Chapter 4: Classification

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

e.g. eye color
cancer diagnosis
which product a customer would purchase.

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. A person arrives in the emergency room w/ set of symptoms that could be attributed to 3 root causes. predict which condition the person has.

2. An online banking service must be able to determine if a transaction is fraudulent or not on the basis of IP address, past transaction history, etc.

3. Something is in the street in front of a self-driving car you are riding in. The car must determine if it is a human or another car.

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**).

fit a model.

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.

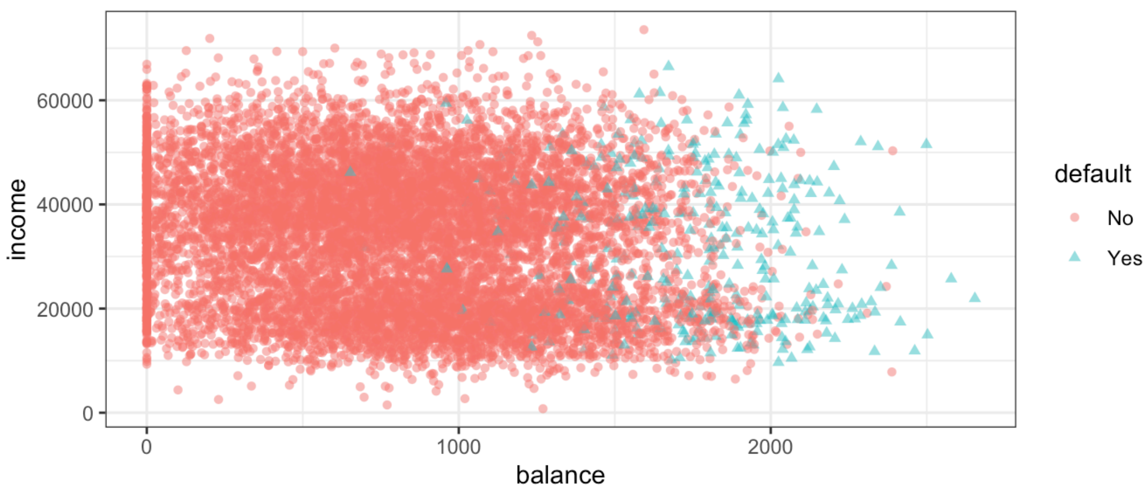
↓ yes or no => categorical.

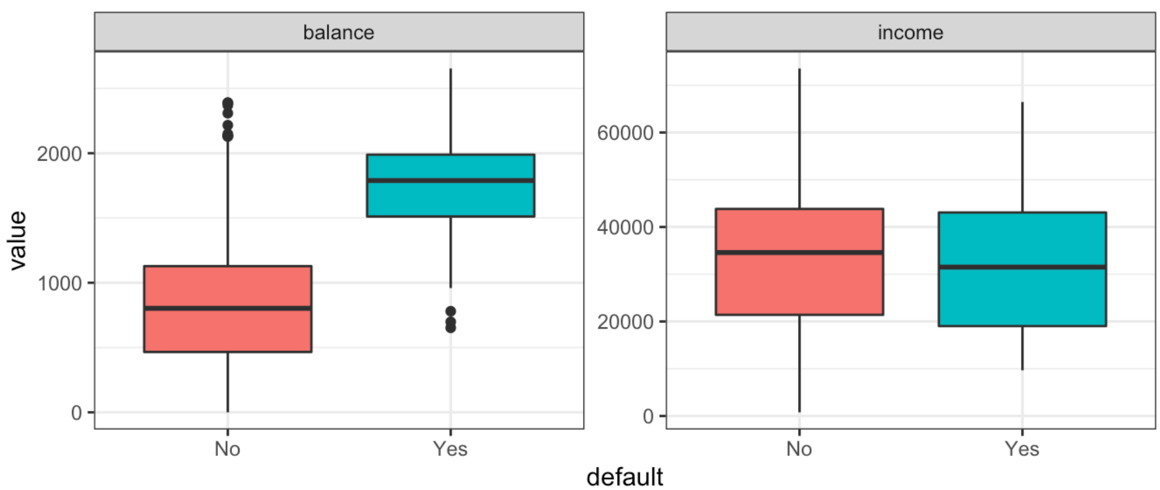
head(Default).

y features.

```
##   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
```

okay separation





relationship between balance and default

(in most real world problems the relationship is not so clear).

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.

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

$Y = \begin{cases} 1 & \text{if default} \\ 10 & \text{otherwise.} \end{cases}$

there is no natural reason to choose 0/1, but it has an advantage:

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

predictions don't have to be between 0 and 1 but will provide an ordering.

Additional problem: this cannot be easily extended to more than 2 classes.

We can instead use methods specifically formulated for categorical responses.

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.

e.g. $P(\text{default} = \text{Yes} \mid \text{balance})$

which can be abbreviated as $p(\text{balance}) \in [0,1]$.

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

e.g. predict default = Yes if $p(\text{balance}) > 0.5$

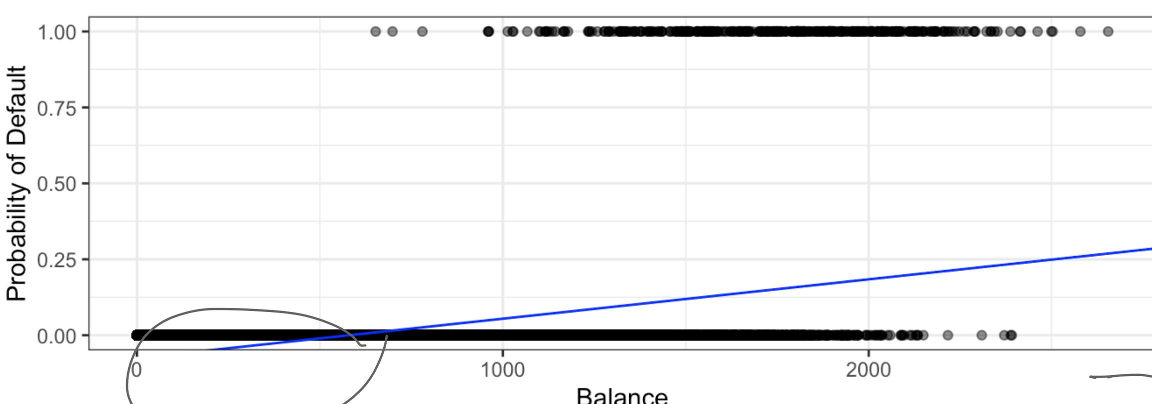
or the company could be more conservative and predict default = Yes if $p(\text{balance}) > 0.1$ threshold.

2.1 The Model

using 0/1 encoding — define as success (e.g. default = Yes).

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

$$p(X) = \beta_0 + \beta_1 X$$



problem: for balances close to 0, we predict negative prob. of default.

If we had a very large balance, would predict prob ≥ 1 of defaulting

neither of these make sense!

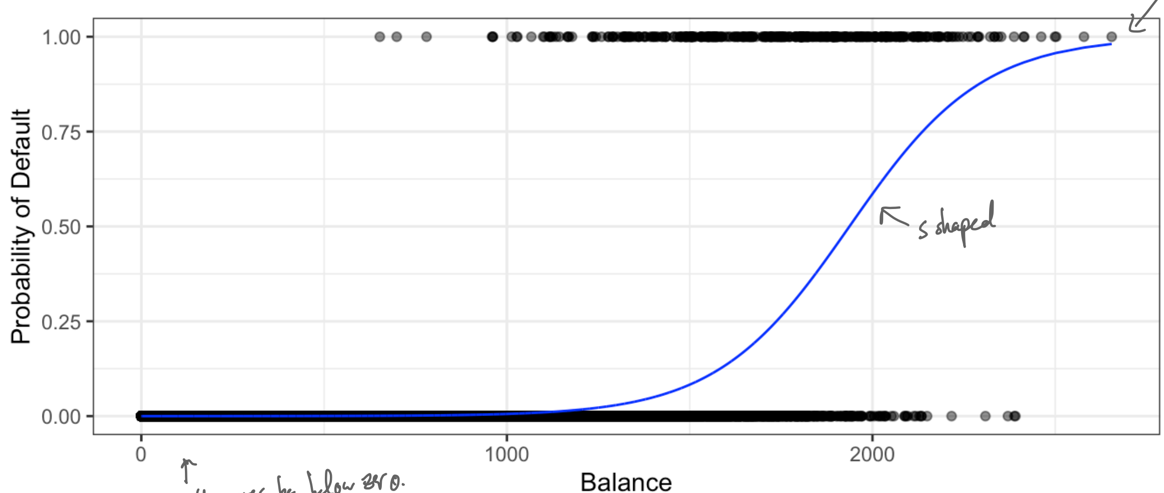
To avoid this, we must model $p(X)$ using a function that gives outputs between 0 and 1 for all values of X. Many functions meet this description, but in *logistic* regression, we use the *logistic* function,

standard logistic function $f(x) = \frac{e^x}{1+e^x}$

$$p(x) = \frac{e^{\beta_0+\beta_1 X}}{1+e^{\beta_0+\beta_1 X}}$$

We will use maximum likelihood to estimate parameters (β_0, β_1) — later.

will never be above 1



s shaped

will never be below zero.

will always get sensible prediction for $p(X)$.

After a bit of manipulation,

$$\underbrace{\frac{p(x)}{1-p(x)}}_{\text{"odds"}} = e^{\beta_0+\beta_1 X}$$

"odds" → can take any value between 0 and ∞

low prob of default

high prob of default.

ex: $p(x) = 0.2$ (1 in 5 people default) $\Rightarrow$ odds $= \frac{0.2}{1-0.2} = \frac{1}{4}$

By taking the logarithm of both sides we see,

$$\underbrace{\log\left(\frac{p(x)}{1-p(x)}\right)}_{\substack{\text{"log-odds"} \\ \text{"logit"}}} = \beta_0 + \beta_1 x$$

log-odds is linear in X.

"log-odds"

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,

increasing X by one-unit changes the log-odds by β_1

$$\Longleftrightarrow$$

increasing X by one unit multiplies the odds by e^{β_1}

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.

Regardless of the value of X,

if β_1 is positive $\Rightarrow$ increasing X increases $p(X)$.

if β_1 is negative $\Rightarrow$ increasing X reduces $p(X)$.

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.

function of parameter; given training data

to do this, use the likelihood $L(\beta_0, \beta_1 \mid \{y_i, \underline{x}_i\}_{i=1}^n) = \prod_{i:y_i=1} p(\underline{x}_i) \prod_{i:y_i=0} (1 - p(\underline{x}_i))$.

$\hat{\beta}_0$ and $\hat{\beta}_1$ chosen to maximize $L(\beta_0, \beta_1)$. (use calculus: derivatives wrt β_0, β_1, set $=0$, solve). use numeric optimization

Aside: in linear regression model w/ $\varepsilon_i \overset{iid}{\sim} N(0, \sigma^2)$ $\Rightarrow$ $\hat{\beta}_{MLE} = \hat{\beta}_{OLS}$

```
logistic_spec <- logistic_reg()

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

$y \sim X$; Y takes values in $\{0,1\}$.

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

$\hat{\beta}_0, \hat{\beta}_1$; accuracy of estimates ; Hypothesis test $H_0: \beta_i = 0$, $H_a: \beta_i \neq 0$

```
##
## 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
```

if $H_0: \beta_1 = 0$ true, implies $p(X) = \frac{e^{\beta_0}}{1+e^{\beta_0}}$ (doesn't depend on X $\Rightarrow$ no relationship).

$\hat{\beta}_1 = 0.0055 \Rightarrow$ increase in balance associated w/ increase in prob. of default.

$\Rightarrow$ one unit increase in balance associated w/ average increase of $\boxed{\text{log-odds}}$ by .0055 units.

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

$$\hat{p}(x) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 x}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 x}}$$

$$\hat{p}(1000) = \frac{e^{-10.6513 + 0.0055 \times 1000}}{1 + e^{-10.6513 + 0.0055 \times 1000}} = 0.00576$$

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

$$\hat{p}(2000) = \frac{e^{-10.6513 + 0.0055 \times 2000}}{1 + e^{-10.6513 + 0.0055 \times 2000}} = 0.586 > 0.5$$

maybe we would predict default = yes based on a threshold of 0.5.

(tidymodels: augment
predict)

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,

$$\log\left(\frac{p(x)}{1-p(x)}\right) = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$$

$$\Downarrow$$

$$p(x) = \frac{e^{\beta_0 + \beta_1 x_1 + \dots + \beta_p x_p}}{1 + e^{\beta_0 + \beta_1 x_1 + \dots + \beta_p x_p}}$$

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

logistic regression specification.

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

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

$Y \sim$ every other variable in data

Y is in $\{0,1\}$.

$\hat\beta_0, \hat\beta_1, \hat\beta_2, \hat\beta_3$ SE$(\hat\beta_i)$ $H_0: \beta_i = 0$ $H_a: \beta_i \neq 0$

```
##
## 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
```

dummy variable for categorical predictor

no significant relationship

$\hat\beta_{student(Yes)} < 0 \Rightarrow$ if you are a student LESS likely to default holding balance & income constant.

student confounded w/ income. (see "restricted regression" for more).

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

$$\hat{p}(\underline{x} = \{\text{Yes}, 1500, 40000\}) = \frac{\exp(-10.689 + (-0.6468)\times 1 + 0.00574\times 1500 + 0.000003\times 40000)}{1 + \exp(-10.689 + (-0.6468)\times 1 + 0.00574\times 1500 + 0.000003\times 40000)}$$

$$= 0{,}058$$

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

$$\hat{p}(\underline{x} = \{\text{No}, 1500, 40000\}) = 0{,}105$$

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 "linear discriminant analysis"

Logistic regression involves directly 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:

Model the distribution of the predictors X separately in each of the response classes (given Y). and then use Bayes theorem to flip these and get $P(Y=k|X=x)$.

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

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

1. Classes well separated, parameter estimates of predictors are surprisingly unstable

2. n is small (& X $\overset{apx}{\sim}$ Normal) → LDA more stable

3. if we have > 2 response classes

3.1 Bayes' Theorem for Classification

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

Y - response (K distinct)

π_k

→ prior → overall probability that an observation is in class K

$$f_k(x) = \begin{cases} P(X = x \mid Y = k) & \rightarrow \text{discrete} \\ P(X \text{ in some small interval} \mid Y = k) & \rightarrow \text{continuous} \end{cases}$$

"density of X in class k"

$$\underbrace{P(Y = k|X = x)}_{p_k(x)} = \frac{P(X=x \mid Y=k)\,P(Y=k)}{P(X=x)} = \frac{f_k(x)\cdot\pi_k}{\sum_{l=1}^{K}\pi_l f_l(x)}$$

"posterior probability"

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

prior

$$\pi_k = \frac{\text{\# of obs. in class } k}{\text{Total \# of observations}}$$

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

If we can estimate $f_k(x)$ → we can develop a classifier close to the "BEST" classifier.

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

$$x \sim N(\mu_k, \sigma_k^2)$$

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

Assume for now $\sigma_k^2 = \sigma^2$ for all k

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

$$p_k(x) = P(Y=k|X=x) = \frac{\overset{\text{prior}}{\pi_k} \overbrace{\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu_k)^2\right\}}^{\to f_k(x)}}{\underbrace{\sum_{l=1}^{K} \pi_l \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu_l)^2\right\}}_{P(X=x) = \sum_k P(X=x|Y=k)\pi_k \text{ (Total prob)}}} \quad \text{prop } \propto \text{ Numerator}$$

Forgot to add this in class

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

maximizing $\delta_k(x) = x\frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k) \leftarrow$

Example 3.1 Let $K = 2$ and $\pi_1 = \pi_2$. When does the Bayes classifier assign an observation to class 1? $\boxed{\mu_1 > \mu_2}$

$$\delta_1(x) > \delta_2(x)$$

$$\delta_1(x) = x\frac{\mu_1}{\sigma^2} - \frac{\mu_1^2}{2\sigma^2} + \cancel{\log(\pi_1)} > x\frac{\mu_2}{\sigma^2} - \frac{\mu_2^2}{2\sigma^2} + \cancel{\log(\overset{\pi_1}{\pi_2})}$$

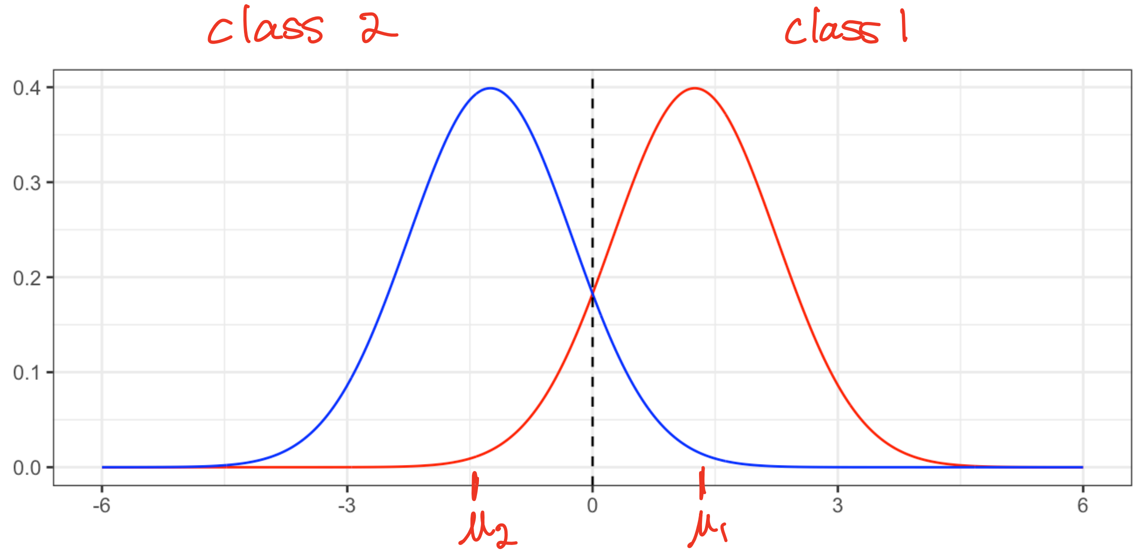
$$= 2x(\mu_1 - \mu_2) > \mu_1^2 - \mu_2^2$$

$\mu_1 > \mu_2$

$$2x(\cancel{\mu_1 - \mu_2}) > (\cancel{\mu_1 - \mu_2})(\mu_1 + \mu_2)$$

$$x > \frac{\mu_1 + \mu_2}{2}$$

Note: if $\mu_1 < \mu_2$ $x < \frac{\mu_1 + \mu_2}{2}$ is the boundary



$\mu_1 = 1.5$
$\mu_2 = -1.5$

$x \to$ class 1 when $\frac{1.5 - 1.5}{2} < x$

$0 < x$

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.

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

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

weighted avg. of class variances

n = Total # of observations
n_k = # obs. in class K

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.

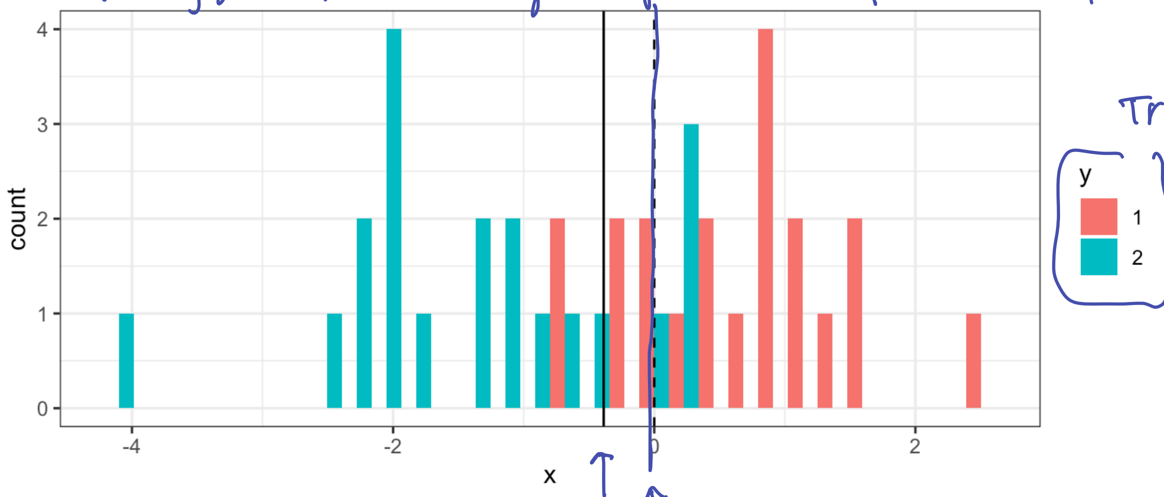
$$\hat{\pi}_k = \frac{n_k}{n}$$

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

$$\hat{\delta}_k(x) = x \frac{\hat{\mu}_k}{\hat{\sigma}^2} - \frac{\hat{\mu}_k^2}{2\hat{\sigma}^2} + \log(\hat{\pi}_k)$$

linear

Histogram of Randomly Sampled Points from Class 1 & 2



True value

LDA Boundary

$\frac{\hat{\mu}_1 + \hat{\mu}_2}{2}$

Bayes classifier

$\frac{\mu_1 + \mu_2}{2}$

LDA confusion Matrix

```
##      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%.

$$\frac{1034 + 3855}{18966 + 1034 + 3855 + 16145} = \text{error}$$

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

$\underline{X} = (X_1, \dots, X_p) \sim MVN(\underline{\mu}, \Sigma)$

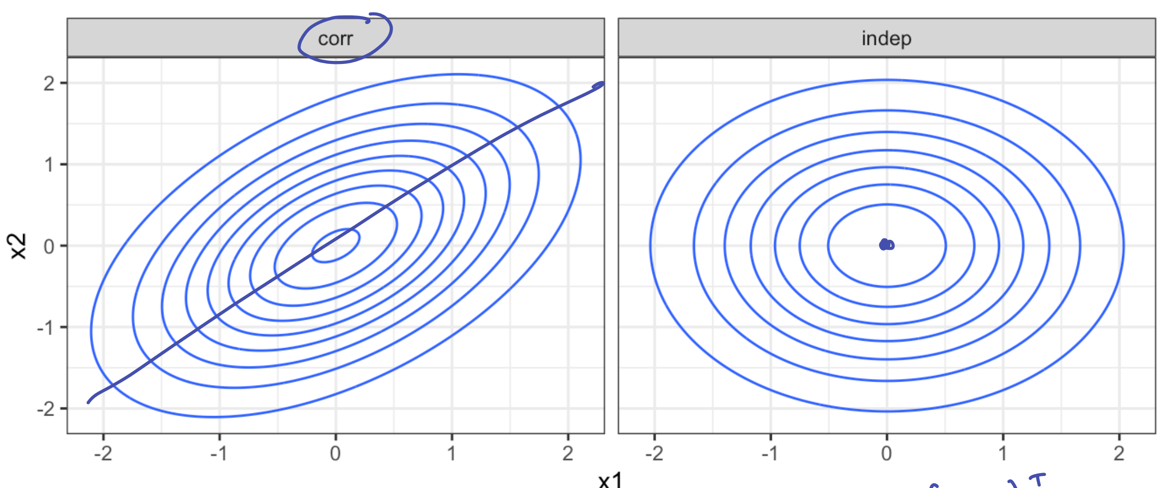
Formally the multivariate Gaussian density is defined as

$$f(\underline{x}) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\underline{x}-\underline{\mu})^T \Sigma^{-1} (\underline{x}-\underline{\mu})\right)$$

"trace"

↳ sum of elements on diagonal

$p = 2$



$\underline{\mu} = (0, 0)^T$

$\Sigma = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}$

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

$$\delta_k(x) = \underline{x}^T \Sigma^{-1} \underline{\mu}_k - \frac{1}{2}\underline{\mu}_k^T \Sigma^T \underline{\mu}_k + \log \pi_k$$

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

$$\hat{\delta}_k(x) = \underline{x}^T \hat{\Sigma}^{-1} \hat{\underline{\mu}}_k - \frac{1}{2}\underline{\mu}_k^T \hat{\Sigma}^T \underline{\mu}_k + \log \hat{\pi}_k$$

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.

```
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
```

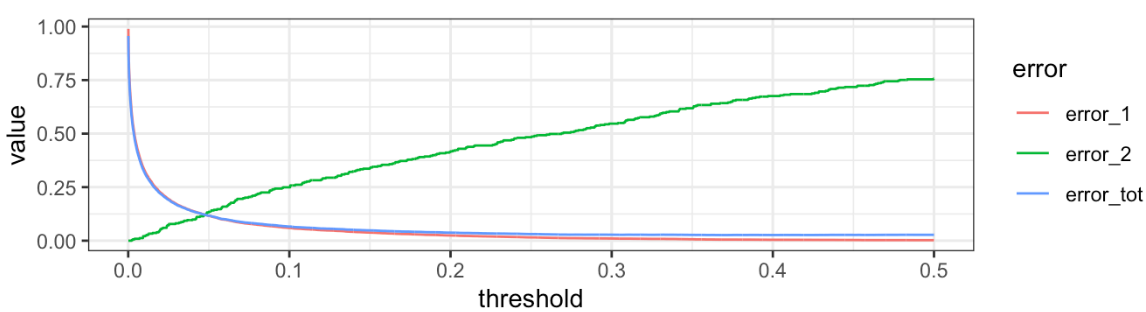
```r
# training data confusion matrix
lda_fit |>
  augment(new_data = Default) |>
  conf_mat(truth = default, estimate = .pred_class)
```

```
##           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
```



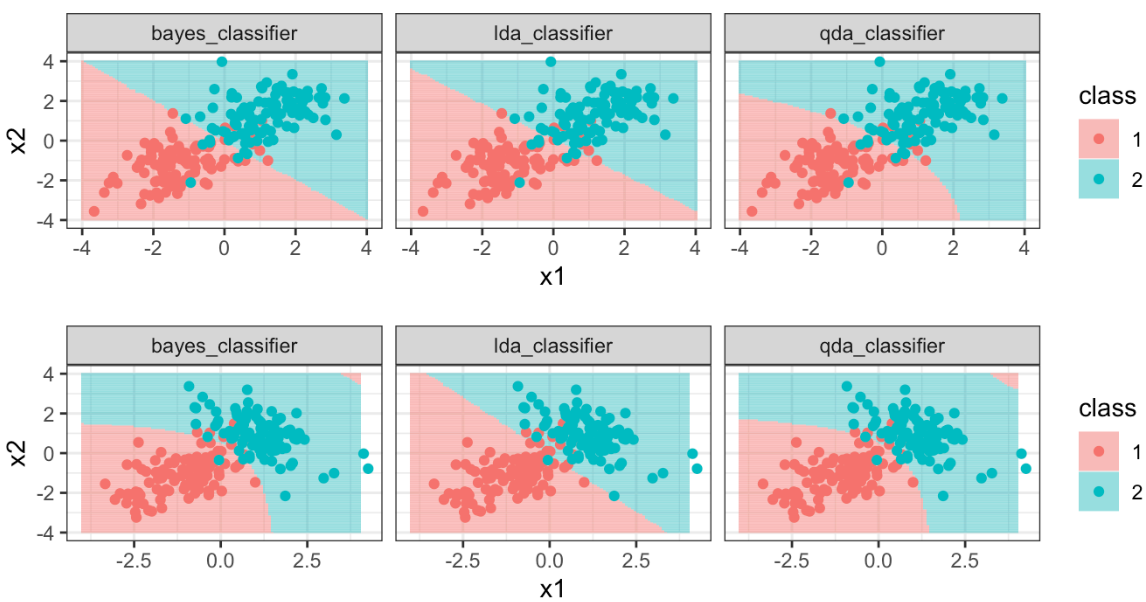
3.4 QDA

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?

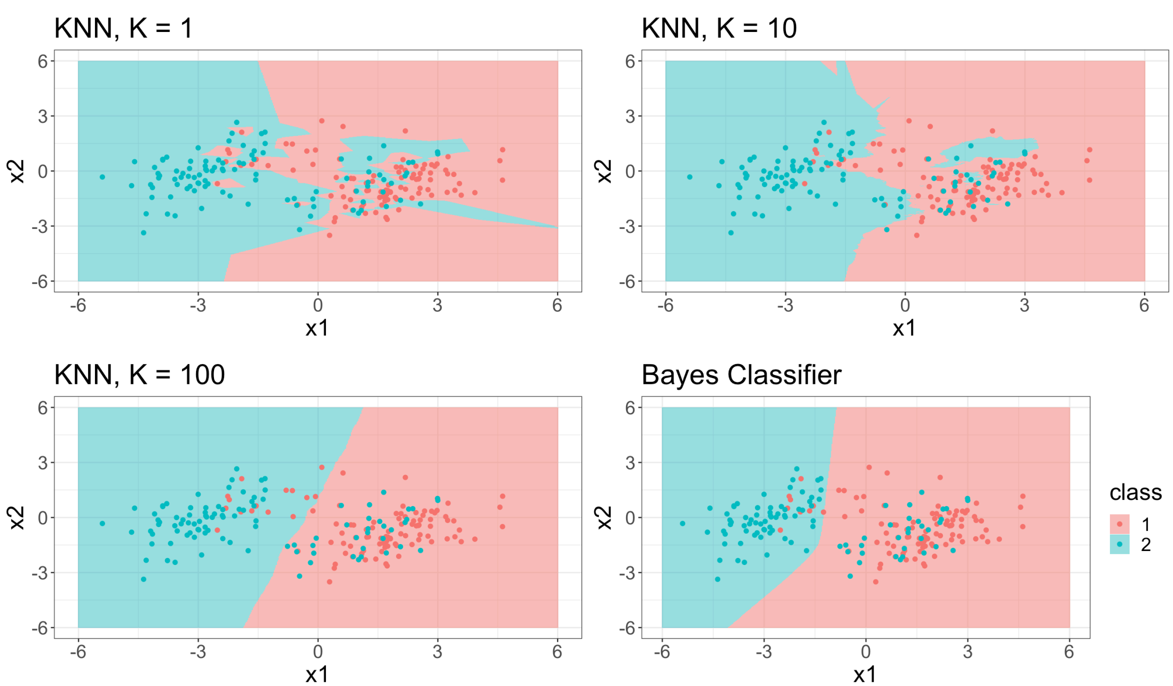


4 KNN

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