6. More Loops, Control Structures, and Bootstrapping

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In this session

We will introduce additional looping procedures as well as control structures that are useful in R. We also provide applications to bootstrapping.

- Repeat and While loops,
- If-Then and If-Then-Else structures
- Introduction to the bootstrap, with examples
Repeat loops

The repeat loop is an infinite loop that is often used in conjunction with a **break** statement that terminates the loop when a specified condition is satisfied. The basic structure of the repeat loop is:

```plaintext
repeat{
    expression
    expression
    expression
    if(condition) break
}
```
Repeat loops

Below is a repeat loop for printing the square of integers from 1 to 10.

```plaintext
i <- 1
repeat {
    print(i^2)
    i <- i+1
    if(i > 10) break
}
```

6.3
**While loops**

The while loop is often used for executing a set of commands or statements repeatedly until a specific condition is satisfied.

The structure of a while loop consists of a boolean condition and statements that are written inside while loop brackets, for which repetitive execution is to be carried out until the condition of interest is satisfied:

```java
while (condition) {
    expression
    expression
    expression
}
```

It is important to note that the while loop will first check that the condition is satisfied prior to executing a first iteration of the commands.
While loops

Below is a while loop for printing out the first few Fibonacci numbers: 0, 1, 1, 2, 3, 5, 8, 13, ..., where each number is the sum of the previous two numbers in the sequence.

```python
a = 0
b = 1
print(a)
while (b < 50) {
    print(b)
    temp = a + b
    a = b
    b = temp
}
```
While loops

Below is a while loop that creates a vector containing the first 20 numbers in the Fibonacci sequence

\[
x = c(0, 1)
n = 20
\]
\[
\text{while (length(x) < n) {}
\text{   position = length(x)}
\text{   new = x[position] + x[position-1]}
\text{   x = c(x, new)}
\text{}}
\]
If-Then and If-Then-Else structures

Sometimes a block of code in a program should only be executed if a certain condition is satisfied. For these situations, *if-then* and *if-then-else* structures can be used:

The *if-then* structure has the following general form:

```java
if (condition) {
    expression
    expression
}
```

The *if-then-else* structure extends the same idea:

```java
if (condition) {
    expression
    expression
} else {
    expression
    expression
}
```
If-Then and If-Then-Else structures

An example: an *if-then-else* statement that takes the square root of the product of two numbers x and y, if the product is positive:

```r
x <- 3
y <- 7
if( (x<0 & y<0) | (x>0 & y>0) ){
  myval <- sqrt(x*y)
}
else{
  myval <- NA
}
```

And the value of myval when x=3 and y=7 is:

```r
> myval
[1] 4.582576
```

What is myval if x=2 and y=-10?

```r
> myval
[1] NA
```
**Introduction to bootstrapping**

Bootstrapping is a very useful tool when the distribution of a statistic is unknown or very complex.

Bootstrapping is a *non-parametric* (i.e. assumption-lite) re-sampling method for estimating standard errors, computing confidence intervals, and hypothesis testing.

The method is often used when sample sizes are small and *asymptotic* (i.e. large-$n$) approximations, may be difficult to apply.

Introduction to bootstrapping

Bootstrapping uses three steps:

- Resample a given data set with replacement a specified number of times, where each bootstrap sample is the same size as the original sample.

- Calculate a statistic of interest for each of the bootstrap samples.

- The distribution of the statistic from the bootstrap samples can then be used to estimate standard errors, create confidence intervals, and to perform hypothesis testing with the statistic.
Example: bootstrapping the median

We can bootstrap in R by going round a loop, using the `sample(x, size, replace, prob)` function at each iteration:

- **x** is a vector containing the items to be resampled.
- **size** specifies how many resamples to take: the default is the length of **x**
- **replace** determines if the sample will be drawn with or without replacement. The default value, FALSE i.e. sampling is performed without replacement
- **prob** lets us specify unequal probabilities of resampling each element of **x** – not needed here

Bootstrapping uses resamples of the same size as the original data, sampling with replacement – so `sample(x, replace=TRUE)`
Example: bootstrapping the median

Let's consider the airquality dataset again. Below is a histogram of the daily ozone concentrations in New York, summer 1973.

```r
hist(airquality$Ozone, col="lightblue", xlab="Ozone Concentrations", main="Ozone Concentrations in NY (Summer 1973)")
```

What’s the median ozone level?

How accurately do we know the median?
Example: bootstrapping the median

First, let's work out the median;

> median(airquality$Ozone)
[1] NA

Several ozone concentration values are missing, but if we take the median of the 116 observed values;

> median(airquality$Ozone, na.rm=TRUE)
[1] 31.5

How might this value differ, in other similar experiments? We will use the bootstrap to estimate its distribution, and to provide a 95% confidence interval for the median.
Example: bootstrapping the median

To make the code easier to read, make a vector of the ozone concentrations with missing values excluded:

\[
ozone <- \text{airquality}\$Ozone[ \!\text{is.na(airquality}\$Ozone) ]\]

Using a `for()` loop, we can create 10,000 bootstrap samples and calculate the median for each sample:

\[
\text{nboot} <- 10000 \quad \# \text{number of bootstrap samples}
\]
\[
\text{bootstrap.medians} <- \text{rep(NA, nboot)}
\]
\[
\text{set.seed(10)}
\]
\[
\text{for}(i \in 1:\text{nboot}){
\quad \text{bootstrap.medians}[i] <- \text{median(sample(ozone, replace=TRUE))}
\}
\]
Example: bootstrapping the median

What do the medians look like? How do they compare with original ‘raw’ data?

```
hist(bootstrap.medians, col="lightblue", xlab="Bootstrap Medians", main="Bootstrap Medians for Ozone Concentrations in NY", cex.main=.8)
```

10,000 of them, not 116

Much less skewed than raw data

Much less variable than raw data
Example: bootstrapping the median

The 95% confidence interval is given by the .025 and .975 quantiles of those bootstrap medians;

> quantile(bootstrap.medians, c(0.025, 0.975) )
2.5%  97.5%
 23.5  39.0

- Could read off from the previous graph
- (23.5, 39.0) is a range of median values we might expect to see (i.e. the uncertainty in the medians) if repeating the experiment many times
- This method does assume that the ozone measurement on different days is independent so probably understates uncertainty, here!
Example: bootstrap for lowess curve

The bootstrap is a very powerful idea. For a more sophisticated example, recall the cars data, and the line we put through it:

```r
data(cars)
plot(dist ~ speed, data = cars)
with(cars, lines(lowess(speed, dist), col = "tomato", lwd = 2))
```
Example: bootstrap for lowess curve

To bootstrap the *curve*, we resample entire observations;

```r
m <- dim(cars)[1] # obtain the sample size
nboot <- 20
for(i in 1:nboot){
  mysample <- sample(1:m, replace=T) # i.e. which rows are resampled?
  with(cars[mysample,],
      lines(lowess(speed, dist), col=(i+1), lwd=2)
  )
}
```

![Graph showing multiple lines representing the lowess curve bootstrap]
Example: bootstrap for lowess curve

For a smoother version, note `lowess()` only produces output at the sampled points – so we extrapolate to the others using `approx()`;

```r
nboot <- 1000
boot.speed <- matrix(NA, 1000, m) # for storing the curve’s value at all m points
set.seed(1314) # Battle of Bannockburn
for(i in 1:nboot){
  mysample <- sample(1:m,replace=T)
  low1 <- with(cars, lowess(speed[mysample], dist[mysample]))
  low.all <- approx(low1$x, low1$y, xout=cars$speed, rule=2)
  boot.speed[i,] <- low.all$y
}
```

Now work out the lower and upper ranges of the lines, at all \( m \) values of speed;

```r
upper <- rep(NA, m)
lower <- rep(NA, m)
for(j in 1:m){
  upper[j] <- quantile(boot.speed[,j], 0.975)
  lower[j] <- quantile(boot.speed[,j], 0.025)
}```
Example: bootstrap for lowess curve

Finally, make a cool blue picture, using transparency;

```r
plot(dist~speed, data=cars)
for(i in 1:nboot){
    lines(x=cars$speed, y=boot.speed[i,], col="#0000FF05") }
with(cars, lines(lowess(speed, dist), col="tomato", lwd=2)) # raw data lowess
polygon(x=c(cars$speed, rev(cars$speed)), y=c(upper, rev(lower)),
    density=0, col="red", lty=2) # pointwise 95% conf ints
```
Summary

- `while{}` and `repeat{}` are useful tools for looping until a condition is satisfied.

- *if-then* and *if-then-else* structures allow blocks of code to be executed under different specified conditions.

- Bootstrapping is a powerful statistical technique for expressing accuracy/inaccuracy. *(Almost all other methods used for this can be thought of as approximations to some form of bootstrap)*.

- Bootstrapping can be implemented in a few lines of R, using loops and the `sample()` function.