Lecture 7: Hypothesis testing and classification

CME/STATS 195

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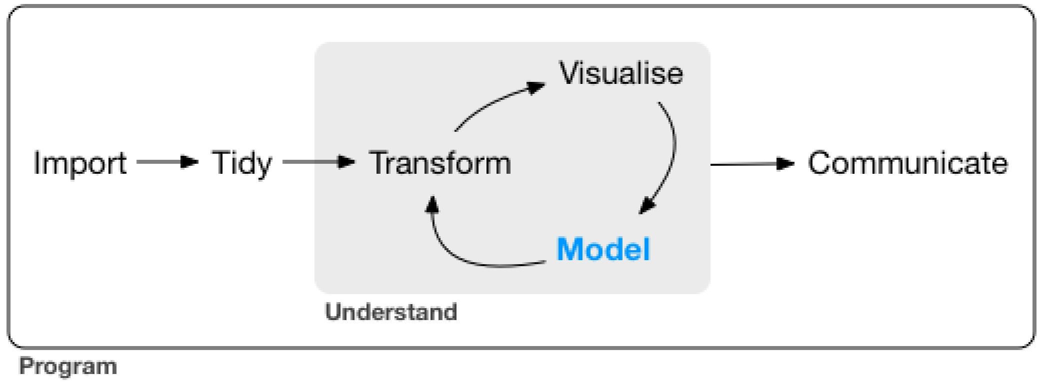


Hypothesis testing

Hypothesis testing can answer questions:

- **Is the measured quantity equal to/higher/lower than a given threshold?** e.g. is the number of faulty items in an order statistically higher than the one guaranteed by a manufacturer?
- **Is there a difference between two groups or observations**? e.g. Do treated patient have a higher survival rate than the untreated ones?
- **Is the level of one quantity related to the value of the other quantity?** e.g. Is hyperactivity related to eating sugar? Is lung cancer related to smoking?

To perform a hypothesis test you need to:

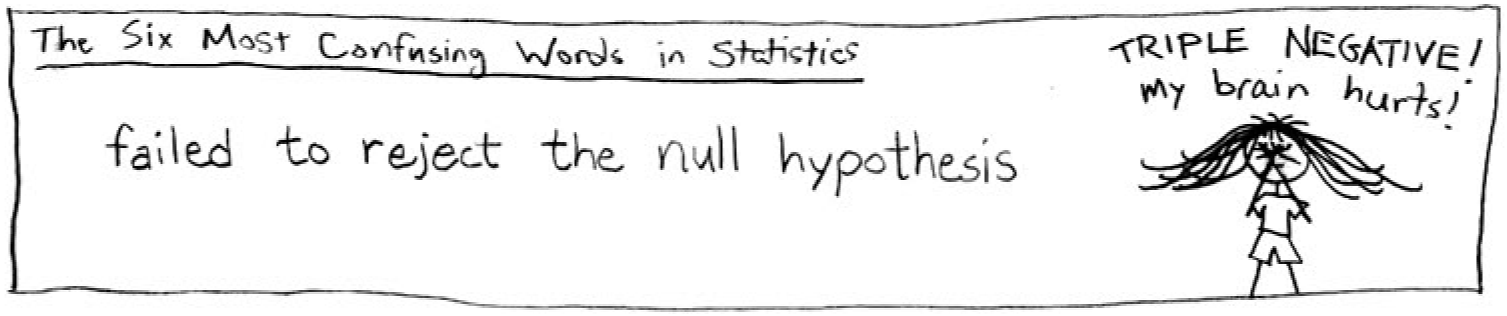
1. Define the null and alternative hypotheses.
2. Choose level of significance α.
3. Pick and compute test statistics.
4. Compute the p-value.
5. Check whether to reject the null hypothesis by comparing p-value to α.
6. Draw conclusion from the test.

Null and alternative hypotheses

The null hypothesis (H_0): A statement assumed to be true unless it can be shown to be incorrect beyond a reasonable doubt. This is something one usually attempts to disprove or discredit.

The alternate hypothesis (H_1): A claim that is contradictory to H0 and what we conclude when we reject H0.

H0 and H1 are on purpose set up to be contradictory, so that one **can collect and examine data to decide if there is enough evidence to reject the null hypothesis or not.**


The Six Most Confusing Words in Statistics
failed to reject the null hypothesis
TRIPLE NEGATIVE! my brain hurts!

Student’s t-test

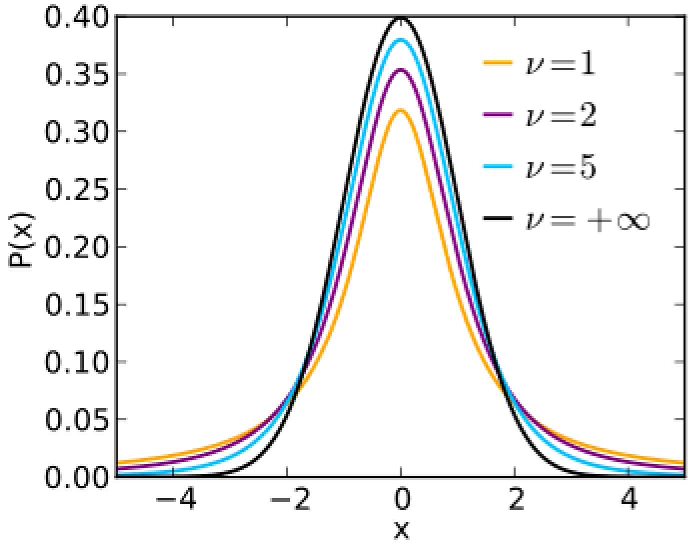
- William Gosset (1908), a chemist at **the Guiness brewery**.
- Published in Biometrika under a **pseudonym Student**.
- Used to select best yielding varieties of barley.
- Now one of the standard/traditional methods for hypothesis testing.

Among the typical applications:

- Comparing population mean to a constant value
- Comparing the means of two populations
- Comparing the slope of a regression line to a constant

In general, used when the test statistic would follow a normal distribution if the value of a scaling term in the test statistic were known.

Distribution of the t-statistic



If $X_i \sim \mathcal{N}(\mu, \sigma^2)$, the empirical estimates for mean and variance are: $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$ and $s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$

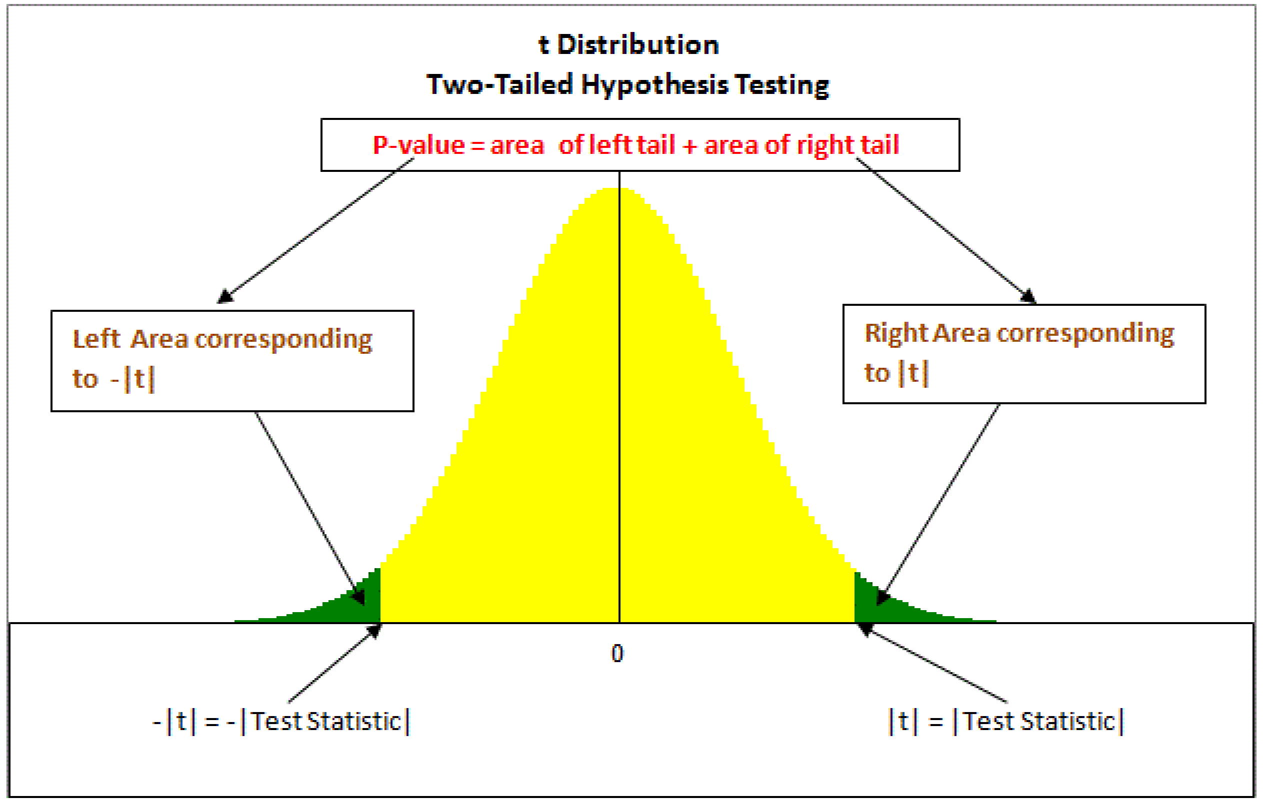
The t-statistic is:

$$T = \frac{\bar{X} - mu}{s/\sqrt{n}} \sim t_{\nu=n-1}$$

p-value

- p-value is the **probability of obtaining the same or “more extreme” event than the one observed, assuming the null hypothesis holds (is true)**.
- A small p-value, typically < 0.05, indicates **strong evidence** against the null hypothesis; in this case you can reject the null hypothesis.
- A large p-value, > 0.05, indicates **weak evidence** against the null hypothesis; in this case, you do NOT reject the null hypothesis.

$$p - value = P[observations \ | \ hypothesis] \neq P[hypothesis \ | \ ovservations]$$



p-values should NOT be used a “ranking”/“scoring” system for your hypotheses

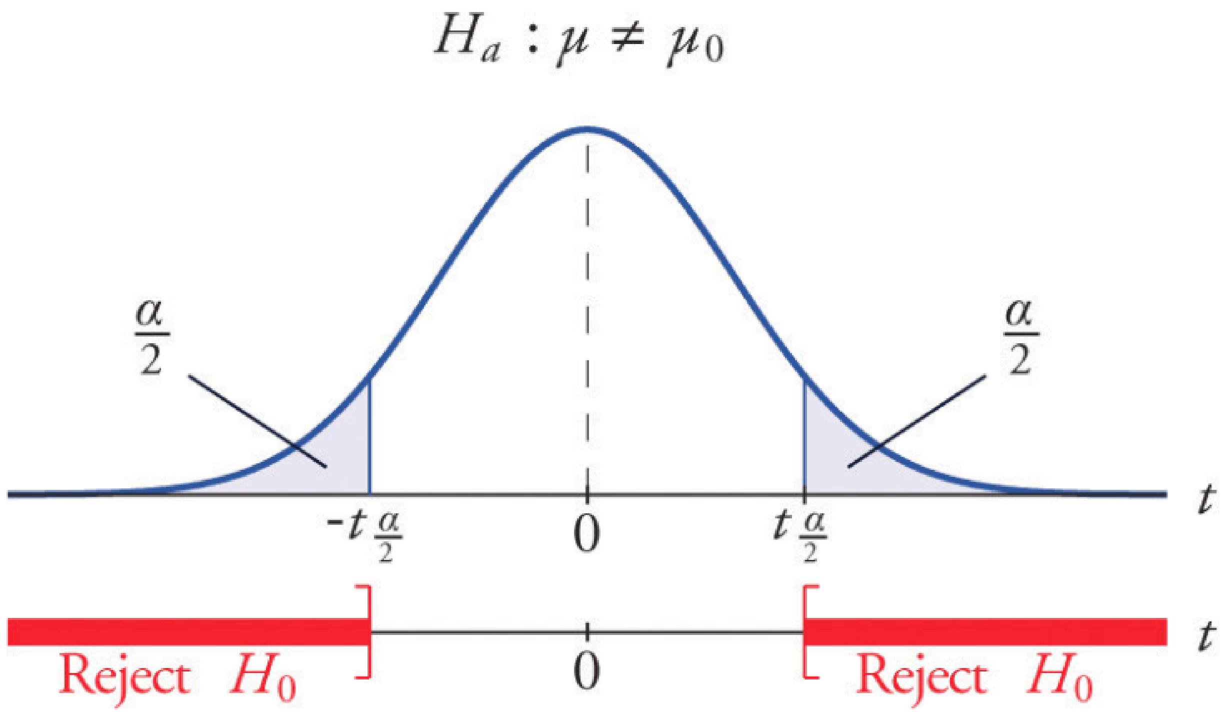
Two-sided test of the mean

Is the mean flight arrival delay statistically equal to 0?

Test the null hypothesis:

$$H_0 : \mu = \mu_0 = 0$$
$$H_a : \mu \neq \mu_0 = 0$$

where μ is where μ is the average arrival delay.



```r
library(tidyverse)
library(nycflights13)
mean(flights$arr_delay, na.rm = T)
```

```
## [1] 6.895377
```

Is this statistically significant?

```r
( tt = t.test(x=flights$arr_delay, mu=0, alternative="two.sided" ) )
```

```
##
##  One Sample t-test
##
## data:  flights$arr_delay
## t = 88.39, df = 327340, p-value < 2.2e-16
## alternative hypothesis: true mean is not equal to 0
## 95 percent confidence interval:
##  6.742478 7.048276
## sample estimates:
## mean of x
##  6.895377
```

The function t.test returns an object containing the following components:

```r
names(tt)
```

```
## [1] "statistic"   "parameter"   "p.value"     "conf.int"    "estimate"   
## [6] "null.value"  "alternative" "method"      "data.name"  
```

```r
# The p-value:
tt$p.value
```

```
## [1] 0
```

```r
# The 95% confidence interval for the mean:
tt$conf.int
```

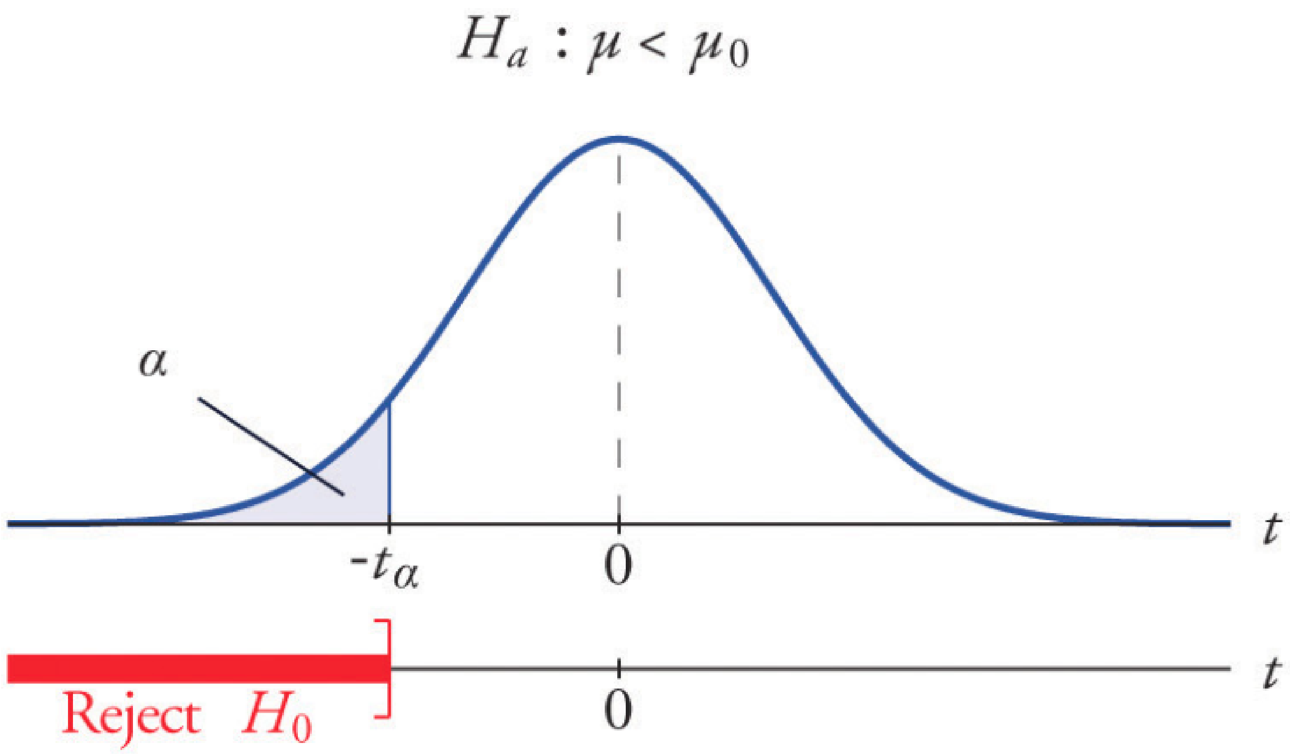
```
## [1] 6.742478 7.048276
## attr(,"conf.level")
## [1] 0.95
```

One-sided test of the mean

One-sided can be more powerful, but the intepretation is more difficult.

Test the null hypothesis:

$$H_0 : \mu = \mu_0 = 0$$
$$H_a : \mu < \mu_0 = 0$$



```r
t.test(x, mu=0, alternative="less")
```

Is the average delay 5 or is it lower?

```r
( tt = t.test(x=flights$arr_delay, mu=5, alternative="less" ) )
```

```
##
##  One Sample t-test
##
## data:  flights$arr_delay
## t = 24.296, df = 327340, p-value = 1
## alternative hypothesis: true mean is less than 5
## 95 percent confidence interval:
##      -Inf 7.023694
## sample estimates:
## mean of x
##  6.895377
```

Failure to reject is not acceptance of the null hypothesis.

Testing difference between groups

Is the average arrival delay the same for the winter and summer?

Test the null hypothesis:

$$
\begin{aligned}
H_0 &: \mu_a = \mu_b \\
H_a &: \mu_a \neq \mu_b
\end{aligned}
$$

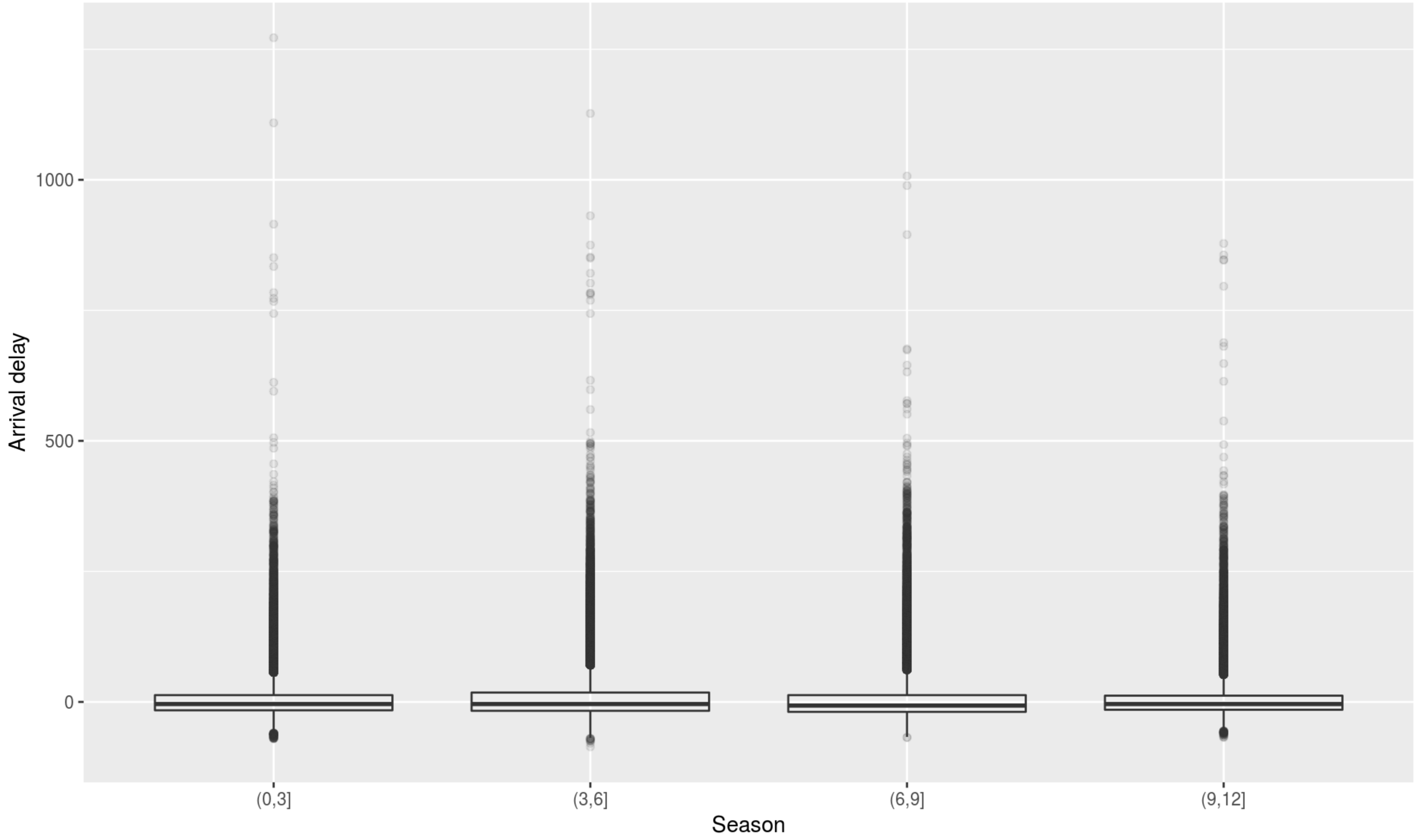
where μ_a mean `arr_delay` in the winter and μ_b is the mean `arr_delay` in the summer.

```
t.test(x, y)
```

Seasonal differences in flight delay

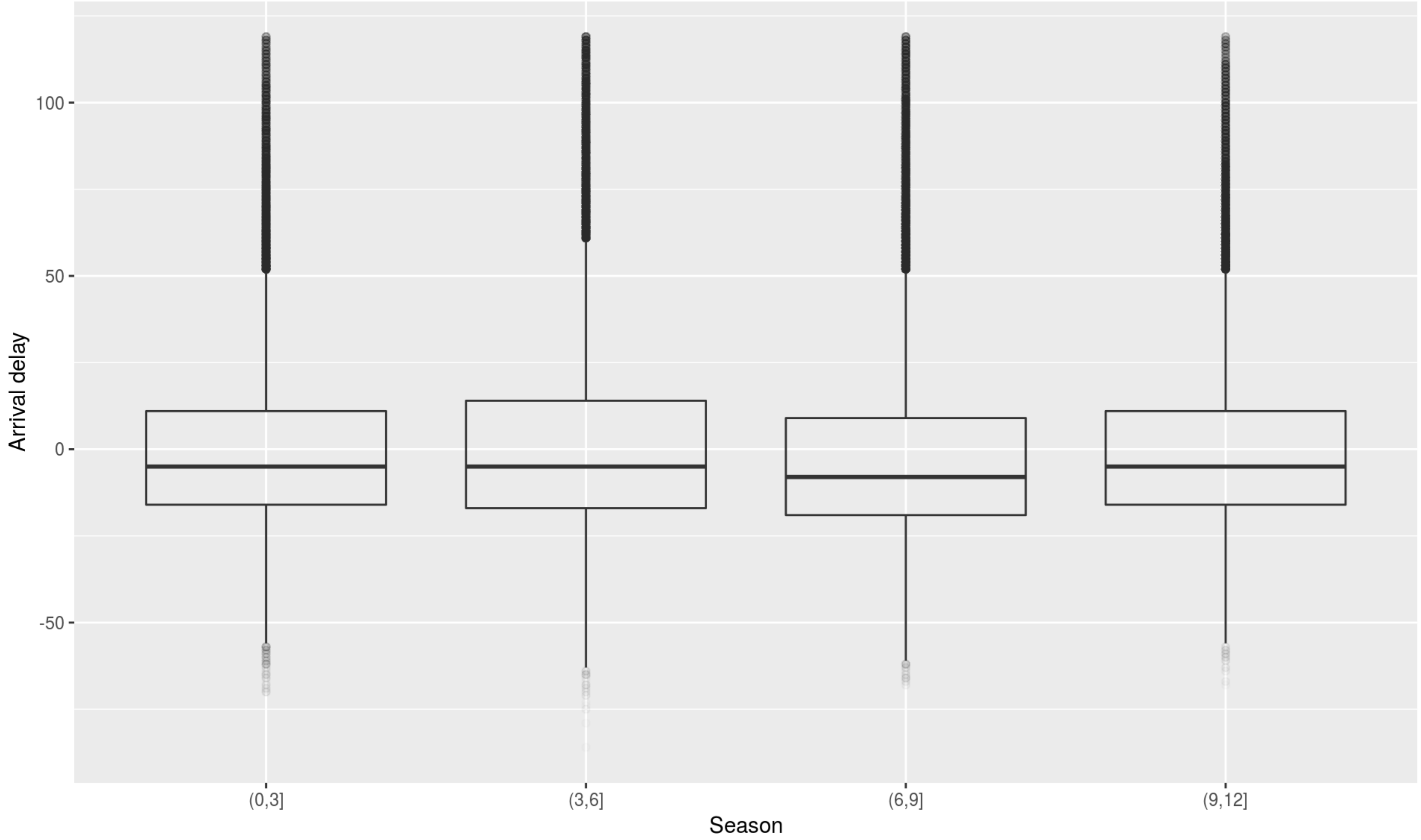
```
flights %>%
  mutate(season = cut(month, breaks = c(0,3,6,9,12))) %>%
  ggplot(aes(x = season, y = arr_delay)) + geom_boxplot (alpha=0.1) +
    xlab("Season" ) + ylab("Arrival delay" )
```

```
## Warning: Removed 9430 rows containing non-finite values (stat_boxplot).
```



Seasonal differences in flight delay

```
flights %>%
  filter(arr_delay < 120) %>%
  mutate(season = cut(month, breaks = c(0,3,6,9,12))) %>%
  ggplot(aes(x = season, y = arr_delay)) + geom_boxplot (alpha=0.01) +
    xlab("Season" ) + ylab("Arrival delay" )
```



Testing seasonal differences in flight delay

```r
flights.winter = filter(flights, month %in% c(1,2,3))
flights.summer = filter(flights, month %in% c(7,8,9))
t.test(x=flights.winter$arr_delay, y=flights.summer$arr_delay)
```

```
##
##  Welch Two Sample t-test
##
## data:  flights.winter$arr_delay and flights.summer$arr_delay
## t = -2.4383, df = 161250, p-value = 0.01476
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
##  -0.9780344 -0.1063691
## sample estimates:
## mean of x mean of y
##  5.857851  6.400052
```

Exercise

- Go to the “Lec7_Exercises.Rmd” file, which can be downloaded from the class website under the Lecture tab.
- Complete Exercise 1.

Classification

- **Classification** is a supervised method which deals with prediction outcomes or **response variables that are qualitative, or categorical**.
- The task is to classify or **assign each observation to a category or a class.**
- Examples of classification problems include:
    - predicting what medical condition or disease a patient has base on their symptoms,
    - determining cell types based on their gene expression profiles (single cell RNA-seq data).
    - detecting fraudulent transactions based on the transaction history

Logistic Regression

Logistic Regression

- Logistic regression is actually used for **classification**, and not regression tasks, $Y \in \{0, 1\}$.
- The name **regression** comes from the fact that the method **fits a linear function to a continuous quantity, the log odds of the response**.

$$p = P[Y = 1 \mid X]$$

$$\log\left(\frac{p}{1-p}\right) = X\beta = \beta_0 + \beta_1^T x$$

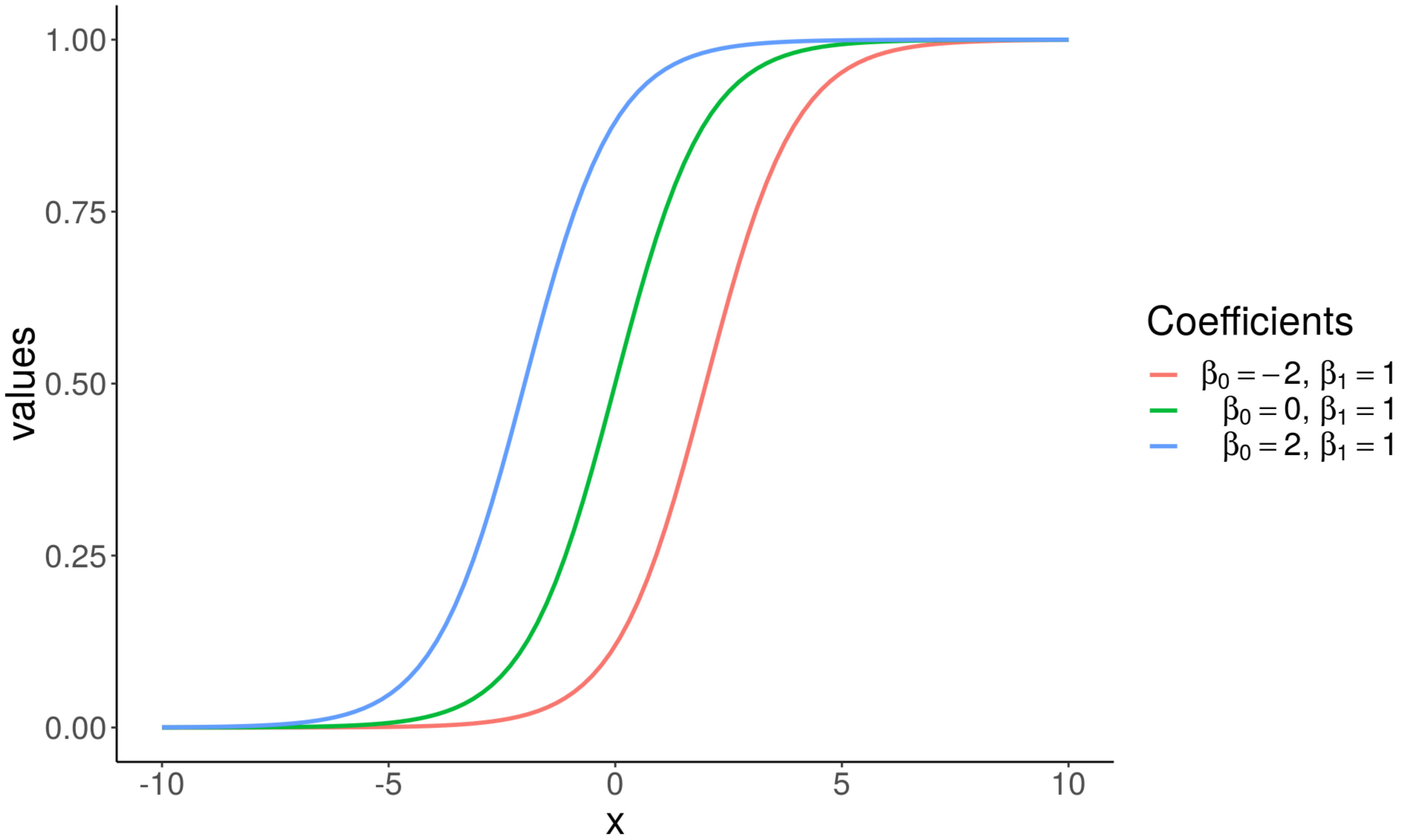
- The method performs **binary classification** (k = 2), but can be generalized to handle $k > 2$ classes (**multinomial logistic regression**).

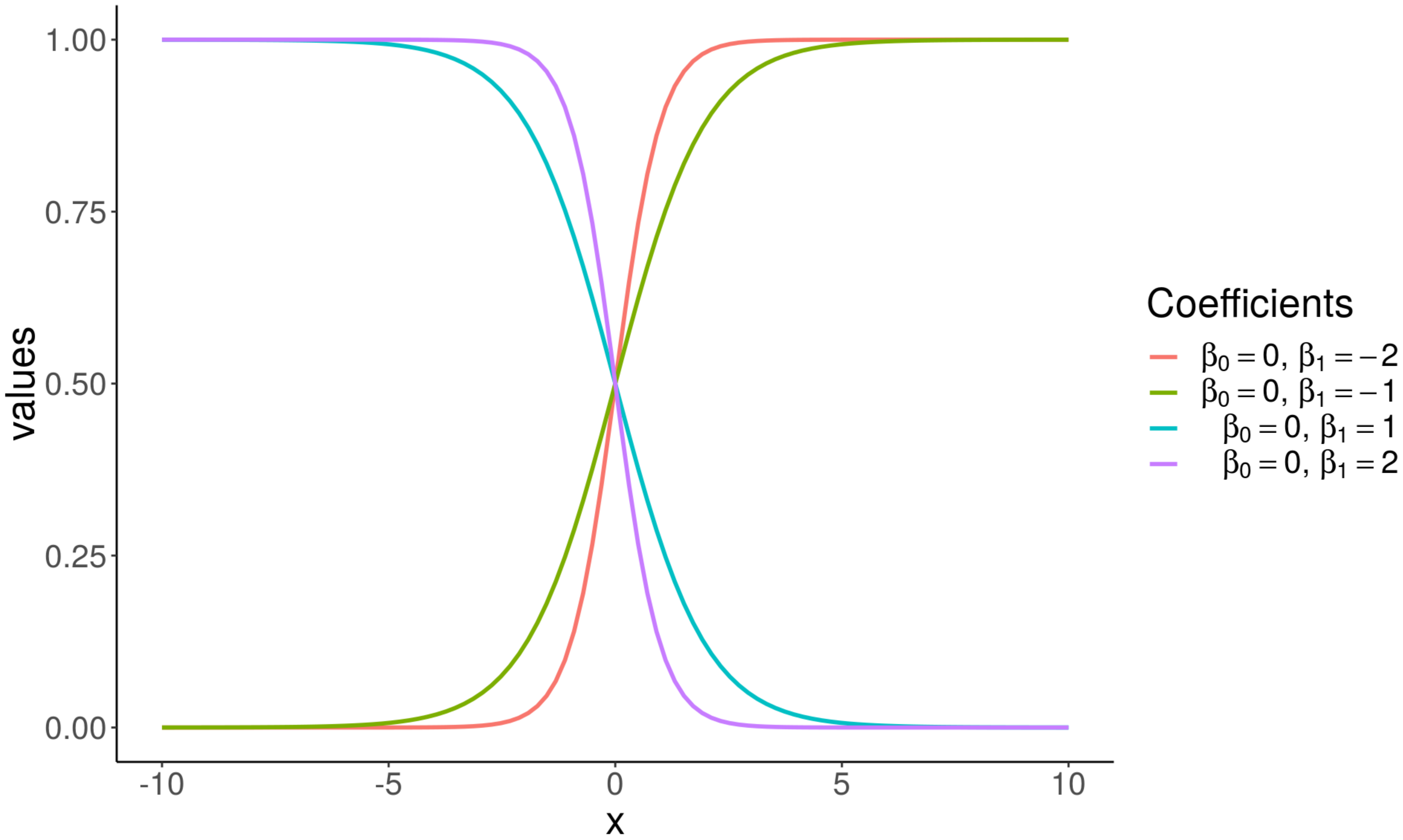
$$g(p) = \log\left(\frac{p}{1-p}\right), \qquad \text{(logit a link function)}$$

$$g^{-1}(\eta) = \frac{1}{1+e^{-\eta}}, \qquad \text{(logistic function)}$$

$$\eta = X\beta, \qquad \text{(linear predictor)}$$

$$\begin{aligned} E[Y] &= P[Y = 1 \mid X = x] \qquad \text{(probability of outcome)} \\ &= p = g^{-1}(\eta) \\ &= \frac{1}{1+e^{-X\beta}} \end{aligned}$$


1.00
0.75
0.50
0.25
0.00
values
-10
-5
0
5
10
x
Coefficients
$\beta_0 = -2,\ \beta_1 = 1$
$\beta_0 = 0,\ \beta_1 = 1$
$\beta_0 = 2,\ \beta_1 = 1$



1.00
0.75
0.50
0.25
0.00
values
-10
-5
0
5
10
x
Coefficients
$\beta_0 = 0,\ \beta_1 = -2$
$\beta_0 = 0,\ \beta_1 = -1$
$\beta_0 = 0,\ \beta_1 = 1$
$\beta_0 = 0,\ \beta_1 = 2$

Grad School Admissions

Suppose we would like to predict students' admission to graduate school based on their GRE, GPA, and the rank of their undergraduate institution.

```
admissions <- read_csv("https://stats.idre.ucla.edu/stat/data/binary.csv")
```

```
## Parsed with column specification:
## cols(
##   admit = col_integer(),
##   gre = col_integer(),
##   gpa = col_double(),
##   rank = col_integer()
## )
```

```
admissions
```

```
## # A tibble: 400 x 4
##    admit   gre   gpa  rank
##    <int> <int> <dbl> <int>
##  1     0   380  3.61     3
##  2     1   660  3.67     3
##  3     1   800  4        1
##  4     1   640  3.19     4
##  5     0   520  2.93     4
##  6     1   760  3        2
##  7     1   560  2.98     1
##  8     0   400  3.08     2
##  9     1   540  3.39     3
## 10     0   700  3.92     2
## # ... with 390 more rows
```

```r
summary(admissions)
```

```
##      admit             gre             gpa             rank
##  Min.   :0.0000   Min.   :220.0   Min.   :2.260   Min.   :1.000
##  1st Qu.:0.0000   1st Qu.:520.0   1st Qu.:3.130   1st Qu.:2.000
##  Median :0.0000   Median :580.0   Median :3.395   Median :2.000
##  Mean   :0.3175   Mean   :587.7   Mean   :3.390   Mean   :2.485
##  3rd Qu.:1.0000   3rd Qu.:660.0   3rd Qu.:3.670   3rd Qu.:3.000
##  Max.   :1.0000   Max.   :800.0   Max.   :4.000   Max.   :4.000
```

```r
sapply(admissions, sd)
```

```
##       admit         gre         gpa        rank
##   0.4660867 115.5165364   0.3805668   0.9444602
```

Check that there are observations included in each subgroup, and whether the data is balanced:

```r
with(admissions, table(admit, rank))
```

```
##      rank
## admit  1  2  3  4
##     0 28 97 93 55
##     1 33 54 28 12
```

Logistic Regression in R

- In R logistic regression can be done using a function `glm()`.
- `glm` stands for Generalized Linear Model.
- The function can fit many other regression models. Use `?glm` to learn more.
- For cases with $k > 2$ classes, `multinom()` function from `nnet` package can be used. To see how go over this example.

Note that currently the column ‘admit’ and ‘rank’ in `admissions` are integers.

```
sapply(admissions, class)
```

```
##     admit       gre       gpa      rank
## "integer" "integer" "numeric" "integer"
```

We convert the two columns to factors.

```
admissions <- mutate(admissions,
  admit = factor(admit, levels = c(0, 1), labels = c("rejected", "admitted")),
  rank = factor(rank, levels = 1:4)
)
admissions
```

```
## # A tibble: 400 x 4
##    admit      gre   gpa rank
##    <fct>    <int> <dbl> <fct>
##  1 rejected   380  3.61 3
##  2 admitted   660  3.67 3
##  3 admitted   800  4    1
##  4 admitted   640  3.19 4
##  5 rejected   520  2.93 4
##  6 admitted   760  3    2
##  7 admitted   560  2.98 1
##  8 rejected   400  3.08 2
##  9 admitted   540  3.39 3
## 10 rejected   700  3.92 2
## # ... with 390 more rows
```

Split data

Divide data into train and test set so that we can evaluate the model accuracy later on. Here we use 60%-20%-20% split.

```r
set.seed(78356)
n <- nrow(admissions)
idx <- sample(1:n, size = n)
train.idx <- idx[seq(1, floor(0.6*n))]
valid.idx <- idx[seq(floor(0.6*n)+1, floor(0.8*n))]

train <- admissions[train.idx, ]
valid <- admissions[valid.idx, ]
test <- admissions[-c(train.idx, valid.idx), ]

nrow(train)
```

```
## [1] 240
```

```r
nrow(valid)
```

```
## [1] 80
```

```r
nrow(test)
```

```
## [1] 80
```

Fitting a logistic regression model

```
logit_fit <- glm(
    admit ~ gre + gpa + rank, data = train, family = "binomial")
```

- The first argument, `formula = admit ~ gre + gpa + rank`, specifies the linear predictor part, $\eta = X\beta$.
- You need to set the family to `family = "binomial"` equivalent to choosing a logistic regression, i.e. using **a logit link function** $g(\cdot)$ in a GLM model.

Logistic regression **coefficients** for continuous predictors (covariates) give **the log fold change in the odds of the outcome corresponding to a unit increase in the predictor**.

$$\beta_{cont} = \log\left(\frac{P[Y = 1 \mid X_{cont} = x + 1]}{P[Y = 1 \mid X_{cont} = x]} \right)$$

Categorical features (factors) are first converted to indicator variables and then the model fits separate coefficients for each level of the factor. Coefficients corresponding to a specific indicator variable give the increase/decrease in the log odds of the outcome in case the observation is recorded with that level.

$$\beta_{factor} = \log\left(\frac{P[Y = 1 \mid X_{fac} = L]}{P[Y = 1 \mid X_{fac} \neq L]} \right)$$

```r
coef(logit_fit)
```

```
##  (Intercept)          gre          gpa        rank2        rank3
## -2.662567353  0.000921435  0.658045298 -0.510004503 -1.560051191
##        rank4
## -1.129252168
```

- For every unit increase in `gre`, the log odds of admitted (versus rejected) increases by ≈ 9.214349810^{-4}.
- For every unit increase in `gpa`, the log odds increases by ≈ 0.6580453.
- There are three coefficients for the rank variable, e.g. a student attending a college with rank 2, one with rank 1 (base level), has the log admission odds decreased by ≈ -0.5100045.

You can get the confidence intervals for the coefficients with the `confint()` fuinction

```r
confint(logit_fit)
```

```
## Waiting for profiling to be done...
```

```
##                     2.5 %       97.5 %
## (Intercept) -5.595691918  0.172732111
## gre         -0.001778273  0.003647635
## gpa         -0.181398218  1.522814525
## rank2       -1.289858306  0.260377700
## rank3       -2.483360377 -0.677844965
## rank4       -2.140151201 -0.167386365
```

The 95% CI are away from zero which indicates significance.

```r
summary(logit_fit)
```

```
##
## Call:
## glm(formula = admit ~ gre + gpa + rank, family = "binomial",
##     data = train)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.4795  -0.9377  -0.7004   1.1883   2.0539
##
## Coefficients:
##               Estimate Std. Error z value Pr(>|z|)
## (Intercept) -2.6625674  1.4651841  -1.817 0.069183 .
## gre          0.0009214  0.0013789   0.668 0.503979
## gpa          0.6580453  0.4329230   1.520 0.128510
## rank2       -0.5100045  0.3935431  -1.296 0.194999
## rank3       -1.5600512  0.4583036  -3.404 0.000664 ***
## rank4       -1.1292522  0.5002488  -2.257 0.023984 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 309.52  on 239  degrees of freedom
## Residual deviance: 289.83  on 234  degrees of freedom
## AIC: 301.83
##
## Number of Fisher Scoring iterations: 4
```

Rank variable effect is given with three different coeffients.

We can sse `wald.test()` function from the `aod` package to test the overall effect of ‘rank’.

```
# install.packages(aod)
library(aod)
wald.test(b = coef(logit_fit), Sigma = vcov(logit_fit), Terms = 4:6)
```

```
## Wald test:
## ----------
##
## Chi-squared test:
## X2 = 14.0, df = 3, P(> X2) = 0.0029
```

- `b` supplies the coefficients,
- `Sigma` supplies the variance covariance matrix of the error terms,
- `Terms` indices of the coefficients to be tested; here 4, 5, and 6, corresponding to ‘rank’.

The p-value indicates that the overall effect of rank is statistically significant.

Fitted values

```
library(modelr)
head(train %>% add_predictions(logit_fit, var = "log_odds"))
```

```
## # A tibble: 6 x 5
##   admit      gre   gpa rank  log_odds
##   <fct>    <int> <dbl> <fct>    <dbl>
## 1 rejected   640  3.67 3        -1.22
## 2 admitted   700  3.52 4        -0.830
## 3 rejected   400  3.35 3        -1.65
## 4 rejected   580  3.51 2        -0.328
## 5 admitted   640  3.19 4        -1.10
## 6 admitted   580  3.58 1         0.228
```

```
(train <- train %>%
    mutate(
        admit_odds = predict(logit_fit),
        admit_prob = predict(logit_fit, type = "response"),
        admit_pred = factor(admit_prob < 0.5, levels = c(TRUE, FALSE),
                            labels = c("rejected", "admitted")),
        admit_pred2 = factor(admit_odds < 0, levels = c(TRUE, FALSE),
                            labels = c("rejected", "admitted"))
    ))
```

```
## # A tibble: 240 x 8
##    admit      gre   gpa rank  admit_odds admit_prob admit_pred admit_pred2
##    <fct>    <int> <dbl> <fct>      <dbl>      <dbl> <fct>      <fct>
##  1 rejected   640  3.67 3          -1.22       0.228 rejected   rejected
##  2 admitted   700  3.52 4          -0.830      0.304 rejected   rejected
##  3 rejected   400  3.35 3          -1.65       0.161 rejected   rejected
##  4 rejected   580  3.51 2          -0.328      0.419 rejected   rejected
##  5 admitted   640  3.19 4          -1.10       0.249 rejected   rejected
##  6 admitted   580  3.58 1           0.228      0.557 admitted   admitted
##  7 rejected   560  3.36 3          -1.50       0.183 rejected   rejected
```

```
##  7 rejected   560  3.36 3         -1.50       0.183 rejected   rejected
##  8 rejected   460  3.77 3         -1.32       0.211 rejected   rejected
##  9 admitted   560  2.98 1         -0.186      0.454 rejected   rejected
## 10 rejected   580  3.02 2         -0.651      0.343 rejected   rejected
## # ... with 230 more rows
```

Predictions

Predictions can be computed using `predict()` function, with the argument `type = "response"`. Otherwise, the default will compute predictions on the scale of the linear predictors.

```r
# Must have the same column names as the variables in the model
new_students <- data.frame(
    gre = c(670, 790, 550),
    gpa = c(3.56, 4.00, 3.87),
    rank = factor(c(1, 2, 2)))

# The output is the probability of admissions for each of the new students.
new_students <- new_students %>%
  mutate(
    admit_odds = predict(logit_fit, newdata = new_students),
    admit_pred = factor(admit_odds < 0, levels = c(TRUE, FALSE),
                   labels = c("rejected", "admitted"))
  )
new_students
```

```
##   gre  gpa rank admit_odds admit_pred
## 1 670 3.56    1  0.2974353   admitted
## 2 790 4.00    2  0.1875430   admitted
## 3 550 3.87    2 -0.1191473   rejected
```

Multiple models

```
logit_fit2 <- glm(
    admit ~ rank, data = train, family = "binomial")

valid <- valid %>%
    mutate(
        admit_odds_fit1 = predict(logit_fit, newdata = valid),
        admit_odds_fit2 = predict(logit_fit2, newdata = valid),
        admit_fit1 = factor(admit_odds_fit1 < 0,
                            levels = c(TRUE, FALSE),
                            labels = c("rejected", "admitted")),
        admit_fit2 = factor(admit_odds_fit2 < 0,
                            levels = c(TRUE, FALSE),
                            labels = c("rejected", "admitted"))
    )
valid
```

```
## # A tibble: 80 x 8
##    admit   gre   gpa rank  admit_odds_fit1 admit_odds_fit2 admit_fit1
##    <fct> <int> <dbl> <fct>           <dbl>           <dbl> <fct>
##  1 reje…   340  2.92 3              -1.99           -1.41  rejected
##  2 reje…   660  3.31 4              -1.01           -1.03  rejected
##  3 admi…   300  2.84 2              -1.03           -0.389 rejected
##  4 reje…   500  4    3              -1.13           -1.41  rejected
##  5 reje…   780  3.87 4              -0.526          -1.03  rejected
##  6 reje…   600  3.63 3              -1.28           -1.41  rejected
##  7 reje…   540  3.78 4              -0.807          -1.03  rejected
##  8 admi…   800  3.74 1               0.536           0.163 admitted
##  9 admi…   800  3.43 2              -0.178          -0.389 rejected
## 10 admi…   740  2.97 2              -0.536          -0.389 rejected
## # ... with 70 more rows, and 1 more variable: admit_fit2 <fct>
```

Evaluating accuracy

```r
# Confusion Matrix for model 1
(confusion_matrix_fit1 <- table(true = valid$admit, pred = valid$admit_fit1))
```

```
##             pred
## true          rejected admitted
##    rejected         56        3
##    admitted         16        5
```

```r
# Confusion Matrix for model 2
(confusion_matrix_fit2 <- table(true = valid$admit, pred = valid$admit_fit2))
```

```
##             pred
## true          rejected admitted
##    rejected         57        2
##    admitted         16        5
```

```r
# Accuracy for model 1
(accuracy_fit1 <- sum(diag(confusion_matrix_fit1))/sum(confusion_matrix_fit1))
```

```
## [1] 0.7625
```

```r
# Accuracy for model 2
(accuracy_fit2 <- sum(diag(confusion_matrix_fit2))/sum(confusion_matrix_fit2))
```

```
## [1] 0.775
```

We choose a simpler model `logit_fit2`

Expected `logit_fit2` performance

Performance of our chosen model, `logit_fit2` can be evaluated on the `test`set

```
test <- test %>%
    mutate(
        admit_odds = predict(logit_fit2, newdata = test),
        admit_pred = factor(admit_odds < 0,
                            levels = c(TRUE, FALSE),
                            labels = c("rejected", "admitted"))
    )

(test_confusion_matrix <- table(pred = test$admit, true = test$admit_pred))
```

```
##              true
## pred          rejected admitted
##    rejected         48        9
##    admitted         15        8
```

```
(test_accuracy <- sum(diag(test_confusion_matrix))/sum(test_confusion_matrix))
```

```
## [1] 0.7
```

So, you should expect your model accuracy to be around 0.7 for a new dataset you collect later.

Exercise

- Go to the “Lec7_Exercises.Rmd” file, which can be downloaded from the class website under the Lecture tab.
- Complete Exercise 2.

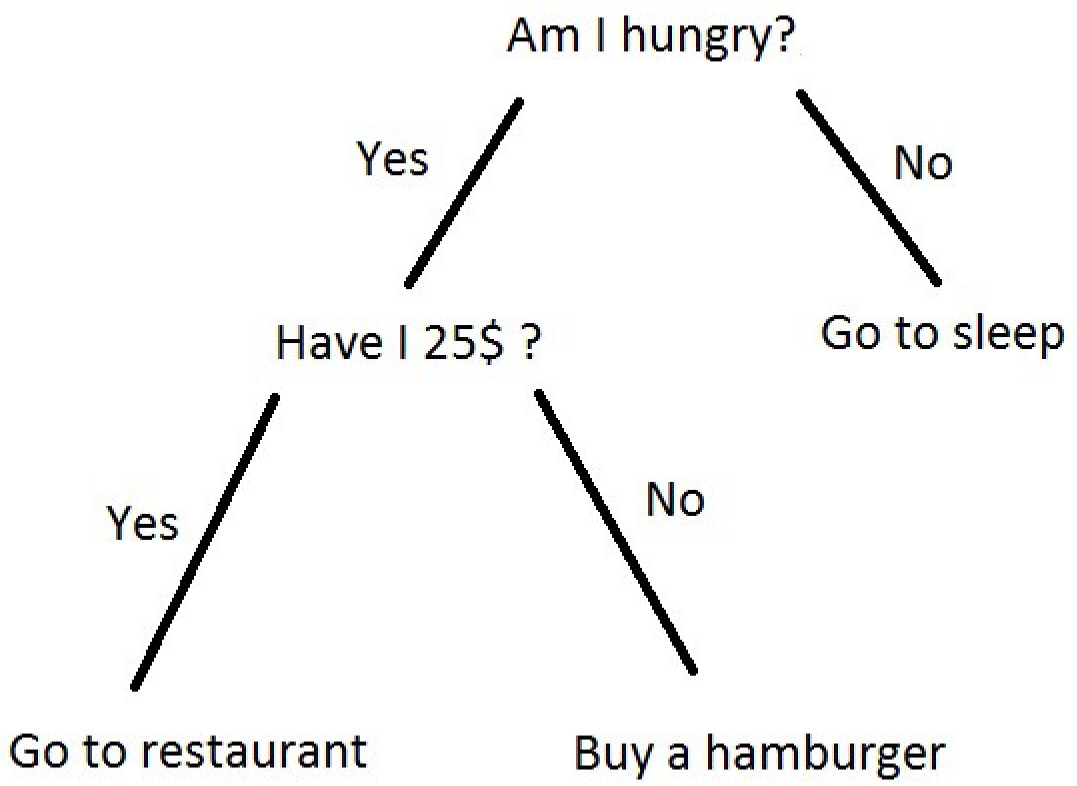
Random Forest

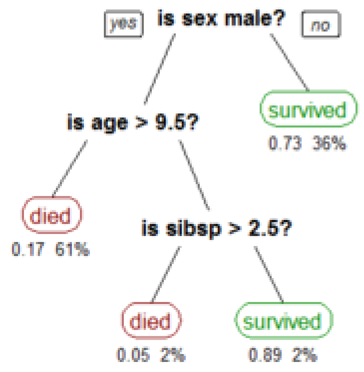
Random Forest

- Random Forest is **an ensemble learning method based on classification and regression trees, CART,** proposed by Breinman in 2001.
- RF can be used to perform **both classification and regression**.
- RF models are robust as they **combine predictions calculated from a large number of decision trees (a forest).**
- Details on RF can be found in Chapter 8 of ISL and Chapter 15 ESL; also a good write-up can also be found here

Decision trees

- Cool visualization explaining what decision trees are: link
- Example of decision trees





Tree bagging Algorithm

Suppse we have an input data matrix, $X \in \mathbb{R}^{N \times p}$ and a response vector, $Y \in \mathbb{R}^{N}$.

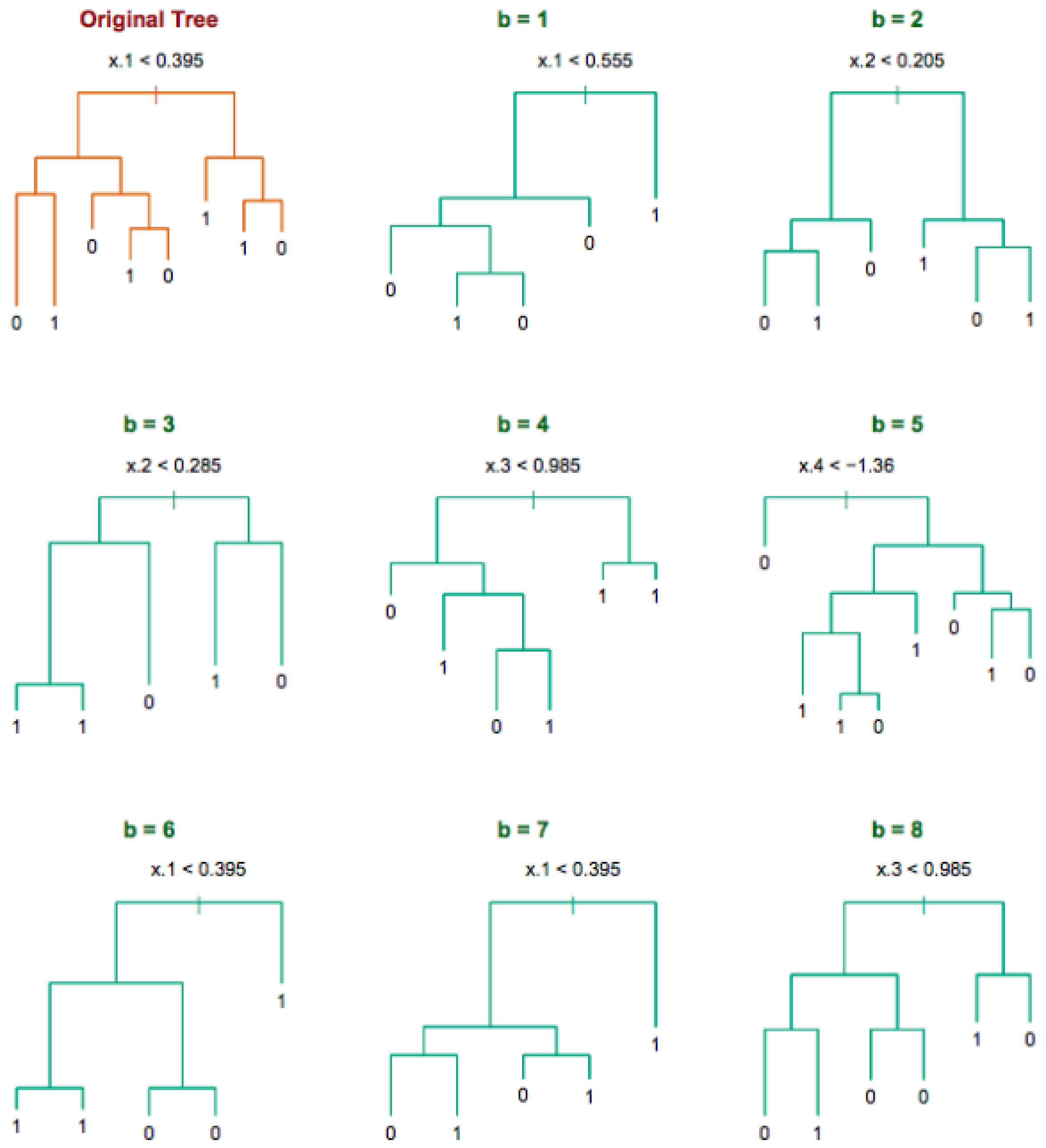
For b = 1, 2, …, B:

1. Generate a random subset of the data (X_b, Y_b) contatining $n < N$ observations sampled with replacement.
2. Train a decision tree T_b on (X_b, Y_b)
3. Predict the outcome for $N - n$ unseen (complement) samples (X_b', Y_b')

Afterwards, combine predictions from all decision trees and compute the average predicted outcome .

Averaging over a collection of decision trees makes the predictions more stable.

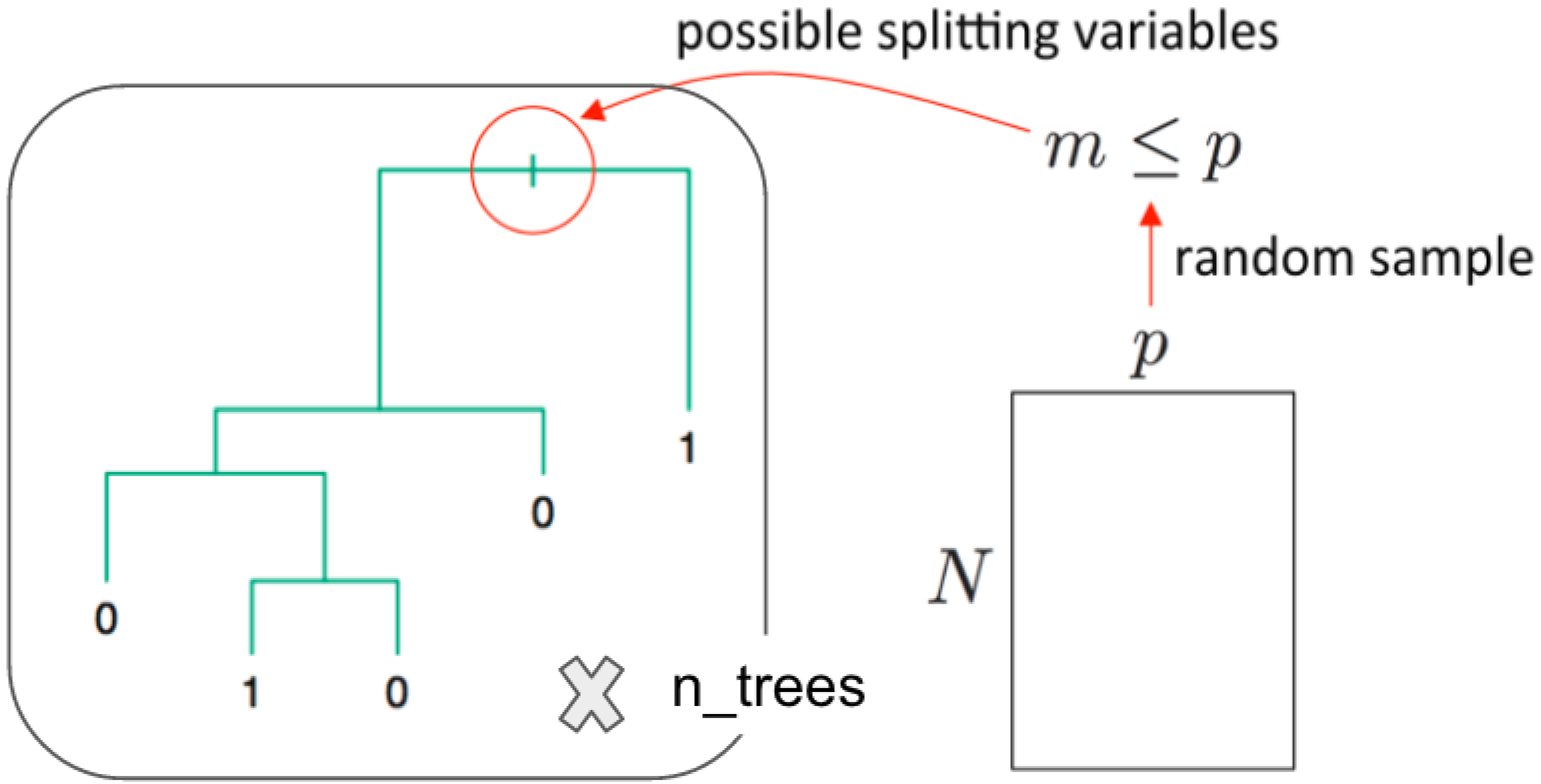
Decision trees for bootrap samples



Source: Chapter 8 ESL

Random Forest Characteristics

- Random forests differ in only one way from tree bagging: it uses a modified tree learning algorithm sometimes called **feature bagging**.
- At each candidate split in the learning process, **only a random subset of the features is included in a pool** from which the variables can be selected for splitting the branch.
- Introducing **randomness** into the candidate splitting variables, **reduces correlation between the generated trees.**



possible splitting variables

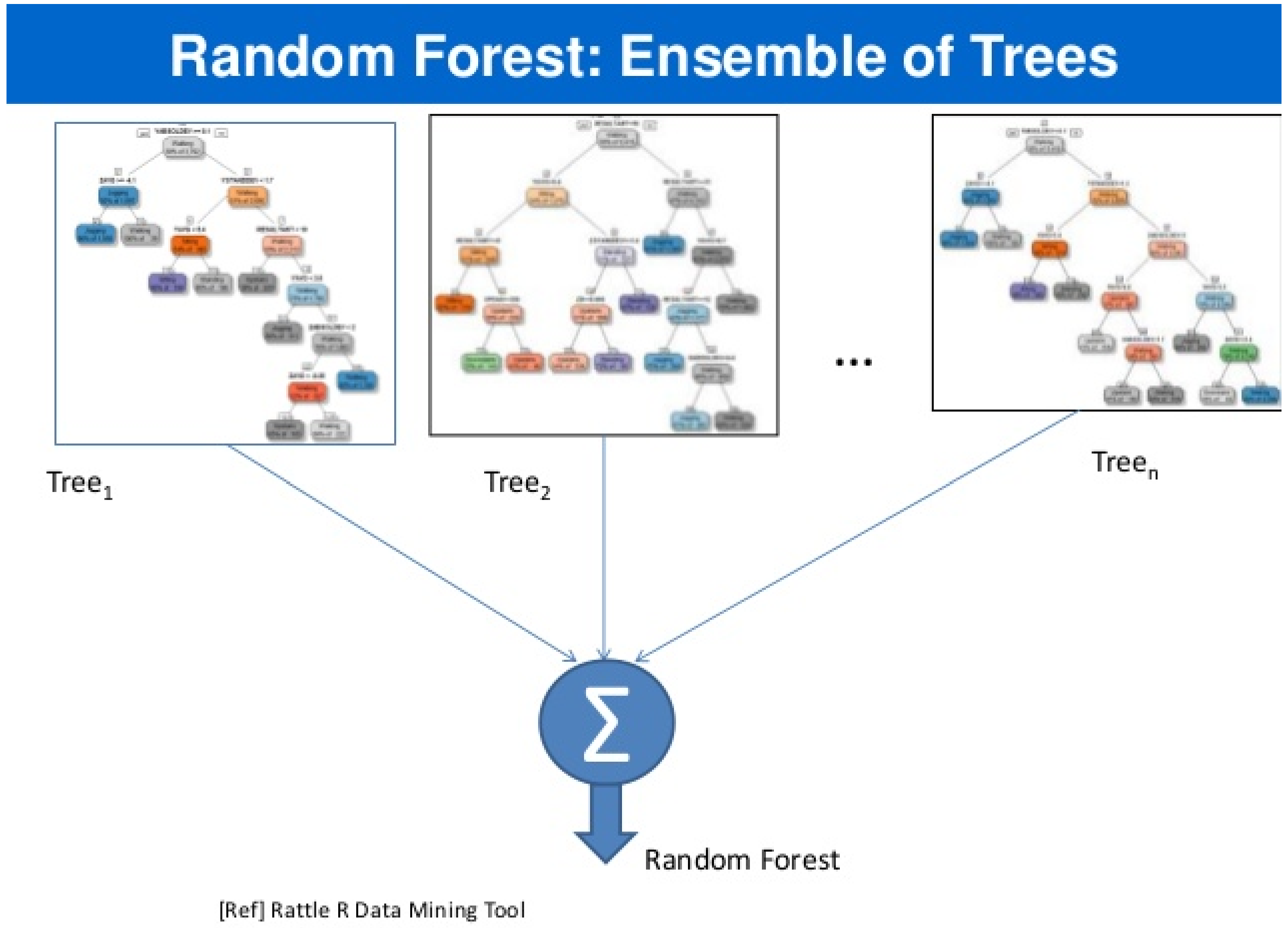
$m \leq p$

random sample

p

N

× n_trees



Random Forest: Ensemble of Trees

[Ref] Rattle R Data Mining Tool

Source: link

Wine Quality

UCI ML Repo includes two datasets on red and white variants of the Portuguese “Vinho Verde” wine. The datasets contain information on physicochemical and sensory characteristics of the wine quality score.

We will use the white wines dataset to classify wines according to their quality classes.

```
url <- 'https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-white
wines <- read.csv(url, sep = ";")
head(wines, 6)
```

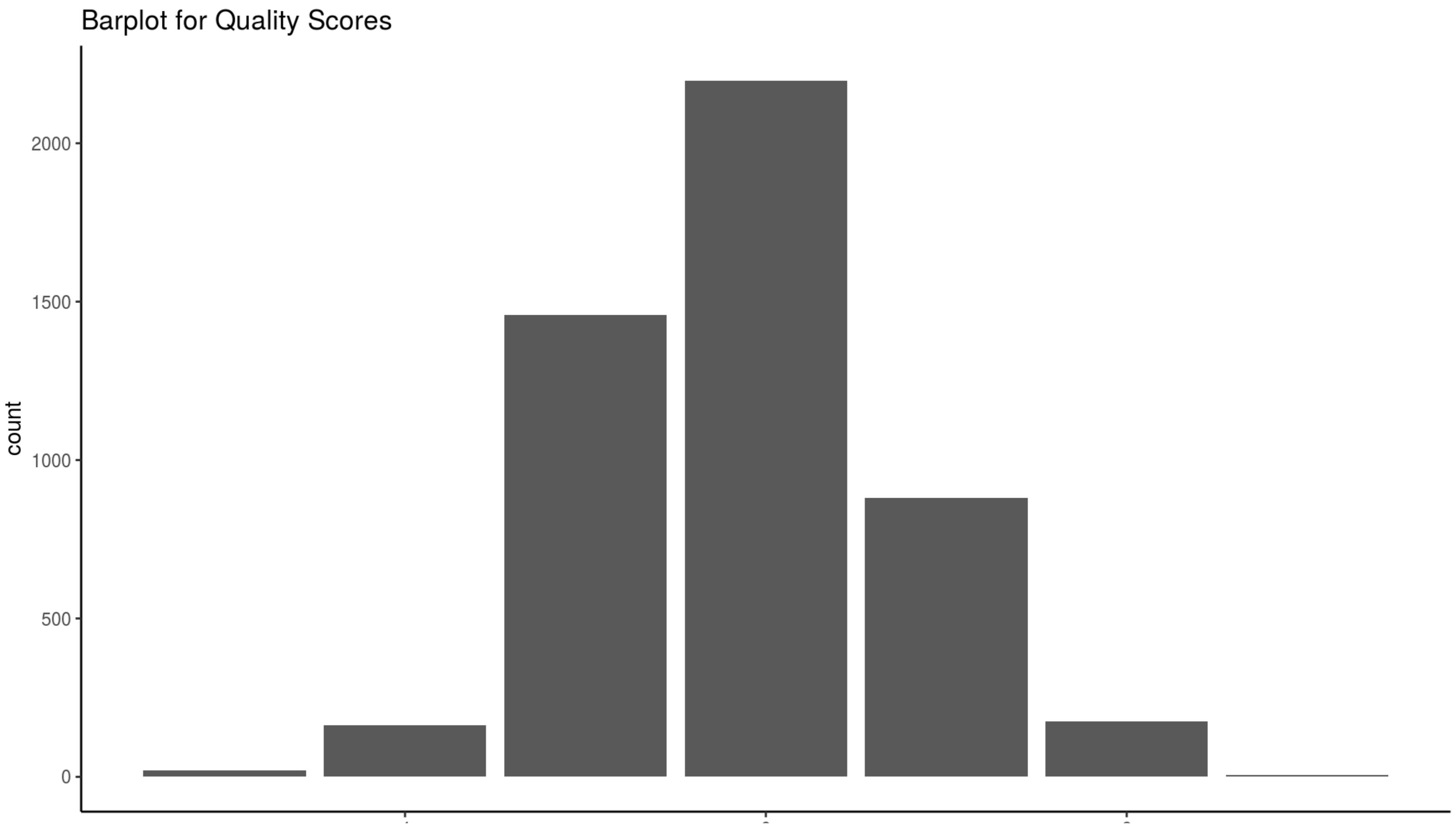
```
##   fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 1           7.0             0.27        0.36           20.7     0.045
## 2           6.3             0.30        0.34            1.6     0.049
## 3           8.1             0.28        0.40            6.9     0.050
## 4           7.2             0.23        0.32            8.5     0.058
## 5           7.2             0.23        0.32            8.5     0.058
## 6           8.1             0.28        0.40            6.9     0.050
##   free.sulfur.dioxide total.sulfur.dioxide density   pH sulphates alcohol
## 1                  45                  170  1.0010 3.00      0.45     8.8
## 2                  14                  132  0.9940 3.30      0.49     9.5
## 3                  30                   97  0.9951 3.26      0.44    10.1
## 4                  47                  186  0.9956 3.19      0.40     9.9
## 5                  47                  186  0.9956 3.19      0.40     9.9
## 6                  30                   97  0.9951 3.26      0.44    10.1
##   quality
## 1       6
## 2       6
## 3       6
## 4       6
## 5       6
## 6       6
```

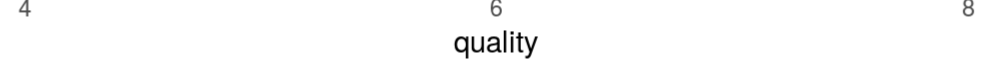
Class Frequency

```
table(wines$quality)
```

```
##
##    3    4    5    6    7    8    9
##   20  163 1457 2198  880  175    5
```

```
ggplot(wines, aes(x = quality)) +
  geom_bar() + theme_classic() +
  ggtitle("Barplot for Quality Scores")
```





The classes are ordered and not balanced (munch more normal wines than excellent/poor ones).

To make things easier, we will wines into **“good”, “average” and “bad”** categories.

The new classes will be more balanced, and it will be easier to fit the model.

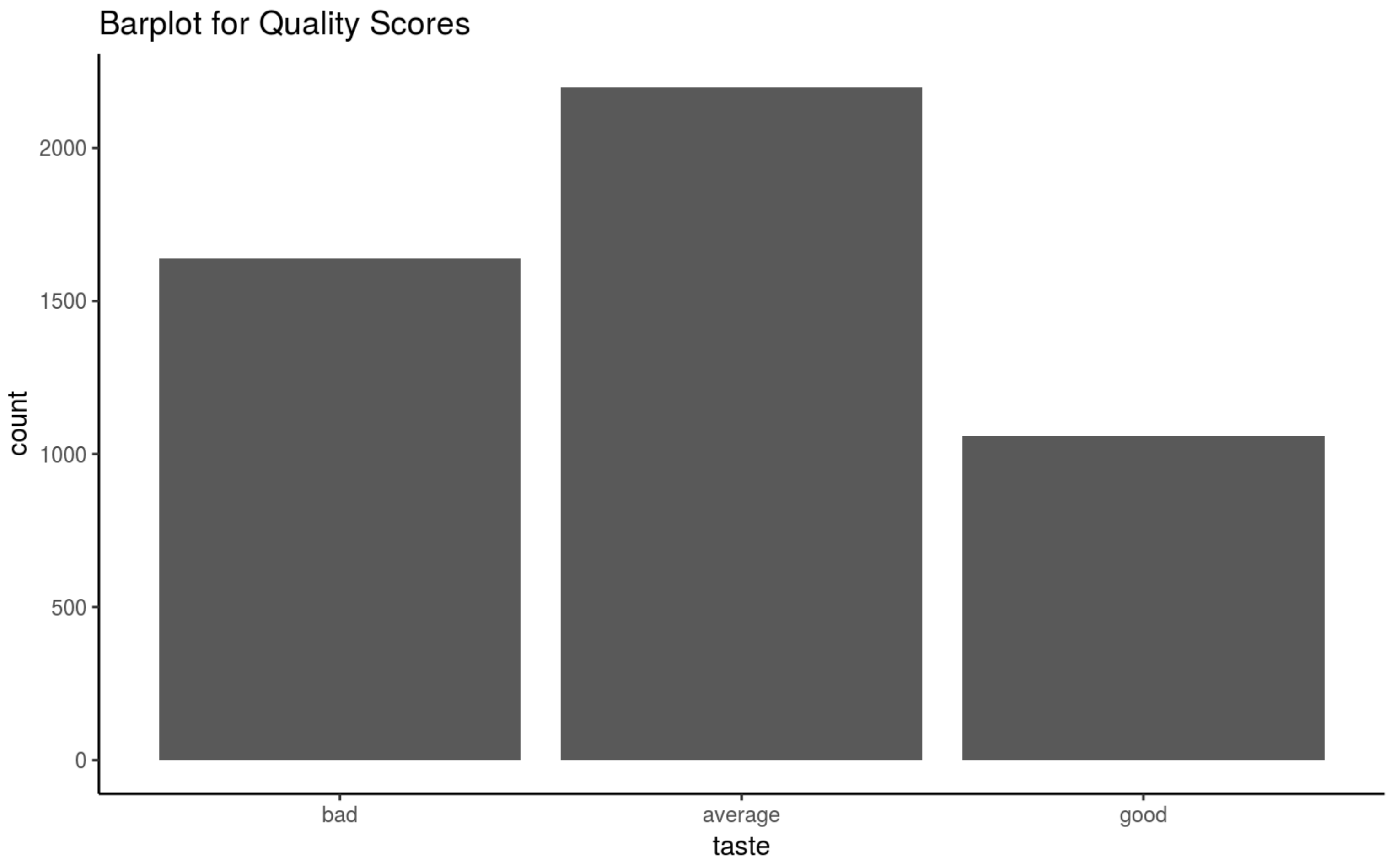
```r
qualClass <- function(quality) {
  if(quality > 6) return("good")
  if(quality < 6) return("bad")
  return("average")
}
wines <- wines %>%
    mutate(taste = sapply(quality, qualClass),
           taste = factor(taste, levels = c("bad", "average", "good")))
head(wines)
```

```
##   fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 1           7.0             0.27        0.36           20.7     0.045
## 2           6.3             0.30        0.34            1.6     0.049
## 3           8.1             0.28        0.40            6.9     0.050
## 4           7.2             0.23        0.32            8.5     0.058
## 5           7.2             0.23        0.32            8.5     0.058
## 6           8.1             0.28        0.40            6.9     0.050
##   free.sulfur.dioxide total.sulfur.dioxide density   pH sulphates alcohol
## 1                  45                  170  1.0010 3.00      0.45     8.8
## 2                  14                  132  0.9940 3.30      0.49     9.5
## 3                  30                   97  0.9951 3.26      0.44    10.1
## 4                  47                  186  0.9956 3.19      0.40     9.9
## 5                  47                  186  0.9956 3.19      0.40     9.9
## 6                  30                   97  0.9951 3.26      0.44    10.1
##   quality   taste
## 1       6 average
## 2       6 average
## 3       6 average
## 4       6 average
## 5       6 average
## 6       6 average
```

```
table(wines$quality)
```

```
##
##    3    4    5    6    7    8    9
##   20  163 1457 2198  880  175    5
```

```
ggplot(wines, aes(x = taste)) +
  geom_bar() + theme_classic() +
  ggtitle("Barplot for Quality Scores")
```



Splitting data

We include 60% of the data in a train set and the remaining into a test set.

```r
set.seed(98475)
idx <- sample(nrow(wines), 0.6 * nrow(wines))
train <- wines[idx, ]
test <- wines[-idx, ]
dim(train)
```

```
## [1] 2938   13
```

```r
dim(test)
```

```
## [1] 1960   13
```

Random Forest in R

In R there is a convenient function `randomForest` from `randomForest` package.

```
# install.packages("randomForest")
library(randomForest)
wines_fit_rf <- randomForest(
    taste ~ . - quality, data = train,
    mtry = 5, ntree = 500, importance = TRUE)
```

- Note that in the formula ‘`taste ~ . - quality`’ means we include all features EXCEPT for ‘quality’ (the response variable).
- `mtry` - the number of variables randomly sampled as candidates at each split. Defaults: for classification – $\sqrt{p}$ and for regression – $p/3$, where p is number of all variables in the model.
- `ntree` - the number of trees in the forest.
- `importance` - whether importance of predictors be computed.

Observe, that RF is good at distinguishing “bad” wines from“good” wines, but still struggles when it comes to “average” wines.

```
wines_fit_rf
```

```
##
## Call:
##  randomForest(formula = taste ~ . - quality, data = train, mtry = 5,      ntree = 500, import
##                Type of random forest: classification
##                      Number of trees: 500
## No. of variables tried at each split: 5
##
##         OOB estimate of  error rate: 31.31%
## Confusion matrix:
##         bad average good class.error
## bad     681     272   15   0.2964876
## average 219     966  135   0.2681818
## good     20     259  371   0.4292308
```

Model Accuracy

- You should always evaluate your model's performance on a test set, which was set aside and not observed by the method at all.
- In case of RF, performance on train and test set should be similar; this is because the method averages predictions computed by individual trees for observations unseen by the tree.
- Inspect the confusion matrix to asses the model accuracy.

```
(confusion_matrix <- table(
    true = test$taste, pred = predict(wines_fit_rf, newdata = test)))
```

```
##            pred
## true        bad average good
##    bad      482     181    9
##    average 149     669   60
##    good      13     143  254
```

```
(accuracy_rf <- sum(diag(confusion_matrix)) / sum(confusion_matrix))
```

```
## [1] 0.7168367
```

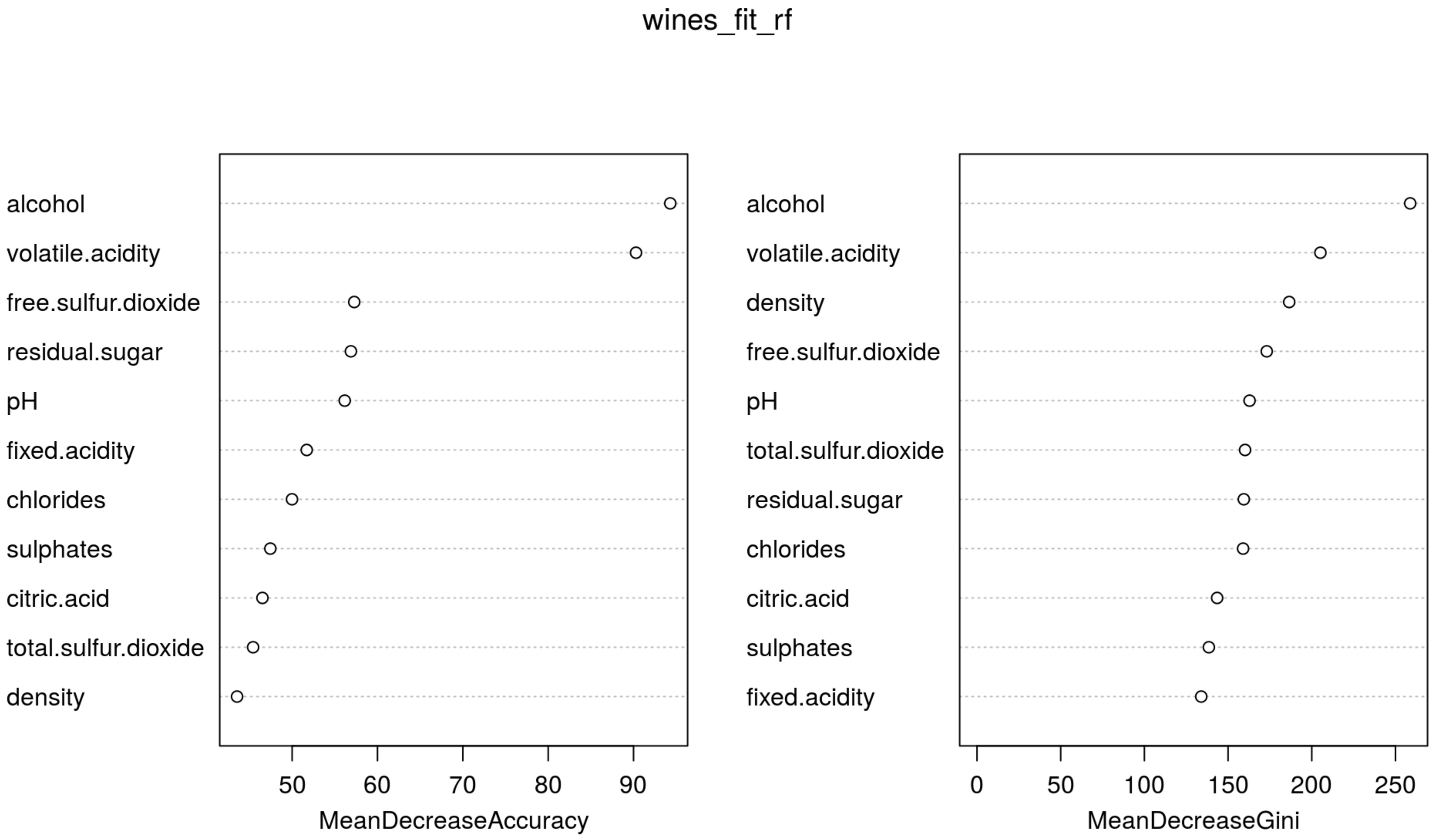
https://stats.stackexchange.com/questions/197827/how-to-interpret-mean-decrease-in-accuracy-and-mean-decrease-gini-in-random-fore

```
## Look at variable importance:
importance(wines_fit_rf)
```

```
##                           bad  average     good MeanDecreaseAccuracy
## fixed.acidity        30.15194 30.17027 29.82500             51.71162
## volatile.acidity     64.10513 51.51792 57.95579             90.28951
## citric.acid          28.54081 32.93660 31.90320             46.52323
## residual.sugar       29.23441 35.39843 27.38350             56.88708
## chlorides            36.06739 26.80210 39.22203             49.98833
## free.sulfur.dioxide  37.74602 35.26059 29.29246             57.27752
## total.sulfur.dioxide 25.84618 23.53196 34.53854             45.42788
## density              26.92925 28.25958 29.45976             43.55052
## pH                   33.72925 31.09405 42.54602             56.16315
## sulphates            29.16720 28.56807 30.09379             47.44873
## alcohol              81.11168 36.20917 66.60965             94.30226
##                      MeanDecreaseGini
## fixed.acidity                133.9582
## volatile.acidity             205.1542
## citric.acid                  143.4607
## residual.sugar               159.3942
## chlorides                    158.9609
## free.sulfur.dioxide          173.0973
## total.sulfur.dioxide         160.1464
## density                      186.5196
## pH                           162.8367
## sulphates                    138.5101
## alcohol                      258.7888
```

What seems to be the conclusion? What are the characteristics that are predictive of the wine quality score?

```r
varImpPlot(wines_fit_rf)
```



Exercise

- Go to the “Lec7_Exercises.Rmd” file, which can be downloaded from the class website under the Lecture tab.
- Complete Exercise 3.