\text{IF}\;\; P(Y_i = k|\mathbf{X}_i) > P(Y_i = l|\mathbf{X}_i) \;\rightarrow\; estimate\ class\ of\ Y_i\ to\ k$$

$$\log\frac{P(Y_i = k|\mathbf{X}_i)}{P(Y_i = l|\mathbf{X}_i)} = \delta_k(\mathbf{X}_i) - \delta_l(\mathbf{X}_i)$$

$$where\;\; \delta_k(\mathbf{X}_i) = -\frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(\mathbf{X}_i - \boldsymbol{\mu}_k)^T{\Sigma_k}^{-1}(\mathbf{X}_i - \boldsymbol{\mu}_k) + \log P(k)$$

LDA and QDA





Loss Function for Classification

- 0-1 Loss

$$L[\tau(\theta), T(X)] = \sum I(Y_i \neq \hat{Y}_i)$$

- The Bayes decision rule for minimizing the loss ($\mathrm{P}\left(Y_i \neq \hat{Y}_i\right)$) is

$$\underset{\mathrm{k}}{argmax}\, P(Y = k|\mathbf{X})$$

Loss Function for Classification

- Categorical Cross Entropy

$$CE_i = -\sum_{k=1}^{C} y_{ik} \log \pi_i(k)$$

- Binary Cross Entropy

$$CE_i = -[y_{i1} \log \pi_i(1) + y_{i0} \log \pi_i(0)]$$

$$= -[y_i \log \pi_i + (1 - y_i) \log(1 - \pi_i)]$$

Loss Function for Classification

- Binary Cross Entropy

$$\sum_{i=1}^{n} CE_i = -\sum_{i=1}^{n}[\, y_i \log\pi_i + (1 - y_i) \log(1 - \pi_i \,)]$$

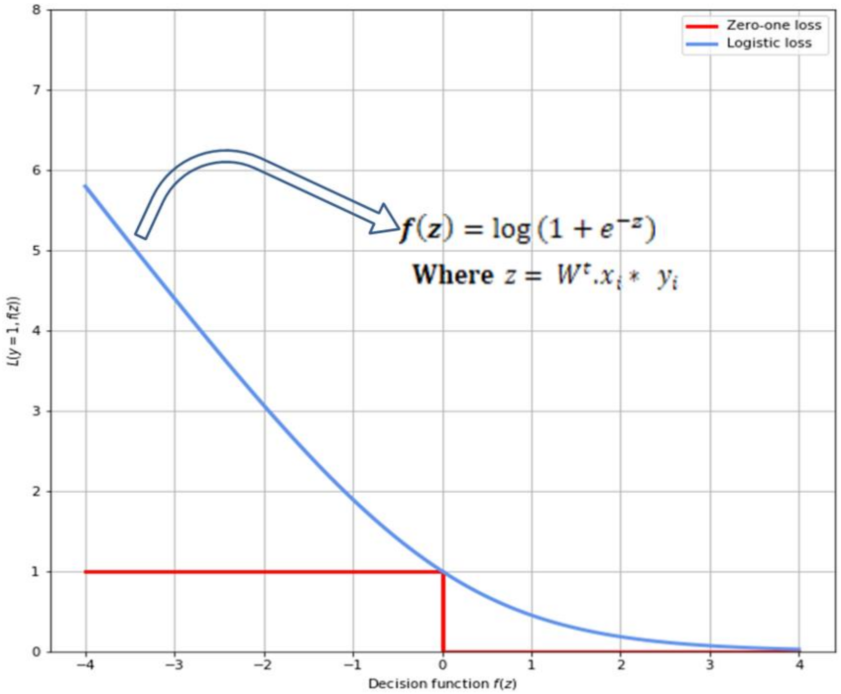
$$l(\boldsymbol{\pi}; \mathbf{X}) = \sum_{i=1}^{n}[\, y_i\log\pi_i + (1 - y_i)\log(1 - \pi_i)]$$

Loss Function for Classification

- For Logistic Regression

$$\underset{\boldsymbol{\beta}}{argmin}\ "Cross\ Entropy" \iff \underset{\boldsymbol{\beta}}{argmax}\ "Likelihood"$$

Loss Function for Classification



Information Theory and Entropy

$$H = -\sum_{i=1}^{N} p_i \log(p_i)$$

reference

자료

19-2 STAT424 통계적 머신러닝 - 박유성 교수님

교재

파이썬을 이용한 통계적 머신러닝 (2020) – 박유성

ISLR (2013) - G. James, D. Witten, T. Hastie, R. Tibshirani

The elements of Statistical Learning (2001) - J. Friedman, T. Hastie, R. Tibshirani

Hands on Machine Learning (2017) - Aurelien Geron