Chapter 4: Classification

The linear model in Ch. 3 assumes the response variable Y is quantitiative. But in many situations, the response is categorical.

In this chapter we will look at approaches for predicting categorical responses, a process known as *classification*.

Classification problems occur often, perhaps even more so than regression problems. Some examples include

1.

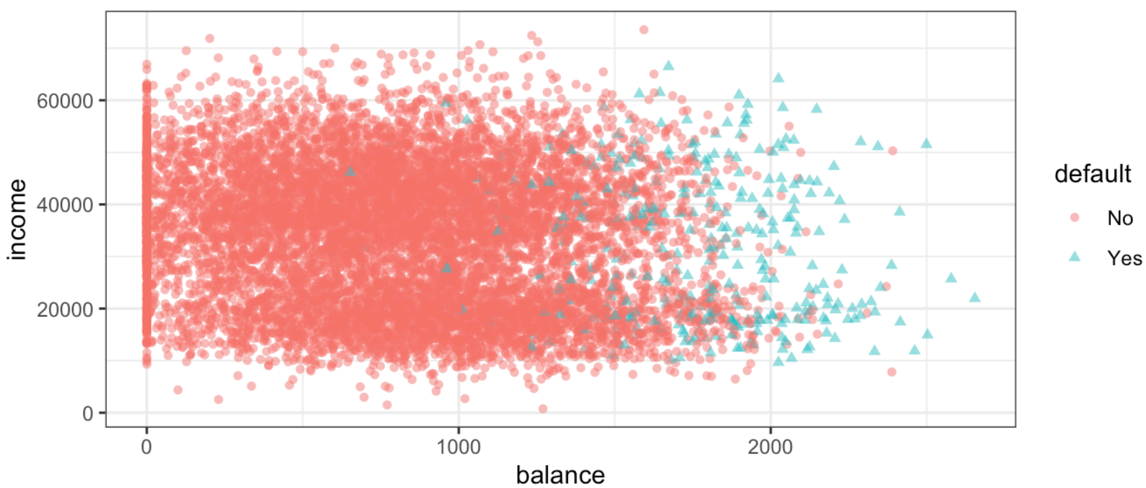
2.

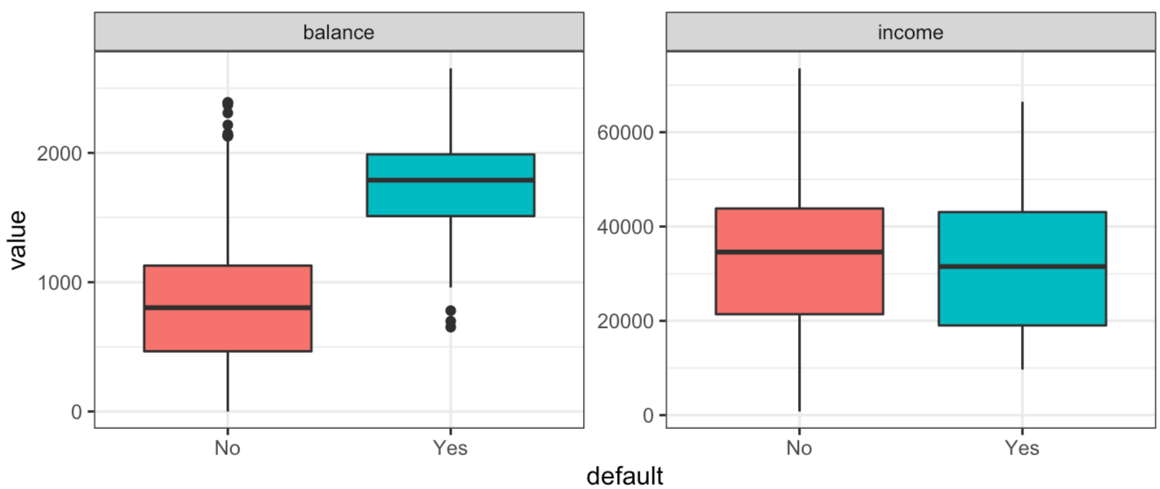
3.

As with regression, in the classification setting we have a set of training observations $(x_1, y_1), \dots, (x_n, y_n)$ that we can use to build a classifier. We want our classifier to perform well on the training data and also on data not used to fit the model (**test data**).

We will use the `Default` data set in the `ISLR` package for illustrative purposes. We are interested in predicting whether a person will default on their credit card payment on the basis of annual income and credit card balance.

```
##   default student   balance    income
## 1      No      No  729.5265 44361.625
## 2      No     Yes  817.1804 12106.135
## 3      No      No 1073.5492 31767.139
## 4      No      No  529.2506 35704.494
## 5      No      No  785.6559 38463.496
## 6      No     Yes  919.5885  7491.559
```





1 Why not Linear Regression?

I have said that linear regression is not appropriate in the case of a categorical response. Why not?

Let's try it anyways. We could consider encoding the values of `default` in a quantitative repsonse variable Y

$$Y = \begin{cases} 1 & \text{if } \texttt{default} \\ 0 & \text{otherwise} \end{cases}$$

Using this coding, we could then fit a linear regression model to predict Y on the basis of `income` and `balance`. This implies an ordering on the outcome, not defaulting comes first before defaulting and insists the difference between these two outcomes is 1 unit. In practice, there is no reason for this to be true.

Using the dummy encoding, we can get a rough estimate of $P(\texttt{default}|X)$, but it is not guaranteed to be scaled correctly.

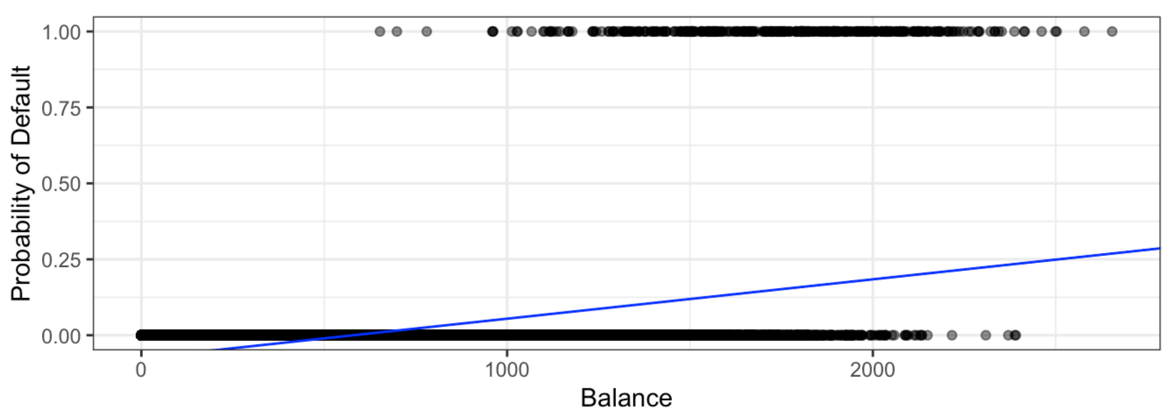
2 Logistic Regression

Let's consider again the `default` variable which takes values `Yes` or `No`. Rather than modeling the response directly, logistic regression models the *probability* that Y belongs to a particular category.

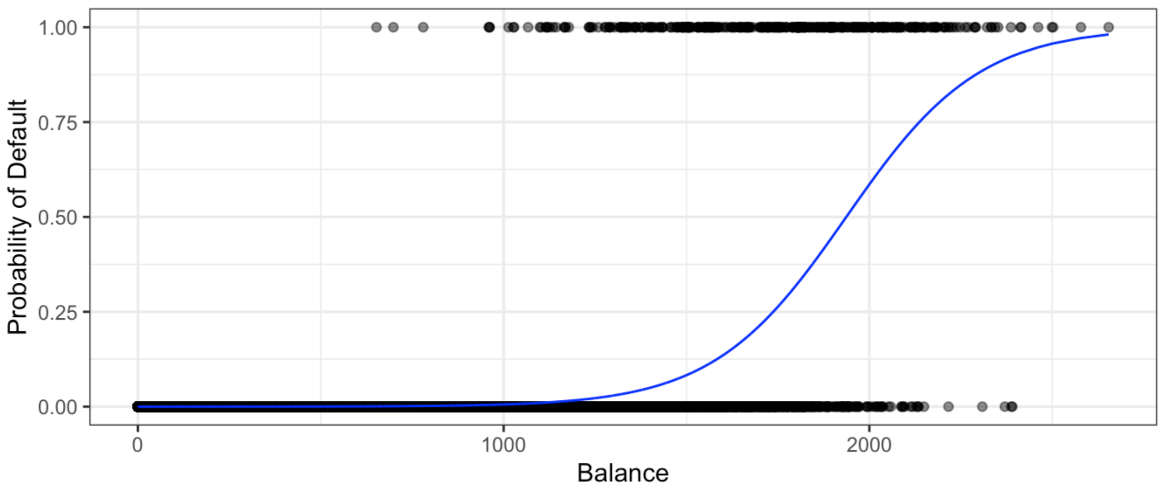
For any given value of `balance`, a prediction can be made for `default`.

2.1 The Model

How should we model the relationship between $p(X) = P(Y = 1|X)$ and X? We could use a linear regression model to represent those probabilities



To avoid this, we must model $p(X)$ using a function that gives outputs between 0 and 1 for all values of X. Many functions meet this description, but in *logistic* regression, we use the *logistic* function,



After a bit of manipulation,

By taking the logarithm of both sides we see,

Recall from Ch. 3 that β_1 gives the "average change in Y associated with a one unit increase in X." In contrast, in a logistic model,

However, because the relationship between $p(X)$ and X is not linear, β_1 does **not** correspond to the change in $p(X)$ associated with a one unit increase in X. The amount that $p(X)$ changes due to a 1 unit increase in X depends on the current value of X.

2.2 Estimating the Coefficients

The coefficients β_0 and β_1 are unknown and must be estimated based on the available training data. To find estimates, we will use the method of *maximum likelihood*.

The basic intuition is that we seek estimates for β_0 and β_1 such that the predicted probability $\hat{p}(x_i)$ of default for each individual corresponds as closely as possible to the individual's observed default status.

```
logistic_spec <- logistic_reg()

logistic_fit <- logistic_spec |>
  fit(default ~ balance, family = "binomial", data = Default)

logistic_fit |>
  pluck("fit") |>
  summary()
```

```
##
## Call:
## stats::glm(formula = default ~ balance, family = stats::binomial,
##     data = data)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -2.2697  -0.1465  -0.0589  -0.0221   3.7589
##
## Coefficients:
##               Estimate Std. Error z value Pr(>|z|)
## (Intercept) -1.065e+01  3.612e-01  -29.49   <2e-16 ***
## balance      5.499e-03  2.204e-04   24.95   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2920.6  on 9999  degrees of freedom
## Residual deviance: 1596.5  on 9998  degrees of freedom
## AIC: 1600.5
##
## Number of Fisher Scoring iterations: 8
```

2.3 Predictions

Once the coefficients have been estimated, it is a simple matter to compute the probability of `default` for any given credit card balance. For example, we predict that the default probability for an individual with `balance` of $1,000 is

In contrast, the predicted probability of default for an individual with a balance of $2,000 is

2.4 Multiple Logistic Regression

We now consider the problem of predicting a binary response using multiple predictors. By analogy with the extension from simple to multiple linear regression,

Just as before, we can use maximum likelihood to estimate $\beta_0, \beta_1, \ldots, \beta_p$.

```
logistic_fit2 <- logistic_spec |>
  fit(default ~ ., family = "binomial", data = Default)

logistic_fit2 |>
  pluck("fit") |>
  summary()
```

```
##
## Call:
## stats::glm(formula = default ~ ., family = stats::binomial, data =
data)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -2.4691  -0.1418  -0.0557  -0.0203   3.7383
##
## Coefficients:
##               Estimate Std. Error z value Pr(>|z|)
## (Intercept) -1.087e+01  4.923e-01 -22.080  < 2e-16 ***
## studentYes  -6.468e-01  2.363e-01  -2.738  0.00619 **
## balance      5.737e-03  2.319e-04  24.738  < 2e-16 ***
## income       3.033e-06  8.203e-06   0.370  0.71152
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2920.6  on 9999  degrees of freedom
## Residual deviance: 1571.5  on 9996  degrees of freedom
## AIC: 1579.5
##
## Number of Fisher Scoring iterations: 8
```

By substituting estimates for the regression coefficients from the model summary, we can make predictions. For example, a student with a credit card balance of $1,500 and an income of $40,000 has an estimated probability of default of

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

2.5 Logistic Regression for > 2 Classes

We sometimes which to classify a response variable that has more than two classes. There are multi-class extensions to logistic regression ("multinomial regression"), but there are far more popular methods of performing this.

3 LDA

Logistic regression involves direction modeling $P(Y = k|X = x)$ using the logistic function for the case of two response classes. We now consider a less direct approach.

Idea:

Why do we need another method when we have logistic regression?

1.

2.

3.

3.1 Bayes' Theorem for Classification

Suppose we wish to classify an observation into one of K classes, where $K \geq 2$.

π_k

$f_k(x)$

$P(Y = k|X = x)$

In general, estimating π_k is easy if we have a random sample of Y's from the population.

Estimating $f_k(x)$ is more difficult unless we assume some particular forms.

3.2 p = 1

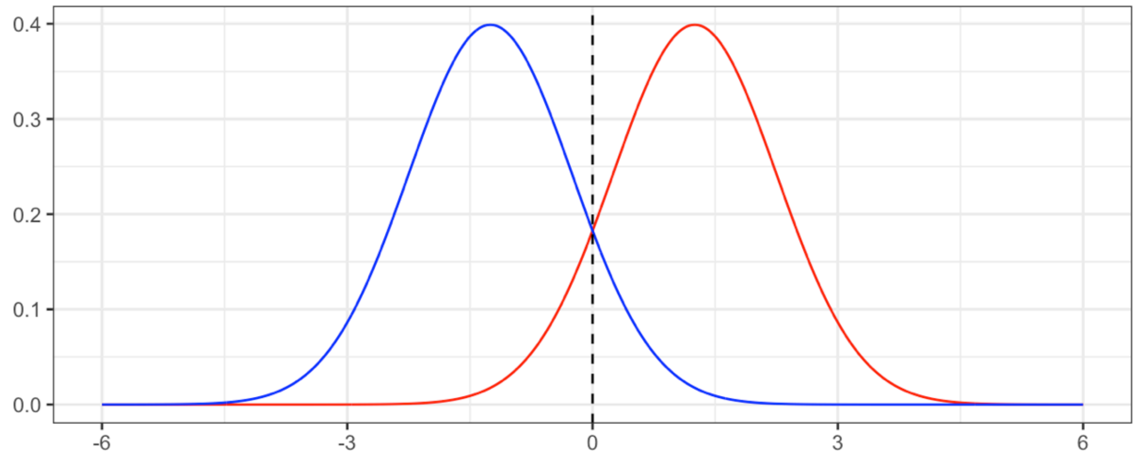
Let's (for now) assume we only have 1 predictor. We would like to obtain an estimate for $f_k(x)$ that we can plug into our formula to estimate $p_k(x)$. We will then classify an observation to the class for which $\hat{p}_k(x)$ is greatest.

Suppose we assume that $f_k(x)$ is normal. In the one-dimensional setting, the normal density takes the form

Plugging this into our formula to estimate $p_k(x)$,

We then assign an observation $X = x$ to the class which makes $p_k(x)$ tthe largest. This is equivalent to

Example 3.1 Let $K = 2$ and $\pi_1 = \pi_2$. When does the Bayes classifier assign an observation to class 1?

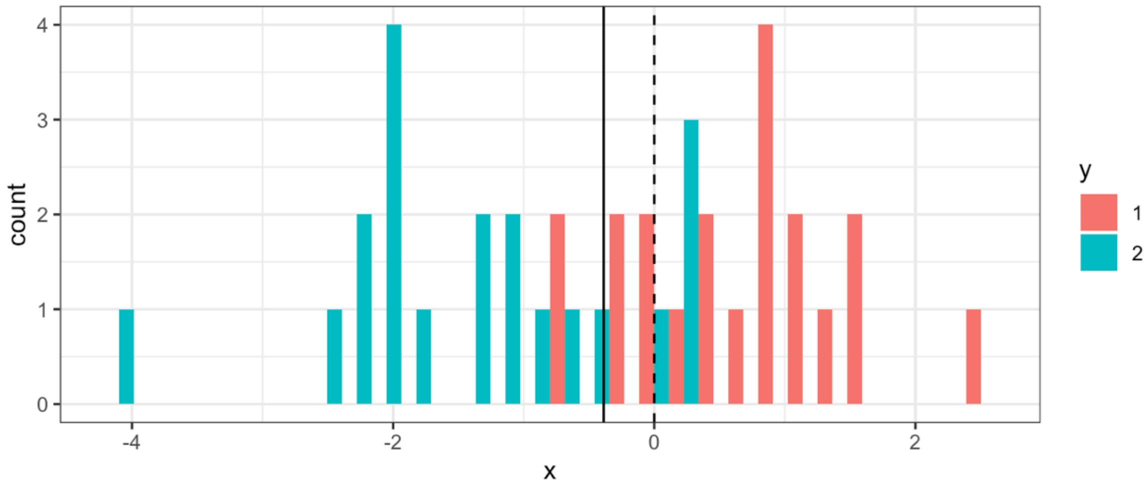


In practice, even if we are certain of our assumption that X is drawn from a Gaussian distribution within each class, we still have to estimate the parameters $\mu_1, \dots, \mu_K, \pi_1, \dots, \pi_K, \sigma^2$.

The *linear discriminant analysis* (LDA) method approximated the Bayes classifier by plugging estimates in for π_k, μ_k, σ^2.

Sometimes we have knowledge of class membership probabilities $\pi_1, \dots, \pi_K$ that can be used directly. If we do not, LDA estimates π_k using the proportion of training observations that belong to the kth class.

The LDA classifier assignes an observation $X = x$ to the class with the highest value of




```
##    pred
## y       1     2
##   1 18966  1034
##   2  3855 16145
```

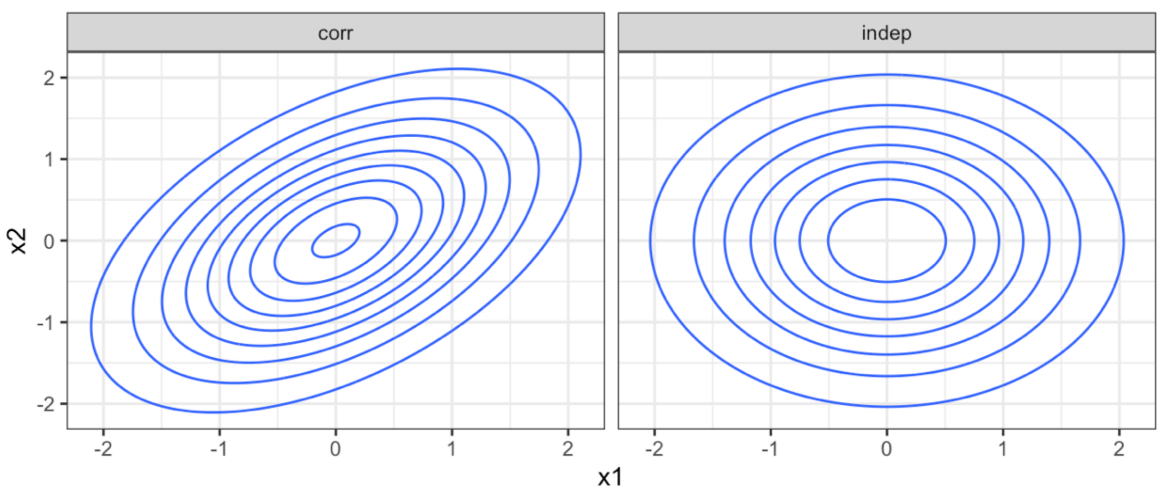
The LDA test error rate is approximately 12.22% while the Bayes classifier error rate is approximately 10.52%.

The LDA classifier results from assuming that the observations within each class come from a normal distribution with a class-specific mean vector and a common variance σ^2 and plugging estimates for these parameters into the Bayes classifier.

3.3 p > 1

We now extend the LDA classifier to the case of multiple predictors. We will assume

Formally the multivariate Gaussian density is defined as



In the case of $p > 1$ predictors, the LDA classifier assumes the observations in the kth class are drawn from a multivariate Gaussian distribution $N(\boldsymbol{\mu}_k, \boldsymbol{\Sigma})$.

Plugging in the density function for the kth class, results in a Bayes classifier

Once again, we need to estimate the unknown parameters $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K, \pi_1, \dots, \pi_K, \boldsymbol{\Sigma}$.

To classify a new value $X = x$, LDA plugs in estimates into $\delta_k(x)$ and chooses the class which maximized this value.

Let's perform LDA on the `Default` data set to predict if an individual will default on their CC payment based on balance and student status.

```r
lda_spec <- discrim_linear(engine = "MASS")

lda_fit <- lda_spec |>
  fit(default ~ student + balance, data = Default)

lda_fit |>
  pluck("fit")
```

```
## Call:
## lda(default ~ student + balance, data = data)
##
## Prior probabilities of groups:
##     No    Yes
## 0.9667 0.0333
##
## Group means:
##     studentYes   balance
## No   0.2914037  803.9438
## Yes  0.3813814 1747.8217
##
## Coefficients of linear discriminants:
##                     LD1
## studentYes -0.249059498
## balance     0.002244397
```

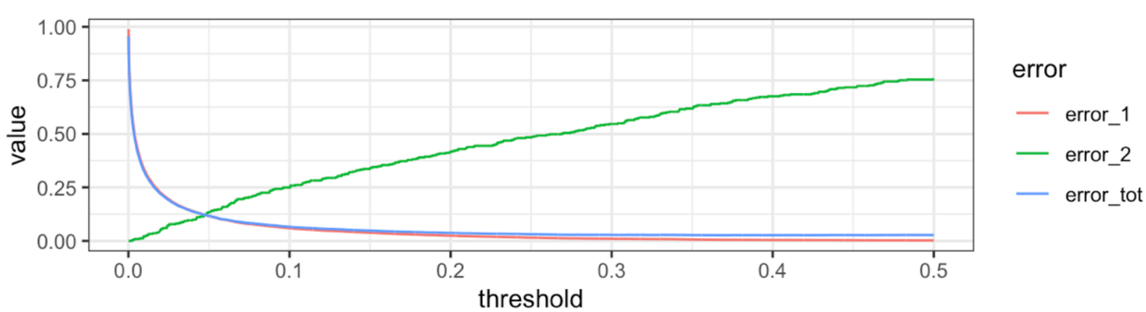
```r
# training data confusion matrix
lda_fit |>
  augment(new_data = Default) |>
  conf_mat(truth = default, estimate = .pred_class)
```

```
##           Truth
## Prediction   No  Yes
##        No  9644  252
##        Yes   23   81
```

Why does the LDA classifier do such a poor job of classifying the customers who default?

```r
lda_fit |>
  augment(new_data = Default) |>
  mutate(pred_lower_cutoff = factor(ifelse(.pred_Yes > 0.2, "Yes",
         "No"))) |>
  conf_mat(truth = default, estimate = pred_lower_cutoff)
```

```
##           Truth
## Prediction   No  Yes
##        No  9432  138
##        Yes  235  195
```



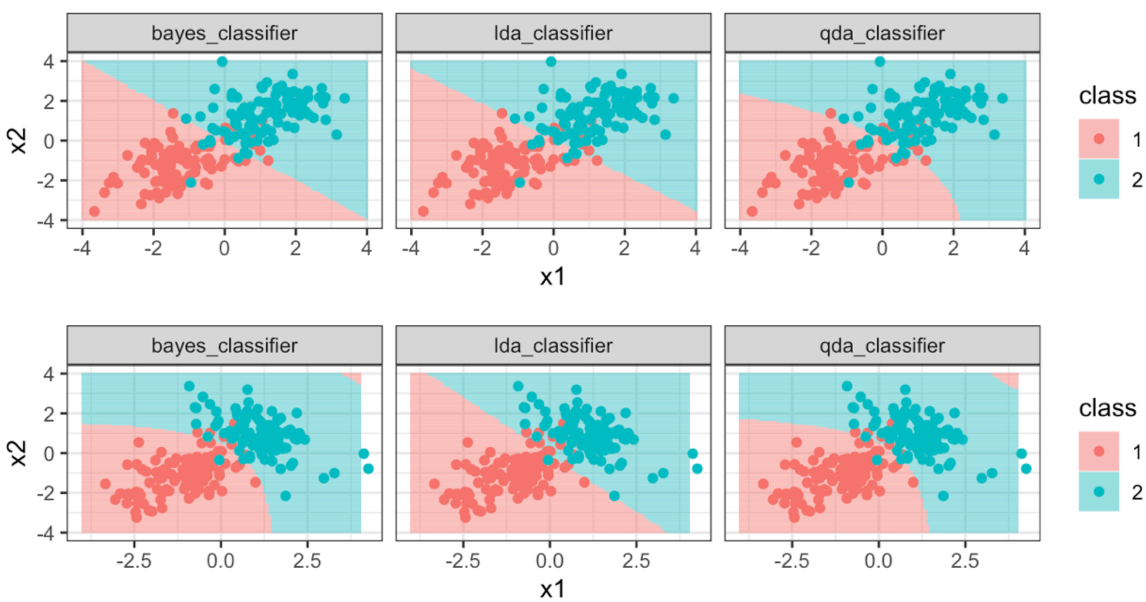
3.4 QDA

LDA assumes that the observations within each class are drawn from a multivariate Gaussian distribution with a class-specific mean vector and a common covariance matrix across all K classes.

Quadratic Discriminant Analysis (QDA) also assumes the observations within each class are drawn from a multivariate Gaussian distribution with a class-specific mean vector but now each class has its own covariance matrix.

Under this assumption, the Bayes classifier assigns observation $X = x$ to class k for whichever k maximizes

When would we prefer QDA over LDA?

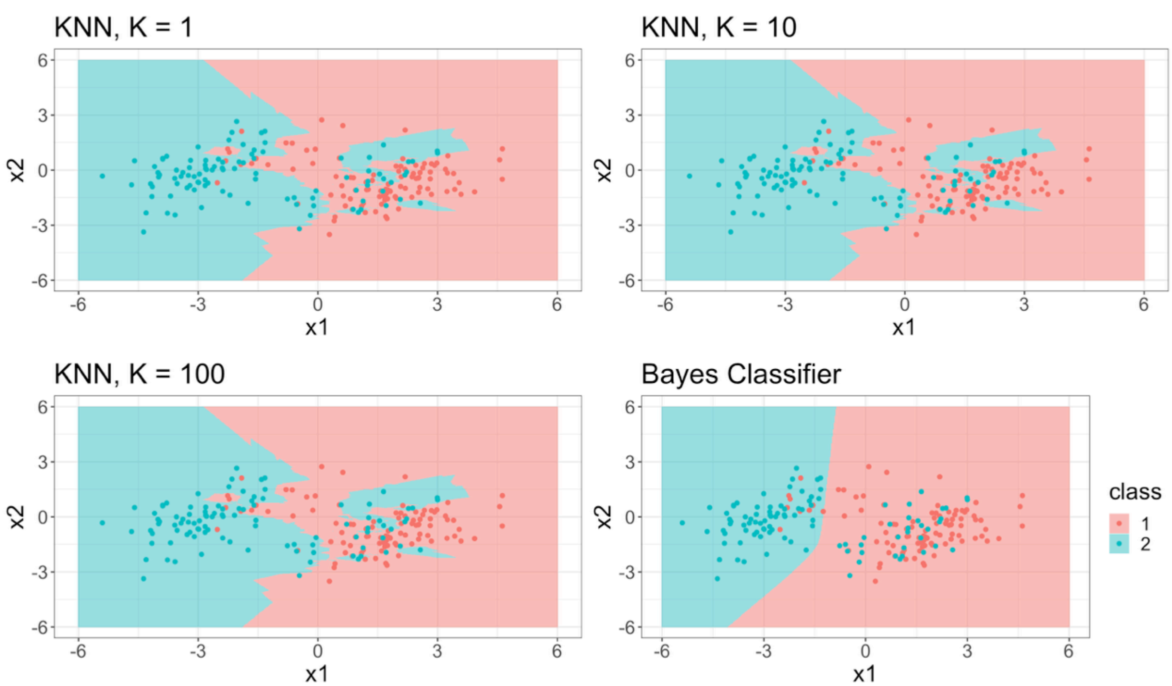


4 KNN

Another method we can use to estimate $P(Y = k|X = x)$ (and thus estimate the Bayes classifier) is through the use of K-nearest neighbors.

The KNN classifier first identifies the K points in the training data that are closest to the test data point $X = x$, called $\mathcal{N}(x)$.

Just as with regression tasks, the choice of K (neighborhood size) has a drastic effect on the KNN classifier obtained.



5 Comparison

LDA vs. Logistic Regression

(LDA & Logistic Regression) vs. KNN

QDA