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
whether a car's hwy mpg is above or below the median ....

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 at an ER w/ set of symptoms that could possibly be attributed to three medical conditions. Which of these three conditions does the person have?
2. An online banking service must be able to determine if a transaction is fraudulent based on user's IP address, past transaction history, etc...
3. Something is in the street in front of the self-driving car you are riding in. The car must decide if it is a human or not.

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
↓
get parameter estimates most likely.

most importantly.

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.

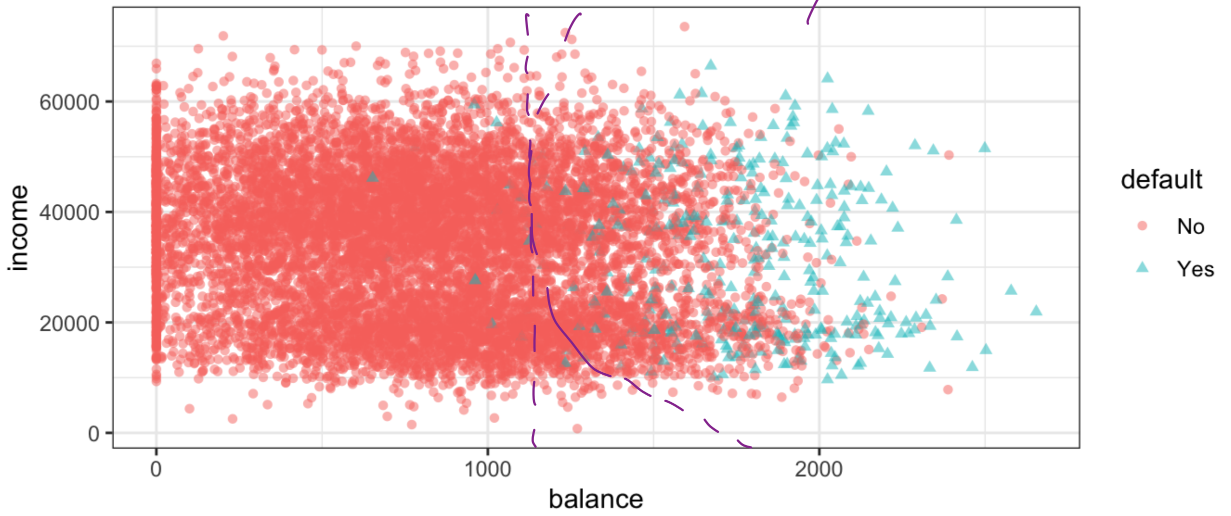
↓
yes or no $\Rightarrow$ categorical predictor $\Rightarrow$ classification

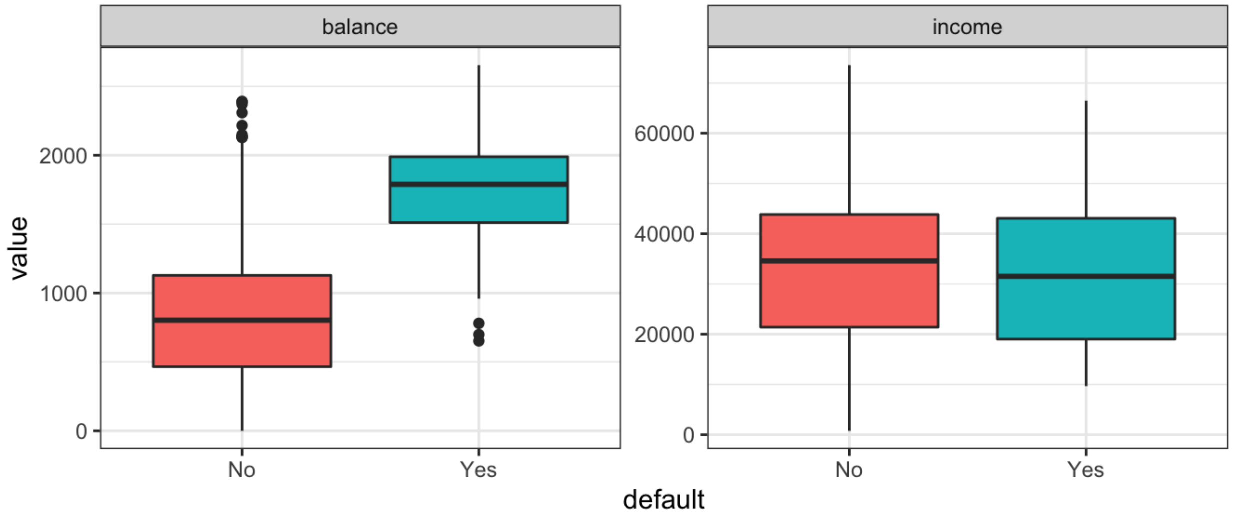
head (Default)

y

```
##   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
```

decent separation not great





pronounced relationship between balance and default

in most real world problems the relationship between predictor 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 for 0/1 encoding, but it does have an advantage:

Using the $\overset{0/1}{\text{dummy}}$ encoding, we can get a rough estimate of $\underline{P(\texttt{default}|X)}$, but it is not guaranteed to be scaled correctly.

↓

doesn't have to be between 0 and 1.
but will provide us an ordering.

Real problem: this cannot be 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 we can abbreviate $p(\text{balance}). \in [0,1]$.

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

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

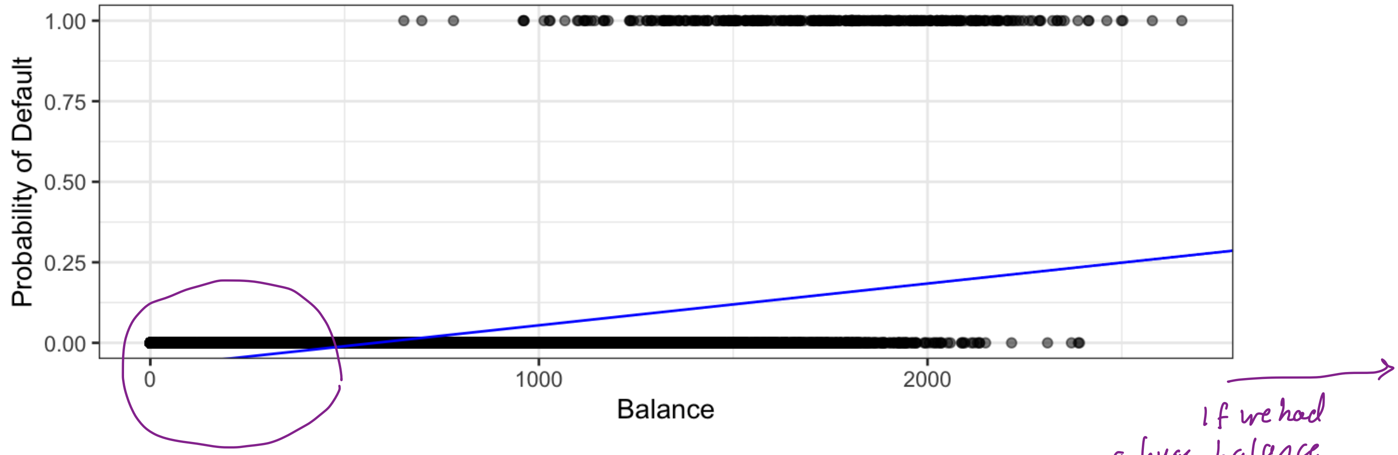
or the company could be more conservative and predict default = Yes if $p(\text{balance}) > 0.1$.

2.1 The Model

using 0/1 encoding.

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 zero, we predict negative probability of default

neither of these make sense!

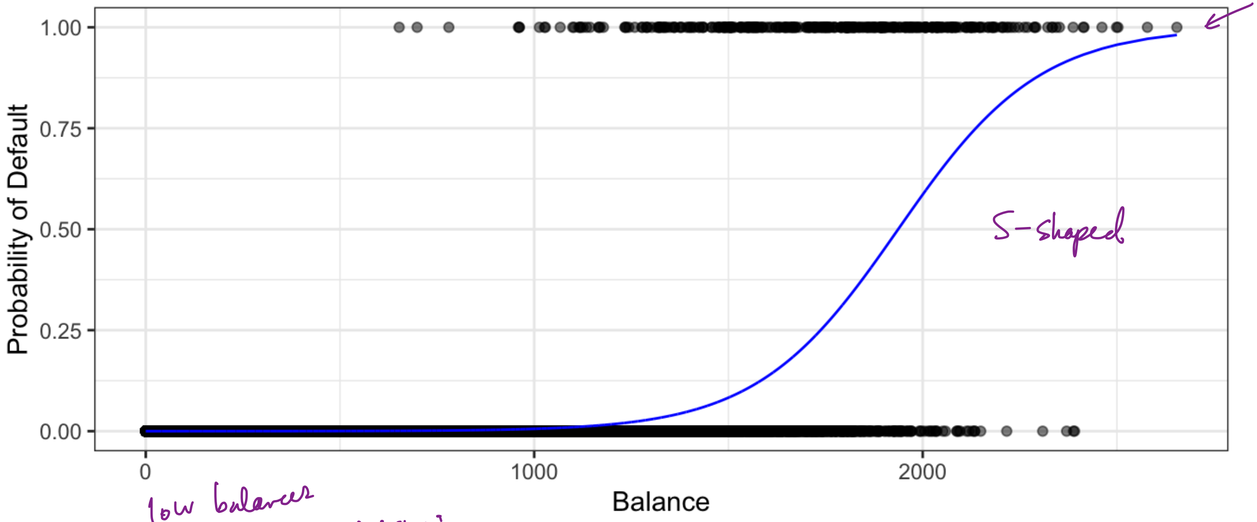
If we had a huge balance we would have probability > 1 of defaulting.

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

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,

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

We will use maximum likelihood to estimate coefficients (more later).



will never be above 1

S-shaped

low balances now predict probabilities close to zero but never below.

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

After a bit of manipulation,

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

$$\Big\downarrow$$

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

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

low prob of default

high prob of default

e.g. $P(X) = 0.2$ (1 in 5 people w/ this balance X will default)

$$\Rightarrow \text{odds} = \frac{0.2}{1-0.2} = \frac{1}{4}$$

By taking the logarithm of both sides we see,

$$\underbrace{\log\left(\frac{p(X)}{1-p(X)}\right)}_{\substack{\text{“log-odds”} \\ \text{“logit”}}} = \beta_0 + \beta_1 X \quad \leftarrow \quad \text{log odds is linear in X.}$$

linear relationship between X and Y

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,

An increase in X by one unit changes the log-odds by β_1

$$\iff$$

An increase in 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 $\Rightarrow$ increase X increases $P(Y=y|X)$

If β_1 is negative $\Rightarrow$ increase X decreases $P(Y=y|X)$.

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.

to do this, we will use the likelihood function $\ell(\beta_0, \beta_1) = \prod_{i:y_i=1} p(x_i) \prod_{i:y_i=0} (1 - p(x_i))$

$\hat{\beta}_0$ and $\hat{\beta}_1$ chosen to maximize $\ell(\beta_0, \beta_1)$.

In fact least squares is a special case of maximum likelihood.

$Y \sim X$

```
m1 <- glm(default ~ balance, family = "binomial", data = Default)
summary(m1)
```

"generalized linear model"

Y takes values in $\{0, 1\}$

$Y | X \sim \text{Binomial}(p(X))$.

accuracy of estimates

$\frac{\hat{\beta}_i}{SE(\hat{\beta}_i)}$.

test

$H_0: \beta_i = 0$

$H_a: \beta_i \neq 0$

H_0 implies $p(X) = \frac{e^{\beta_0}}{1 + e^{\beta_0}}$ $i = 1$.

$\Rightarrow$ does not depend on X

$\Rightarrow$ no sig. relationship w/ X.

```
##
## Call:
## glm(formula = default ~ balance, family = "binomial", data = Default)
##
## 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
```

$\hat{\beta}_0$

$\hat{\beta}_1$

there is a sig. relationship between default & balance.

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

↳ increase in log-odds of default by 0.0055 unit.

↳ multiplicative increase in odds of default by $e^{0.0055}$ units.

2.3 Predictions

predicted

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

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0+\hat{\beta}_1 X}}{1+e^{\hat{\beta}_0+\hat{\beta}_1 X}} = \frac{e^{-10.6513+0,0055\times1000}}{1+e^{-10.6513+0.0055\times1000}} = 0.00576$$

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

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0+\hat{\beta}_1 X}}{1+e^{\hat{\beta}_0+\hat{\beta}_1 X}} = \frac{e^{-10.6513+0.0055\times2000}}{1+e^{-10.6513+0.0055\times2000}} = 0,586$$

58.6% > 50% => maybe we would predict default = Yes based on threshold = 0,5.

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 $\beta_0, \beta_1, \dots, \beta_p$.

0/1 response.

```
m2 <- glm(default ~ ., family = "binomial", data = Default)
summary(m2)
```

$Y \sim$ every other column in our data frame

```
##
## Call:
## glm(formula = default ~ ., family = "binomial", data = Default)
##
## 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
```

$\hat{\beta}_i$ $SE(\hat{\beta}_i)$ $H_0: \beta_i = 0$ $H_a: \beta_i \neq 0$

dummy variable.

no sig. relationship w/ income.

$\hat{\beta}_{\text{student[Yes]}} < 0 \Rightarrow$ If you are a student LESS likely to default holding balance and income constant.

student confounded w/ balance and income. (If you are a student, more likely to have high balance and low income)

but if you have some balance and income as non-student, less likely to default.

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

$$\hat{p}(x) = \frac{e^{-10.869 + 0.00574(1500) + 0.000003 \times 40000 - 0.6468 \times 1}}{1 + e^{-10.869 + 0.00574(1500) + 0.000003 \times 40000 - 0.6468 \times 1}}$$

$$= 0.058$$

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

$$\hat{p}(x) = \frac{e^{-10.869 + 0.00574(1500) + 0.000003 \times 40000 - 0.6468 \times 0}}{1 + e^{-10.869 + 0.00574(1500) + 0.000003 \times 40000 - 0.6468 \times 0}}$$

$$= 0.105$$

in R:

predict(m2, predict-df)

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.