Bio 723

Scientific Computing for Biologists

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1 Getting your feet wet with R

1.1 Getting Acquainted with R

1.1.1 Installing R

The R website is at `http://www.r-project.org/`. I recommend that you spend a few minutes checking out the resources, documentation, and links on this page. Download the appropriate R installer for your computer from the Comprehensive R Archive Network (CRAN). A direct link can be found at: `http://cran.stat.ucla.edu/`. As of mid August 2012 the latest R release is verison 2.15.1.

The R installer will install appropriate icons under the `Start Menu` (Windows) or `Applications` Folder (OS X). On OS X it will install two icons – "R" and "R64", corresponding to 32-bit and 64-bit versions of the executable. The 64 bit version, which allows access to much larger amounts of your comptuer's RAM, is suitable for dealing with very large data sets.

1.1.2 Starting and R Interactive Session

The OS X and Windows version of R provide a simple GUI interface for using R in interactive mode. When you start up the R GUI you'll be presented with a single window, the R console. See the your textbook, The Art of R Programming (AoRP) for a discussion of the difference between R's interactive and batch modes.

1.1.3 Accessing the Help System on R

R comes with fairly extensive documentation and a simple help system. You can access HTML versions of R documentation under the Help menu in the GUI. The HTML documentation also includes information on any packages you've installed. Take a few minutes to browse through the R HTML documentation.

The help system can be invoked from the console itself using the `help` function or the `?` operator.

```
> help(length)
> ?length
> ?log
```

What if you don't know the name of the function you want? You can use the `help.search()` function.

```
> help.search("log")
```

In this case `help.search("log")` returns all the functions with the string 'log' in them. For more on `help.search` type `?help.search`. Other useful help related functions include `apropos()` and `example()`.

1.1.4 Navigating Directories in R

When you start the R environment your 'working directory' (i.e. the directory on your computer's file system that R currently 'sees') defaults to a specific directory. On Windows this is usually the same directory that R is installed in, on OS X it is typically your home directory. Here are examples showing how you can get information about your working directory and change your working directory.

```
> getwd()
[1] "/Users/pmagwene"
> setwd("/Users")
> getwd()
[1] "/Users"
```

Note that on Windows you can change your working directory by using the `Change dir...` item under the `File` menu, while the corresponding item is found under the `Misc` menu on OS X.

To get a list of the file in your current working directory use the `list.files()` function.

```
> list.files()
[1] "Shared" "pmagwene"
```

1.1.5 Using R as a Calculator

The simplest way to use R is as a fancy calculator.

```
> 10 + 2 # addition
[1] 12
> 10 - 2 # subtraction
[1] 8
> 10 * 2 # multiplication
[1] 20
> 10 / 2 # division
[1] 5
> 10 ^ 2 # exponentiation
[1] 100
> 10 ** 2 # alternate exponentiation
[1] 100
> sqrt(10) # square root
[1] 3.162278
> 10 ^ 0.5 # same as square root
[1] 3.162278
> exp(1) # exponential function
[1] 2.718282
```

```
> 3.14 * 2.5^2
[1] 19.625
> pi * 2.5^2 # R knows about some constants such as Pi
[1] 19.63495
> cos(pi/3)
[1] 0.5
> sin(pi/3)
[1] 0.8660254
> log(10)
[1] 2.302585
> log10(10) # log base 10
[1] 1
> log2(10) # log base 2
[1] 3.321928
> (10 + 2)/(4-5)
[1] -12
> (10 + 2)/4-5 # compare the answer to the above
[1] -2
```

Be aware that certain operators have precedence over others. For example multi-plication and division have higher precedence than addition and subtraction. Use parentheses to disambiguate potentially confusing statements.

```
> sqrt(pi)
[1] 1.772454
> sqrt(-1)
[1] NaN
Warning message:
NaNs produced in: sqrt(-1)
> sqrt(-1+0i)
[1] 0+1i
```

What happened when you tried to calculate sqrt(-1)?, -1 is treated as a real number and since square roots are undefined for the negative reals, R produced a warning message and returned a special value called NaN (Not a Number). Note that square roots of negative complex numbers are well defined so sqrt(-1+0i) works fine.

```
> 1/0
[1] Inf
```

Division by zero produces an object that represents infinite numbers.

1.1.6 Comparison Operators

You've already been introduced to the most commonly used arithmetic operators. Also useful are the comparison operators:

```
> 10 < 9   # less than
[1] FALSE
> 10 > 9   # greater than
[1] TRUE
```

```
> 10 <= (5 * 2) # less than or equal to
[1] TRUE
> 10 >= pi # greater than or equal to
[1] TRUE
> 10 == 10 # equals
[1] TRUE
> 10 != 10 # does not equal
[1] FALSE
> 10 == (sqrt(10)^2) # Surprised by the result? See below.
[1] FALSE
> 4 == (sqrt(4)^2) # Even more confused?
[1] TRUE
```

Comparisons return boolean values. Be careful to distinguish between == (tests equality) and = (the alternative assignment operator equivalent to <-).

How about the last two statement comparing two values to the square of their square roots? Mathematically we know that both $(\sqrt{10})^2 = 10$ and $(\sqrt{4})^2 = 4$ are true statements. Why does R tell us the first statement is false? What we're running into here are the limits of computer precision. A computer can't represent $\sqrt{10}$ exactly, whereas $\sqrt{4}$ can be exactly represented. Precision in numerical computing is a complex subject and beyond the scope of this course. Later in the course we'll discuss some ways of implementing sanity checks to avoid situations like that illustrated above.

1.1.7 Working with Vectors in R

Vectors are the core data structure in R. Vectors store an ordered list of items all of the same type. Learning to compute effectively with vectors and one of the keys to efficient R programming. Vectors in R always have a length (accessed with the length () function) and a type (accessed with the typeof() function). The simplest way to create a vector at the interactive prompt is to use the c() function, which is short hand for 'combine' or 'concatenate'.

```
> x <- c(2,4,6,8)
[1] "double"
> length(x)
[1] 4
> y <- c('joe','bob','fred')
> typeof(y)
[1] "character"
> length(y)
[1] 3
> z <- c() # empty vector
> length(z)
[1] 0
> typeof(z)
[1] "NULL"
```

Vector Arithmetic and Comparison

The basic R arithmetic operations work on vectors as well as on single numbers (in fact single numbers *are* vectors).

```
> x <- c(2, 4, 6, 8, 10)
> x * 2
[1]   4   8 12 16 20
> x * pi
[1]   6.283185 12.566371 18.849556 25.132741 31.415927
> y <- c(0, 1, 3, 5, 9)
> x + y
[1]   2   5   9 13 19
> x * y
[1]   0   4 18 40 90
> x/y
[1]      Inf 4.000000 2.000000 1.600000 1.111111
> z <- c(1, 4, 7, 11)
> x + z
[1]   3   8 13 19 11
Warning message:
longer object length
        is not a multiple of shorter object length in: x + z
```

When vectors are not of the same length R 'recycles' the elements of the shorter vector to make the lengths conform. In the example above z was treated as if it was the vector (1, 4, 7, 11, 1).

The comparison operators also work on vectors as shown below. Comparisons involving vectors return vectors of booleans.

```
> x > 5
[1] FALSE FALSE  TRUE  TRUE  TRUE
> x != 4
[1]  TRUE FALSE  TRUE  TRUE  TRUE
```

If you try and apply arithmetic operations to non-numeric vectors, R will warn you of the error of your ways:

```
> w <- c('foo', 'bar', 'baz', 'qux')
> w**2
Error in w^2 : non-numeric argument to binary operator
```

Note, however that the comparison operators can work with non-numeric vectors. The results you get will depend on the type of the elements in the vector.

```
>  w == 'bar'
[1] FALSE  TRUE FALSE FALSE
> w < 'cat'
[1] FALSE  TRUE  TRUE FALSE
```

Indexing Vectors

For a vector of length n, we can access the elements by the indices $1 \ldots n$. We say that R vectors (and other data structures like lists) are 'one-indexed'. Many other programming languages, such as Python, C, and Java, use zero-indexing where the elements of a data structure are accessed by the indices $0 \ldots n - 1$. Indexing errors are a common source of bugs. When moving back and forth between different programming languages keep the appropriate indexing straight!

Trying to access an element beyond these limits returns a special constant called NA (Not Available) that indicates missing or non-existent values.

```
> x <- c(2, 4, 6, 8, 10)
> length(x)
[1] 5
> x[1]
[1] 2
> x[4]
[1] 8
> x[6]
[1] NA
> x[-1]
[1]  4  6  8 10
> x[c(3,5)]
[1]  6 10
```

Negative indices are used to exclude particular elements. x[-1] returns all elements of x except the first. You can get multiple elements of a vector by indexing by another vector. In the example above x[c(3,5)] returns the third and fifth element of x.

Combining Indexing and Comparison

A very powerful feature of R is the ability to combine the comparison operators with indexing. This facilitates data filtering and subsetting. Some examples:

```
> x <- c(2, 4, 6, 8, 10)
> x[x > 5]
[1]  6  8 10
> x[x < 4 | x > 6]
[1]  2  8 10
```

In the first example we retrieved all the elements of x that are larger than 5 (read as 'x where x is greater than 5'). In the second example we retrieved those elements of x that were smaller than four *or* greater than six. The symbol | is the 'logical or' operator. Other logical operators include & ('logical and' or 'intersection') and ! (negation). Combining indexing and comparison is a powerful concept and one you'll probably find useful for analyzing your own data.

Generating Regular Sequences

Creating sequences of numbers that are separated by a specified value or that follow a particular patterns turns out to be a common task in programming. R has some built-in operators and functions to simplify this task.

```
> s <- 1:10
> s
 [1]  1  2  3  4  5  6  7  8  9 10
> s <- 10:1
> s
 [1] 10  9  8  7  6  5  4  3  2  1
> s <- seq(0.5,1.5,by=0.1)
> s
 [1] 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5
# 'by' is the 3rd argument so you don't have to specify it
> s <- seq(0.5, 1.5, 0.33)
> s
[1] 0.50 0.83 1.16 1.49
```

rep() is another way to generate patterned data.

```
> rep(c("Male","Female"),3)
[1] "Male"   "Female" "Male"   "Female" "Male"   "Female"
> rep(c(T,T, F),2)
[1]  TRUE  TRUE FALSE  TRUE  TRUE FALSE
```

1.1.8 Some Useful Functions

You've already seem a number of functions (e.g. `sin()`, `log`, `length()`, etc). Functions are called by invoking the function name followed by parentheses containing zero or more *arguments* to the function. Arguments can include the data the function operates on as well as settings for function parameter values. We'll discuss function arguments in greater detail below.

Creating vectors

An important function that you've used extensively but we've glossed over is the `c()` function. This is short for 'concatenate' or 'combine' and as you've seen it combines it's arguments to form a vector.

For vectors of more than 10 or so elements it gets tiresome and error prone to create vectors using `c()`. For medium length vectors the `scan()` function is very useful.

```
> test.scores <- scan()
1: 98 92 78 65 52 59 75 77 84 31 83 72 59 69 71 66
17:
Read 16 items
> test.scores
 [1] 98 92 78 65 52 59 75 77 84 31 83 72 59 69 71 66
```

When you invoke `scan()` without any arguments the function will read in a list of values separated by white space (usually spaces or tabs). Values are read until `scan()` encounters a blank line or the end of file (EOF) signal (platform dependent).

   Note that we created a variable with the name `test.scores`. If you have previous programming experience you might be surprised that this works. Unlike most languages, R allows you to use periods in variable names. Descriptive variable names generally improve readability but they can also become cumbersome (e.g. `my.long.and.obnoxious.variable.name`). As a general rule of thumb use short variable names when working at the interpreter and more descriptive variable names in functions.

Useful Numerical Functions

Let's introduce some additional numerical functions that are useful for operating on vectors.

```
> sum(test.scores)
[1] 1131
> min(test.scores)
[1] 31
> max(test.scores)
[1] 98
> range(test.scores) # min,max returned as a vec of len 2
[1] 31 98
> sorted.scores <- sort(test.scores)
> sorted.scores
 [1] 31 52 59 59 65 66 69 71 72 75 77 78 83 84 92 98
> w <- c(-1, 2, -3, 3)
> abs(w) # absolute value function
```

1.1.9 Function Arguments in R

Function arguments can specify the data that a function operates on or parameters that the function uses. Some arguments are required, while others are optional and are assigned default values if not specified.

   Take for example the `log()` function. If you examine the help file for the `log()` function you'll see that it takes two arguments, refered to as 'x' and 'base'. The argument x represents the numeric vector you pass to the function and is a required argument (see what happens when you type `log()` without giving an argument). The argument base is optional. By default the value of base is $e = 2.71828$.... Therefore by default the `log()` function returns natural logarithms. If you want logarithms to a different base you can change the base argument as in the following examples:

```
> log(2) # log of 2, base e
[1] 0.6931472
> log(2,2) # log of 2, base 2
[1] 1
> log(2, 4) # log of 2, base 4
```

```
[1] 0.5
```

1.1.10 Simple Input in R

The c() and scan() functions are fine for creating small to medium vectors at the interpreter, but eventually you'll want to start manipulating larger collections of data. There are a variety of functions in R for retrieving data from files.

The most convenient file format to work with are tab delimited text files. Text files have the advantage that they are human readable and are easily shared across different platforms. If you get in the habit of archiving data as text files you'll never find yourself in a situation where you're unable to retrieve important data because the binary data format has changed between versions of a program.

1.1.11 Using scan() to input data

scan() itself can be used to read data out of a file. Download the file algae.txt from the class website and try the following (after changing your working directory):

```
> algae <- scan('algae.txt')
Read 12 items
> algae
 [1] 0.530 0.183 0.603 0.994 0.708 0.006 0.867 0.059 0.349 0.699 0.983
     0.100
```

One of the things to be aware of when using scan() is that if the data type contained in the file can not be coerced to doubles than you must specify the data type using the what argument. The what argument is also used to enable the use of scan() with columnar data. Download algae2.txt and try the following:

```
> algae.table <- scan('algae2.txt', what=list('',double(0)))
                          # note use of list argument to what
> algae.table
[[1]]
 [1] "Jan" "Feb" "Mar" "Apr" "May" "Jun" "Jul" "Aug" "Sep" "Oct" "Nov" "Dec
     "

[[2]]
 [1] 0.530 0.183 0.603 0.994 0.708 0.006 0.867 0.059 0.349 0.699 0.983
     0.100

> algae.table[[1]]
 [1] "Jan" "Feb" "Mar" "Apr" "May" "Jun" "Jul" "Aug" "Sep" "Oct" "Nov" "Dec
     "
> algae.table[[2]]
 [1] 0.530 0.183 0.603 0.994 0.708 0.006 0.867 0.059 0.349 0.699 0.983
     0.100
```

Use help to learn more about scan().

1.1.12 Using `read.table()` to input data

`read.table()` (and it's derivates - see the help file) provides a more convenient inter-
face for reading tabular data. Using the file `turtles.txt`:

```
> turtles <- read.table('turtles.txt', header=T)
> turtles
   sex length width height
1   f     98    81     38
2   f    103    84     38
3   f    103    86     42
  # output truncated
> names(turtles)
[1] "sex"    "length" "width"  "height"
> length(turtles)
[1] 4
> length(turtles$sex)
[1] 48
```

What kind of data structure is `turtles`? What happens when you call the `read.table()`
function without specifying the argument `header=T`?

You'll be using the `read.table()`}function frequently. Spend some time reading
the documentation and playing around with different argument values (for example,
try and figure out how to specify different column names on input).

Note: `read.table()` is more convenient but `scan()` is more efficient for large files.
See the R documentation for more info.

1.1.13 Basic Statistical Functions in R

There are a wealth of statistical functions built into R. Let's start to put these to use.

If you wanted to know the mean carapace width of turtles in your sample you could
calculate this simply as follows:

```
> sum(turtles$width)/length(turtles$width)
[1] 95.4375
```

Of course R has a built in `mean()` function.

```
mean(turtles$width) [1] 95.4375
```

One of the advantages of the built in `mean()` function is that it knows how to operate
on lists as well as vectors:

```
> mean(turtles)
      sex    length     width    height
       NA 124.68750  95.43750  46.33333
Warning message:
argument is not numeric or logical: returning NA in: mean.default(X[[1]],
    ...)
```

Can you figure out why the above produced a warning message? Let's take a look at
some more standard statistical functions:

```
> min(turtles$width)
[1] 74
> max(turtles$width)
[1] 132
> range(turtles$width)
[1]   74 132
> median(turtles$width)
[1] 93
> summary(turtles$width)
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
  74.00   86.00   93.00   95.44  102.00  132.00
> var(turtles$width) # variance
[1] 160.6769
> sd(turtles$width)   # standard deviation
[1] 12.67584
```

1.1.14 Simple Plots in R

One of the advantages of R is it's ability to produce a variety of plots and statistical graphics. Try out the following:

```
> hist(turtles$width)   # histogram plot
> hist(turtles$width,10) # produces a histogram with 10 bins
> hist(turtles$width,breaks=10, xlab="Carapace Width", probability=T)
> boxplot(turtles$width) # simple box plot
# a fancy box plot showing multiple variables
> boxplot(list(turtles$length, turtles$width,  turtles$height),
+         names=c("Carapace\nLength","Carapace\nWidth","Carapace\nHeight"),
+         ylab="millimeters")
> title("Turtle Shell Variables")
> plot(turtles$length, turtles$width)
# how does this differ from the plot above?
> plot(turtles$length ~ turtles$width)
> plot(turtles$length, turtles$width,
+      xlab="Carapace Length(mm)", ylab="Carapace Width(mm)")
> title("Relationship Between\nLength and Width")
```

To get a sense of some of the graphical power of R try the demo() function:

```
> demo(graphics)
```

1.2 Exploring Univariate Distributions in R

1.2.1 Histograms

One of the most common ways to examine a the distribution of observations for a single variable is to use a histogram. The hist() function creates simple histograms in R.

```
> hist(turtles$length) # create histogram with fxn defaults
> ?hist # check out the documentation on hist
```

Note that by default the `hist()` function plots the frequencies in each bin. If you want the probability densities instead set the argument `freq=FALSE`.

```
> hist(turtles$length,freq=F) # y-axis gives probability density
```

Here's some other ways to fine tune a histogram in R.

```
> hist(turtles$length, breaks=12) # use 12 bins
> mybreaks = seq(85,185,8)
> hist(turtles$length, breaks=mybreaks) # specify bin boundaries
> hist(turtles$length, breaks=mybreaks, col='red') # fill the bins with red
```

1.2.2 Density Plots

One of the problems with histograms is that they can be very sensitive to the size of the bins and the break points used. This is due to the discretization inherent in a histogram. A 'density plot' or 'density trace' is a continuous estimate of a probability distribution from a set of observations. Because it is continuous it doesn't suffer from the same sensitivity to bin sizes and break points. One way to think about a density plot is as the histogram you'd get if you averaged many individual histograms each with slightly different breakpoints.

```
> d <- density(turtles$length)
> plot(d)
```

A density plot isn't entirely parameter free – the parameter you should be most aware of is the 'smoothing bandwidth'.

```
> d <- density(turtles$length) # let R pick the bandwidth
> plot(d,ylim=c(0,0.020)) # gives ourselves some extra headroom on y-axis
> d2 <- density(turtles$length, bw=5) # specify bandwidth
> lines(d2, col='red') # use lines to draw over previous plot
```

The bandwidth determines the standard deviation of the 'kernel' that is used to calculate the density plot. There are a number of different types of kernels you can use; a Gaussian kernel is the R default and is the most common choice. See the documentation for more info.

The `lattice` package is an R library that makes it easier to create graphics that show conditional distributions. Here's how to create a simple density plot using the `lattice` package.

```
> library(lattice)
> densityplot(turtles$length) # densityplot defined in lattice
```

Notice how by default the `lattice` package also drew points representing the observations along the x-axis. These points have been 'jittered' meaning they've been randomly shifted by a small amount so that overlapping points don't completely hide each other. We could have produced a similar plot, without the lattice package, as so:

```
> d <- density(turtles$length)
> plot(d)
> nobs <- length(turtles$length)
> points(jitter(turtles$length), rep(0,nobs))
```

Notice that in our version we only jittered the points along the x-axis. You can also combine a histogram and density trace, like so:

```
> hist(turtles$length, 10, xlab='Carapace Length (mm)',freq=F)
> d <- density(turtles$length)
> lines(d, col='red', lwd=2) # red lines, with pixel width 2
```

Notice the use of the `freq=F` argument to scale the histogram bars in terms of probability density.

Finally, let's some of the features of `lattice` to produce density plots for the 'length' variable of the turtle data set, conditional on sex of the specimen.

```
> densityplot(~length | sex, data = turtles)
```

There are a number of new concepts here. The first is that we used what is called a 'formula' to specify what to plot. In this case the formula can be read as 'length conditional on sex'. We'll be using formulas in several other contexts and we discuss them at greater length below. The `data` argument allows us to specify a data frame or list so that we don't always have to write arguments like `turtles$length` or `turtles$sex` which can get a bit tedious.

1.2.3 Box Plots

Another common tool for depicting a univariate distribution is a 'box plot' (sometimes called a box-and-whisker plot). A standard box plot depicts five useful features of a set of observations: the median (center most line), the upper and lower quartiles (top and bottom of the box), and the minimum and maximum observations (ends of the whiskers).

There are many variants on box plots, particularly with respect to the 'whiskers'. It's always a good idea to be explicit about what a box plot you've created depicts.

Here's how to create box plots using the standard R functions as well as the lattice package:

```
> boxplot(turtles$length)
> boxplot(turtles$length, col='darkred', horizontal=T) # horizontal version
> title(main = 'Box plot: Carapace Length', ylab = 'Carapace length (mm)')
> bwplot(~length,data=turtles) # using the bwplot function from lattice
```

Note how we used the `title()` function to change the axis labels and add a plot title.

Historical note – The box plot is one of many inventions of the statistician John W. Tukey. Tukey made many contributions to the field of statistics and computer science, particularly in the areas of graphical representations of data and exploratory data analysis.
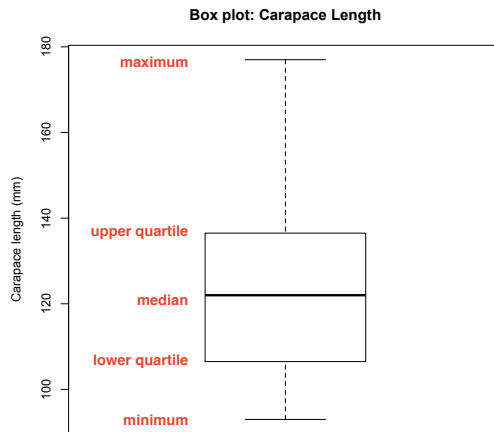
Box plot: Carapace Length

Figure 1.1: A box plot represents a five number summary of a set of observations.

1.2.4 Bean Plots

My personal favorite way to depict univariate distributions is called a 'beanplot'. Beanplots combine features of density plots and boxplots and provide information rich graphical summaries of single variables. The standard features in a beanplot include the individual observations (depicted as lines), the density trace estimated from the observations, the mean of the observations, and in the case of multiple beanplots an overall mean.
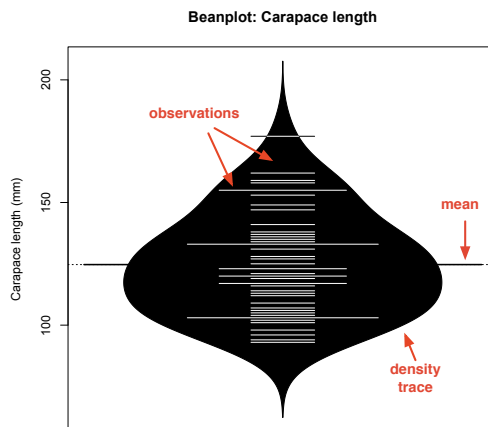
Beanplot: Carapace length

Figure 1.2: Beanplots combine features of density and box plots.

The `beanplot` package is not installed by default. To download it and install it use the R package installer under the `Packages & Data` menu (standard R GUI) or in

`Tools > Install Packages...` in RStudio (see also the `Packages` tab in the lower-right window in RStudio). If this is the first time you use the package installer you'll have to choose a CRAN repository from which to download package info (I recommend you pick one in the US). Once you've done so you can search for 'beanplot' from the Package Installer window. You should also check the 'install dependencies' check box.

Once the beanplot package has been installed check out the examples to see some of the capabilities:

```
> library(beanplot)
> example(beanplot)
```

If you ran the examples in RStudio, use the `Clear All` option in the `Plots` tab after running the examples in order to reset parameters that the examples changed.

Note the use of the `library()` function to make the functions in the `beanplot` library available for use. Here's some examples of using the `beanplot` function with the turtle data set:

```
> beanplot(turtles$length) # note the message about log='y'
> beanplot(turtles$length, log='') # DON'T do the automatic log transform
> beanplot(turtles$length, log='', col=c('white','blue','blue','red'))
```

In the final version we specified colors for the parts of the beanplot. See the explanation of the `col` argument int he beanplot function for details.

We can also compare the carapace length variable for male and female turtles.

```
> beanplot(length ~ sex, data = turtles, col=list(c('red'),c('black')),
names = c('females','males'),xlab='Sex', ylab='Caparace length (mm)')
```

Note the use of the formula notation to compare the carapace length variable for males and females. There is also a asymmetrical version of the beanplot which can be used to more directly compare distributions between two groups. We explore this below. Note too the use of the list argument to `col`, and the use of vectors within the list to specify the colors for female and male beanplots.

We can also create a beanplot with multiple variables in the same plot if the variables are measured on the same scale.

```
> beanplot(turtles$length, turtles$width, turtles$height, log='',
names=c('length','width','height'), ylab='carapace dimensions (mm)')
```