6. More Loops, Control Structures, and Bootstrapping

Ken Rice
Tim Thornton

University of Washington

Seattle, July 2019
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.

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

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.

```plaintext
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

```r
x <- c(0,1)
n <- 20
while (length(x) < n) {
    position <- length(x)
    new <- x[position] + x[position-1]
    x <- c(x,new)
}
```
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:

\[
x \leftarrow 3 \\
y \leftarrow 7 \\
\text{if}( (x<0 \land y<0) \lor (x>0 \land y>0) )\{
    \text{myval} \leftarrow \sqrt{x*y}
\} \text{ else}\{
    \text{myval} \leftarrow \text{NA}
\}
\]

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

\[> \text{myval} \]
\[[1] 4.582576\]

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

\[> \text{myval} \]
\[[1] \text{NA}\]
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 time, 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.
- \( \text{size} \) specifies how many resamples to take: the default is the length of \( x \)
- \( \text{replace} \) determines if the sample will be drawn with or without replacement. The default value, FALSE i.e. sampling is performed without replacement.
- \( \text{prob} \) 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;

```r
> median(airquality$Ozone)
[1] NA
```

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

```r
> 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:

```r
ozone <- airquality$Ozone[!is.na(airquality$Ozone)]
```

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

```r
nboot <- 10000 # number of bootstrap samples
bootstrap.medians <- rep(NA, nboot)
set.seed(10)
for(i in 1:nboot){
  bootstrap.medians[i] <- 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)
```

Medians of Bootstrapping Samples for Ozone Concentration in NY

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;

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

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=TRUE)
    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$speed, y=boot.speed[i,], col= adjustcolor("blue", alpha.f=0.02)) }
with(cars, lines(lowess(speed, dist), col="tomato", lwd=2)) # raw data lowess
polygon(x=c(cars$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