





DCMB BioComputing BootCamp Day 3, Session II: R Control Structures and Functions

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Overview

- 1. Working Directory
- 2. Reading and Writing Data in R
- 3. Factors
- 4. Using Indexes
- 5. Merging Data Frames
- 6. Functions
- 7. Program Control Structures

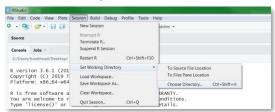
Use Directory Structure to Organize Your Work

- Imagine if all of your input data, code, output data, images files were all in the same directory!
- Sounds like a mess!
- There is no perfect/standard directory structure, but here are a few suggestions:
 - 1. Create a unique directory for each project
 - 2. Break your code up into parts
 - 3. Write output (i.e. tables, images) to a separate sub-directory



The R Working Directory

- R executes commands from a 'working directory'
 - scripts, input files, output files
 - absolute and relative directories may be specified
- Use getwd() to display current working directory
- > getwd()
 [1] "C:/Users/bankhead/Documents"



- Use Session->Set Working Director->Choose Directory or setwd() to change your working directory
- > setwd("../Desktop/armandsFolder")
- Use dir() to list files and folders in your working directory

Exercise: Create a directory/folder outside of R and change R's working directory to that directory

Writing Data To Text Files

First lets create something to write as a text file

```
> m4 = matrix(1:300,nrow=100,ncol=3)
> colnames(m4) = c('A','B','C')
> m4 = data.frame(m4,D = c(rep('X',50),rep('Y',50)))
```

- Use write.table() to write data to a file
 - Many arguments! Use ?write.table to find out more

```
> write.table(m4, 'myData.txt', quote=F, row.names=F, sep="\t")
> dir()
[1] "myData.txt"
```

Reading Data From Text Files

• Use read.delim() to read data from a file

```
> m5 = read.delim('myData.txt')
> dim(m5)
> head(m5)
```

- By default the first row is read in as column names
- Our data appears to be read in correctly but R has converted our text data into something called a factor
- > m5\$D



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Factors in R

- Factors are used to break complex data up into discrete categories
- This comes in handy when we need to group samples for statistical analysis (e.g. fitting linear models)
- Adding new values can generate errors!
- By default R will convert non-numeric data into factors
 - Use options(stringsAsFactors=FALSE) in your scripts to over-ride!

```
> options(stringsAsFactors = FALSE)
```

```
> m5 = read.delim('myData.txt')
```

> m5\$D

Using Indexes

- Indexing is a powerful tool for filtering large data frames or matrices
- There are two commonly used ways to index:
 - 1. Logical vectors:

```
> m5$A < 10
```

- [1] TRUE TRUE TRUE
- 2. Integer vectors:

```
> which(m5$A < 10)
[1] 1 2 3 4 5 6 7 8 9</pre>
```

Using Indexes

 We can combine multiple conditions use the &, |, and parens

```
> m5\$A < 10 \& M5\$B > 205
> m5\$A < 10 \& M5\$B > 205 | M5\$D == 'Y'
> m5\$A < 10 | m5\$D == 'Y' \& m5\$A < 55
```

- Be aware of operator precedence
- Use the sum command to count how many positive values survive
- Indexes can be used to index vectors, matrices, or data frames

```
> idx = m5$A < 10 & m5$B > 205
> subMatrix = m5[idx,]
```

Operator Precedence in R							
Operator	Description	Associativity					
۸	Exponent	Right to Left					
-x, +x	Unary minus, Unary plus	Left to Right					
%%	Modulus	Left to Right					
*, /	Multiplication, Division	Left to Right					
+, -	Addition, Subtraction	Left to Right					
<, >, <=, >=, !=	Comparisions	Left to Right					
!	Logical NOT	Left to Right					
&, &&	Logical AND	Left to Right					
1.11	Logical OR	Left to Right					
->, ->>	Rightward assignment	Left to Right					
<-, <<-	Leftward assignment	Right to Left					
=	Leftward assignment	Right to Left					

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Merging Data Frames

 A common programming task in bioinformatics is to "join" two tables:

	Table X		Table Y			Table Z			
20,000 rows	Gene	RPKM		Gene	Entrez		Gene	Entrez	RPKM
	AKT1	100.03		AKT1	207		AKT1	207	100.03
	EGFR	32.18		EGFR	1956		EGFR	1956	32.18
	•••	•••		•••	•••		•••	•••	
	ZXDA	78.34		ZXDA	7789		ZXDA	7789	78.34

- Joins are performed in R using the merge() function
 - Requires a common column between tables (e.g. gene) be specified using the "by" parameter
 - Multiple types of joins (e.g. inner, outer) are possible, use ?merge to find out more

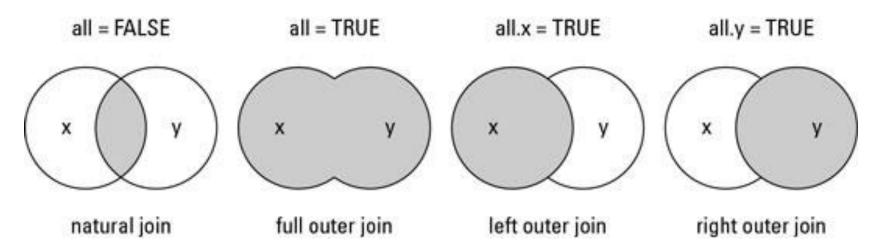
Merging Data Frames

- Use merge() to join together data from two different matrices or data frames
- Important: both matrices must contain unique row identifiers to join on!

```
> df1 = data.frame(gene = c('AKT1', 'ERBB2', 'EGFR'),
log2rpkm = c(5,.5,10))
> df2 = data.frame(gene = c('AKT1', 'ERBB2', 'EGFR'),
entrez = c(207,2064,1956))
> combined = merge(df1,df2,by='gene')
```

Exercise: Execute the code above. Using the dim() function, what are the number of rows and columns of the 'combined' data frame?

Merging Data Frames: Types of Joins



- <u>natural join:</u> intersection of common rows
- <u>full outer join</u>: union of rows
- left outer join: all x rows represented
- right outer join: all y rows represented

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Functions

- Functions allow us to break our R scripts up into modular pieces
- Modular program design has already been discussed in unix (day1) and python (day2)
- Benefits to our code include:
 - Program design
 - Readability
 - Re-use
 - Trouble-shooting
- Functions are specified using the 'function' key word

```
myFunction = function(arg1,arg2,...) {
   statements
}
```

 When multiple arguments are specified R will match first by name, prefix matching arguments, then by position

Functions

```
> sq1 = function(x) return(x * x)
> sq1 = function(x) x * x
> randomValues = rnorm(1000)
> randomValuesSquared = sq1(randomValues)
> myAnalysis = function(randomValues,
randomValuesSquared) {
     vector1 = randomValues
     vector2 = randomValuesSquared
     result = cor(vector1, vector2)
```

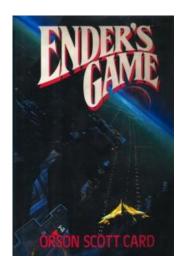
Exercise: Create an R script that contains the myAnalysis function What correlation value is generated?

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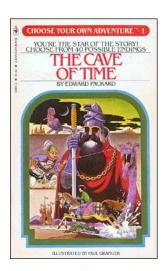
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What is a Control Structure?

- Control structures allow programmers to change the flow of a program
- As programmers we may want code to repeat or be skipped
- Example: if/else statements allow conditional execution of code



VS.

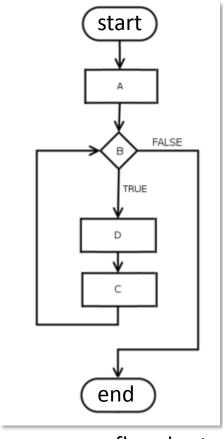


One single linear path

Multiple branching linear paths

Program Control Structures

- R program flow is not always a linear sequence of operations
- Besides functions, program flow may be modified using control structures
 - 1. apply
 - 2. if/else/else if
 - 3. for
 - 4. while
- Other important R commands that can alter program flow:
 - 1. break exit loop
 - 2. next skip to the next iteration



program flowchart

Program Control Structures: apply

- Use the apply function to iterate through a data.frame, matrix, or arrays
 - Use lapply() to iterate through lists or vectors
- apply function takes at least 3 values
 - 1. data frame/matrix
 - 2. 1 or 2 indicating rows or columns respectively
 - function to 'apply' to each value (standard or custom)

```
> m4 = matrix(1:300, nrow=100, ncol=3)
```

- > rowMeans = apply(m4,1,mean)
- > columnMeans = apply(m4,2,mean)

Exercise: Run the code above.

What data structures are rowMeans and columnMeans?

Are rows on average larger or columns?

Program Control Structures: if/else/else if

- 'if' statements allow us to condition our program flow
- basic syntax:

```
if(condition) {
    statement1
}
else if(condition) {
    statement2
}
else {
    statement3
}
```

- conditions must be TRUE or FALSE
- statements are a series of R commands

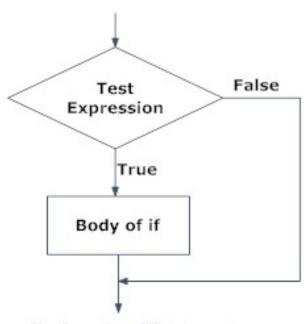


Fig: Operation of if statement

Program Control Structures: if/else/else if

Example if statement

```
m5 = read.delim('myData.txt')
if(ncol(m5) == 4 && is.factor(m5$D)) {
   print('factors!')
}
else {
   print('no factors!')
}
```

- Multiple conditions can be combined using:
 - II OR
 - && AND
 - ! NOT
 - () parens

Program Control Structures: for

- 'for' loops allow us to iterate our code
- Basic syntax:

```
for(counter in vector) {
   statements
}
```

• 'vector' can represent a list of numbers (e.g. 1:10) or arbitrary data types (e.g. c('mon','tues','wed',...))

Program Control Structures: for

• Example #1:

for(i in 1:5) {

```
print(i)
}
• Example #2:
m5 = read.delim('myData.txt')
for(column in 1:ncol(m5)) {
   print(mean(m5[,column]))
```

- 'break' can be used to exit loop structure
- We could have used apply!

Program Control Structures: while

- while() loops allow iteration until a condition is met
- Basic syntax:

```
while(condition) {
  statements
}
```

To exit the loop structure

- 'break' can be used to exit loop structure
- set condition to be false

In Class Exercise.

Exercises

- 1. Write a function that converts Fahrenheit to Celsius
 - input: temperature in Fahrenheit
 - output: temperature in Celsius
- 2. Write a program that builds a data frame containing degrees Fahrenheit to Celsius for -30 to 130 degrees Fahrenheit

HINT: celsius = (fahrenheit – 32) X 5/9

3. Write the table from #2 to a tab-delimited text file

References

- Gentleman, Robert. R Programming for Bioinformatics. CRC Press, 2009.
- Slides source in part from Barry Grant and Hui Jiang

Bonus Exercise (if time!)

- The unique() function can be used to get the unique values in a vector
- The CO2 data set contains 84 measurements from an experiment comparing the CO2 uptake of Echinochloa crus-galli sourced from Quebec and Mississippi. Plants were measured chilled and nonchilled.
- Using the CO2 data set determine if the average expression of chilled plants from Quebec is higher than plants from Mississippi.