Topic 3. Classification

Overview

- **Classification**: predicting a qualitative response
- A classification technique is called a *classifier*.

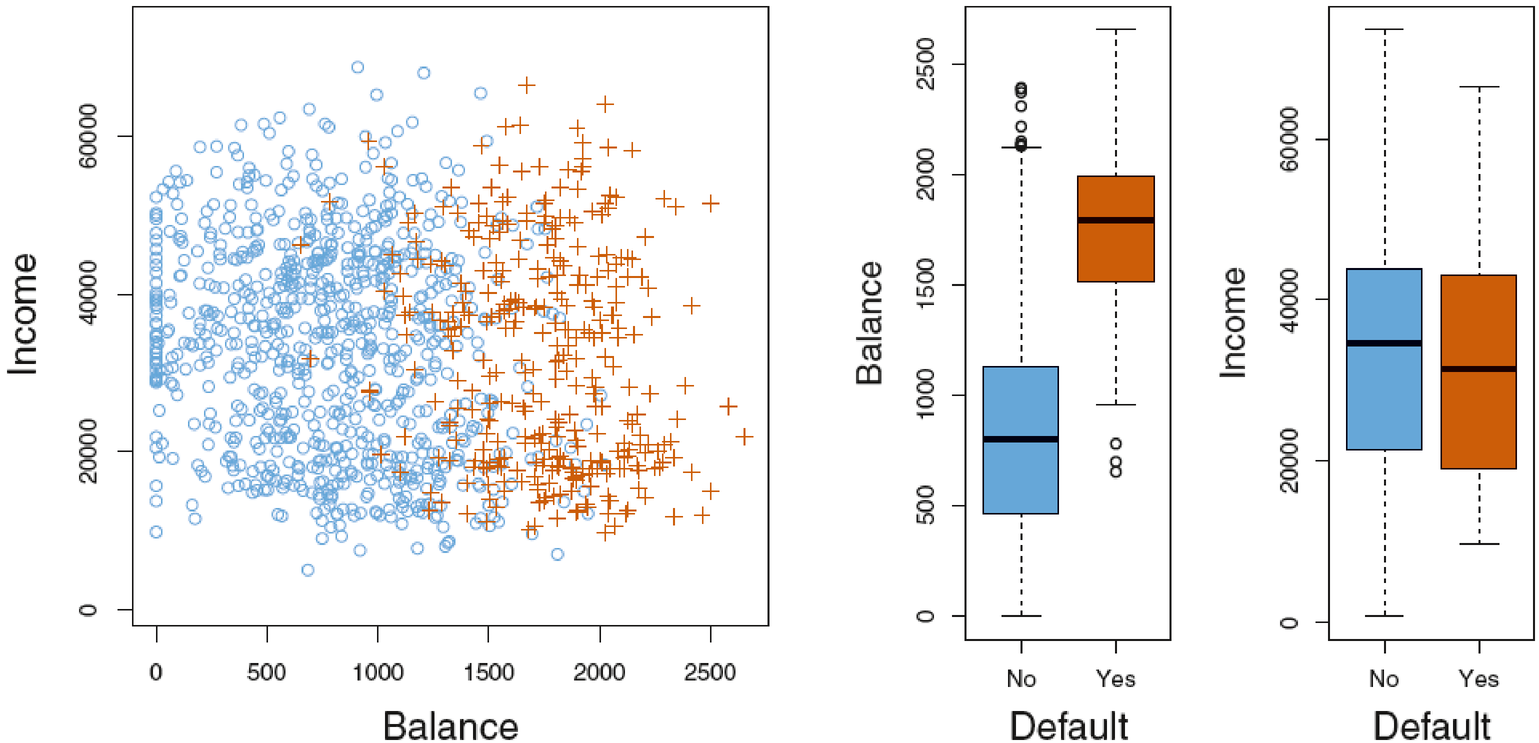
- **Popular classifiers**
  - Logistic regression
  - Linear discriminant analysis (LDA) & QDA
  - K-Nearest Neighbors (KNN)

- **Performance assessment and comparison**

Logistic Regression

Motivating Example

- Predicting whether an individual will default on his/her credit card payment
- Default data set: $Y = default\ (yes/no)$, $X_1 = balance$, $X_2 = income$



Why Not Linear Regression?

$$Y = \begin{cases} 0 & default = No \\ 1 & default = Yes \end{cases}$$

- Linear regression model using the binary response

$$Y = \beta_0 + \beta_1 X_1 + \varepsilon$$

- Problem: the prediction ($\hat{Y} = \hat{\beta}_0 + \hat{\beta}_0 X_1$) can take any value between negative and positive infinity. How do we interpret values greater than 1? Or values between 0 and 1?

Why Not Linear Regression?

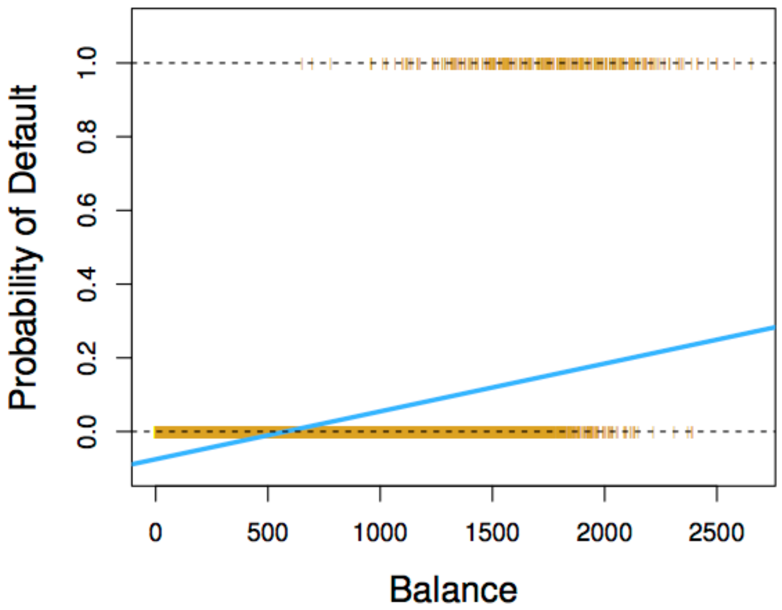
$$Y = \begin{cases} 0 & default = No \\ 1 & default = Yes \end{cases}$$

- Linear regression model using the probability as response

  $$P(Y=1) = \beta_0 + \beta_1 X_1$$

  the probability of default

- Problem: now the values between 0 and 1 makes sense. But it is still difficult to interpret negative values and values greater than 1.

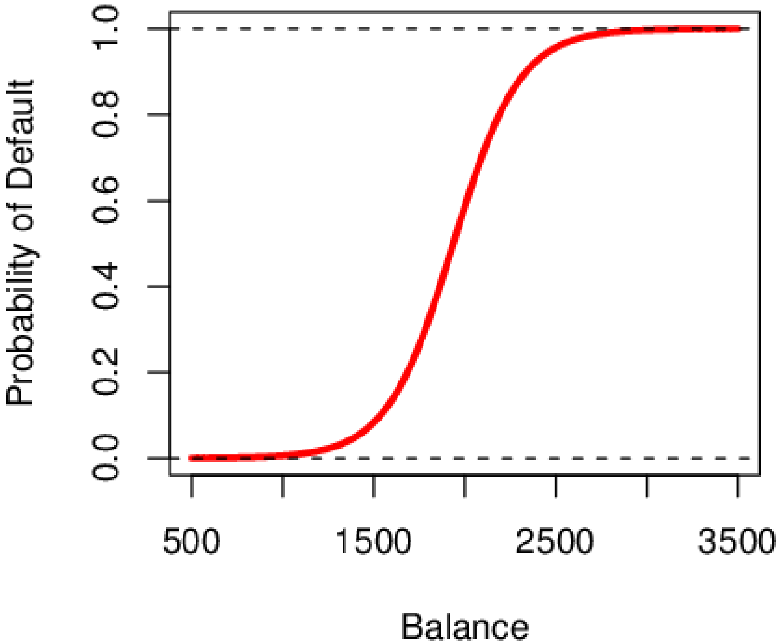


Solution: Logistic Function

$$P(Y = 1) = \beta_0 + \beta_1 X_1$$

- Left side: $[0,1]$ Right side: $(-\infty, \infty)$
- **Question**: is there a transformation of the right side such that it has the same range as the left side?
- The logistic function

$$P(Y = 1) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}$$



Logistic Regression

- Logistic regression is very similar to linear regression

$$\text{logistic regression:} \quad log\left(\frac{P(Y=1)}{1-P(Y=1)}\right) = \beta_0 + \beta_1 X$$

$$\text{linear regression:} \quad Y \approx \beta_0 + \beta_1 X$$

- In linear regression, β_1 represents the average change in Y for one-unit increase in X. However, this simple interpretation does not work for logistic regression because we are predicting the probability $P(Y)$, not the response Y.

Interpreting β_1

$$log\left(\frac{P(Y=1)}{1-P(Y=1)}\right) = \beta_0 + \beta_1 X \leftrightarrow P(Y=1) = \frac{e^{\beta_0+\beta_1 X}}{1+e^{\beta_0+\beta_1 X}}$$

- If β_1= 0, this means that there is no relationship between the response and the predictor(s).
- If β_1 > 0, this means that when X gets larger so does the probability of default.
- If β_1 < 0, this means that when X gets larger, the probability of default gets smaller.
- How much bigger or smaller depends on value of the slope.

Estimating Coefficients

- Find estimates of the parameters β_0, β_1 based on training data

$$\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$$

- Maximum likelihood method

  Likelihood function

$$l(\beta_0, \beta_1) = \prod_{i:y_i=1} P(y_i = 1) \prod_{i':y_{i'}=0} 1 - P(y_{i'} = 1)$$

$$P(y_i = 1) = \frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}} \qquad P(y_{i'} = 0) = \frac{1}{1+e^{\beta_0+\beta_1 x_{i'}}}$$

- The estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ are chosen to maximize this function.

Results of the Default Example

	Coefficient	Std. Error	Z-statistic	P-value
Intercept	-10.6513	0.3612	-29.5	< 0.0001
balance	0.0055	0.0002	24.9	< 0.0001

- Predicting default using balance
- Use a z test instead of t test (as used in linear regression) to see whether β_0 and β_1 are significantly different from zero
- Here the p-value for balance is very small, and $\hat{\beta}_1$ is positive. That means if the balance increases, then the probability of default will increase as well.

Making Predictions

- Suppose an individual has an average balance of \$1000. What is their probability of default?

$$P(Y=1) = \frac{e^{\hat{\beta}_0+\hat{\beta}_1 X}}{1+e^{\hat{\beta}_0+\hat{\beta}_1 X}} = \frac{e^{-10.6513+0.0055\times 1000}}{1+e^{-10.6513+0.0055\times 1000}} = 0.00576$$

- The predicted probability of default for an individual with a balance of \$1000 is less than 1%.

- For a balance of \$2000, the probability is much higher, and equals to 0.586 (58.6%).

Qualitative Predictors

- We can predict if an individual default by checking if she is a student or not. Thus we can use a qualitative variable "student" coded as a dummy variable (student=1, non-student=0).

	Coefficient	Std. Error	Z-statistic	P-value
Intercept	-3.5041	0.0707	-49.55	< 0.0001
student[Yes]	0.4049	0.1150	3.52	0.0004

$$\widehat{\Pr}(\texttt{default}=\texttt{Yes}|\texttt{student}=\texttt{Yes}) = \frac{e^{-3.5041+0.4049\times 1}}{1+e^{-3.5041+0.4049\times 1}} = 0.0431,$$

$$\widehat{\Pr}(\texttt{default}=\texttt{Yes}|\texttt{student}=\texttt{No}) = \frac{e^{-3.5041+0.4049\times 0}}{1+e^{-3.5041+0.4049\times 0}} = 0.0292.$$

- The estimate is positive, which indicates that students tend to have higher default probabilities than non-students.

Multiple Logistic Regression

- Predicting a binary response using multiple predictors

$$log\left(\frac{P(Y=1)}{1-P(Y=1)}\right)=\beta_0+\beta_1X_1+\cdots+\beta_pX_p$$

$$P(Y=1)=\frac{e^{\beta_0+\beta_1X_1+\cdots+\beta_pX_p}}{1+e^{\beta_0+\beta_1X_1+\cdots+\beta_pX_p}}$$

Default Example

- Predict default using balance, income, and student (qualitative)

	Coefficient	Std. Error	Z-statistic	P-value
Intercept	-10.8690	0.4923	-22.08	< 0.0001
balance	0.0057	0.0002	24.74	< 0.0001
income	0.0030	0.0082	0.37	0.7115
student[Yes]	-0.6468	0.2362	-2.74	0.0062

- The p-values of balance and student are very small, indicating that they are associated with the probability of default.
- The coefficient for student is negative, indicating that students are less likely to default than non-students.

Predictions

- A student with a credit card balance of $1,500 and an income of $40,000 has an estimated probability of default

$$P(Y=1) = \frac{e^{-10.869+0.00574\times 1500+0.003\times 40-0.6468\times 1}}{1+e^{-10.869+0.00574\times 1500+0.003\times 40-0.6468\times 1}} = 0.058$$

- A non-student with the same balance and income has an estimated probability of default

$$P(Y=1) = \frac{e^{-10.869+0.00574\times 1{,}500+0.003\times 40-0.6468\times 0}}{1+e^{-10.869+0.00574\times 1{,}500+0.003\times 40-0.6468\times 0}} = 0.105$$

An Apparent Paradox!

- Predicting default using only student

	Coefficient	Std. Error	Z-statistic	P-value
Intercept	-3.5041	0.0707	-49.55	< 0.0001
student[Yes]	0.4049	0.1150	3.52	0.0004

Conclusion: students tend to have higher probability of default than non-students.

- Predicting default using balance, income, and student

	Coefficient	Std. Error	Z-statistic	P-value
Intercept	-10.8690	0.4923	-22.08	< 0.0001
balance	0.0057	0.0002	24.74	< 0.0001
income	0.0030	0.0082	0.37	0.7115
student[Yes]	-0.6468	0.2362	-2.74	0.0062

Conclusion: students tend to have lower probability of default than non-students.

Interpretation

- Students tend to have higher balance. Higher balance tends to have higher probability of default. So, if not consider balance, students tend to have higher probability of default.

	Coefficient	Std. Error	Z-statistic	P-value
Intercept	-3.5041	0.0707	-49.55	< 0.0001
student[Yes]	0.4049	0.1150	3.52	0.0004

Interpretation

- However, given the balance (i.e., after adjusting for the effect of balance), students tend to have lower probability of default.

	Coefficient	Std. Error	Z-statistic	P-value
Intercept	-10.8690	0.4923	-22.08	< 0.0001
balance	0.0057	0.0002	24.74	< 0.0001
income	0.0030	0.0082	0.37	0.7115
student[Yes]	-0.6468	0.2362	-2.74	0.0062

Useful Inference for Credit Card Company

- **Question:** to whom should they offer credit card?
- A student is risker than a non-student if no information about the student's credit card balance is available
- However, that student is less risky than a non-student with the same credit card balance!

Multinomial Logistic Regression

- **Question:** How to extend logistic regression to response variables with more than two classes?
- Multinomial Logistic Regression
- Two ways:
  - Select a single class as baseline
  - Treat all classes symmetrically

Linear Discriminant Analysis (LDA)

Assumptions of LDA

- Each predictor variable is normally distributed.
- If there are more than one predictor, the predictors follow a multivariate normal distribution.

Why Not Logistic Regression?

- In the case where n is small and the distribution of predictors $\boldsymbol{X}$ is approximately normal in each of the classes, LDA is more stable than Logistic regression.

- LDA is more popular when the response has more than two classes (Logistic regression is usually used when there are only two classes).

Review: Bayes Theorem

$$P(A_i|B) = \frac{P(A_i \cap B)}{P(B)} = \frac{P(A_i)P(B|A_i)}{\sum_{k=1}^{K} P(A_k)P(B|A_k)}$$

The Bayes Classifier

- According to the **Bayes theorem**

$$\Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}$$

  - K: the total number of response classes
  - π_k: the overall or prior probability of the kth class
  - $f_k(x)$: the density function of observations from the kth class

- **Rule of classification**: Given an observation $X = x$, calculate $P(Y = 1|X = x), P(Y = 2|X = x), \ldots, P(Y = K|X = x)$. Assign this observation to the class with the largest probability.

Example

- Default data set, $Y = \text{default}(\text{No/Yes})$, $X = \text{balance}$
- The number of classes $K = 2$

$$P(Y = 0|X = x) = P(\text{default} = \text{No}|\text{balance} = x)$$
$$= \frac{\pi_0 f_0(x)}{\pi_0 f_0(x) + \pi_1 f_1(x)}$$

$$P(Y = 1|X = x) = P(\text{default} = \text{Yes}|\text{balance} = x)$$
$$= \frac{\pi_1 f_1(x)}{\pi_0 f_0(x) + \pi_1 f_1(x)}$$

- Given $\text{balance} = \$1000$, if we find $P(Y = 0|X = 1000) = 0.7$, $P(Y = 1|X = 1000) = 0.3$, the predicted class is $Y = 0$, i.e., no default.

Gold Standard for Classification

- In theory, the Bayes classifier has the best performance in classification, so we would always like to use it.
- However, for real data, we do not know the distribution of predictor(s) in each class, so computing the Bayes classifier is impossible.
- The Bayes classifier serves as an unattainable gold standard against which to compare other classifiers.

Idea of LDA

- Assume in each class the predictor follows a normal distribution

  Predictor in class k: $X \sim N\left(\mu_k, \sigma_k^2\right)$

- Assume those normal distributions have equal variance

$$\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_K^2 = \sigma^2$$

- So the density function in class k is

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_k)^2\right)$$

Idea of LDA

- Plugging the normal density function into the Bayes classifier

$$\boxed{\log P(Y = k|X = x)} = \boxed{\frac{\mu_k}{\sigma^2}} \cdot x + \boxed{\left[\log(\pi_k) - \frac{\mu_k^2}{2\sigma^2}\right]}$$

$$\delta_k(x) = a \cdot x + b$$

Discriminant function

- **Rule of classification**: Given an observation $X = x$, calculate $\delta_1(x), \delta_2(x), \dots, \delta_K(x)$. Assign this observation to the class with the largest δ.

Estimates Used in LDA

- To calculate $\delta_k(x)$, we need to find estimates for the prior probabilities π_k and parameters μ_k, σ^2 of the normal distribution

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_i$$

$$\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)^2$$

$$\hat{\pi}_k = n_k/n$$

- μ_k is estimated by the average of the training data from the kth class.
- σ^2 is estimated by the weighted average of the sample variances for the K classes.
- π_k is estimated by the proportion of the training data that belong to the kth class.

LDA for Binary Response

- A binary response Y, single predictor
- Discriminant function for class 1

$$\delta_1(x) = \frac{\mu_1}{\sigma^2} \cdot x + \left[\log(\pi_1) - \frac{\mu_1^2}{2\sigma^2}\right]$$

- Discriminant function for class 2

$$\delta_2(x) = \frac{\mu_2}{\sigma^2} \cdot x + \left[\log(\pi_2) - \frac{\mu_2^2}{2\sigma^2}\right]$$

- Decision boundary (assume $\pi_1 = \pi_2 = 0.5$)

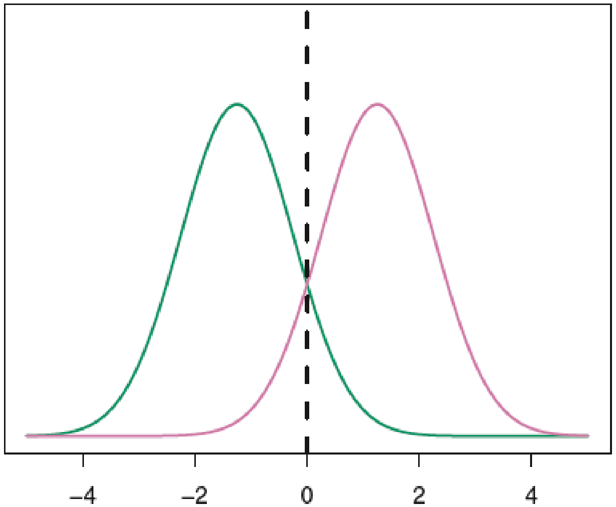
$$\delta_1(x_0) = \delta_2(x_0) \rightarrow x_0 = \frac{\mu_1 + \mu_2}{2}$$

- Rule of classification: assume $\mu_2 > \mu_1$,

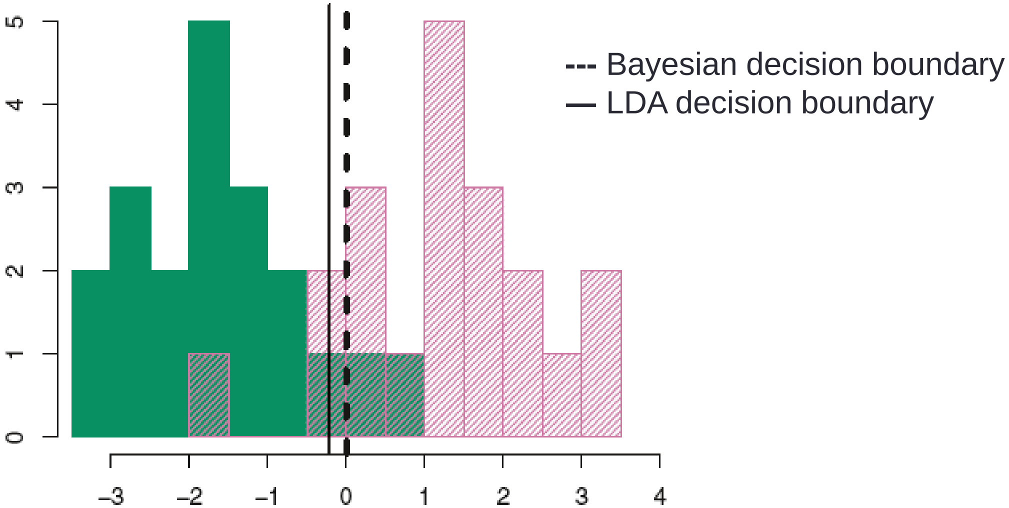
$$y(x) = \begin{cases} \text{class } 2, if\ x > x_0 \\ \text{class } 1, if\ x < x_0 \end{cases}$$

A Simple Example

- Normal density functions $f_1(x)$ and $f_2(x)$ from the two classes
- The two density functions overlap, so there is some uncertainty to classify an observation with unknown class.
- 20 observations were drawn from each of the two classes.
- LDA performs pretty well in prediction: LDA error rate=11.1% vs. Bayes error rate=10.6%



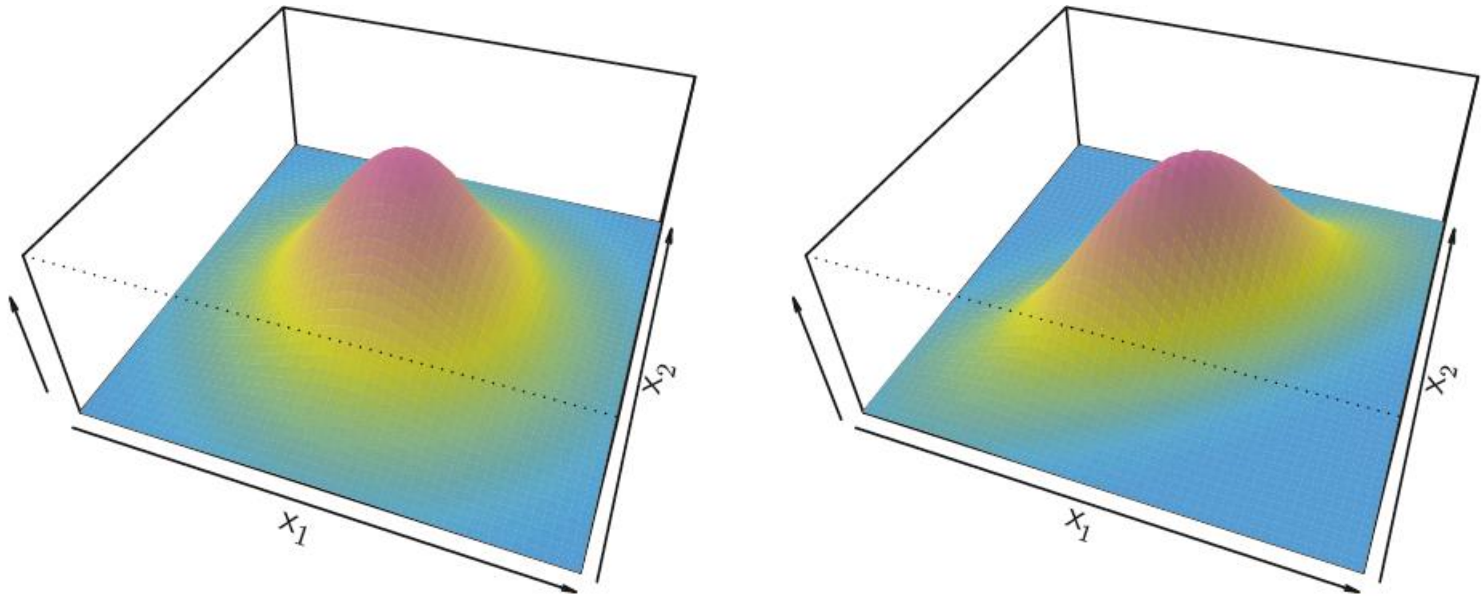
Left: normal density functions



Right: histograms of observations

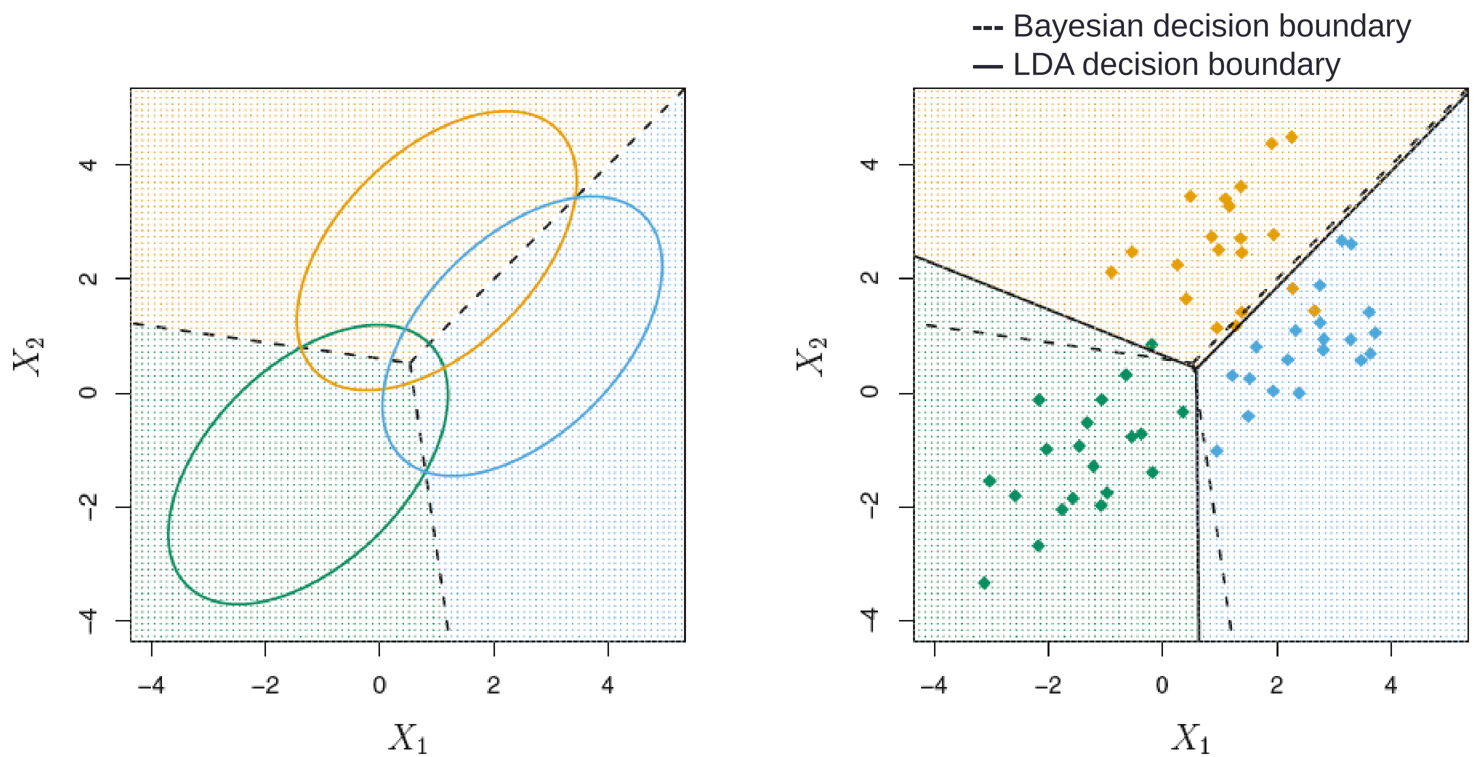
Cases with Multiple Predictors ($p > 1$)

- When there are multiple predictors (i.e., $p > 1$), we use exactly the same approach except that the density function of the predictors is modeled as a multivariate normal density.



An Example with Two Predictors ($p = 2$)

- Bivariate normal density functions $f_1(\boldsymbol{x})$, $f_2(\boldsymbol{x})$ and $f_3(\boldsymbol{x})$ from three classes



Left: Ellipses that contain 95% of the probability

Right: 20 observations generated from each class

Quadratic Discriminant Analysis (QDA)

- LDA assumes that all the classes have the same variance (or variance-covariance matrix in the case of multiple predictors).
- LDA may perform poorly if this assumption is far from truth.
- QDA works identically as LDA except that it estimates separate variance (or variance-covariance matrix in the case of multiple predictors) for each class.
- The discriminant function of QDA takes a quadratic form.

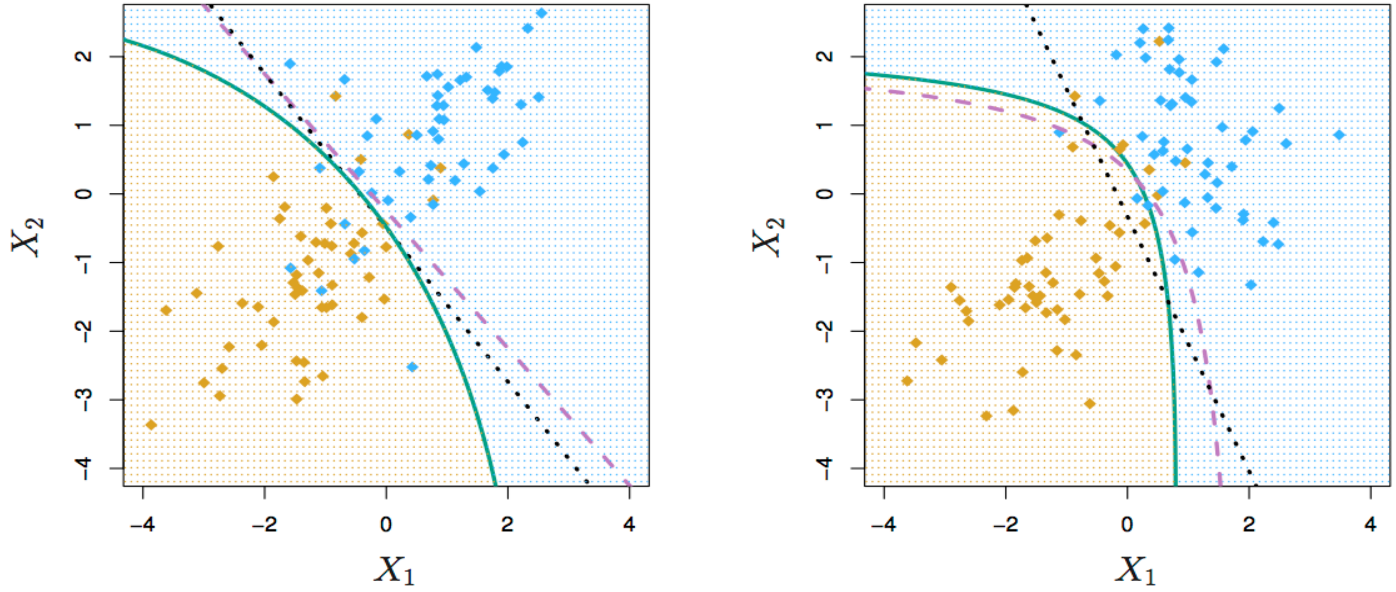
Which Is Better?

- Since QDA allows for different variances among classes, the resulting boundaries become quadratic.

- Which approach is better: LDA or QDA?
  - QDA is more flexible than LDA.
  - QDA works best when the variances are very different between classes and we have enough observations to accurately estimate the variances.
  - LDA works best when the variances are similar among classes or we don't have enough data to accurately estimate the variances.

Comparing LDA and QDA

- Two simulated examples with binary response
  Left: variances of the two classes are equal (LDA is better)
  Right: variances of the two classes are not equal (QDA is better)



- **Black** dotted: LDA boundary
- Purple dashed: Bayes' boundary
- Green solid: QDA boundary

K-Nearest Neighbors (KNN)

K-Nearest Neighbors (KNN) Classifier

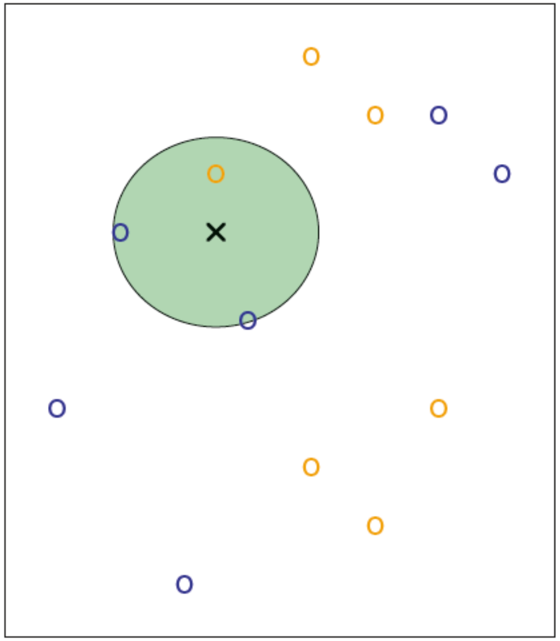
- Given a test observation $X = x_0$, KNN works in the following steps to find its predicted class:
- **Step 1**: identify the K points in the training data that are closest to x_0, i.e., the "K nearest neighbors".
- **Step 2**: calculate the fraction of observations belonging to each class among the K points.
- **Step 3**: assign this observation to the class with the largest fraction.

A Simple Example

- Training data set includes 6 blue points and 6 orange points.

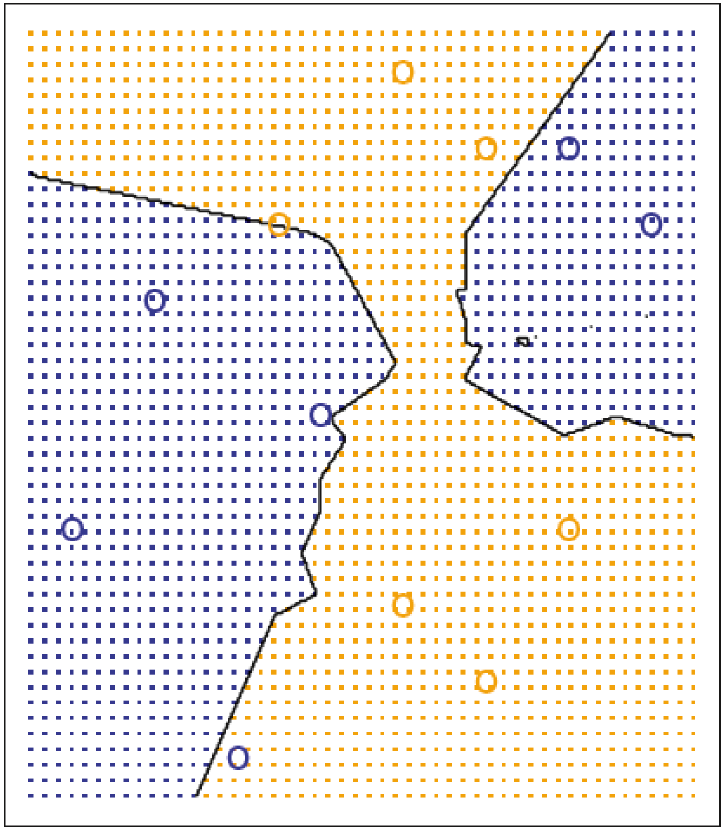
- KNN method ($K = 3$):

  (1) find the 3 nearest neighbors of the test point
  (2) among the 3 points, 2/3 belong to blue class, 1/3 orange class.
  (3) the test point is assigned to blue class.



KNN Decision Boundary

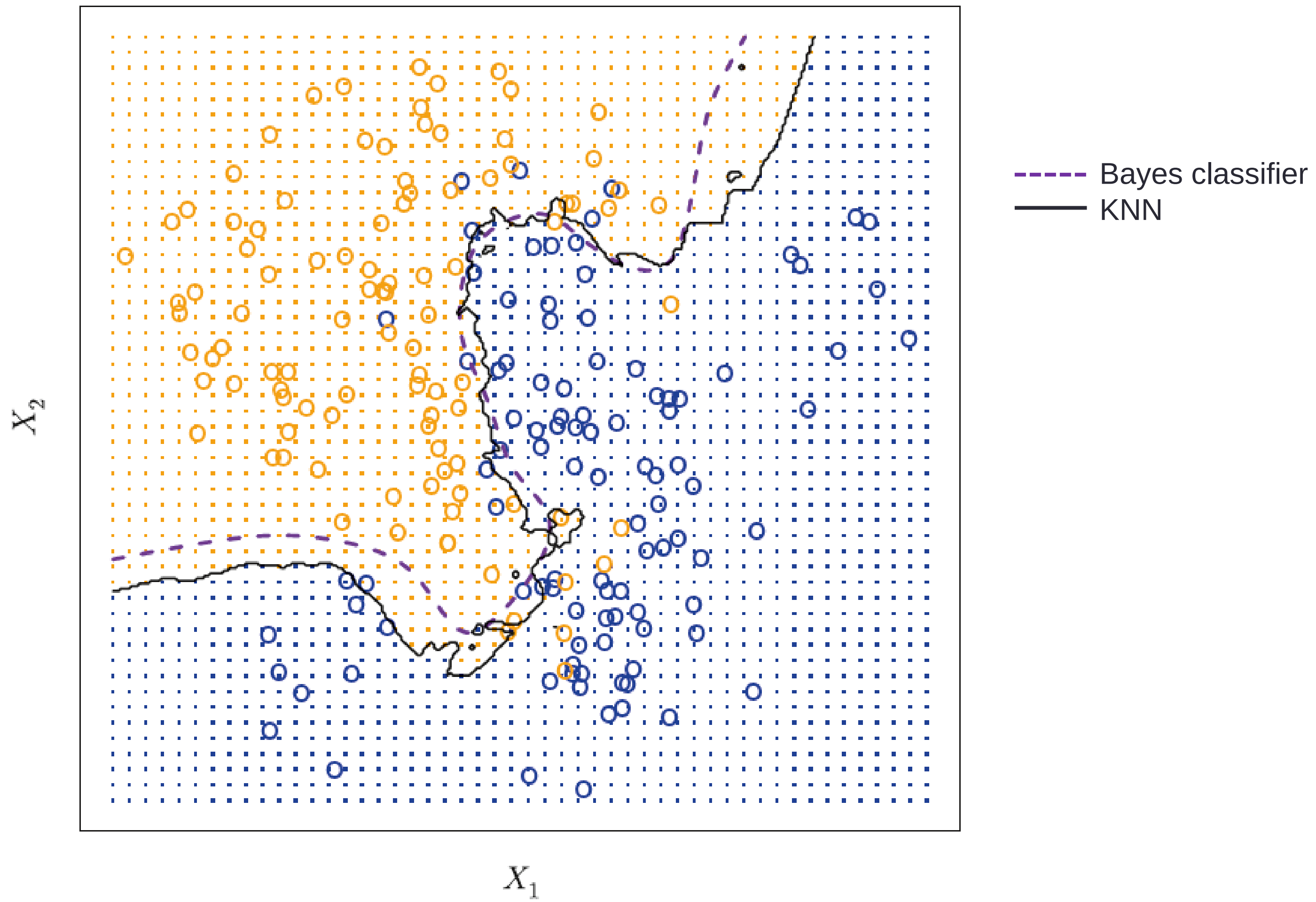
- Blue grid: region of the blue class
- Orange grid: region of the orange class



KNN Can Work Pretty Well!

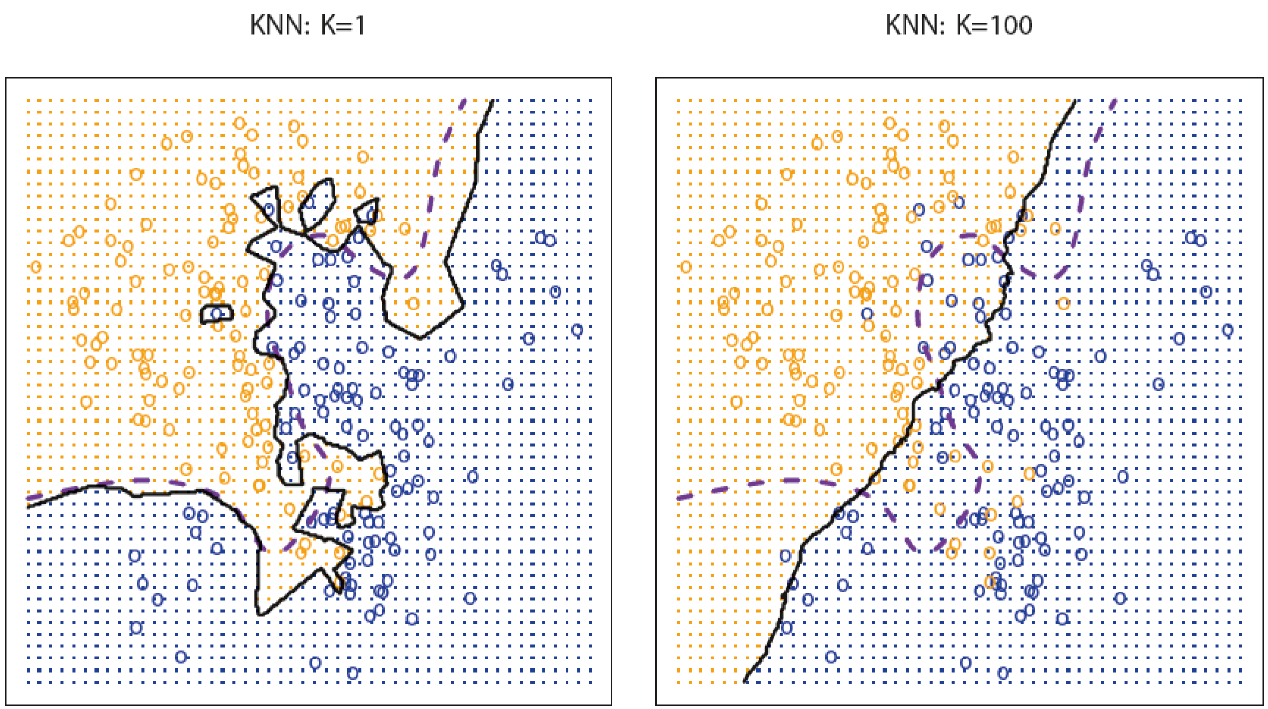
- Though KNN is a very simple approach, it can often perform surprisingly well, close to the Bayes classifier.

KNN: K=10



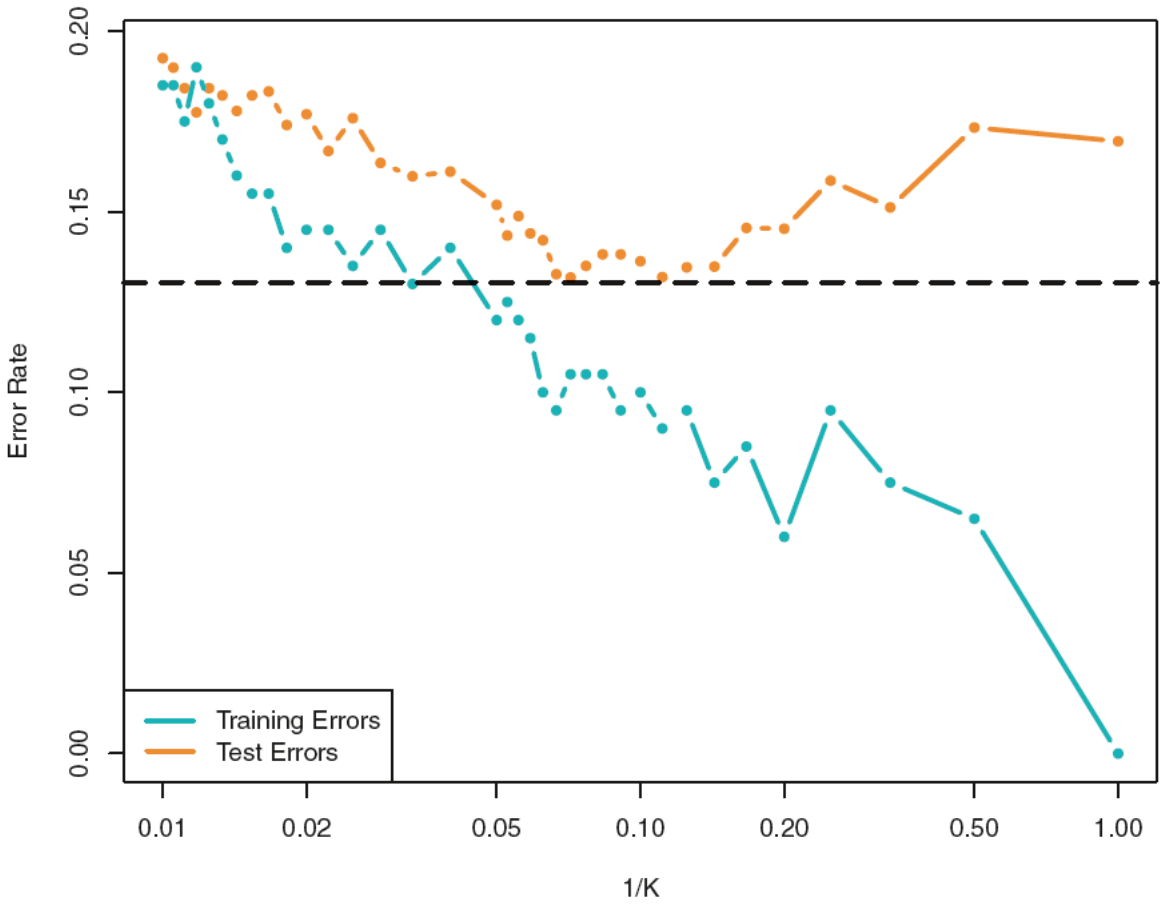
Choice of K

- $K = 1$: decision boundary is flexible
- As K grows, the boundary becomes less flexible and gets close to linear.
- $1/K$ represents the level of flexibility.



Training/Test Error vs. Flexibility

- Optimal choice to minimize test error rate: $K = 10$



Performance Assessment and Comparison

Classifiers

- Logistic regression (linear boundary)
- LDA (linear boundary)
- QDA (nonlinear boundary)
- KNN (highly nonlinear boundary)

Logistic Regression vs. LDA

- **Similarity**: both logistic regression and LDA produce linear boundaries

- **Difference**
  - LDA assumes that the observations are drawn from the normal distribution with common variance in each class, while logistic regression does not have this assumption.
  - LDA would do better than logistic regression if the normality assumption holds, otherwise logistic regression can outperform LDA.

KNN vs. (Logistic regression and LDA)

- KNN is completely *non-parametric*: No assumptions are made about the shape of the decision boundary!

- **Advantage of KNN**: We can expect KNN to dominate both LDA and logistic regression when the decision boundary is highly non-linear

- **Disadvantage of KNN**: KNN does not tell us which predictors are important (no table of coefficients)

QDA vs. (Logistic regression, LDA, KNN)

- QDA is a compromise between non-parametric KNN method and the linear LDA and logistic regression

Choosing A Classifier

- If the true decision boundary is:
  - Linear: LDA and logistic regression outperform
  - Moderately non-linear: QDA outperforms
  - More complicated: KNN is superior

Assessing Performance of Classification

- **Performance measures for all classifiers**

  Accuracy

  Error rate

  Sensitivity

  Specificity

- **Performance measures for logistic regression/LDA/QDA**

  Receiver operating characteristics (ROC)

  Area under curve (AUC)

Confusion Matrix

- Example: Default data set (training)

		True Default Status		
		No	Yes	Total
Predicted Default Status	No	9644	252	9896
	Yes	23	81	104
	Total	9667	333	10000

$$\text{Accuracy} = \frac{(\quad\quad)}{(\quad\quad)} \qquad \text{Error rate} = \frac{(\quad\quad)}{(\quad\quad)}$$

$$\text{Sensitivity} = \frac{(\quad\quad)}{(\quad\quad)} \qquad \text{Specificity} = \frac{(\quad\quad)}{(\quad\quad)}$$

Performance Measures

$$\text{True positive rate} = \frac{\text{TP}}{\text{P}} \qquad \text{False positive rate} = \frac{\text{FP}}{\text{N}}$$

$$\text{Accuracy} = \frac{(\text{TN} + \text{TP})}{\text{N} + \text{P}} \qquad \text{Error rate} = \frac{(\text{FN} + \text{FP})}{\text{N} + \text{P}}$$

$$\text{Sensitivity} = \frac{\text{TP}}{\text{P}} \qquad \text{Specificity} = \frac{\text{TN}}{\text{N}}$$

		Predicted class		
		− or Null	+ or Non-null	Total
True class	− or Null	True Neg. (TN)	False Pos. (FP)	N
	+ or Non-null	False Neg. (FN)	True Pos. (TP)	P
	Total	N*	P*	

$$\text{Error rate} = 1 - \text{Accuracy}$$

$$\text{Sensitivity} = \text{True positive rate}$$

$$\text{Specificity} = 1 - \text{False positive rate}$$

Interpretation

		True Default Status		
		No	Yes	Total
Predicted	No	9644	252	9896
Default Status	Yes	23	81	104
	Total	9667	333	10000

- Accuracy: fraction of people that are correctly classified (97.25%).
- (Training) Error rate: fraction of people that are incorrectly classified (2.75%)
- Sensitivity (true positive rate): fraction of defaulters that are correctly identified (24.3%)
- Specificity: fraction of non-defaulters that are correctly identified as non-defaulters (99.76%)
- False positive rate (1– Specificity): fraction of non-defaulters that are incorrectly classified as defaulters (0.24%)

Threshold in Class Prediction

- Recall that logistic regression and LDA/QDA produce a probability estimate for each observation, and then a threshold is used to determine its predicted class.
- Usually 0.5 is used as threshold.
- If we use a different value for the threshold, the performance of classification will be different.

Example

- Use LDA for the Default data set
- Threshold = 0.5: the training error rate is 2.75%, but the sensitivity is only 24.3%.
- Threshold = 0.2: the training error rate is 3.73%, while the sensitivity increases to 58.6%.

Threshold = 0.5

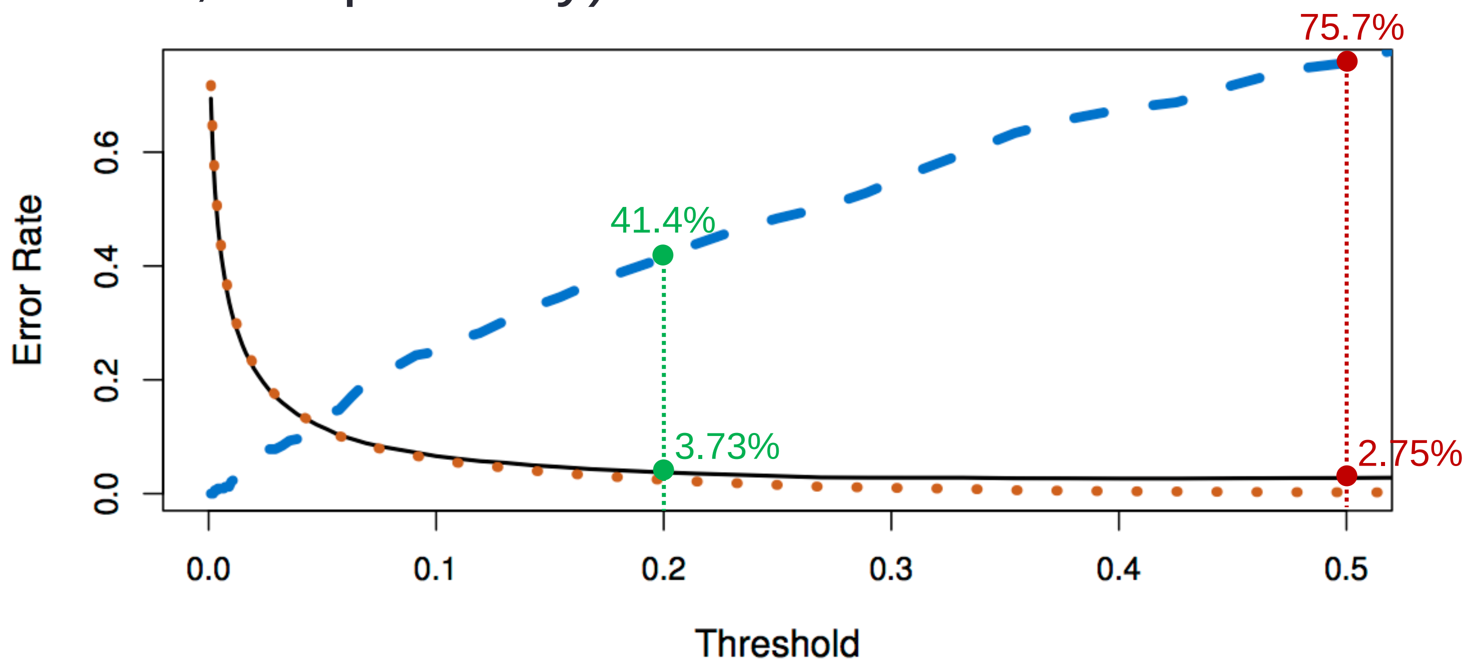
		True Default Status		
		No	Yes	Total
Predicted	No	9644	252	9896
Default Status	Yes	23	81	104
	Total	9667	333	10000

Threshold = 0.2

		True Default Status		
		No	Yes	Total
Predicted	No	9432	138	9570
Default Status	Yes	235	195	430
	Total	9667	333	10000

Threshold Values vs. Error Rates

- **Black** solid: overall error rate
- Blue dashed: fraction of defaulters missed (1–Sensitivity)
- Orange dotted: non-defaulters incorrectly classified (False positive rate, 1–Specificity)



- Decide the threshold based on domain knowledge, such as detailed information about the cost associated with default.

Receiver Operating Characteristics (ROC)

- **Ideal**: top left corner.
- **Diagonal**: “no information” classifier or random guessing
- **Overall performance**: area under the curve (AUC)