

# R for Data Science

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# Material for this class

All the material for the HPC Summer School can be found here:

`https:`

`//wiki.scinet.utoronto.ca/wiki/index.php/2016_Ontario_Summer_School_for_High_Performance_Computing_Central`

The slides for this class can be found here:

`http://tinyurl.com/ss2016-R1`

and at the SciNet education website:

`http://support.scinet.utoronto.ca/education`

# An introduction to R

Our adventure in R will cover the following:

- Getting R started.
- Primitive types
- Lists
- Vectors
- Matrices, Arrays
- Data frames
- Statistics
- Functions
- \*pply: lapply, apply, tapply

If you have questions, please ask.

# R history

R has been around for a while, and is well-developed:

- Introduced in 1996 as an evolution of the S language.
- R is designed for exploring and analysing data.
- Home page: <http://www.r-project.org>.
- Community packages are stored at CRAN - Comprehensive R Archive Network.
- A new full version of R is released each year. We're currently on release 3.3.1.

# About R

Some important things to know about R:

- R is a scripting language, meaning an interpreter executes commands one line at a time (not a compiled language).
- R can be used interactively, with or without IDE (RStudio).
- R has a large repository of community packages.
- R is all about data analysis: it is not a general purpose language.
  - ▶ Several important features (numerics, visualization) are baked into the language, not add-ons.
  - ▶ Not as useful outside of number crunching.
- R is designed with interactive data exploration in mind.
  - ▶ Lots of surprising things "just work" interactively.
  - ▶ But this design can make it a little difficult to debug large non-interactive programs.
- R is closer to functional in approach.

# Starting R

How you start the R interpreter depends upon your system:

- Windows: several graphical R interfaces exist (RCommander, Rgui, RStudio). Launch whichever one you have installed.
- Mac: similar to Windows, but running from the command line is also an option.
- Linux: open a terminal. Type "R". Use "q()" to quit.

Open up your R interface now. Raise your hand if you don't think it's working. Please follow along by entering the commands on the slides, and playing with the output.

# Starting R on SciNet

Alternatively, you can log into SciNet and run R there.

```
ejspence@mycomp ~>
ejspence@mycomp ~> ssh ejspence@login.scinet.utoronto.ca -X
ejspence@scinet01-ib0 ~>
ejspence@scinet01-ib0 ~> ssh -X gpc03
ejspence@gpc-f103n084-ib0 ~>
ejspence@gpc-f103n084-ib0 ~> module load intel/15.0.2 curl/7.49.1
ejspence@gpc-f103n084-ib0 ~> module load R/3.3.0
ejspence@gpc-f103n084-ib0 ~>
ejspence@gpc-f103n084-ib0 ~> R
>
```

We won't be using parallel R capabilities until this afternoon, so you should be able to just work either on your own laptop, or on a SciNet devel node for this morning.

# R data types

Once you start your session you will get an interactive prompt:

- Enter commands at the prompt, the interpreter interprets them.
- The "!" is the NOT operator.
- "paste" converts the input to strings, and then concatenates them.
- The "class" function returns names of the classes from which the object inherits.
- Like Python, R uses the # symbol to start comments.

```
>
> a <- 1
> b <- 1.73
> d <- "hello"
> e <- FALSE
> f <- "world"
>
> a + b
[1] 2.73
> !e
[1] TRUE
> paste(d,f)
[1] "hello world"
> class(b)
[1] "numeric"
>
> # a comment
>
```



# R data types, continued

R and Python have similar primitive types:

- integer
- "numeric": floating types (as with Python, double precision)
- logicals
- character strings

But there are some differences:

- R: idiomatic assignment operator is "`<-`".
- logical literals are shoutier (TRUE/FALSE, or T/F).
- variables can have periods in their names.

The strength of R lies in its data structures. Note that, like Python, R is case sensitive ("A" is not the same as "a").

# R lists

Lists are the most basic "container" data type in R:

- The "list" function will generate a list from the inputs.
- "str" stands for "structure". It gives a description of the argument.
- In R, the "start:finish" notation returns a sequence running from start to finish, inclusive.

```
> l <- list(a, b, d, e, f, pi)
> str(l)
List of 6
 $ : num 1
 $ : num 1.73
 $ : chr "hello"
 $ : logi FALSE
 $ : chr "world"
 $ : num 3.14
>
> l[[6]]
[1] 3.141593
> l[1:2]
[[1]]
[1] 1

[[2]]
[1] 1.73
>
```

# R lists, continued

As with Python lists, the values can be of various types - including lists.  
Note:

- Indexing individual items in a list is done with `[[ ]]`.
- Indexing starts at 1, as with most scientific computing languages. (Indices, not offsets.)
- Slicing is done with `[start:finish]`, and the last item is included (unlike Python).
- Note that `[[ -1]]` will return an error message.
- What does slicing with a negative number do - eg, `l[-1]`? This is very different behaviour than Python.

# R vectors

Unlike Python, vectors are built into the language:

- Homogeneous (same type)
- Compact
- Not nested
- Like numpy vectors

```
> a <- c(1,2,3)
> b <- c("Hello", "World", "From", "A", "Vector")
> str(b)
chr [1:5] "hello" "World" "From" "A" "Vector"
> d <- 1:17
> str(d)
int [1:17] 1 2 3 4 5 6 7 8 9 10 ...
>
```

The "c" command combines values in to a vector or list.

# R vectors, continued

There are many ways to create vectors in R:

```
>
> 1:10
[1] 1 2 3 4 5 6 7 8 9 10
> seq(2, 20, 4)
[1] 2 6 10 14 18
> paste("A", 1:5, sep = "")
[1] "A1" "A2" "A3" "A4" "A5"
> rep(letters[1:5], 3)
[1] "a" "b" "c" "d" "a" "b" "c" "d" "a" "b" "c" "d"
> is.vector(1:10)
[1] TRUE
>
```

And others.

# Using sample to create vectors

The "sample" function samples from a vector:

- By default, sample removes the previously sampled elements from the set.
- As such, you can't sample more than the set size.
- To keep sampled elements in the set, use the "replace = TRUE" argument.
- If you want consistent samples (for testing and debugging purposes), set the seed to the same value before sampling.

```
>
-----
> sample(1:10, 4)
[1] 10 5 4 7
-----
> sample(1:10, 4)
[1] 2 6 10 3
-----
> sample(1:10, 4, replace = TRUE)
[1] 7 10 3 7
-----
>
-----
> set.seed(2)
-----
> sample(1:10, 4, replace = TRUE)
[1] 2 8 6 2
-----
> set.seed(2)
-----
> sample(1:10, 4, replace = TRUE)
[1] 2 8 6 2
-----
>
```

# Diagnostic functions

R is loaded with functions for figuring out what things are:

- The "typeof" function returns the type or storage mode of the object.
- To check to see if something is a vector, use "is.vector".
- The "summary" function returns a summary of the object's properties. It is often used in the context of summarizing the results of model-fitting functions.

```
> typeof(l)
[1] "list"


---


> is.vector(l)
[1] TRUE


---


> summary(d)
  Min. 1st Qu.  Median  Mean 3rd Qu.  Max.
    1         5         9      9      13      17


---


>
```

Note that lists are considered vectors in R.

# Appending to vectors

Unlike numpy arrays in Python, you can add elements to the end of existing vectors:

- Use sparingly! It's better to fill the whole length you need first, using `seq()` or `rep()`, rather than set elements as needed.
- Increasing length of vector/list one at a time is:
  - ▶ slow
  - ▶ at risk of causing memory problems

```
>
-----
> # probably bad, certainly slow
-----
> a <- c(1,2,3)
-----
> a <- c(a,4)
-----
> a <- c(a,5)
-----
> a
[1] 1 2 3 4 5
-----
>
-----
> # probably bad,
> # certainly funny-looking
-----
> a[length(a) + 1] <- 6
-----
> a
[1] 1 2 3 4 5 6
-----
>
```



# Appending to vectors, continued

It's much better to allocate your vector once, and then set the elements as you go.

```
>  
-----  
> # good  
-----  
> a <- rep(0,5)  
-----  
> a[4] <- 4  
-----  
> a[5] <- 5  
-----  
> a  
[1] 0 0 0 4 5  
-----  
>
```

If you extend your vector one element at a time, the contents of the vector must be copied each time the vector is extended. This is slow.

# R vectors behave intuitively

As with numpy vectors, most operations happen automatically on vectors:

```
> a <- 1:5 + 1
> a
[1] 2 3 4 5 6
> b <- rep(2.,5)
> a * b
[1] 4 6 8 10 12
> sin(a)
[1] 0.9092974 0.1411200 -0.7568025 -0.9589243 -0.2794155
>
> d <- sample(c(TRUE,FALSE), 5, replace = TRUE)
> d
[1] TRUE FALSE FALSE TRUE FALSE
> !d
[1] FALSE TRUE TRUE FALSE TRUE
> a[d]
[1] 2 5
>
```

# More slicing

You can slice with:

- vectors of integers
- ranges (which are really just vectors of integers)
- vectors of booleans (which pull out the values corresponding to TRUE, as in the last example on the last slide)

```
>  
_____  
> a[2:4]  
[1] 3 4 5  
_____  
> a[c(1,2,4)]  
[1] 2 3 5  
_____  
> a[-c(1,2,3)]  
[1] 5 6  
_____  
> a[seq(1,5,2)]  
[1] 2 4 6  
_____  
>
```

# Boolean operators

- The statement "a < 3" returns where this statement is TRUE.
- The "==" is the equivalence test ("is this equal to this?"). "!=" does the opposite.
- The & symbol is the "AND" operator.
- The | symbol is the "OR" operator.
- The "which" command will give the indices of the TRUE entries.

```
> a < 4
[1] TRUE TRUE FALSE FALSE FALSE
> a[a < 4]
[1] 2 3
>
> b <- seq(1, 60, 13)
> b
[1] 1 14 27 40 53
>
> b == 38
[1] FALSE FALSE FALSE FALSE FALSE
> (b > 5) & (b < 50)
[1] FALSE TRUE TRUE TRUE FALSE
> (b < 10) | (b > 30)
[1] TRUE FALSE FALSE TRUE TRUE
>
> which((b < 10) | (b > 30))
[1] 1 4 5
```

# Not Available (NA)

Let's try extending the "a" vector by another 3 items, and only set the last one:

```
> a
[1] 2 3 4 5 6
>
> length(a)
[1] 5
>
> a[length(a) + 3] <- 9
>
> a
[1] 2 3 4 5 6 NA NA 9
>
```

NA (Not Available) is used to represent missing or invalid data. The right thing to do with NAs will depend on the application, but we will often need to deal with NAs specifically.

# NA, continued

We can use the "is.na" function to pick out NAs:

```
>
> is.na(a)
[1] FALSE FALSE FALSE FALSE FALSE TRUE TRUE FALSE
>
> a[!is.na(a)]
[1] 2 3 4 5 6 9
>
> a[is.na(a)] <- -1
>
> a
[1] 2 3 4 5 6 -1 -1 9
>
```

Recall that the "!" symbol is the "NOT" operator.

# NA, continued more

Most math operations on NAs will return NA; but most generally have built-in optional ways of dealing with them.

```
>
> a[a == -1] <- NA
>
> a
[1] 2 3 4 5 6 NA NA 9
>
> sum(a)
[1] NA
>
> sum(a, na.rm = TRUE)
[1] 29
>
```

# Help!

But what if you don't know how to use the function, or don't know the optional arguments? You can use the help function, which is also accessed using '?':

```
>
> help(sum)
:
>
> ? sum
:
>
```

Press 'q' to exit the help page (on a Linux system).



# Help, continued

Some authors of functions have even been kind enough to give you examples of how to use their functions:

```
>
> example(sum)

sum> ## Pass a vector to sum, and it will add the elements together.
sum> sum(1:5)
[1] 15

sum> ## Pass several numbers to sum, and it also adds the elements.
sum> sum(1, 2, 3, 4, 5)
[1] 15
:
sum> ## ... unless we exclude missing values explicitly:
sum> sum(1:5, NA, na.rm = TRUE)
[1] 15
>
```

# Pop quiz!

Create a vector of 100 elements whose elements are randomly drawn from a normal distribution with a mean of 200 and a standard deviation of 20. The function that you are looking for is called 'rnorm'. Use 'help' to figure out how to use it.

# Pop quiz!

Create a vector of 100 elements whose elements are randomly drawn from a normal distribution with a mean of 200 and a standard deviation of 20. The function that you are looking for is called 'rnorm'. Use 'help' to figure out how to use it.

```
>  
> mynorm <- rnorm(100, 200, 20)  
>  
> length(mynorm)  
[1] 100  
>  
> mean(mynorm)  
[1] 199.5294  
>  
> sd(mynorm)  
[1] 19.12821  
>
```

# Matrices, arrays

Vectors are generalized into matrix and array types - matrices are 2D and are created by specifying at least one of the two dimensions:

- The "matrix" function returns a 1D vector by default.
- To make it 2D, specify either "nrow" or "ncol", but make sure it divides the number of elements evenly.
- The "rnorm" function draws from the normal distribution.

```
> A <- matrix(rnorm(9), nrow = 3)
>
> class(A)
[1] "matrix"
> A
      [,1]      [,2]      [,3]
[1,] -0.02574689  0.1676856 -1.2806814
[2,]  0.17226639 -0.7561610 -1.0730775
[3,] -0.35919061  0.2674792 -0.6362443
>
```

# Matrices, continued

As you might expect, you can use matrices to do matrix math:

- The "solve" function solves the equation  $\mathbf{Ax} = \mathbf{b}$ , where  $\mathbf{A}$  is a matrix and  $\mathbf{x}$  and  $\mathbf{b}$  are vectors.
- If available, "solve" will use a LAPACK routine on your machine to solve this system. That means it's fast.
- What's with the `%*%` symbol?

```
>
> b <- 1:3
>
> A %*% b
      [,1]
[1,] -3.532420
[2,] -4.559288
[3,] -1.732965
>
> solve(A,b)
[1] -8.943326 -3.229387 -1.023876
>
```

# R special operators

R contains a number of "special operators":

- `%*%` is matrix multiply.
- `%o%` is outer product.
- `%x%` is Kronecker product.
- `%/%` is the modulus.
- `%/%` is integer division.
- And there are others as well.

```
> A
      [,1]      [,2]      [,3]
[1,] -0.02574689  0.1676856 -1.2806814
[2,]  0.17226639 -0.7561610 -1.0730775
[3,] -0.35919061  0.2674792 -0.6362443
```

```
> a <- 1:3;   b <- 3:5
```

```
> a * b
[1] 3 8 15
```

```
> a %*% b
      [,1]
[1,]    26
```

```
> a %o% b
      [,1] [,2] [,3]
[1,]    3    4    5
[2,]    6    8   10
[3,]    9   12   15
```

```
> a %x% b
[1] 3 4 5 6 8 10 9 12 15
```

```
> 9 %% 4
[1] 1
```

```
> 9 / 4
[1] 2.25
```

```
> 9 %/% 4
[1] 2
```

# More matrix operations

A few more miscellaneous matrix operations:

- The "dim" command can be used to change the dimensions of a matrix.
- Note that R is column major. Do you see how this manifests itself in the way the elements get arranged?
- The "t" command gives the transpose of a matrix.

```
> a = sample(c(T,F), 6, replace = T)
> a
[1] FALSE TRUE TRUE TRUE FALSE FALSE
> dim(a) <- c(3,2)
> a
      [,1] [,2]
[1,] FALSE TRUE
[2,]  TRUE FALSE
[3,]  TRUE FALSE
> dim(a) <- c(2,3)
> a
      [,1] [,2] [,3]
[1,] FALSE TRUE FALSE
[2,]  TRUE TRUE FALSE
> t(a)
      [,1] [,2]
[1,] FALSE TRUE
[2,]  TRUE TRUE
[3,] FALSE FALSE
```

# R is column major

A 1D array is linear in memory, but so is a 2D array.

```
> a <- 1:9
> dim(a) <- c(3,3)
> a
  [,1] [,2] [,3]
[1,]  1   4   7
[1,]  2   5   8
[2,]  3   6   9
> a[2,3]
[1] 8
>
```



This is how the numbers are stored in memory. If you loop over the 2D array, which index should you loop over (first or second)?



# Arrays

Arrays can have any rank (not necessarily just 2D).

Arrays are just high-dimension versions of matrices.

```
> B <- array(1:12, c(2, 3, 2))
```

```
> class(B)
```

```
[1] "array"
```

```
> B
```

```
, , 1
      [,1] [,2] [,3]
[1,]    1    3    5
[2,]    2    4    6
```

```
, , 2
```

```
      [,1] [,2] [,3]
[1,]    7    9   11
[2,]    8   10   12
```

```
> C <- array(1:12, c(2, 6))
```

```
> class(C)
```

```
[1] "matrix"
```

```
>
```

# Built-in datasets

R contains built-in datasets that can be used for practicing.

```
> data()
Data sets in package datasets:

AirPassengers      Monthly Airline Passenger Numbers 1949-1960
BJsales            Sales Data with Leading Indicator
BJsales.lead (BJsales) Sales Data with Leading Indicator
BOD                Biochemical Oxygen Demand
CO2                Carbon Dioxide Uptake in Grass Plants
:
>
> str(faithful)
data.frame': 272 obs. of 2 variables:
 $ eruptions: num 3.6 1.8 3.33 2.28 4.53 ...
 $ waiting  : num 79 54 74 62 85 55 88 85 51 85 ...
>
```

Type 'q' to get out of the 'data' menu.

# Data frames

Data frames are a building block for data analysis in R; in Python, pandas data frames are based on them.

A data frame is a list of vectors. Each vector (a column of the frame) has the same length, but different columns may have different types.

Thus every row of the frame is a list.

```
> data <- trees
> class(data)
[1] "data.frame"
> str(data)
'data.frame':  31 obs.  of 3 variables:
 $ Girth : num  8.3 8.6 8.8 10.5 10.7 10.8 11 11 11.1 11.2 ...
 $ Height: num  70 65 63 72 81 83 66 75 80 75 ...
 $ Volume: num  10.3 10.3 10.2 16.4 18.8 19.7 15.6 18.2 22.6 19.9 ...
>
```

# Slicing data frames

Accessing parts of the data frame makes a lot more sense when you remember it's just a list of vectors.

```
>
> names(data)
[1] "Girth" "Height" "Volume"
>
> data[1:3,"Girth"]
[1] 8.3 8.6 8.8
>
> data[2,]
  Girth Height Volume
2   8.6    65   10.3
>
> data$Height[4:5]
[1] 72 81
>
```

# Updating data frames

Performance tip: While you can update individual items in a data frame via slicing:

```
> data[1, "Girth"] <- 8.7
```

It turns out this is extremely slow and memory intensive, for boring reasons. If you have to do a number of such updates, try to minimize the number of updates to the data frame.

It's better to extract a column, update it, and then update the whole column at once:

```
> Girth <- data$Girth  
_____  
> Girth <- 2. * Girth + 1  
_____  
> data$Girth <- Girth
```

# Getting external data

Getting data from online is as simple as putting in the URL:

```
> data = read.csv("http://tinyurl.com/DentalData-csv")
> str(data)
 $ Quarter: Factor w/ 3 levels "Q1","Q2","Q3":  1 1 1 1 1 1 1 1 ...
      :
 $ Total  : num 9317 14948 23136 18546 40536 ...
> colnames(data)
 [1] "Quarter"          "Year"
 [3] "Data"             "CCG_Code"
 [5] "AT_CODE"          "Region_Code"
 [7] "Patient_type"     "Band_1"
 [9] "Band_2"           "Band_3"
[11] "Urgent_Occasional" "Free___Arrest_of_Bleeding"
[13] "Free___Bridge_Repairs" "Free___Denture_Repair"
[15] "Free___Prescription_Issue" "Free___Removal_of_sutures"
[17] "Total"
```

The original URL for this data is

<http://www.hscic.gov.uk/catalogue/PUB07163/nhs-dent-stat-udas-eng-2011-2012-anx5.csv>.

# Getting external data, continued

We can do some initial exploration of the data by plotting it.

- `boxplot`, shockingly, creates a boxplot.
- The tilde symbol indicates that we are creating a "formula".
- The boxplot uses this to determine what to plot against what.

```
>  
_____  
> boxplot(data$Total ~ data$Patient_Type)  
_____  
>  
_____  
> boxplot(data$Urgent_Occasional ~ data$Patient_Type)  
_____  
>
```

# R and statistics

Without a doubt, one of R's strongest features is its statistical libraries.

- Every distribution is there.
- Everything is baked in.
- If it's not baked in, someone's already written your function or distribution for you. Go find it.
- Many of the standard functions are written in R itself, so you can go read the source code and determine exactly what has been done.
- (The name of the project is "The R Project for Statistical Computing".)

You could make a worse choice for statistical programming language.



# R and statistics, the normal distribution

We start with our old friend, the normal distribution:

- 'dnorm(x)' returns the value of the normal distribution at x.
- 'pnorm(x)' returns the cumulative distribution function.
- 'qnorm(x)' returns the quantile function.

```
>
> x <- seq(-4, 4, 0.01)
>
> plot(x, dnorm(x), type = "l")
>
> plot(x, pnorm(x))
>
> qnorm(0.25)
[1] -0.6744898
>
> qnorm(c(0.025, 0.975))
[1] -1.959964 1.959964
>
```

# R and statistics, a t-test example

Let's perform a Student's t test:

- Consider the two samples, given by 'A' and 'B'.
- Question: what is the probability that these two samples are drawn from the same distribution?
- The answer: about 8%.

```
> A <- array(c(97, 98, 78, 80, 81, 84,  
+ 85, 85, 86, 94, 100, 102, 103, 104))  
_____  
> B <- array(c(76, 87, 89, 90, 94, 96,  
+ 98, 99, 100, 106, 109, 112, 113, 105))  
_____  
>  
_____  
> t.test(A, B, var.equal = T)
```

Two Sample t-test

```
data: A and B  
t = -1.8423, df = 26, p-value = 0.07686  
alternative hypothesis: true difference  
in means is not equal to 0  
95 percent confidence interval:  
-14.6589062 0.8017634  
sample estimates:  
mean of x mean of y  
91.21429 98.14286  
_____  
>
```

# Functions in R

R tends towards functional programming; functions aren't normally called for side effects.

Functions return whatever values are needed.

Typical upsides/downsides to functional programming:

- Easy to read, understand, debug.
- Makes parallelism somewhat easier.
- Requires lots of temporary memory (copies being made).

# R functions

What do the following do?

```
> a <- 1:5  
_____  
> doubleVector <- function(x) {x <- x * 2}  
_____  
> doubleVector2 <- function(x) {x * 2}  
_____  
> a  
[1] 1 2 3 4 5  
_____  
> doubleVector(a)  
_____  
> a
```

# R functions

What do the following do?

```
> a <- 1:5  
_____  
> doubleVector <- function(x) {x <- x * 2}  
_____  
> doubleVector2 <- function(x) {x * 2}  
_____  
> a  
[1] 1 2 3 4 5  
_____  
> doubleVector(a)  
_____  
> a  
[1] 1 2 3 4 5  
_____  
>
```

# R functions

What do the following do?

```
> a <- 1:5  
_____  
> doubleVector <- function(x) {x <- x * 2}  
_____  
> doubleVector2 <- function(x) {x * 2}  
_____  
> a  
[1] 1 2 3 4 5  
_____  
> doubleVector(a)  
_____  
> a  
[1] 1 2 3 4 5  
_____  
> a <- doubleVector2(a)  
_____  
> a
```

# R functions

What do the following do?

```
> a <- 1:5
> doubleVector <- function(x) {x <- x * 2}
> doubleVector2 <- function(x) {x * 2}
> a
[1] 1 2 3 4 5
> doubleVector(a)
> a
[1] 1 2 3 4 5
> a <- doubleVector2(a)
> a
[1] 2 4 6 8 10
>
```

R passes by value, not by reference, unless the argument is not being modified.

# R return statement

Did you notice the lack of "return" statement in the function definition?

- R tends toward functional programming.
- The "return" statement tends to be unnecessary in this context, as state changes are discouraged.
- However, you may include it for clarity.

```
>
> doubleVector2 <- function(x)
+ {x * 2}
>
> doubleVector3 <- function(x) {
+ return(x * 2)
+ }
>
> doubleVector2(a)
[1] 2 4 6 8 10
> doubleVector3(a)
[1] 2 4 6 8 10
>
```



# R iterators

Iterators are a fundamental part of Python, but are a recent addition to R.

- An iterator allows a programmer to traverse a list/array/container without loading the entire container into memory first.
- If I need to loop over one million elements, I don't want to load all of the elements into memory unless I really need to.
- Use the 'iterators' package.

```
>
> library(iterators)
>
> names <- c("Bob", "Mary",
+ "Jack", "Jane")
>
> str(names)
chr [1:4] "Bob" "Mary" "Jack" "Jane"
>
> inames <- iter(names)
> str(inames)
List of 4
 $ state      :<environment: 0x1a5496b8>
 $ length    : int 4
 $ checkFunc: function (...)
 $ recycle   : logi FALSE
 - attr(*, "class")= chr [1:2]
 "containeriter" "iter"
>
```

# R iterators

Once you have your iterator you can advance to the next element using "nextElem".

In what can only be described as a bizarre design decision, iterators do not work with for loops. Nor is there an easy way to create your own iterating functions.

You can, however, use iterators with "foreach". We'll discuss that this afternoon.

```
>
> nextElem(inames)
[1] "Bob"
>
> nextElem(inames)
[1] "Mary"
>
> people <- data.frame(names = names,
+ ages = c(17, 23, 41, 19))
>
> ipeople <- iter(people, by = "row")
>
> nextElem(ipeople)
[1] "Bob" 17
>
```

# R loops

R has three types of loops:

- The "for" loop. Note that the list or vector being looped over can be of any type.
- The "while" loop.
- The "repeat" loop (not illustrated here). The repeat loop requires the use of a "break" statement; you may as well use a while loop.

```
>
> for (i in list('cow', 1, F)) {
+ print(i) }
[1] "cow"
[1] 1
[1] FALSE
>
> i <- 1
> while(i < 4) {
+ print(i)
+ i <- i + 1 }
[1] 1
[1] 2
[1] 3
>
```

# Conditionals

R has the usual types of conditionals:

- The "if" conditional.
- The "switch" conditional. This is analogous to the "case" conditional seen in other languages.

```
>
> for (i in 1:3) {
+ if (i < 2) {
+ print(i) }
}
[1] 1
>
> for (animal in c('cow', 'pig', 'sheep')) {
+ switch(animal,
+ cow = { print('moo') },
+ sheep = { print('baaa') },
+ pig = { print('oink') },
+ stop("Wrong type of animal.")
+ )
+ }
[1] "moo"
[1] "oink"
[1] "baaa"
>
```

# The 'apply' family of functions

The apply family of functions make it very easy, and fast, to repeatedly apply a function to a lot of individual elements.

Many parallel routines are parallel versions of these higher-level functions.

- `lapply`: apply a function to each element of a list/vector.
- `sapply`: simplify the `lapply` return list to a vector or array if possible.
- `apply`: apply a function to rows, columns, or elements of an array.
- `tapply`: apply a function to subsets of a list/vector.
- `mapply`: apply a function to the "transpose" of a list. Pass two lists of length three; apply function to first items of lists, then second, then third.

# lapply

The function "lapply" repeatedly applies a function to each element of a list or vector. Let's say we wanted to show that as  $N$  grows larger, the mean of  $N$  normally distributed random numbers tended to zero.

```
> mean.n.rnorm <- function(n) return(mean(rnorm(n)))  
> ns <- c(1, 10, 100, 1000)  
> lapply(ns, mean.n.rnorm)  
[[1]]  
[1] -0.2720619  
  
[[2]]  
[1] 0.1122716  
  
[[3]]  
[1] 0.1562597  
  
[[4]]  
[1] -0.0007317103  
>
```

# lapply, continued

We could even do this in two steps, applying `rnorm` to the list of `ns`, and then `mean` to the list of vectors:

```
> ns <- c(1, 10, 100, 1000)
> random.nums <- lapply(ns, rnorm)
> means <- lapply(random.nums, mean)
> means
[[1]]
[1] -1.143101

[[2]]
[1] 0.1152926

[[3]]
[1] -0.02110213

[[4]]
[1] 0.004479629
```

# sapply

And we can get that final result as a sometimes-more-convenient vector rather than list with "sapply":

```
>
> ns <- c(1, 10, 100, 1000)
> random.nums <- lapply(ns, rnorm)
> means <- sapply(random.nums, mean)
> means
[1] -1.143100822 0.115292582 -0.021102134 0.004479629
> means * means
[1] 1.306679e+00 1.329238e-02 4.453001e-04 2.006707e-05
>
```



# sapply/vapply

Performance tip: if you know the size and type that sapply will return, create such a vector/matrix and use vapply, passing it the example object as the third parameter (everything else stays the same). This can be substantially faster, and more memory-efficient for large outputs.

# apply

The 'apply' function is used on matrices and arrays. In this case, it's just easier to demonstrate:

```
>
> A <- matrix(1:9, nrow = 3, ncol = 3)
> A
      [,1] [,2] [,3]
[1,]    1    4    7
[2,]    2    5    8
[3,]    3    6    9
> apply(A, MARGIN = 1, max)  # max of each row
[1] 7 8 9
> apply(A, MARGIN = 2, max)  # max of each col
[1] 3 6 9
>
```

# apply, continued

Apply applies a function to the rows ( $MARGIN = 1$ ) or columns ( $MARGINS = 2$ ) of an array (also relevant: `rowSums`, `colSums`).

You can also apply it to each element by using  $MARGIN = 1:2$ .

Here we square each element of the array:

```
> A <- matrix(1:9, nrow = 3, ncol = 3)
> A
      [,1] [,2] [,3]
[1,]    1    4    7
[2,]    2    5    8
[3,]    3    6    9
> apply(A, MARGIN = 1:2, function(x) {x**2}) # square of each item
      [,1] [,2] [,3]
[1,]    1   16   49
[2,]    4   25   64
[3,]    9   36   81
>
```

# tapply

Finally, tapply is also a lot easier to just demonstrate than explain:

```
> data <- morley
>
> str(data)
'data.frame': 100 obs. of 3 variables:
 $ Expt : int 1 1 1 1 1 1 1 1 1 1 ...
 $ Run  : int 1 2 3 4 5 6 7 8 9 10 ...
 $ Speed: int 850 740 900 1070 930 850 950 980 980 880 ...
>
> tapply(data$Speed, data$Expt, mean)
 1      2      3      4      5
909.0 856.0 845.0 820.5 831.5
>
```

In the above, tapply takes the Speed values, splits them up into a list of vectors by value of Expt, and then applies mean to each vector.

# tapply/split

Try playing with 'split' to understand splitting:

```
>  
-----  
> split(data$Speed, data$Expt)
```

# tapply/split

Try playing with 'split' to understand splitting:

```
>
> split(data$Speed, data$Expt)
$`1`
 [1] 850 740 900 1070 930 850 950 980 980 880 1000 980 930 650 760 810 1000
 [18] 1000 960 960

:

$`5`
 [1] 890 840 780 810 760 810 790 810 820 850 870 870 810 740 810 940 950 800
 [19] 810 870
>
```

# Pop quiz!

Consider the "DNase" dataset, which contains data obtained during the development of an ELISA assay for the recombinant protein DNase.

```
>
> str(DNase)
Classes nfnGroupedData, nfGroupedData, groupedData and 'data.frame': 176 obs.
of 3 variables:
 $ Run      : Ord.factor w/ 11 levels "10"<"11"<"9"<...: 4 4 4 4 4 4 4 4 4 4 ...
 $ conc     : num 0.0488 0.0488 0.1953 0.1953 0.3906 ...
 $ density  : num 0.017 0.018 0.121 0.124 0.206 0.215 0.377 0.374 ...
:
>
```

Using `tapply`, calculate the mean and standard deviation of the optical density measurements for the given values of protein concentration.

# Pop quiz!, continued

Using tapply, calculate the mean and standard deviation of the optical density measurements for the given values of protein concentration.



# Pop quiz!, continued

Using `tapply`, calculate the mean and standard deviation of the optical density measurements for the given values of protein concentration.

```
>
> tapply(DNase$density, DNase$conc, mean)
0.04882812 0.1953125 0.390625 0.78125 1.5625 3.125
0.05331818 0.15095455 0.23972727 0.40677273 0.66631818 1.03772727
 6.25 12.5
1.42859091 1.76986364
>
> tapply(DNase$density, DNase$conc, sd)
0.04882812 0.1953125 0.390625 0.78125 1.5625 3.125
0.02756358 0.02429085 0.02628268 0.02755243 0.03057604 0.03789985
 6.25 12.5
0.06917036 0.08462258
>
```

# Saving your results

Inevitably you will need to save the results of your analysis. Let's take a look at the humble ".csv" file.

```
ejspence@gpc-f103n084-ib0 ejspence> ls -sh1 airOT2010.*
151M airOT2010.RDS
154M airOT2010.Rdata
1.4G airOT2010.csv
```

---

```
ejspence@gpc-f103n084-ib0 ejspence>
```

---

```
ejspence@gpc-f103n084-ib0 ejspence> Rscript timeexamples.R
[1] "Reading Rdata file"
   user  system  elapsed
 8.564   0.634   9.225
[1] "Reading RDS file"
   user  system  elapsed
11.045   0.598  11.685
[1] "Reading CSV file"
   user  system  elapsed
141.143  3.167  144.440
```

---

```
ejspence@gpc-f103n084-ib0 ejspence>
```

# A note on file formats

CSV (Comma Separated Value) – or any text-based format – is the worst possible format for quantitative data. It manages the trifecta of being:

- Slow to read.
- Huge in size.
- Inaccurate.

Converting floating point numbers back and forth between internal representations and strings is slow and prone to truncation errors.

Use binary formats whenever possible. The ".Rdata" format is a bit prone to change; ".RDS" is modestly better. Portable formats like HDF5 (for data frames) or NetCDF4 (for matrices and arrays) are compact, accurate, fast (though not as fast as .Rdata/.RDS), portable, and can be read by tools other than R.

# Using 'save' and 'load'

The simplest way to save and retrieve data:

- You can save variables using the 'save' function.
- To load saved data, use 'load'.
- Note that your loaded data will overwrite any existing variables of the same name.

```
>
> save(label.names, days.of.week, file = "mydata.Rdata")
>
exit and come back
>
> load("mydata.Rdata")
> print(label.names)
[1] "1" "2" "3" "4" "5" "6" "7"
>
```

# Workspace management

You can also save the state of your R session:

- You are working in a "workspace". To save your workspace for next time, use `save.image()`. This will put your image in a file named ".Rdata".
- To load a previous workspace, use 'load'.
- Note that your loaded image will append to, and overwrite, your current workspace.
- R will ask if you want to save your workspace when you try to exit.

```
> # do a bunch of stuff
> save.image()
> # or alternatively
> save.image(file = 'myimage.Rdata')
>
> load("myimage.Rdata")
>
```

# Installing R packages

R makes it crazy-easy to install packages which you don't already have.

- To load a non-default library, use the 'library' function.
- To install non-standard packages, use 'install.packages'.

```
> library('fun')
Error in library("fun") : there is no package called fun
>
> install.packages("fun")
Installing package into '/home/s/scinet/ejspence/R'
(as 'lib' is unspecified)
--- Please select a CRAN mirror for use in this session ---
:
** testing if installed package can be loaded
* DONE (fun)
>
> library('fun')
>
```

# Plotting in R

R has a tonne of plotting options.  
Let's start with 'plot':

- If one argument is specified, it plots the argument against value index. With two arguments it takes the first as the 'x' axis.
- By default, every time 'plot' is run it writes over the previous plot.
- To add a line to an existing plot, use "lines".
- If you want customized axis labels, they can add them after you make the plot, or at plot time.

```
>  
-----  
> x <- 1:100 / 100.  
-----  
>  
-----  
> plot(sin(x * 4 * pi))  
-----  
>  
-----  
> plot(x, sin(x * 4 * pi))  
-----  
>  
-----  
> plot(x, sin(x * 4 * pi),  
+ type = "o", col = "blue",  
+ axes = F)  
-----  
>  
-----  
> lines(x, sin(x * 2 * pi),  
+ col = 'red', type = 'o')  
-----  
>  
-----  
> title(xlab = "time [s]")  
-----  
>
```

# Plotting in R, continued

The plotting parameters can be set before plotting using the 'par' function. Some useful options include

- `par(new = TRUE)`. This will keep R from overwriting your previous plot, which is the default behaviour.
- `par(family = 'HersheySans')`, change the font family to a vector-drawn font. Always use vector-drawn fonts for publication-quality plots.
- `par(font = 2)`, change the font format. 1 - default, 2 - bold, 3 - italic, 4 - bold italic.
- `par(ann = FALSE)`, do not annotate the plot. In this case you must label your axes after the plotting function is called.
- `par(mfrow = c(2,2))`, make a 2 x 2 plots. Allows you to put several plots together.
- Many other options.



# Plotting in R, continued more

Name it and you can plot it:

- hist: plot a histogram.
- pie: plot a pie chart.
- Note that 'hist' will bin your data, but 'pie' won't.
- The 'table' function creates a table, which gives counts of entries.
- scatterplots, 3D plots, box plots, log plots, contour plots...

```
> data <- airquality
> hist(data$Ozone)
>
> bad.days <- data$Ozone > 20.0
> table(data$Month[bad.days])
 5  6  7  8  9
11  6 22 23 17
> bad.months <- names(table(data$Month[bad.days]))
> bad.month.counts <- as.vector(table(data$Month[bad.days]))
> pie(bad.month.counts, label = bad.months)
```

# Saving your plots

Once you have your plot, you will eventually need to save it. The commands for saving your files depends upon the type of file you want:

- `bmp(filename = 'myfile.bmp')`.
- `jpeg(filename = 'myfile.jpeg')`.
- `png(filename = 'myfile.jpeg')`.
- `tiff(filename = 'myfile.tiff')`.
- `pdf(file = 'myfile.pdf')`.

The problem with these functions is that you need to invoke them before you start making your plot. You then invoke `"dev.off()"` to stop saving the image.

Alternatively, you can create your image and then use one of the `dev.copy(...)`, `dev.copy2pdf(...)`, etc. commands.

# R data analysis, an example

Let's use an R package to build a decision tree. Let's use the Iris dataset.

- We first randomly split the iris dataset, 70/30, into training and test datasets.
- We then separate the relevant values from the dataset.

```
>
> str(iris)
'data.frame': 150 obs. of 5 variables:
 $Sepal.Length: num 5.1 4.9 4.7 4.6 5 ...
 $Sepal.Width : num 3.5 3 3.2 3.1 3.6 ...
 $Petal.Length: num 1.4 1.4 1.3 1.5 1.4 ...
 $Petal.Width : num 0.2 0.2 0.2 0.2 0.2 ...
 $Species      : Factor w/ 3 levels ...
>
> ind <- sample(1:2, nrow(iris),
+ replace = T, prob = c(0.7, 0.3))
> trainData <- iris[ind == 1,]
> testData <- iris[ind == 2,]
>
```

# R analysis, an example, continued

Now that the data's split up, we're ready to generate the tree.

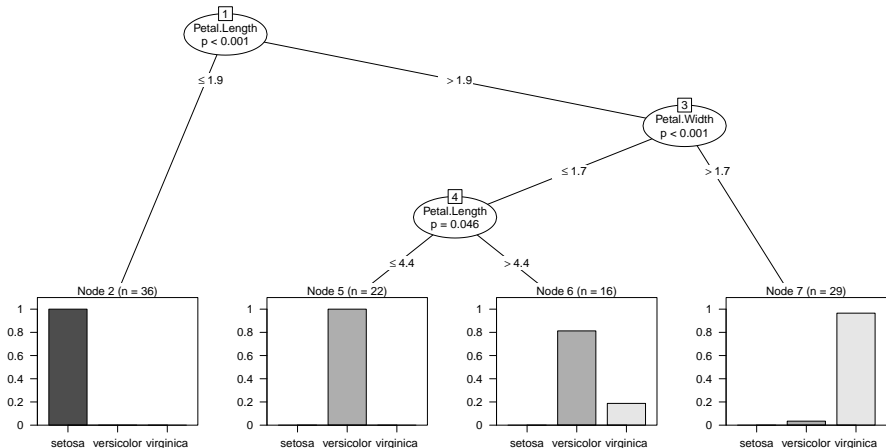
- Load the 'party' library.
- Create our 'formula'.
- Generate the decision tree.
- Check the result against the training data.
- Pretty good fit!
- Plot the result.

```
> library(party)
>
> myFormula <- Species ~ Sepal.Length +
+ Sepal.Width + Petal.Length + Petal.Width
>
> iris_tree <- ctree(myFormula,
+ data = trainData)
>
> table(predict(iris_tree),
+ trainData$Species)
```

	setosa	versicolor	virginica
setosa	36	0	0
versicolor	0	35	3
virginica	0	1	28

```
>
> plot(iris_tree)
>
```

# Our decision tree



# R analysis, an example, continued more

Ok, but how does the decision tree do on the test data?

- Test the built tree with the test data.
- Print out the table of results.
- Not bad!

```
>
-----
> testPred <- predict(iris_tree,
+ newdata = testData)
-----
>
-----
> table(testPred, testData$Species)
      setosa versicolor virginica
setosa      14          0          0
versicolor   0         14          2
virginica    0          0         17
-----
>
```

# Enough to get started

There's obviously a lot more to learn about using R. Nonetheless, this is enough to get you started.

We'll discuss implementing R functions in parallel this afternoon.