09 - Classification

Logistic Regression, Discriminant Analysis, and Naive Bayes

SYS 6018 | Fall 2019

09-classification.pdf

Contents

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1 Classification Intro

1.1 Credit Card Default data (`Default`)

The textbook *An Introduction to Statistical Learning (ISL)* has a description of a simulated credit card default dataset. The interest is on predicting whether an individual will default on their credit card payment.

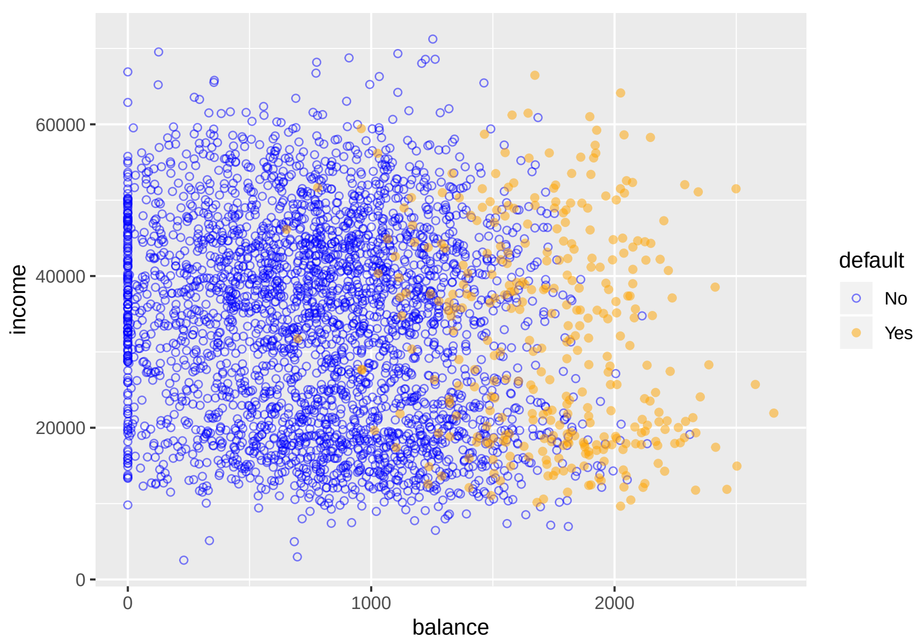
```
data(Default, package="ISLR")
```

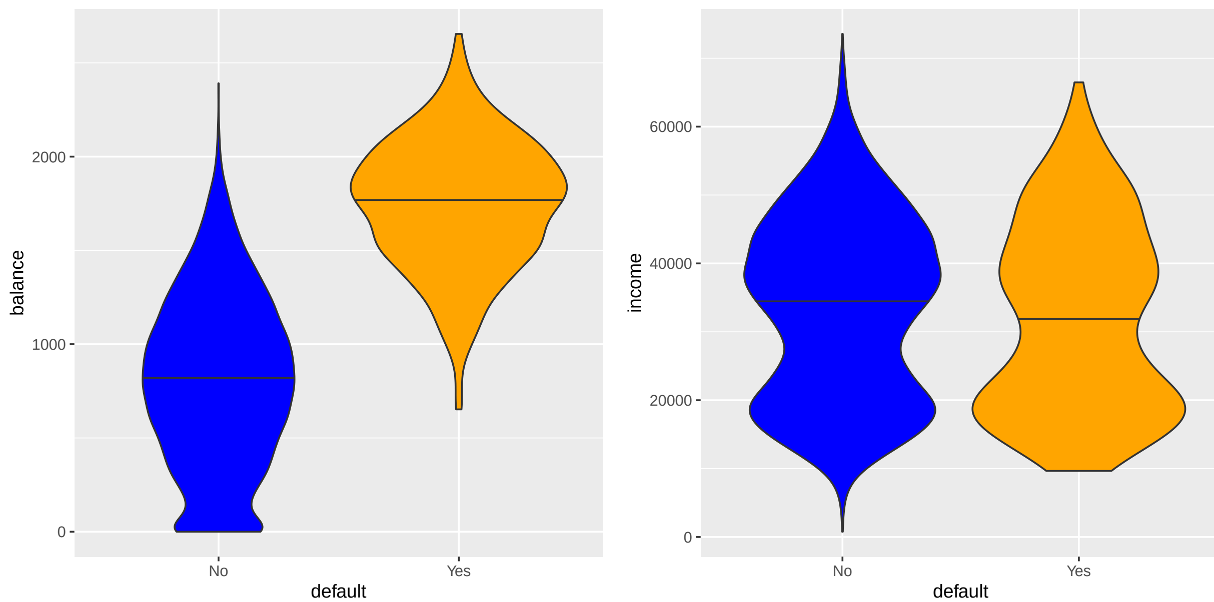
The variables are:

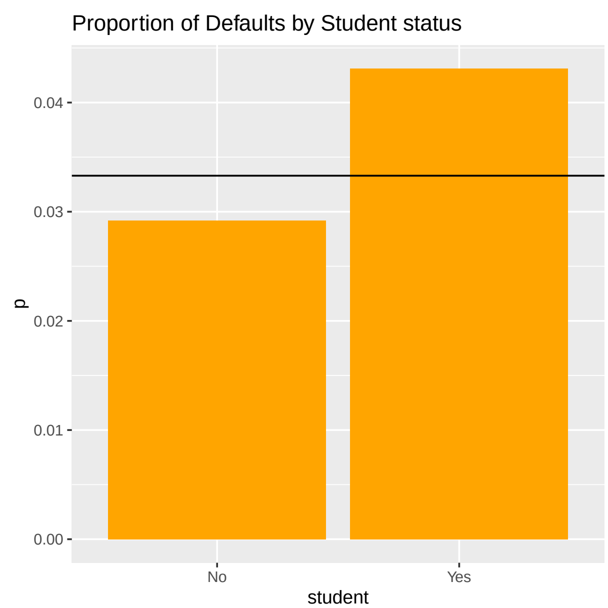
- *response variable* is categorical (factor) `Yes` and `No`, (`default`)
- the categorical (factor) variable (`student`) is either `Yes` or `No`
- the average balance a customer has after making their monthly payment (`balance`)
- the customer's income (`income`)

default	student	balance	income
No	No	729.5	44362
No	Yes	817.2	12106
No	No	1073.5	31767
No	No	529.3	35704
No	No	785.7	38463
No	Yes	919.6	7492

```
summary(Default)
#>  default    student       balance         income     
#>  No :9667   No :7056   Min.   :   0   Min.   :  772  
#>  Yes: 333   Yes:2944   1st Qu.: 482   1st Qu.:21340  
#>                        Median : 824   Median :34553  
#>                        Mean   : 835   Mean   :33517  
#>                        3rd Qu.:1166   3rd Qu.:43808  
#>                        Max.   :2654   Max.   :73554  
```




balance
2000
1000
0
No
Yes
default
income
60000
40000
20000
0
No
Yes
default


Proportion of Defaults by Student status
p
0.04
0.03
0.02
0.01
0.00
No
Yes
student

Your Turn #1 : Credit Card Default Modeling

How would you construct a model to predict defaults?

2 Classification and Pattern Recognition

- The response variable is categorical and denoted $G \in \mathcal{G}$
  - Default Credit Card Example: $\mathcal{G} = \{$"Yes", "No"$\}$
  - Medical Diagnosis Example: $\mathcal{G} = \{$"stroke", "heart attack", "drug overdose", "vertigo"$\}$
- The training data is $D = \{(X_1, G_1), (X_2, G_2), \ldots, (X_n, G_n)\}$
- The optimal decision/classification is often based on the posterior probability $\Pr(G = g \mid \mathbf{X} = \mathbf{x})$

2.1 Binary Classification

- Classification is simplified when there are only 2 classes.
  - Many multi-class problems can be addressed by solving a set of binary classification problems (e.g., one-vs-rest).
- It is often convenient to *code* the response variable to a binary $\{0, 1\}$ variable:

$$Y_i = \begin{cases} 1 & G_i = \mathcal{G}_1 \quad \text{(outcome of interest)} \\ 0 & G_i = \mathcal{G}_2 \end{cases}$$

- In the `Default` data, it would be natural to set `default=Yes` to 1 and `default=No` to 0.

2.1.1 Linear Regression

- In this set-up we can run linear regression

$$\hat{y}(\mathbf{x}) = \hat{\beta}_0 + \sum_{j=1}^{p} \hat{\beta}_j x_j$$

```
#-- Create binary column (y)
Default = Default %>% mutate(y = ifelse(default == "Yes", 1L, 0L))

#-- Fit Linear Rergression Model
fit.lm = lm(y~student + balance + income, data=Default)
```

term	estimate	std.error	statistic	p.value
(Intercept)	-0.0812	0.0084	-9.685	0.0000
studentYes	-0.0103	0.0057	-1.824	0.0682
balance	0.0001	0.0000	37.412	0.0000
income	0.0000	0.0000	1.039	0.2990

Your Turn #2 : OLS for Binary Responses

1. For the binary Y, what is linear regression estimating?

2. What is the *loss function* that linear regression is using?

3. How could you create a *hard classification* from the linear model?

4. Does is make sense to use linear regression for binary classification?

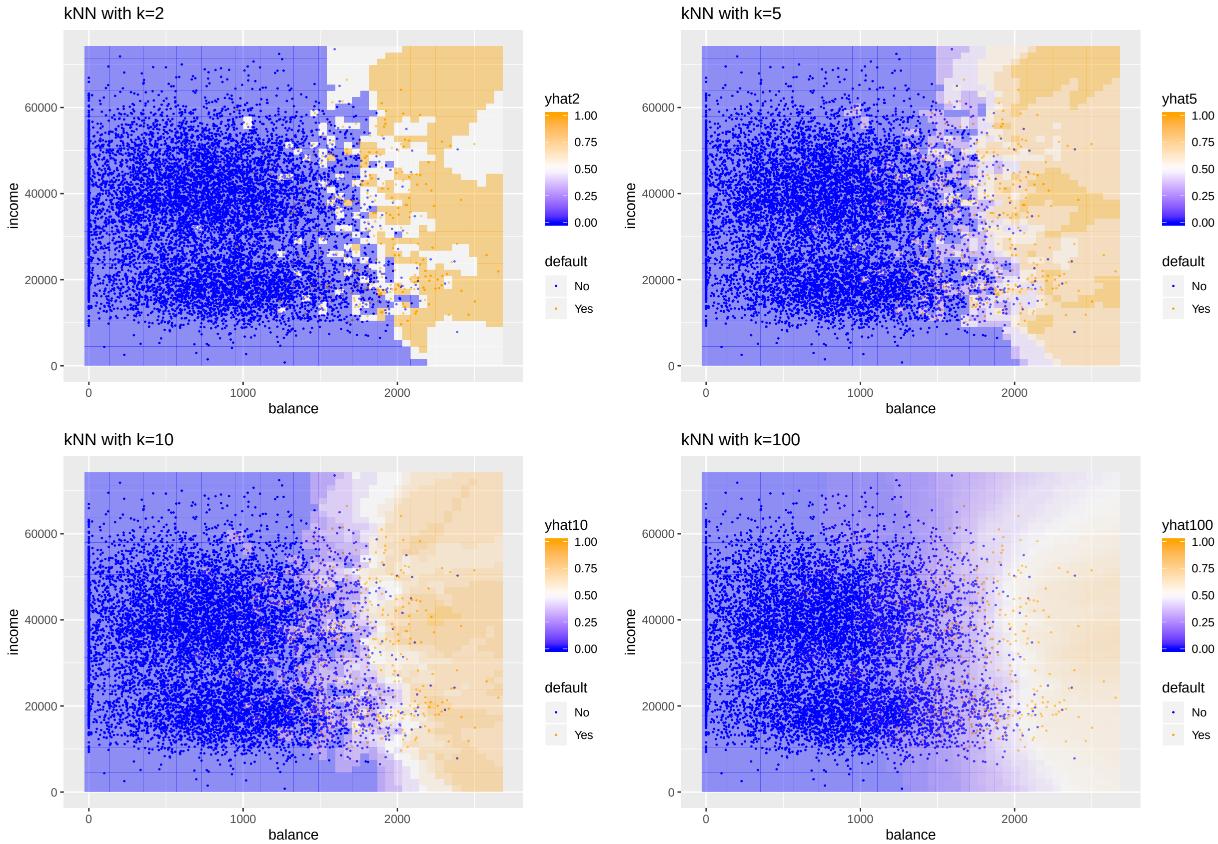
2.1.2 k-nearest neighbor (kNN)

- The k-NN method is a non-parametric *local* method, meaning that to make a prediction $\hat{y}|x$, it only uses the training data in the *vicinity* of x.
  - contrast with OLS linear regression, which uses all X's to get prediction.
- The model (for regression and binary classification) is simple to describe

$$
\begin{aligned}
f_{\text{knn}}(x;k) &= \frac{1}{k} \sum_{i:x_i \in N_k(x)} y_i \\
&= \text{Avg}(y_i \mid x_i \in N_k(x))
\end{aligned}
$$

  - $N_k(x)$ are the set of k nearest neighbors
  - only the k closest y's are used to generate a prediction
  - it is a *simple mean* of the k nearest observations
- When y is binary (i.e., $y \in \{0, 1\}$), the kNN model estimates

$$f_{\text{knn}}(x;k) \approx p(x) = \Pr(Y = 1|X = x)$$



Your Turn #3 : Thoughts about kNN

The above plots show a kNN model using the *continuous* predictors of `balance` and `income`.

- How could you use kNN with the categorical `student` predictor?

- The k-NN model also has a more general description when the response variables is categorical $G_i \in \mathcal{G}$

$$
\begin{aligned}
f_g^{\text{knn}}(x; k) &= \frac{1}{k} \sum_{i: x_i \in N_k(x)} \mathbb{1}(g_i = g) \\
&= \widehat{\Pr}(G_i = g \mid x_i \in N_k(x))
\end{aligned}
$$

  - $N_k(x)$ are the set of k nearest neighbors
  - only the k closest y's are used to generate a prediction
  - it is a *simple proportion* of the k nearest observations that are of class g

3 Logistic Regression

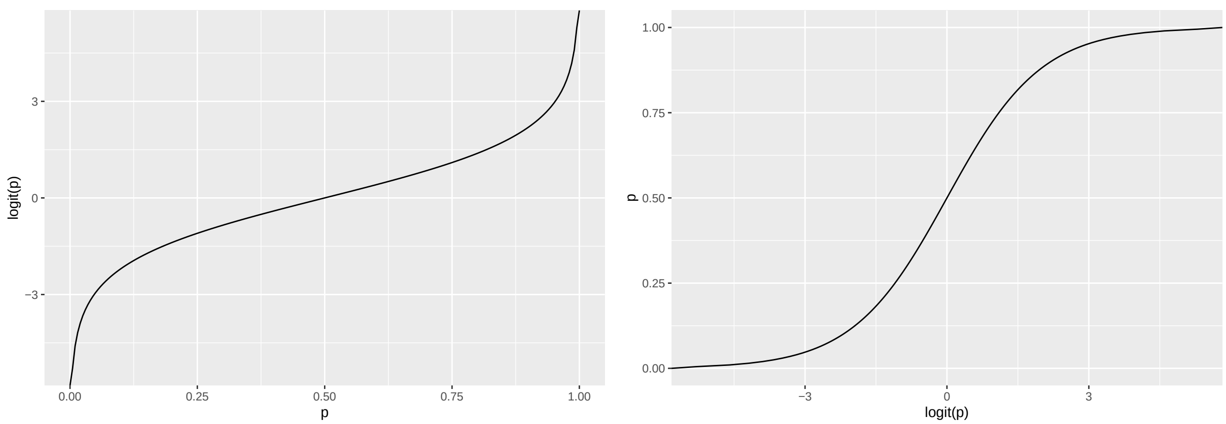
3.1 Basics

- Let $0 \leq p \leq 1$ be a probability.
- The log-odds of p is called the *logit*

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

- The inverse logit is the *logistic function*. Let $f = \text{logit(p)}$, then

$$\begin{aligned} p &= \frac{e^f}{1+e^f} \\ &= \frac{1}{1+e^{-f}} \end{aligned}$$



- For binary response variables $Y \in \{0, 1\}$, linear regression models estimate

$$\text{E}[Y \mid X = x] = \Pr(Y = 1 \mid X = x) = \beta^\mathsf{T} x$$

- Logistic Regression models alternatively estimate

$$\log\left(\frac{\Pr(Y = 1 \mid X = x)}{1 - \Pr(Y = 1 \mid X = x)}\right) = \beta^\mathsf{T} x$$

and thus,

$$\begin{aligned} \Pr(Y = 1 \mid X = x) &= \frac{e^{\beta^\mathsf{T} x}}{1 + e^{\beta^\mathsf{T} x}} \\ &= \left(1 + e^{-\beta^\mathsf{T} x}\right)^{-1} \end{aligned}$$

3.2 Estimation

- The data for logistic regression is: $(\mathbf{x}_i, y_i)_{i=1}^n$ where $y_i \in \{0, 1\}$, $\mathbf{x}_i = (x_{i0}, x_{i1}, \ldots, x_{ip})^\mathsf{T}$.
- $y_i \mid \mathbf{x}_i \sim \text{Bern}(p_i(\beta))$
  - $p_i(\beta) = \Pr(Y = 1 \mid \mathbf{X} = \mathbf{x}_i; \beta) = \left(1 + e^{-\beta^\mathsf{T} \mathbf{x}_i}\right)^{-1}$

  - $\beta^{\mathsf{T}}\mathbf{x}_i = \mathbf{x}_i^{\mathsf{T}}\beta = \beta_0 + \sum_{j=1}^{p} x_{ij}\beta_j$
- Bernoulli Likelihood Function

$$L(\beta) = \prod_{i=1}^{n} p_i^{y_1} + (1-p_i)^{1-y_i}$$

$$\log L(\beta) = \sum_{i=1}^{n} \{y_i \ln p_i + (1-y_i)\ln(1-p_i)\}$$

- The usual approach to estimating the Logistic Regression coefficients is *maximum likelihood*

$$\begin{aligned}\hat{\beta} &= \arg\max_{\beta} L(\beta) \\ &= \arg\max_{\beta} \log L(\beta)\end{aligned}$$

- We can also view this as the coefficients that minimize the *loss function*, where the loss function is the negative log-likelihood

$$\begin{aligned}\hat{\beta} &= \arg\min_{\beta} \ell(\beta) \\ &= -C\sum_{i=1}^{n} \{y_i \ln p_i + (1-y_i)\ln(1-p_i)\}\end{aligned}$$

  - where C is some constant, e.g., $C = 1/n$
- This view facilitates *penalized logistic regression*

$$\hat{\beta} = \arg\min_{\beta} \ell(\beta) + \lambda P(\beta)$$

  - Ridge Penalty

$$P(\beta) = \sum_{j=1}^{p} |\beta_j|^2 = \beta^{\mathsf{T}}\beta$$

  - Lasso Penalty

$$P(\beta) = \sum_{j=1}^{p} |\beta_j|$$

  - Best Subsets

$$P(\beta) = \sum_{j=1}^{p} |\beta_j|^0 = \sum_{j=1}^{p} 1_{(\beta_j \neq 0)}$$

3.3 Logistic Regression in Action

- In **R**, logistic regression can be implemented with the `glm()` function since it is a type of *Generalized Linear Model*.
- Because logistic regression is a special case of *Binomial* regression, use the `family=binomial()` argument

```
#-- Fit logistic regression model
fit.lr = glm(y~student + balance + income, data=Default,
             family="binomial")
```

term	estimate	std.error	statistic	p.value
(Intercept)	-10.8690	0.4923	-22.0801	0.0000
studentYes	-0.6468	0.2363	-2.7376	0.0062
balance	0.0057	0.0002	24.7376	0.0000
income	0.0000	0.0000	0.3698	0.7115

Your Turn #4 : Interpreting Logistic Regression

1. What is the estimated probability of default for a Student with a balance of $1000?

2. What is the estimated probability of default for a *Non-Student* with a balance of $1000?

3. Why does `student=Yes` appear to lower risk of default, when the plot of student status vs. default appears to increase risk?

4 Linear/Quadratic Discriminant Analysis (LDA/QDA)

- Discriminant analysis seeks to find a function that will *discriminate* between class boundaries.
  - *Linear Discriminant Analysis (LDA)* finds *linear* boundaries between classes
  - *Quadratic Discriminant Analysis (QDA)* finds *quadratic* boundaries between classes

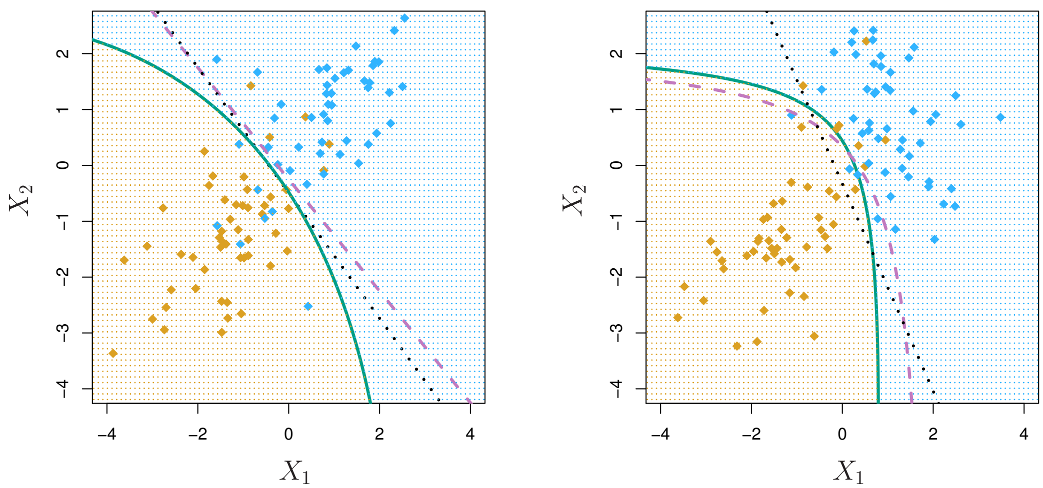


FIGURE 4.9 (from ISLR). Left: The Bayes (purple dashed), LDA (black dotted), and QDA (green solid) decision boundaries for a two-class problem with $\Sigma_1 = \Sigma_2$. The shading indicates the QDA decision rule. Since the Bayes decision boundary is linear, it is more accurately approximated by LDA than by QDA. Right: Details are as given in the left-hand panel, except that $\Sigma_1 \neq \Sigma_2$. Since the Bayes decision boundary is non-linear, it is more accurately approximated by QDA than by LDA.

- Suppose there are $K = |\mathcal{G}|$ classes in the training data, $D = \{(\mathbf{X}_i, G_i)\}_{i=1}^n$
  - where $\mathbf{X}_i \in \mathbf{R}^p$, $G_i \in \mathcal{G}$
- Consider the posterior probability of class g, given $X = x$,

$$\begin{aligned}\Pr(G = g \mid \mathbf{X} = \mathbf{x}) &= \frac{f(x \mid G = g)\Pr(G = g)}{f(x)} \\ &= \frac{f_g(x)\pi_g}{\sum_{k=1}^K f_k(x)\pi_k}\end{aligned}$$

  - $f_k(x)$ is the *class conditional density*
  - $0 \leq \pi_k \leq 1$ are the *prior class probabilities*
  - $\sum_{k=1}^K \pi_k = 1$
- The challenge is to estimate the densities $\{f_k(\cdot)\}$
  - Note: $\hat{\pi}_k = n_k/n$ is a natural estimate for the class priors if we think the testing data will have the same proportions as the training data

4.1 Estimation

- LDA and QDA have strong connections to model based clustering.
  - But easier, since we have the true class labels in the supervised setting
- Both LDA and QDA model the class conditional densities $f_k(x)$ with *Gaussians*
  - Thus, they model the observations as coming from a *Gaussian mixture model*
  - Each class has its own mean vector μ_k
  - The difference between LDA and QDA is what they use for their covariance matrix

- **LDA**

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

  - $\Sigma_k = \Sigma \quad \forall k$ (*uses the same variance-covariance for all classes*)
- **QDA**

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

  - Σ_k is different for each classes

Your Turn #5 : Model Complexity

The LDA model uses a common covariance matrix while QDA allows each class to have a different covariance (which permits quadratic boundaries). But this flexibility comes at a cost.

1. How many parameters have to be estimated in an LDA model with K classes and p dimensions?

2. How many parameters have to be estimated in an QDA model with K classes and p dimensions?

- There are a few methods to maintain some flexibility, yet protect the model from high variance
- One is to use a *regularlized covariance matrix* (see ESL 4.3.1)

$$\hat{\Sigma}_k(\alpha,\gamma) = \alpha\hat{\Sigma}_k + (1-\alpha)\{\gamma\hat{\Sigma} + (1-\gamma)\hat{\sigma}^2 I_p\}$$

- Another is to fit an LDA model in an *enlarged feature space*
  - E.g., for $p = 2$ dimensions, use $X_1, X_2, X_1 \cdot X_2, X_1^2, X_2^2$ instead of QDA in X_1, X_2.
  - Think basis expansion like what we say with polynomial regression or B-splines

4.2 LDA/QDA in Action

- In **R**, LDA and QDA can be implemented with the `lda()` and `qda()` functions from the `MASS` package.
- See ISLR 4.6 for details

5 Evaluation Classification Models

- Training Data: $\{X_i, G_i\}$
  - $G_i \in \{1, \ldots, K\}$ (i.e., there are K classes)
- Predictor: $\hat{G}(X)$
- Loss function: $L(G, \hat{G}(X))$ is the loss incurred by estimating G with $\hat{G}$

- Risk is the expected loss (or expected prediction error EPE)

$$
\begin{aligned}
\mathrm{Risk}(\hat{G}) &= \mathrm{EPE} \\
&= \mathrm{E}_{XG}\left[L(G, \hat{G}(X))\right] \\
&= \mathrm{E}_{X}\left[\mathrm{E}_{G|X}\left[L(G, \hat{G}(X)) \mid X\right]\right] \\
&= \mathrm{E}_{X}\left[R_X(\hat{G})\right]
\end{aligned}
$$

- The Risk at input $X = x$ is

$$
\begin{aligned}
R_x(\hat{G}) &= \mathrm{E}_{G|X}\left[L(G, \hat{G}(x)) \mid X = x\right] \\
&= \sum_{k=1}^{K} L(K, \hat{G}(x)) \Pr(G = k \mid X = x)
\end{aligned}
$$

- Thus the optimal class label, given $X = x$, is

$$
\hat{G}(x) = \arg\min_{g} R_x(g)
$$

5.1 Evaluation of Binary Classification Models

- We are considering *binary* outcomes, so use the notation $Y \in \{0, 1\}$
- Let $p(x) = \Pr(Y = 1 \mid X = x)$
- The Risk (for a binary outcome) is:

$$
\begin{aligned}
R_x(g) &= L(1, g) \Pr(Y = 1 \mid X = x) + L(0, g)(1 - \Pr(Y = 1 \mid X = x)) \\
&= L(1, g)p(x) + L(0, g)(1 - p(x))
\end{aligned}
$$

- Decision: choose $\hat{G}(x) = 1$ if

$$
\begin{aligned}
R_x(1) &< R_x(0) \\
L(1,1)p(x) + L(0,1)(1 - p(x)) &< L(1,0)p(x) + L(0,0)(1 - p(x)) \\
p(x)\left(L(1,1) - L(1,0)\right) &< (1 - p(x))\left(L(0,0) - L(0,1)\right) \\
\frac{p(x)}{1 - p(x)} &< \frac{L(0,0) - L(0,1)}{L(1,1) - L(1,0)} \\
\frac{p(x)}{1 - p(x)} &\geq \frac{L(0,1) - L(0,0)}{L(1,0) - L(1,1)}
\end{aligned}
$$

5.1.1 Example

- Say we have a goal of estimating if a patient has cancer using medical imaging
  - Let $G = 1$ for cancer and $G = 0$ for no cancer
- Suppose we have solicited a loss function with the following values
  - $L(G = 0, \hat{G} = 0) = 0$: There is no loss for correctly diagnosis a patient without cancer
  - $L(G = 1, \hat{G} = 1) = 0$: There is no loss (for our model) for correctly diagnosis a patient with cancer
  - $L(G = 0, \hat{G} = 1) = FP$: There is a cost of FP units if the model issues a *false positive*, estimating the patient has cancer when they don't
  - $L(G = 1, \hat{G} = 0) = FN$: There is a cost of FN units if the model issues a *false negative*, estimating the patient does not have cancer when they really do

  - In these scenarios $FN >> FP$ because the patient can have serious effects if not treated promply (and correctly)
- Our model should decide for a positive cancer if $R_x(1) < R_x(0)$ which becomes

$$\begin{aligned}\frac{p(x)}{1-p(x)} &\geq \frac{FP}{FN}\\ p(x) &\geq \frac{FP}{FP+FN}\end{aligned}$$

- The ratio of FP to FN is all that matter to make the decision. Let's say that FP=1 and FN=10. Then if $p(x) \geq 1/11$, our model will diagnose cancer.
  - Note: $p(x) = \Pr(Y = 1|X = x)$ is affected by the class prior $Pr(Y = 1)$ (e.g., the portion of the population tested with cancer), which is usually going to be small.

5.2 Common Binary Loss Functions

- Suppose we are going to estimate a binary reponse $Y \in \{0, 1\}$ with a (possibly continuous) predictor $\hat{y}(x)$
- **0-1 Loss** or **Misclassification Error**

$$L(y, \hat{y}(x)) = \mathbb{1}(y \neq \hat{y}(x)) = \begin{cases} 0 & y = \hat{y}(x) \\ 1 & y \neq \hat{y}(x) \end{cases}$$

  - This assumes $L(0, 1) = L(1, 0)$ (i.e., false positive costs the same as a false negative)
  - Requires that a *hard classification* is made
  - The optimal prediction is $y^*(x) = \mathbb{1}(p(x) > 1 - p(x))$
- **Squared Error**

$$L(y, \hat{y}(x)) = (y - \hat{y}(x))^2$$

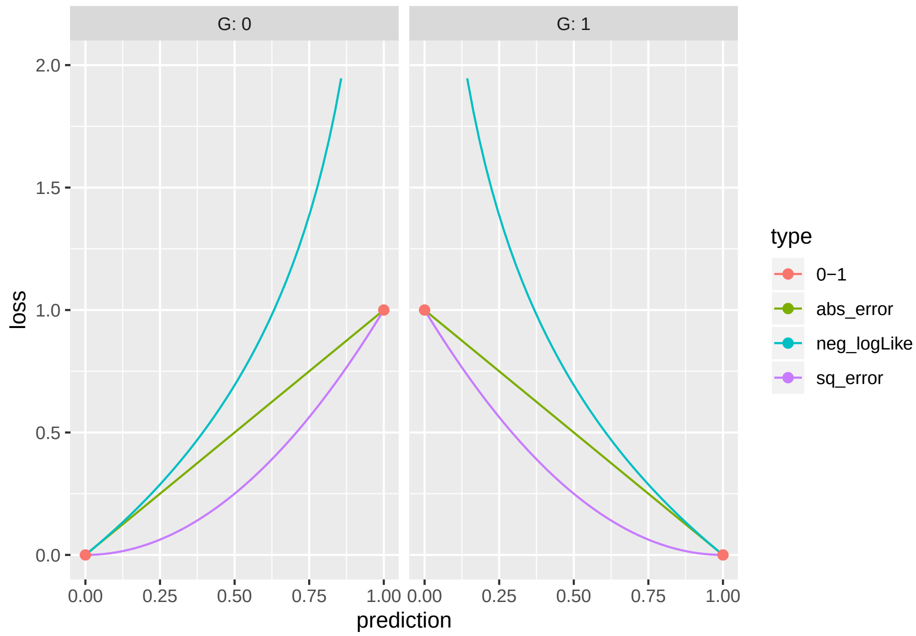
  - The optimal prediction is $y^*(x) = \mathrm{E}[Y \mid X = x] = \Pr(Y = 1 \mid X)$
- **Absolute Error**

$$L(y, \hat{y}(x)) = |y - \hat{y}(x)|$$

- **Bernoulli negative log-likelihood**

$$\begin{aligned}L(y, \hat{y}(x)) &= -\{y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)\}\\ &= \begin{cases} -\log \hat{y} & y = 1 \\ -\log(1 - \hat{y}) & y = 0 \end{cases}\end{aligned}$$

  - Requires $\hat{y}(x) \in [0, 1]$



5.3 Evaluating Binary Classification Models

- Recall, the optimal (*hard classification*) decision is to choose $\hat{G} = 1$ if:

$$\frac{p(x)}{1 - p(x)} \geq \frac{L(0,1) - L(0,0)}{L(1,0) - L(1,1)}$$

- Denote $\gamma(x)$ as the *logit* of $p(x)$:

$$\gamma(x) = \log \frac{p(x)}{1 - p(x)} = \frac{\Pr(G = 1 \mid X = x)}{\Pr(G = 0 \mid X = x)}$$

- Then we get

$$\begin{aligned} p(x) &= \Pr(G = 1 \mid X = x) \\ &= \frac{e^{\gamma(x)}}{1 + e^{\gamma(x)}} \end{aligned}$$

- And the optimal (*hard classification*) decision becomes

$$\boxed{\text{Choose } \hat{G}(x) = 1 \text{ if } \hat{\gamma}(x) > t, \quad \text{where } t \text{ is a threshold}}$$

- If the loss/cost is known, then

$$t^* = \log \left(\frac{L(0,1) - L(0,0)}{L(1,0) - L(1,1)} \right)$$

- For a given threshold t and input x, the hard classification is $\hat{G}_t(x) = \mathbb{1}(\hat{\gamma}(x) \geq t)$

5.4 Evaluation Metrics

5.4.1 Metrics

Metric	Definition	Estimate
Mis-classification Rate	$P_{XG}(\hat{G}_t(X) \neq G(X)) =$ $P_X(\hat{G}_t(X) = 0, G(X) = 1) +$ $P_X(\hat{G}_t(X) = 1, G(X) = 0)$	$\frac{1}{n} \sum_{i=1}^{n} \mathbb{1}(\hat{G}_t(x_i) \neq G_i)$
False Positive Rate (FPR)	$P_X(\hat{G}_t(X) = 1 \mid G(X) = 0)$	$\frac{1}{n_0} \sum_{i:G_i=0} \mathbb{1}(\hat{G}_t(x_i) = 1)$
True Positive Rate (TPR) {Hit Rate, Recall, Sensitivity}	$P_X(\hat{G}_t(X) = 1 \mid G(X) = 1)$	$\frac{1}{n_1} \sum_{i:G_i=1} \mathbb{1}(\hat{G}_t(x_i) = 1)$
Precision	$P_X(G(X) = 1 \mid \hat{G}_t(X) = 1)$	$\frac{1}{\hat{n}_1} \sum_{i:\hat{G}(x_i)=1} \mathbb{1}(G(x_i) = 1)$

- Note: Performance estimate is best carried out on *hold-out* data!

5.4.2 Confusion Matrix

- Given a threshold t, we can get *confusion matrix*

		Model Outcome		
		$\hat{G}_t = 1$	$\hat{G}_t = 0$	**total**
True Outcome	$G = 1$	True Positive	False Negative	N_1
	$G = 0$	False Positive	True Negative	N_0
	total	$\hat{N}_1(t)$	$\hat{N}_0(t)$	

Table from: https://tex.stackexchange.com/questions/20267/how-to-construct-a-confusion-matrix-in-latex

- See Wikipedia Page: Confusion Matrix for more metrics