
AS YOU CAN CLEARLY SEE IN SLIDE 397...
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GAAAAH!
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"POWERPOINT" POISONING.
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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

Do it Yourself!

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 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 use the setwd() function to navigate to that directory

Writing Data To Text Files

Do it Yourself!

- 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"
```

Do it Yourself!

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

```
> m5$D
 [1] X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X Y Y Y Y Y Y Y Y
[59] Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y Y
Levels: X Y
```

Do it Yourself!

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
```

```
> m5$D
 [1] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X"
[30] "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "X" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y"
[59] "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y"
[88] "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y" "Y"
```

Using Indexes

- Indexing is a powerful tool for filtering large data frames or matrices
- There are two central 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

```
> m5$A < 10
  [1]  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
 [20] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
 [39] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
 [58] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
 [77] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
 [96] FALSE FALSE FALSE FALSE FALSE
> which(m5$A < 10)
[1] 1 2 3 4 5 6 7 8 9
```

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
^	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
|, ||	Logical OR	Left to Right
->, ->>	Rightward assignment	Left to Right
<-, <<-	Leftward assignment	Right to Left
=	Leftward assignment	Right to Left

https://www.programiz.com/r-programming/precedence-associativity

Merging Data Frames

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

20,000 rows

Table X

Gene	RPKM
AKT1	100.03
EGFR	32.18
…	…
ZXDA	78.34

Table Y

Gene	Entrez
AKT1	207
EGFR	1956
…	…
ZXDA	7789

Table Z

Gene	Entrez	RPKM
AKT1	207	100.03
EGFR	1956	32.18
…	…	…
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

Do it Yourself!

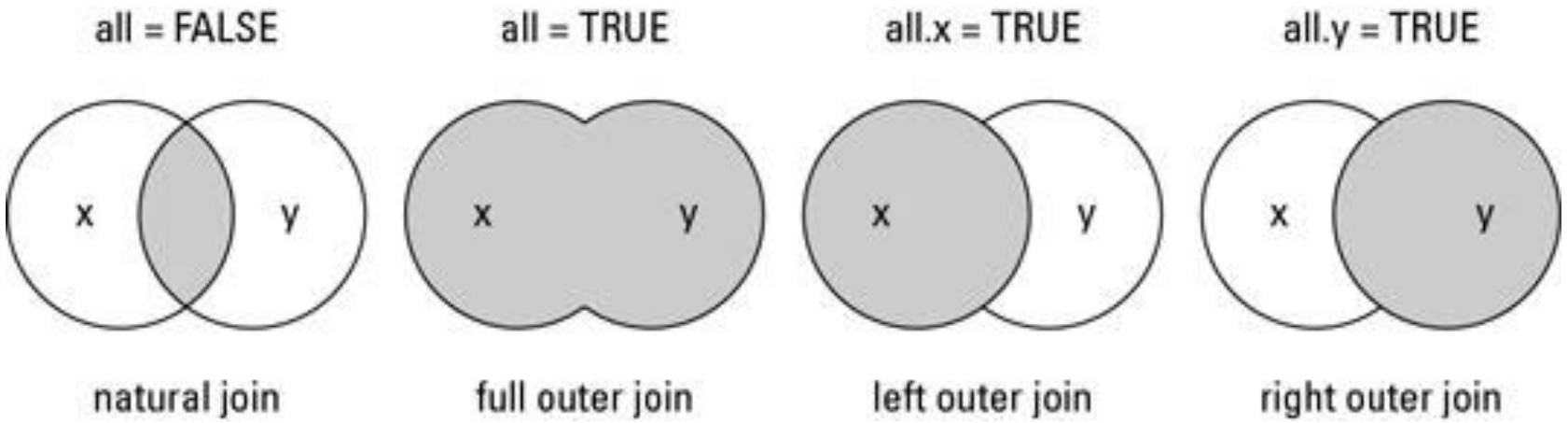
- Use merge() to join together data from two different matrices or data frames
- **Important: both matrices must contain unique row identifiers to join on!**

```
> 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: What happens if gene is not unique?

Add a duplicate gene name and find out.

Merging Data Frames: Types of Joins



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

https://www.dummies.com/programming/r/how-to-use-the-merge-function-with-data-sets-in-r/

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

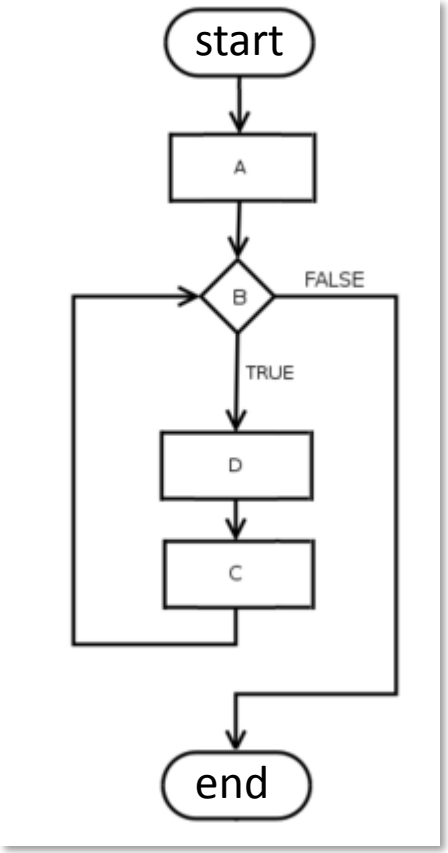
Do it Yourself!

```
>  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 contains the myAnalysis function
What correlation value is generated?

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

Do it Yourself!

- 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
  3. 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 are 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

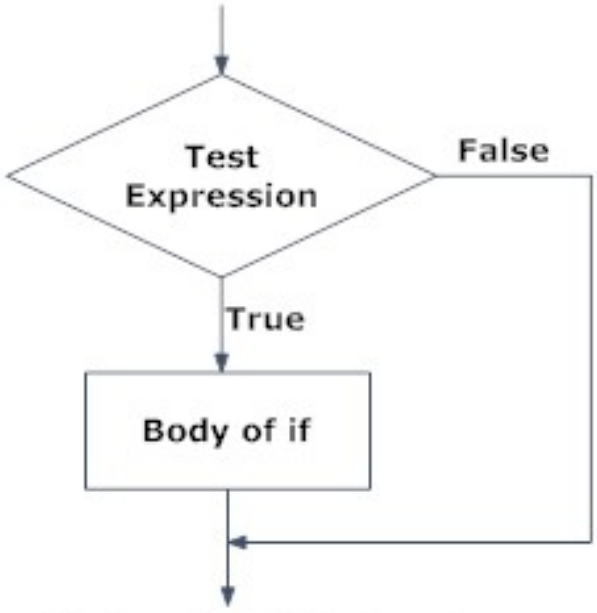


Fig: Operation of if statement

https://www.programiz.com/r-programming/if-else-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

https://www.programiz.com/r-programming/if-else-statement

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

Exercises

Do it Yourself!

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

Do it Yourself!

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 C02 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.

Closing Remarks/Advice

- Comment your code
- Short programs are better
- Plan!
- Be prepared to iterate
  - Make a change
  - Run
  - Make another change
  - Run
  - …

References

- Gentleman, Robert. R Programming for Bioinformatics. CRC Press, 2009.
- Slides Partially Sourced from Barry Grant and Hui Jiang