

### **Introduction To R**

Introduction to Bioinformatics

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NBIS • SciLifeLab

#### **Contents**



- Getting Started
- Variables & Operators
- Data Types
- Datatype Conversion
- Functions
- Control Structures
- R Packages
- Base Graphics
- Grid Graphics
- Input & Output
- Rmarkdown
- Tidyverse
- Bioconductor
- Help & Learning R

### **Topics**



- Familiarise with R & RStudio environment
- Running code, scripting, sourcing script
- Variables and operators
- Data types & datatype conversion
- Creating and running functions
- Base and grid graphics
- Input & output of text & graphics
- Reproducible analyses, Rmarkdown, notebooks and reports
- Tidyverse: Modern R programming paradigm

## What? Why R?



R is a language and environment for statistical computing and graphics.

Command line interface

#### **Pros**

- Data analysis
- Statistics
- High quality graphics
- Huge number of packages
- R is popular
- Reproducible research
- RStudio IDE
- FREE! Open source

#### Cons

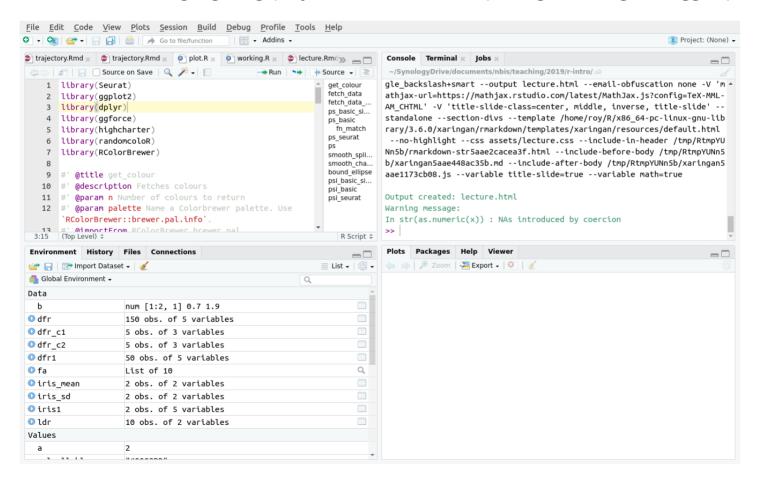
- Steep learning curve
- Not elegant/consistent
- Slow



#### **Getting Started • Installation**



- Install R from r-project.org.
- Install RStudio IDE
- Code editor, highlighting, projects, version control, package building, debugger, profiler



### **Getting Started • Interaction**



- Execute commands directly in Console
- Ready console shows >
- Console shows + when waiting for information
- Press Esc to escape from + to >
- Save commands by writing scripts
- Run lines using Ctrl + Enter
- Run entire script using Ctrl + Shift + Enter

### **Variables & Operators**



Assign variables using <- , = or ->

```
x <- 4
x = 4
x
```

Arithmetic operators

```
x <- 4; y <- 2;

x + y # add
x - y # subtract
x * y # multiply
x / y # divide
x %% y # modulus
x ^ y # power</pre>
```

```
## [1] 6
## [1] 2
## [1] 8
## [1] 0
## [1] 16
```

• Logical operators return TRUE or FALSE

```
x == y # equal to?
x != y # not equal to?
x > y # greater than?
x < y # less than?
x >= y # greater than or equal to?
x <= y # less than or equal to?</pre>
```

```
## [1] FALSE
## [1] TRUE
## [1] TRUE
## [1] FALSE
## [1] TRUE
## [1] FALSE
```

```
T | F # OR
T & F # AND
```

```
## [1] TRUE
## [1] FALSE
```

• [], &&, !, any(), all for logical vectors

#### **Variables & Operators**



- perator is used for generating regular sequences
- :: & ::: are used for accessing functions
- %\*% used for matrix multiplication
- %in% used as a set operator

```
"a" %in% c("x","p","a","c")
## [1] TRUE
```

- Avoid conflicting variable names like c, t etc
- Variable names cannot start with a number

### Data Type • Overview



• Use typeof() to find type of a variable

```
x <- 4; typeof(x)

## [1] "double"

y <- "this"; typeof(y)

## [1] "character"

mode(x); class(x)
str(x); structure(x)

## [1] "numeric"
## [1] "numeric"
## num 4
## [1] 4</pre>
```

## Data Type • Basic



Mode

```
mode(1.0)
mode(1L)
mode("hello")
mode(factor(1))
mode(T)

## [1] "numeric"
## [1] "numeric"
## [1] "character"
## [1] "numeric"
## [1] "logical"
```

#### Type

```
typeof(1.0)
typeof(1L)
typeof("hello")
typeof(factor(1))
typeof(T)

## [1] "double"
## [1] "integer"
## [1] "character"
## [1] "integer"
## [1] "logical"
```

### Data Type • Missing Values



- R explicitly handles missing data as NA and undefined data as NULL (NA vs NULL)
- NA is not 0
- NA is not ""
- NA is not FALSE
- NA is not NULL
- Operations that involve NA may or may not result in an NA

```
NA==1
sum(c(2,6,NA,6))
sum(c(2,6,NA,6),na.rm=TRUE)
NA|NA
NA|TRUE
NA&TRUE
NULL|TRUE
```

```
## [1] NA
## [1] NA
## [1] 14
## [1] NA
## [1] TRUE
## [1] NA
## [1] NA
```

#### Data Type • Vector • Create



- Vector stores multiple values
- Concatenate variables, values and vectors using the function c()

```
x <- c(2,3,4,5,6)
y <- c("a","c","d","e")
x
y</pre>
```

```
## [1] 2 3 4 5 6
## [1] "a" "c" "d" "e"
```

• Few different ways to create vectors.

```
c(2,3,5,6)
2:8
seq(2,5,by=0.5)
rep(1:3,times=2)
```

```
## [1] 2 3 5 6
## [1] 2 3 4 5 6 7 8
## [1] 2.0 2.5 3.0 3.5 4.0 4.5 5.0
## [1] 1 2 3 1 2 3
```

#### Data Type • Vector • Access



• Access vectors using the [] operator.

```
x[1]; y[3]

## [1] 2
## [1] "d"
```

• Function c() to specify multiple positions.

```
x[c(1,3)]
## [1] 2 4
```

Vectorised operation

```
x <- c(2,3,4,5); y <- c(9,8,7,6)
x+y
z <- c("a","an","a","a"); k <- c("boy","apple","girl","mess")
paste(z,k)</pre>
```

```
## [1] 11 11 11 11
## [1] "a boy" "an apple" "a girl" "a mess"
```

#### Data Type • Vector



Verify data type

```
x < -c(2,3,4,5)
z <- c("a", "an", "a", "a")
mode(x)
mode(z)
str(x)
str(z)
## [1] "numeric"
## [1] "character"
## num [1:4] 2 3 4 5
## chr [1:4] "a" "an" "a" "a"
is.atomic(x)
is.numeric(x)
is.character(z)
## [1] TRUE
## [1] TRUE
## [1] TRUE
```

#### Data Type • Factor



Factors store categorical data

```
x <- factor(c("a","b","c","c"))
class(x)
str(x)</pre>
```

```
## [1] "factor"
## Factor w/ 3 levels "a","b","c": 1 2 2 3 3
```

• Factor x has 3 categories (3 levels)

```
levels(x)
```

```
## [1] "a" "b" "c"
```

• Verify if an R object is a factor

```
is.factor(x)
```

```
## [1] TRUE
```

### Data Type • Matrix • Create



• Create a matrix from vector

```
x <- matrix(c(2,3,4,5,6,7))
x</pre>
```

```
## [,1]
## [1,] 2
## [2,] 3
## [3,] 4
## [4,] 5
## [5,] 6
## [6,] 7
```

Matrix has rows and columns

```
dim(x) # dimensions
nrow(x) # number of rows
ncol(x) # number of columns
```

```
## [1] 6 1
## [1] 6
## [1] 1
```

• Specify rows and columns

```
## [,1] [,2]
## [1,] 2 3
## [2,] 4 5
## [3,] 6 7
```

```
str(x)
```

```
## num [1:3, 1:2] 2 4 6 3 5 7
```

• Verify if an R object is a matrix

```
is.matrix(x)
```

```
## [1] TRUE
```

### Data Type • Matrix • Access



• Access matrix using [] operator as [row,col]

```
x[2,2]
## [1] 5
```

• Get whole row/col using [row,] or [,col]

```
x[1,]
x[,2]
```

```
## [1] 2 3
## [1] 3 5 7
```

• Use drop=FALSE to retain a matrix as [row,col,drop=FALSE]

```
x[1,,drop=F]
x[,2,drop=F]
```

```
## [,1] [,2]
## [1,] 2 3
## [,1]
## [1,] 3
## [2,] 5
## [3,] 7
```

## Data Type • Matrix • Label



• Add row/column names

Access using labels

```
x["b",]
x[,"p"]

## k p
## 4 5
## a b c
## 3 5 7
```

#### Data Type • List



• Create using <a href="list(">list()</a>.

```
## [[1]]
## [1] 2 3 4 5
##
## [[2]]
## [1] "a" "b" "c" "d"
##
## [[3]]
## [1] a a b
## Levels: a b
##
## [[4]]
## [,1] [,2]
## [1,] 3 5
## [2,] 2 6
## [3,] 3 7
```

```
typeof(x); class(x);
```

```
## [1] "list"
## [1] "list"
```

Access lists using [] and [[]]

```
x[1]
```

```
## [[1]]
## [1] 2 3 4 5
```

Lists are recursive

```
x <- list(list(list())))
str(x)</pre>
```

```
## List of 1
## $:List of 1
## ...$:List of 1
## ...$: list()
```

## Data Type • data.frame • Create



```
dfr <- data.frame(x = 1:3, y = c("a", "b", "c"))
dfr
str(dfr)
## 'data.frame': 3 obs. of 2 variables:
## $ x: int 1 2 3
## $ y: Factor w/ 3 levels "a", "b", "c": 1 2 3
 • Use <a href="stringsAsFactors=FALSE">stringsAsFactors=FALSE</a> to avoid auto factor conversion
dfr <- data.frame(x = 1:3, y = c("a", "b", "c"), stringsAsFactors = F)</pre>
str(dfr)
is.data.frame(dfr)
## 'data.frame': 3 obs. of 2 variables:
## $ x: int 1 2 3
## $ y: chr "a" "b" "c"
## [1] TRUE
```

## Data Type • data.frame • Access



• Access using [] or \$ operator

```
dfr$x
dfr$y
```

```
## [1] 1 2 3
## [1] "a" "b" "c"
```

- head() / tail() functions show first/last six lines
- Subset a data.frame using subset()

```
subset(dfr,dfr$y=="a")
```

#### **Data Type • Conversion**



```
x <- c(1,2,3); str(x)

## num [1:3] 1 2 3
```

Convert to character

```
y <- as.character(x); str(y)

## chr [1:3] "1" "2" "3"
```

Character coerced (if possible) to number

```
x <- c("1","2","hello"); str(x)

## chr [1:3] "1" "2" "hello"

str(as.numeric(x))

## num [1:3] 1 2 NA</pre>
```

• Few other conversion functions

```
as.matrix(), as.data.frame(), as.integer(), as.Date()
```

#### Functions • Built-In • Math

# generate 10 random numbers between 1 and 200

## [1] 80 130 196 42 83 105 37 168 89 116 ## [1] 37 42 80 83 89 105 116 130 168 196

x <- sample(x=1:200,10); x;



```
## [1] 80 130 196 42 83 105 37 168 89 116
sum(x) # sum
mean(x) # mean
median(x) # median
min(x) # min
log(x) # log
exp(x) # exponent
sqrt(x) # square-root
round(x) # round
sort(x) # sort
## [1] 1046
## [1] 104.6
## [1] 97
## [1] 37
## [1] 4.382027 4.867534 5.278115 3.737670 4.418841 4.653960 3.610918
## [8] 5.123964 4.488636 4.753590
## [1] 5.540622e+34 2.872650e+56 1.323483e+85 1.739275e+18 1.112864e+36
## [6] 3.989520e+45 1.171914e+16 9.151093e+72 4.489613e+38 2.388691e+50
## [1] 8.944272 11.401754 14.000000 6.480741 9.110434 10.246951 6.082763
## [8] 12.961481 9.433981 10.770330
```

### Functions • Built-In • String



```
paste("hello","kitty") # join
grep("hell","hello") # find a pattern
nchar("hello") # number of characters
toupper("hello") # to uppercase
tolower("HELLO") # to lowercase
sub("ell","ipp","hello") # replace pattern
substr("hello",start=1,stop=3) # substring
strsplit("sunny&bunny&funny","&") # split a character
```

```
## [1] "hello kitty"
## [1] 1
## [1] 5
## [1] "HELLO"
## [1] "hello"
## [1] "hippo"
## [1] "hel"
## [1] "sunny" "bunny" "funny"
```

- print() & cat() are useful for printing messages
- newline character

#### **Functions • Custom**



```
a <- 1:6; b <- 8:10

d <- a*b
e <- log(d)
f <- sqrt(e)
f</pre>
```

```
## [1] 1.442027 1.700109 1.844234 1.861649 1.951067 2.023449
```

Custom function definition

```
my_function <- function(a,b){
  d <- a*b
  e <- log(d)
  f <- sqrt(e)
  return(f)
}</pre>
```

• Re-use function

```
my_function(a=2:4,b=6:8)
## [1] 1.576359 1.744856 1.861649
```

• Function names must not start with number

#### Control Structure • if



• Conditional statements using <a href="tip:15">tf()</a>

```
a <- 2; b <- 5;
if(a < b) print(paste(a,"is smaller than",b))
## [1] "2 is smaller than 5"</pre>
```

• Use else for alternative output

```
if(a < b) {
  print(paste(a,"is smaller than",b))
}else{
  print(paste(b,"is smaller than",a))
}

## [1] "2 is smaller than 5"</pre>
```

• Chain if else statements

```
if(grade == "A"){
  print("Grade is Excellent!")
}else if(grade == "B"){
  print("Grade is Good.")
} else if (grade == "C") {
  print("Grade is Alright.")
}
```

```
## [1] "Grade is Good."
```

#### Control Structure • for



• Use for() loop for known number of iterations

```
for (i in 1:5){
  print(i)
}

## [1] 1
## [1] 2
## [1] 3
## [1] 4
## [1] 5
```

• Use <a href="https://while">while</a>() loop for unknown number of iterations

```
i <- 1
while(i < 5){
  print(i)
  i <- i+1
}</pre>
```

```
## [1] 1
## [1] 2
## [1] 3
## [1] 4
```

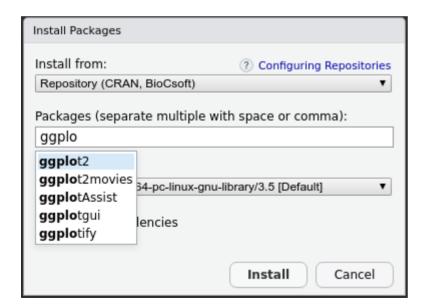
#### **R** Packages



• CRAN (The Comprehensive R Archive Network); Use install.packages()

```
install.packages("ggplot2",dependencies=TRUE)

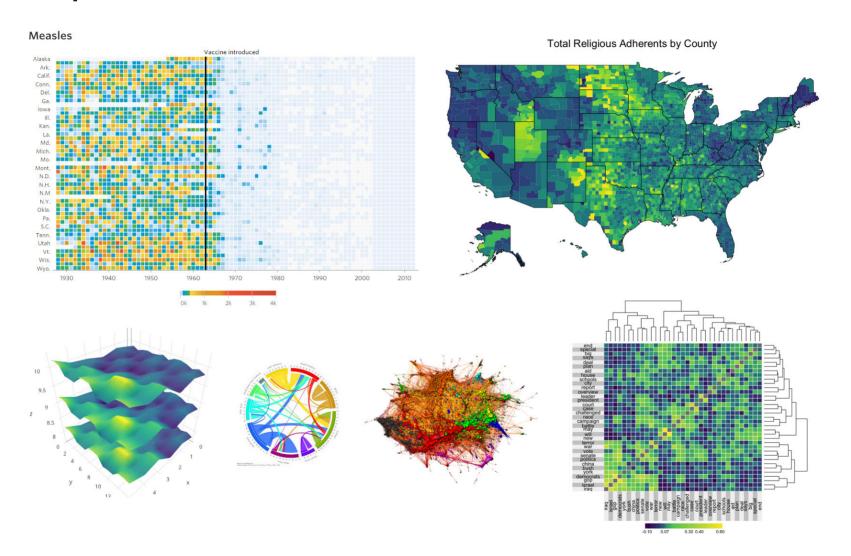
• For local packages, use type="source"
install.packages(path="./dir/package.zip",type="source")
```



- Bioconductor for Biology/Bioinformatics packages; Use BiocManager::install()
- For GitHub packages, Use devtools::install\_github()

# **Graphics**

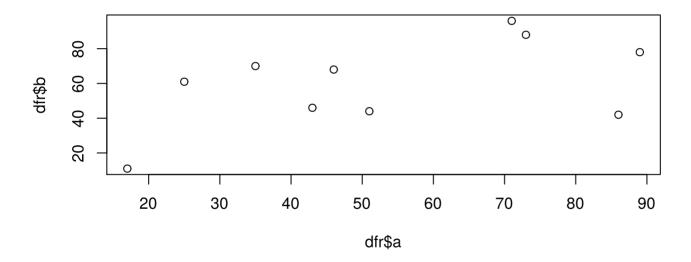




### **Graphics** • Base



```
dfr <- data.frame(a=sample(1:100,10),b=sample(1:100,10))
plot(dfr$a,dfr$b)</pre>
```

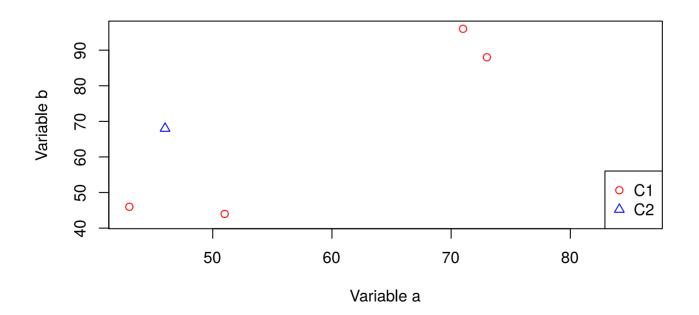


• Add axes labels etc

```
plot(dfr$a,dfr$b,xlab="Variable a",ylab="Variable b")
plot(dfr$a,dfr$b,xlab="Variable a",ylab="Variable b",type="b")
```

#### **Graphics** • Base



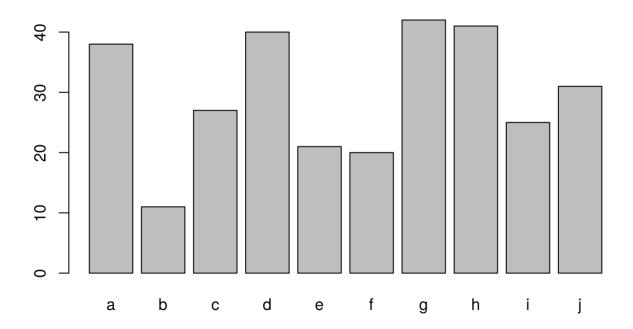


## **Graphics** • Base



• Barplot

```
ldr <- data.frame(a=letters[1:10],b=sample(1:50,10))
barplot(ldr$b,names.arg=ldr$a)</pre>
```

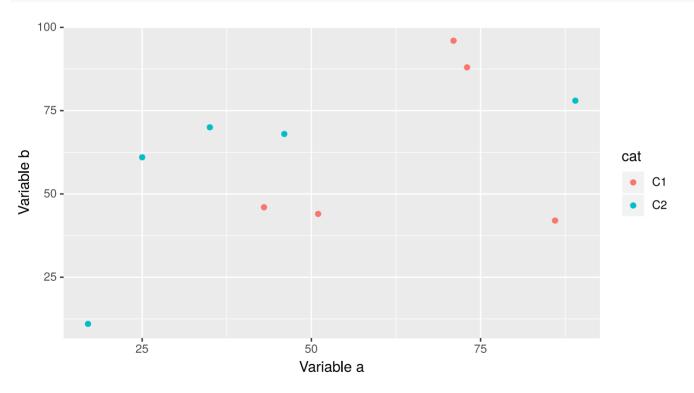


# **Graphics** • ggplot2



```
library(ggplot2)

ggplot(dfr,aes(x=a,y=b,colour=cat))+
  geom_point()+
  labs(x="Variable a",y="Variable b")
```

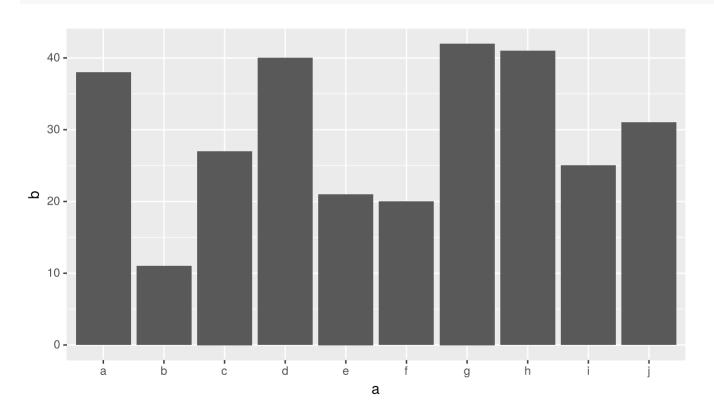


# **Graphics** • ggplot2



• Barplot

```
ggplot(ldr,aes(x=a,y=b))+
  geom_bar(stat="identity")
```



#### Input & Output • Text



```
dfr <- read.table("iris.txt",header=TRUE,stringsAsFactors=F)
head(dfr)

str(dfr)

## 'data.frame': 150 obs. of 5 variables:
## $ Sepal.Length: num 5.1 4.9 4.7 4.6 5 5.4 4.6 5 4.4 4.9 ...
## $ Sepal.Width : num 3.5 3 3.2 3.1 3.6 3.9 3.4 3.4 2.9 3.1 ...
## $ Petal.Length: num 1.4 1.4 1.3 1.5 1.4 1.7 1.4 1.5 1.4 1.5 ...
## $ Petal.Width : num 0.2 0.2 0.2 0.2 0.4 0.3 0.2 0.2 0.1 ...
## $ Species : chr "setosa" "setosa" "setosa" "setosa"

dfr1 <- dfr[dfr$Species == "setosa",]
write.table(dfr1,"iris-setosa.txt",sep="\t",row.names=F,quote=F)</pre>
```

sep="\t" sets tab delimiter, row.names=F avoids printing rownames, quote=F avoids quotes
around strings.

#### Input & Output • Image



Create data

```
dfr <- data.frame(a=sample(1:100,10),b=sample(1:100,10))</pre>
```

• Base plot

```
png(filename="plot-base.png")
plot(dfr$a,dfr$b)
dev.off()
```

• ggplot method 1

```
p <- ggplot(dfr,aes(a,b)) + geom_point()

png(filename="plot-ggplot-1.png")
print(p)
dev.off()</pre>
```

• ggplot method 2

```
ggsave(filename="plot-ggplot-2.png",plot=p)
```

# **R** objects



- Save R objects as compressed native R formats
- Save/Read a single object as .Rds format

```
dfr <- data.frame(a=sample(1:100,10),b=sample(1:100,10))
saveRDS(dfr,"data.Rds")
dfr <- readRDS("data.Rds")</pre>
```

• Save one or more objects as .Rda/.Rdata format

```
save(dfr,"data.Rdata")
save(dfr,dfr2,"data.Rdata")
load("data.Rdata")
```

• Save entire workspace

```
save.image(file="workspace.Rdata")
load("workspace.Rdata")
```

# Reproducible Analyses



- Manually steps = poor reproducibility
- Rerunning analyses
- Adding new data
- Transferring projects
- Collaborative work
- Eliminate copy-paste errors

#### Recommendations

- Single document with analyses, code and results
- Self-contained portable project
- Avoid manual steps
- Results are linked to code used to produce them
- Contexual narrative to workflow
- Version control of documents

### **Data Management Ecosystem**





- Track edits and collaborate coding. Eg: Git
- Share and track code. Eg: GitHub
- Notebooks, documentation and reports. Eg: Latex, Jupyter, Rmarkdown
- Package and environment manager. Eg: Packrat, Conda, Virtualenv
- Workflow manager Eg: Snakemake, Nextflow
- Virtual machines. Eg: VMWare, VirtualBox
- Containerised computing environment. Eg: *Docker, Singularity, Vagrant*
- Big data analyses. Eg: *Hadoop, Spark*
- Workflow orchestration. Eg: Openstack, Kubernetes, Terraform

# Reproducibility in R



- Manage R versions carefully
- Install packages from repositories

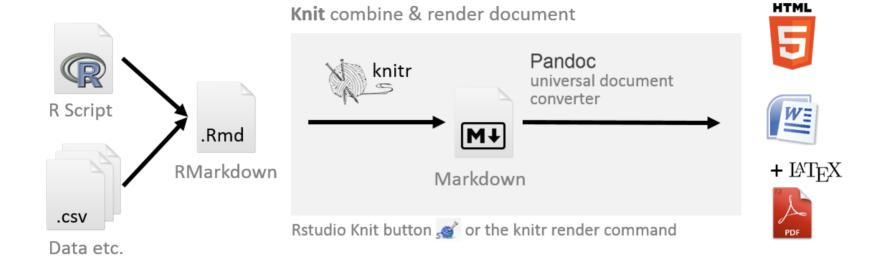
```
install.packages(); devtools::install_github(); BiocManager::install()
```

- Package management using packrat (RStudio integrated)
- Version control using git (RStudio integrated)
- RStudio (Syntax highlighting, Debugging, Projects etc)
- Running external programs from R

```
system("./plink --file --flag1 --flag2 --out bla")
```

#### **Document Converter**



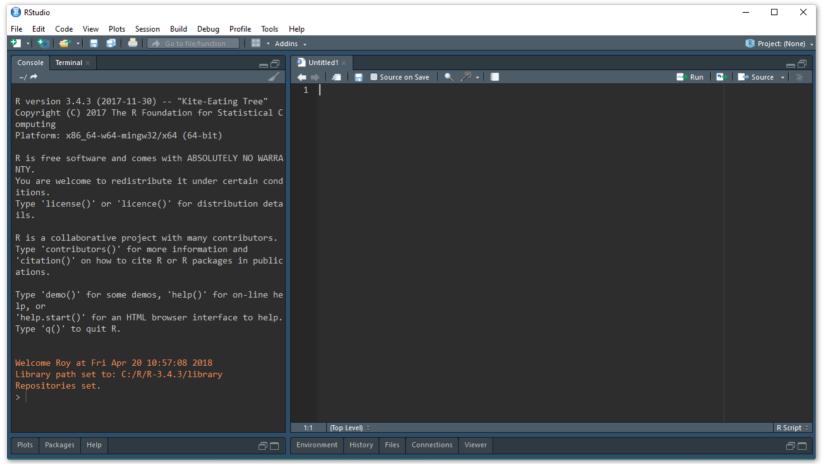


- Document converter (Reports, Presentations, Articles etc)
- Rmd -> md -> HTML|PDF|docx

#### **RStudio Notebook**



#### Create a new .Rmd document



- Text and code can be written together
- Inline R output (text and figures)

### Rmarkdown Guide



- Plain text format for readability
- Support of pure language (HTML, Latex etc) for complex formatting
- Rmarkdown = Markdown + R chunks
- Create a file that ends in .Rmd
- Add YAML matter to top

```
title: "This is a title"
output:
   rmarkdown::html_document
---
```

- In RStudio File > New File > R Markdown opens up an Rmd template
- Render interactively using the Knit button Knit
- Render using command rmarkdown::render("report.Rmd")

### **Rmarkdown Guide**



```
### Heading 3
#### Heading 4

_italic text_
__bold text__
`code text`
~~strikethrough~~
2^10^
2~10^
- bullet point

Link to [this](somewhere.com)
![](https://www.r-project.org/Rlogo.png)
```

Heading 3

Heading 4

italic text
bold text

code text

strikethrough

 $2^{10}$ 

2<sub>10</sub>

bullet point

Link to this



#### Rmarkdown Guide



• R code can be executed inline

```
Today's date is 'r date()'
Today's date is Thu Nov 7 20:46:11 2019
```

R code can be executed in code chunks

```
```{r}
date()
```

• By default shows input code and output result.

```
date()
## [1] "Thu Nov 7 20:46:11 2019"
```

- Many arguments to customise chunks
  - Set eval=FALSE to not evaluate a code chunk
  - Set echo=FALSE to hide input code
  - Set results="hide" to hide output
- R Markdown reference

# **Tidyverse**



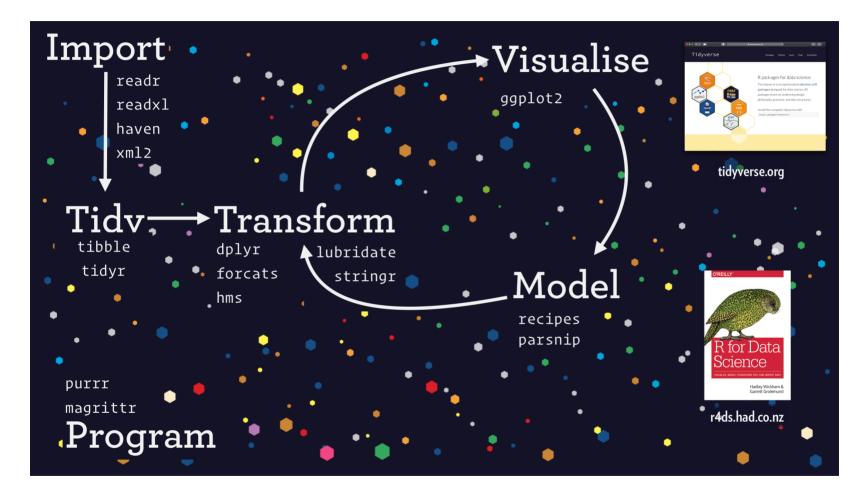


"Language for solving data science challenges using R"

- Collection of R packages that share underlying design and grammar
- Modern, consistent and optimised functions
- Additional features compared to base R
- New code structure using new operators (Eg: pipe %>%)
- Tidy data & tidy evaluation

# **Tidyverse**





# **Tidyverse**



- magrittr : Piping commands using %>%
- tibble: A better data.frame
- readr: Functions to import/export data
- tidyr: Data structuring: wide & long formats, splitting, fill missing values etc
- dplyr: Data selection, filtering, summarising, merging etc
- lubridate: Working with time
- stringr: Working with strings
- forcats: Working with factors
- purrr : Simpler control structures for programming
- broom: Model building
- ggplot2 : Plotting

# Tidyverse • Examples

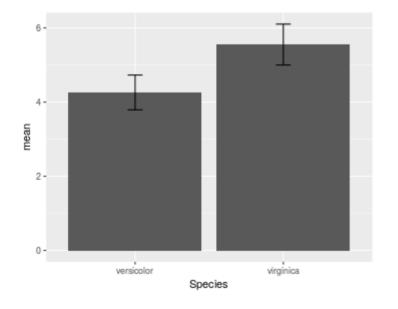


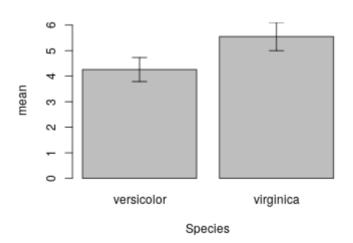
#### **Tidyverse**

```
iris %>%
 filter(Species!="setosa") %>%
  select(Species,Petal.Length) %>%
 group by(Species) %>%
  summarise(mean=mean(Petal.Length),sd=sd(Petal.L iris1$Species <- factor(iris1$Species)</pre>
 mutate(ymin=mean-sd,ymax=mean+sd) %>%
  qqplot(aes(x=Species,y=mean,ymin=ymin,ymax=yma)
 geom bar(stat="identity")+
 geom errorbar(width=0.1)
```

#### Base R

```
iris mean <- aggregate(Petal.Length~Species.data=</pre>
iris sd <- aggregate(Petal.Length~Species,data=si</pre>
iris1 <- merge(iris mean,iris sd,by="Species")</pre>
colnames(iris1) <- c("Species", "mean", "sd")</pre>
iris1$ymin <- iris1$mean-iris1$sd</pre>
iris1$ymax <- iris1$mean+iris1$sd</pre>
{b <- barplot(iris1$mean,names.arg=iris1$Species,</pre>
arrows(x0=b,y0=iris1$ymin,y1=iris1$ymax, length=6
```





# Tidyverse • Examples



#### **Tidyverse**

```
# extract columns from a data.frame
select(iris, Species, Petal.Width)
select(iris, 5, 4)
# extract rows
filter(iris, Petal.Width > 0.5 & Species == "setc iris[iris$Petal.Width > 0.5 & iris$Species == "setc
# ordering a data.frame
arrange(iris, desc(Species), Petal.Width)
# add new computed variable
iris %>% mutate(cent=Petal.Length-mean(Petal.Length - iris$petal.Length-mean(iris$petal.Length-mean()
# grouped summarisation
iris %>% group by(Species) %>% summarise(mean=mea aggregate(Petal.Length~Species,data=iris,FUN=mear
```

#### Base R

```
# extract columns from a data.frame
iris[, c("Species", "Petal.Width")]
iris[, c(5, 4)]
# extract rows
# ordering a data.frame
iris[order(rev(iris$Species), iris$Petal.Width),
# add new computed variable
# grouped summarisation
```

### **Bioconductor**





- NGS/Genomics/Biology related packages
- Package management using BiocManager
- Complex objects (Classes) to hold related objects
- Workflows for common tasks

# Help



- Use <a href="function">: function</a> to get function documentation
- Use ??name to search for a function
- Use args(function) to get the arguments to a function
- Go to the package CRAN page/webpage for vignettes
- R bloggers: Great blog to follow to keep updated with the latest in the R world as well as tutorials.
- Stackoverflow: Online community to find solutions to your problems.



# **Learning R**



There are lots of resources for getting help in R.

#### **Tutorials**

- Introduction to R: Tutorial by Datacamp with excellent tutorials.
- R programming tutorial: Youtube video tutorial by Derek Banas.
- R for data science Data science tutorial by Hadley wickham.
- Data carpentry Data carpentry R workshop (Medium-Advanced)

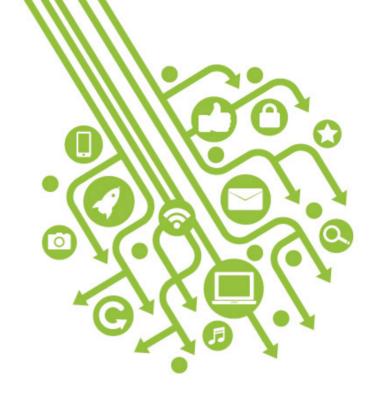
#### Reference

- R Cookbook: General purpose reference.
- Quick R: General purpose reference.
- Awesome R: Curated list of useful R packages.
- RStudio cheatsheets: Useful cheatsheets.
- Advanced R by Hadley Wickham (Medium-Advanced)

#### Links

• Tutorialspoint List: Good list of resources.





# Thank you

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