

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 version 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 computer’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 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 multiplication 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"

```

You can also use `c()` to concatenate two or more vectors together.

```
> v <- c(1,3,5,7)
> w <- c(-1, -2, -3)
> vwx <- c(v,w,x)
> vwx
[1] 1 3 5 7 -1 -2 -3 2 4 6 8
```

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 $1 \dots n$. 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 $0 \dots n - 1$. 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 seen a number of functions (`c()`, `length()`, `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 longer vectors

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). We'll see how to read in data from files below.

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 66 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 (type `?log` now) you'll see that it takes two arguments, referred 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 $e = 2.71828\dots$. 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
```

Because base 2 and base 10 logarithms are fairly commonly used, there are convenient aliases for calling log with these bases.

```
> log2(8)
[1] 3
> log10(100)
[1] 2
```

1.1.10 Lists in R

R lists are like vectors, but unlike a vector where all the elements are of the same type, the elements of a list can have arbitrary types (even other lists).

```
> l <- list('Bob', pi, 10, c(2,4,6,8))
```

Indexing of lists is different than indexing of vectors. Double brackets (`x[[i]]`) return the element at index *i*, single bracket return a list containing the element at index *i*.

```
> l[1] # single brackets
[[1]]
[1] "Bob"

> l[[1]] # double brackets
[1] "Bob"
> typeof(l[1])
[1] "list"
> typeof(l[[1]])
[1] "character"
```

The elements of a list can be given names, and those names objects can be accessed using the `$` operator. You can retrieve the names associated with a list using the `names()` function.

```
> l <- list(name='Bob', age=27, years.in.school=10)
> l
$name
[1] "Bob"

$age
[1] 27

$years.in.school
[1] 10

> l$years.in.school
[1] 10
> l$name
```

```
[1] "Bob"
> names(1)
[1] "name"          "age"          "years.in.school"
```

1.1.11 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.

1.1.12 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 then 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
> algae.table
[[1]]
[1] "Jan" "Feb" "Mar" "Apr" "May" "Jun" "Jul" "Aug" "Sep" "Oct" "Nov"
[12] "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
[12] 0.100

> algae.table[[1]]
[1] "Jan" "Feb" "Mar" "Apr" "May" "Jun" "Jul" "Aug" "Sep" "Oct" "Nov"
[12] "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
[12] 0.100
```

Use `help` to learn more about `scan()`.

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

`read.table()` (and its derivatives - see the help file) provides a more convenient interface for reading tabular data. Download the `turtles.txt` data set from the class wiki. The data in `turtles.txt` are a set of linear measurements representing dimensions of the carapace (upper shell) of painted turtles (*Chrysemys picta*), as reported in Jolicœur and Mosimmann, 1960; Growth 24: 339-354.

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.

1.1.14 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
```

1.2 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 fn 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. You probably noticed that in the example above as we changes the number of bins and the breakpoints to generate the histograms for the `turtles$length` variable. 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. In the example above, R picked a bandwidth of 8.5 (the black line in our plot). When we specified a smaller bandwidth of 5, the resulting density plot (red) is less smooth. There exists a statistical literature on picking ‘optimum’ kernel sizes. In general, larger data sets support the use of smaller kernels. See the R documentation for more info on the `density()` function and references to the literature on density estimators.

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 see 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).

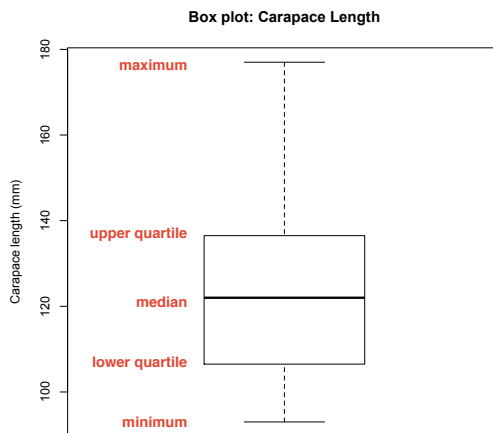


Figure 1.1: A box plot represents a five number summary of a set of observations.

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.

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.

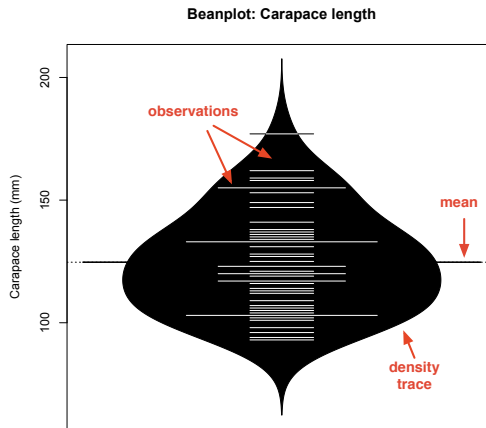


Figure 1.2: Beanplots combine features of density and box plots.

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

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 `turtles` 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 in the `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. Note 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.

There is also an asymmetrical version of the `beanplot` which can be used to more directly compare distributions between two groups. This can be specified by using the argument `side='both'` to the `beanplot` function.

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

Plots like this one are very convenient for comparing distributions between samples grouped by treatment, sex, species, etc.

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)')
```

1.2.5 Demo Plots in R

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

```
> demo(graphics)
```

2 Vector Operations and Exploring Bivariate Relationships in R

2.1 Vector Operations in R

As you saw last week R vectors support basic arithmetic operations that correspond to the same operations on geometric vectors. For example:

```
> x <- 1:15
> y <- 10:24
> x
[1] 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
> y
[1] 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

> x + y           # vector addition
[1] 11 13 15 17 19 21 23 25 27 29 31 33 35 37 39
> x - y           # vector subtraction
[1] -9 -9 -9 -9 -9 -9 -9 -9 -9 -9 -9 -9 -9 -9 -9
> x * 3           # multiplication by a scalar
[1] 3 6 9 12 15 18 21 24 27 30 33 36 39 42 45
```

R also has an operator for the dot product, denoted `%*%`. This operator also designates matrix multiplication, which we will discuss next week. By default this operator returns an object of the R matrix class. If you want a scalar (or the R equivalent of a scalar, i.e. a vector of length 1) you need to use the `drop()` function.

```
> z <- x %*% x
> class(z)           # note use of class() function
[1] "matrix"
> z
      [,1]
[1,] 1240
> drop(z)
[1] 1240
```

In lecture we saw that many useful geometric properties of vectors could be expressed in the form of dot products. Let's start with some two-dimensional vectors where the geometry is easy to visualize:

```
> a <- c(1, 0) # the point (1,0)
> b <- c(0, 1) # the point (0,1)
```

Now let's draw our vectors:

```
# create empty plot w/specified x- and y- limits
# the 'asp=1' argument maintains the scaling of the x- and y-axes
# so that units are equivalent for both axes (i.e. squares remain squares)
> plot(c(-2,2),c(-1,2),type='n', asp=1)

# draw an arrow from origin (0,0) to x,y coordinates of vector "a"
# the length argument changes the size of the arrowhead
# use the R help to read more about the arrows function
> arrows(0, 0, a[1], a[2], length=0.1)

# and now for the vector "b"
> arrows(0, 0, b[1], b[2], length=0.1)
```

You should now have a figure that looks like the one below: Let's see what the dot

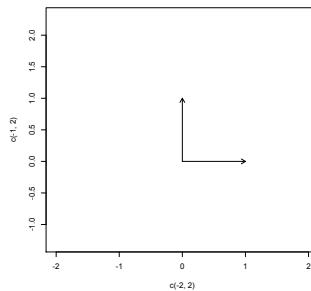


Figure 2.1: A simple vector figure.

product can tell us about these vectors. First recall that we can calculate the length of a vector as the square-root of the dot product of the vector with itself ($|\vec{a}|^2 = \vec{a} \cdot \vec{a}$)

```
> len.a <- drop(sqrt(a %*% a))
> len.a
[1] 1
> len.b <- drop(sqrt(b %*% b))
```

How about the angle between a and b ?

```
> dot.ab <- a %*% b
> dot.ab
[1,]
[1,] 0
> cos.ab <- (a %*% b)/(len.a * len.b)
> cos.ab
[1,]
[1,] 0
```

A key point to remember dot product of two vectors is zero if, and only if, they are orthogonal to each other (regardless of their dimension).

2.2 Writing Functions in R

So far we've been mostly using R's built in functions. However the power of a true programming language is the ability to write your own functions.

The general form of an R function is as follows:

```
funcname <- function(arg1, arg2) {
  # one or more expressions
  # last expression is the object returned
  # or you can explicitly return an object
}
```

To make this concrete, here's an example where we define a function in the interpreter and then put it to use:

```
> myfunc <- function(x,y){
+ # don't type the '+' symbols, these show continuation lines
+   x^2 + y^2
+ }

> a <- 1:5
> b <- 6:10
> a
[1] 1 2 3 4 5
> b
[1] 6 7 8 9 10
> myfunc(a,b)
[1] 37 53 73 97 125
> myfunc
function(x,y){
  x^2 + y^2
}
```

If you type a function name without parentheses R shows you the function's definition. This works for built-in functions as well (though sometimes these functions are defined in C code in which case R will tell you that the function is a 'Primitive').

2.2.1 Putting R functions in Scripts

When you define a function at the interactive prompt and then close the interpreter your function definition will be lost. The simple way around this is to define your R functions in a script that you can then access at any time.

Choose File > New Script (or File > New Document in OS X) in the R GUI . This will bring up a blank editor window. Enter your function into the editor and save the source file in your R working directory with a name like vecgeom.R.

```
# functions defined in vecgeom.R

veclength <- function(x) {
  # Given a numeric vector, returns length of that vector
}
```

```

sqrt(drop(x %*% x))
}

unitvector <- function(x) {
  # Return a unit vector in the same direction as x
  x/vecLength(x)
}

vec.cos <- function(x,y) {
  # Calculate the cos of the angle between vectors x and y
  len.x <- vecLength(x)
  len.y <- vecLength(y)
  return( (x %*% y)/(len.x * len.y) )
}

```

There are two functions defined above, one of which calls the other. Both take single vector arguments. At this point there is no error checking to insure that the argument is reasonable but R's built in error handling will do just fine for now.

Once your functions are in a script file you can make them accessible by using the `source()` function (See also the File > Source R code... menu item in the R GUI):

```

> source("vecgeom.R")
> x <- c(1,0.4)
> vecLength(x)
[1] 1.077033
> ux <- unitvector(x)
> ux
[1] 0.9284767 0.3713907
> vecLength(ux)
[1] 1

```

Assignment 2.1

Write a function that uses the dot product and the `acos()` function to calculate the angle (in radians) between two vectors of arbitrary dimension. By default, your function should return the angle in radians. Also include a logical (Boolean) argument that will return the answer in degrees. Test your function with the following two vectors: $x = [-3, -3, -1, -1, 0, 0, 1, 2, 2, 3]$ and $y = [-8, -5, -3, 0, -1, 0, 5, 1, 6, 5]$. The expected angle for these test vectors is 0.441 radians (25.3 degrees).

Let's also add the following function to `vecgeom.R` to aid in visualizing 2D vectors:

```

draw.vectors <- function(a, b, colors=c('red', 'blue'), clear.plot=TRUE){

```

```

  # figure out the limits such that the origin and the vector
  # end points are all included in the plot
  xhi <- max(0, a[1], b[1])
  xlo <- min(0, a[1], b[1])
  yhi <- max(0, a[2], b[2])
  ylo <- min(0, a[2], b[2])

```

```

xlims <- c(xlo, xhi)*1.10 # give a little breathing space around
                           vectors
ylims <- c(ylo, yhi)*1.10

if (clear.plot){
  plot(xlims, ylims, type='n', asp=1, xlab="x-coord", ylab="y-coord")
}
arrows(0, 0, a[1], a[2], length=0.1, col=colors[1])
arrows(0, 0, b[1], b[2], length=0.1, col=colors[2])
}

```

You can use this new function as follows:

```

# you need to source the file everytime you change it
> source("/Users/pmagwene/Downloads/vecgeom.R")
> x <- c(1,0.4)
> y <- c(0.2, 0.8)
> draw.vectors(x,y) # draw the original vectors

```

The resulting figure should resemble the one below.

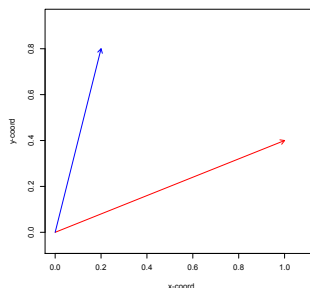


Figure 2.2: Another vector figure.

Notice that we included a `clear.plot` argument in our `draw.vectors` function. I included this so we could add additional vectors to our plot, without overwriting the old vectors, as demonstrated below:

```

# draw the unit vectors that point in the same directors as the original
  vectors
> ux <- unitvector(x)
> uy <- unitvector(y)
> draw.vectors(ux, uy, colors=c('black', 'green'), clear.plot=F)

```

Assignment 2.2

Write a function, `vproj()`, that takes two vectors, \vec{x} and \vec{y} , and returns a list containing the projection of \vec{y} on \vec{x} and the component of \vec{y} in \vec{x} :

$$P_{\vec{x}}(\vec{y}) = \left(\frac{\vec{x} \cdot \vec{y}}{|\vec{x}|} \right) \frac{\vec{x}}{|\vec{x}|}$$

and

$$C_{\vec{x}}(\vec{y}) = \frac{\vec{x} \cdot \vec{y}}{|\vec{x}|}$$

Use the test vectors from Assignment 2.1 to test your function. The list returned by your function for these test vectors should resemble that shown below:

```
> vproj(x, y)

$proj
[1] -6 -6 -2 -2  0  0  2  4  4  6

$comp
[1] 12.32883
```

2.3 Exploring Bivariate Relationships in R

Let's use a dataset called `iris` (included in the standard R distribution) to explore bivariate relationships between variables. This data set was made famous by R. A. Fisher who used it to illustrate many of the fundamental statistical methods he developed. The data set consists of four morphometric measurements for specimens from three different iris species. Use the R help to read about the iris data set (`?iris`). We'll be using this data set repeatedly in future weeks so familiarize yourself with it.

```
> ?iris
> names(iris)
[1] "Sepal.Length" "Sepal.Width"  "Petal.Length" "Petal.Width"
[5] "Species"
> unique(iris$Species)
[1] setosa      versicolor virginica
Levels: setosa versicolor virginica
> dim(iris)
[1] 150  5
```

For now let's just work with the *I. setosa* specimens. Read the help file for `subset()`.

```
> setosa <- subset(iris, Species == 'setosa', select = -Species)
> dim(setosa)
[1] 50  4
> names(setosa)
[1] "Sepal.Length" "Sepal.Width"  "Petal.Length" "Petal.Width"
```


Notice how we used the `select` argument to `subset()` in order to drop the `Species` column. Let's explore the `setosa` subset with some graphs.

```
> plot(setosa$Sepal.Length, setosa$Sepal.Width)
> plot(setosa$Sepal.Width ~ setosa$Sepal.Length)
```

Did you notice what is different between the two versions above? You can also use the `data` argument with `plot`, like so:

```
> plot(Sepal.Width ~ Sepal.Length, data = setosa)
```

The `xyplo()` function from the `lattice` package does pretty much the same thing:

```
> library(lattice)
> xyplot(Sepal.Width ~ Sepal.Length, data = setosa)
```

Let's also explore a number of the other bivariate relationships in this data set:

```
# an alternate way to generate such a plot, using the data argument to
# specify where the variables are defined
> plot(Petal.Length ~ Sepal.Length, data = setosa)

# same form as the first plot, but changing the character used for the plot
# using the 'pch' argument. The 'cex' argument increases the size of the
# characters by the specified factor (1.5x in this case)
> plot(setosa$Sepal.Length, setosa$Petal.Width, pch = 20, cex=1.5)
```

Often times it's useful to look at many bivariate relationships simultaneously. The `pairs()` function allows you to do this:

```
> pairs(setosa)
```

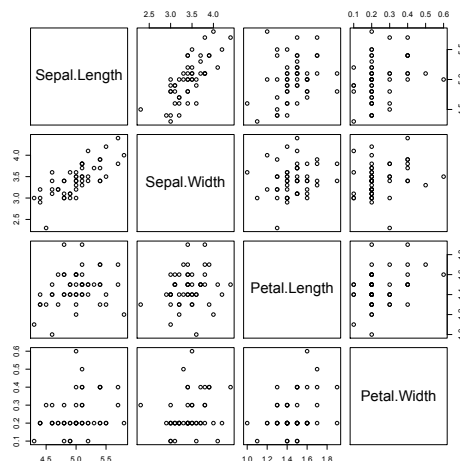


Figure 2.3: Output of the `pairs()` function for the *I. setosa* specimens in the `iris` dataset.

Let's return to our use of the dot product to explore the relationship between variables. First let's add a function to `vecgeom.R` to calculate the cosine of the angle between to vectors.

```
# add to vecgeom.R

vec.cos <- function(x,y) {
  # Calculate the cos of the angle between vectors x and y
  len.x <- veclength(x)
  len.y <- veclength(y)
  return( (x %%% y)/(len.x * len.y) )
}
```

We can then use this function to examine the relationships between the variables in the `setosa` dataset. First we'll center the `setosa` dataset using the `scale()` function. `scale()` has two logical arguments `center` and `scale`. By default both are `TRUE` which will center *and* scale the variables. But for now we just want to center the data. `scale()` returns a matrix object so we use the `data.frame` function to cast the object back to a data frame.

```
> source("/Users/pmagwene/Downloads/vecgeom.R")
> ctrd <- scale(setosa,center=T,scale=F)
> class(ctrd)
[1] "matrix"
> names(ctrd)
NULL
> ctrd <- data.frame(scale(setosa,center=T,scale=F))
> class(ctrd)
[1] "data.frame"
> names(ctrd)
[1] "Sepal.Length" "Sepal.Width" "Petal.Length" "Petal.Width"
> vec.cos(ctrd$Sepal.Length, ctrd$Sepal.Width)
[1,]
[1,] 0.7425467
> vec.cos(ctrd$Sepal.Length, ctrd$Petal.Length)
[1,]
[1,] 0.2671758
> vec.cos(ctrd$Sepal.Length, ctrd$Petal.Width)
[1,]
[1,] 0.2780984
```

Consider the values above in the context of the scatter plots you generated with the `pairs()` function; and then recall that for mean-centered variables, $\text{cor}(X,Y) = r_{XY} = \cos \theta = \frac{\vec{x} \cdot \vec{y}}{|\vec{x}| |\vec{y}|}$. So our `vec.cos()` function, when applied to centered data, is equivalent to calculating the correlation between x and y . Let's confirm this using the built in `cor()` function in R:

```
> cor(setosa$Sepal.Length, setosa$Sepal.Width)
[1] 0.7425467
> cor(setosa) # called like this will calculate all pairwise correlations
Sepal.Length Sepal.Width Petal.Length Petal.Width
```

Sepal.Length	1.0000000	0.7425467	0.2671758	0.2780984
Sepal.Width	0.7425467	1.0000000	0.1777000	0.2327520
Petal.Length	0.2671758	0.1777000	1.0000000	0.3316300
Petal.Width	0.2780984	0.2327520	0.3316300	1.0000000

2.3.1 Bivariate Regression in R

R has a flexible built in function, `lm()` for fitting linear models. Bivariate regression is the simplest case of a linear model.

```
> setosa.lm <- lm(Sepal.Width ~ Sepal.Length, data=setosa)
> class(setosa.lm)
[1] "lm"
> names(setosa.lm)
[1] "coefficients" "residuals"      "effects"        "rank"
[5] "fitted.values" "assign"         "qr"             "df.residual"
[9] "xlevels"      "call"          "terms"         "model"
```

Call:

```
lm(formula = Sepal.Width ~ Sepal.Length, data = setosa)
```

Residuals:

Min	1Q	Median	3Q	Max
-0.72394	-0.18273	-0.00306	0.15738	0.51709

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-0.5694	0.5217	-1.091	0.281
Sepal.Length	0.7985	0.1040	7.681	6.71e-10 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.2565 on 48 degrees of freedom

Multiple R-squared: 0.5514, Adjusted R-squared: 0.542

F-statistic: 58.99 on 1 and 48 DF, p-value: 6.71e-10

As demonstrated above, the `summary()` function spits out key diagnostic information about the model we fit. Now let's create a plot illustrating the fit of the model.

```
> plot(Sepal.Width ~ Sepal.Length, data=setosa, xlab="Sepal Length (cm)",
       ylab="Sepal Width (cm)", main="Iris setosa")
> abline(setosa.lm, col='red', lwd=2, lty=2) # see ?par for info about lwd
and lty
```

Your output should resemble the figure below. Note the use of the function `abline()` to plot the regression line. Calling `plot()` with an object of class `lm` shows a series of diagnostic plots. Try this yourself.

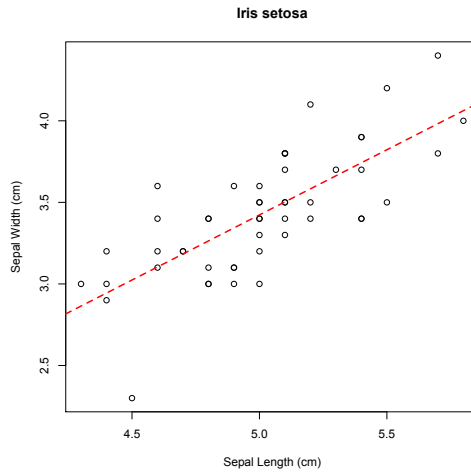


Figure 2.4: Linear regression of Sepal Width on Sepal Length for *I. setosa*.

Assignment 2.3

Write your own regression function (i.e. your code shouldn't refer to the built in regression functions) for mean centered vectors in R. The function will take as it's input two vectors, \vec{x} and \vec{y} . The function should return:

1. a list containing the mean-centered versions of these vectors
2. the regression coefficient b in the mean centered regression equation $\vec{\hat{y}} = b\vec{x}$
3. the coefficient of determination, R^2

Demonstrate your regression function by using it to carry out regressions of Sepal.Length on Sepal.Width separately for the 'versicolor' and 'virginica' specimens from the iris data set. Include plots in which you use the `plot()` and `abline()` functions to illustrate your calculated regression line. To test your function, compare your regression coefficients and coefficient of determination to the same values returned by the built in `lm()` function.