R tutorial - I

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Introduction to NGS Data and Analysis Week 16; v2020





R is a programming environment

- It's free
 - Hence R is supported by a large user network
 - R is open source
- Can be run on Windows, Linux and Mac
- Provides an unparalleled platform for programming new statistical methods in an easy and straightforward manner.
- Excellent graphics capabilities
- Lots and lots of analysis packages
- It is also old, hence you need to know new functions which do things much faster



Recommended textbook

http://r4ds.had.co.nz/



VISUALIZE, MODEL, TRANSFORM, TIDY, AND IMPORT DATA

Hadley Wickham & Garrett Grolemund

R for Data Science

Garrett Grolemund Hadley Wickham

Welcome

This is the website for **"R for Data Science"**. This book will teach you how to do data science with R: You'll learn how to get your data into R, get it into the most useful structure, transform it, visualise it and model it. In this book, you will find a practicum of skills for data science. Just as a chemist learns how to clean test tubes and stock a lab, you'll learn how to clean data and draw plots—and many other things besides. These are the skills that allow data science to happen, and here you will find the best practices for doing each of these things with R. You'll learn how to use the grammar of graphics, literate programming, and reproducible research to save time. You'll also learn how to manage cognitive resources to facilitate discoveries when wrangling, visualising, and exploring data.

Download R (ver4.0.1) and Rstudio

Studio

http://www.r-project.org https://www.rstudio.com/

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		PLOTS
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RStudio

RStudio makes R easier to use. It includes a code editor, debugging & visualization tools.

📥 Download 👘 🚯 Learn More



knitr ggplot2

Shiny

Shiny helps you make interactive web applications for visualizing data. Bring R data analysis to life.

Learn More

R Packages

Our developers create popular packages to expand the features of R. Includes ggplot2, dplyr, R Markdown & more.

Learn More

Rstudio interface



Slide annotation

#code box
Comment

function(x)

R as a calculator

Assignment

Boolean assignment

student <- 30000 phd <- 56000

Vector is the simplest data structure in R

x<- c(1,2,3,4,5,6,7,8,9,10)

c = combine or concatenate In this case, we assign a vector of 10 numbers into x

x * 2 x /10 + 1 Different types of vectors

```
x<- c(1,2,3,4,5,6,7,8,9,10)
strings <- c("AS","BRC")
```

typeof(x)
typeof(strings)

This matters when one data type is numbers, and you want to sort them categorically (factors)

> typeof(x)
[1] "double"
> typeof(char)
[1] "character"
> typeof(strings)
[1] "character"

Data frames

- Think of these like Excel spreadsheets
- All the values of the same variable must go in the same column
 - E.g., age, sex, RPKM, numbers
- Rows represent samples
 - E.g., sample A collected in Taiwan, sample B collected in Japan
- Like matrices but different types of data are allowed
- Tibble from the dplyr package ; basically like data frame but much easier to manipulate

R has some pre-installed data frames

The data set consists of **50 samples from** each of three species of Iris (Iris setosa, Iris virginica and Iris versicolor). Four features were measured from each sample: the length and the width of the sepals and petals, in centimetres. Based on the combination of these four features, Fisher developed a linear discriminant model to distinguish the species from each other.

This data set became a typical test case for many statistical classification techniques in machine learning such as support vector machines

iris **head**(iris)

https://en.wikipedia.org/wiki/Iris_flower_data_set

THE USE OF MULTIPLE MEASUREMENTS IN TAXONOMIC PROBLEMS

By R. A. FISHER, Sc.D., F.R.S.

I. DISCRIMINANT FUNCTIONS

WHEN two or more populations have been measured in several characters, x_1, \ldots, x_s , special interest attaches to certain linear functions of the measurements by which the populations are best discriminated. At the author's suggestion use has already been made of this fact in craniometry (a) by Mr E. S. Martin, who has applied the principle to the sex differences in measurements of the mandible, and (b) by Miss Mildred Barnard, who showed how to obtain from a series of dated series the particular compound of cranial measurements showing most distinctly a progressive or secular trend. In the present paper the application of the same principle will be illustrated on a taxonomic problem; some questions connected with the precision of the processes employed will also be discussed.

II. ARITHMETICAL PROCEDURE

Table I shows measurements of the flowers of fifty plants each of the two species *Iris* setosa and *I. versicolor*, found growing together in the same colony and measured by Dr E. Anderson, to whom I am indebted for the use of the data. Four flower measurements are given. We shall first consider the question: What linear function of the four measurements $X = \lambda_1 x_1 + \lambda_2 x_2 + \lambda_3 x_3 + \lambda_4 x_4$

will maximize the ratio of the difference between the specific means to the standard deviations within species? The observed means and their differences are shown in Table II. We may represent the differences by d_p , where p = 1, 2, 3 or 4 for the four measurements.

The sums of squares and products of deviations from the specific means are shown in Table III. Since fifty plants of each species were used these sums contain 98 degrees of freedom. We may represent these sums of squares or products by S_{pq} , where p and q take independently the values 1, 2, 3 and 4.

Then for any linear function, X, of the measurements, as defined above, the difference between the means of X in the two species is

$$D = \lambda_1 d_1 + \lambda_2 d_2 + \lambda_3 d_3 + \lambda_4 d_4,$$

while the variance of X within species is proportional to

$$S = \sum_{p=1}^{4} \sum_{q=1}^{4} \lambda_p \lambda_q S_{pq}$$

The particular linear function which best discriminates the two species will be one for

Selection in data frames

Square brackets

- dat[i,] would select the *i*-th row (which is a **vector**)
- dat[, j] would select the *j*-th column (which is a **vector**)
- dat[i, j] would select the value from the *i*-th row and *j*-th column

iris[,1] iris[1,] iris[1,1]

dollar (\$) operation (for columns only)

iris\$Petal.Width

Function

function (arg1, arg2, arg3..., option1=,option2=...)

x<- c(1,2,3,4,5,6,7,8,9,10) y<- c(3,6,9,10,13,30,20,100)

mean(x) mean(y) median(x) max(x) > x<- c(1,2,2,3,5,6,7,10)
> y<- c(3,6,9,10,13,30,20,100)
> mean(x)
[1] 4.5
> mean(y)
[1] 23.875
> median(x)
[1] 4
> median(y)
[1] 11.5
> max(x)
[1] 10
> min(y)
[1] 3

- Must have **assigned names**
- Applies using **round brackets**
- Takes **argument** and options

Useful base functions here

y<- **abs**(-20) x<- **Sum**(y+5) $Z \le Log(x)$ round(x,1) summary(iris) **head**(iris) tail(iris) **ncol**(iris) **nrow**(iris)

R base function **plot**

x<- c(1,2,3,4,5,6,7,8,9,10) y<- c(3,6,9,10,13,30,20,100,220,100)

plot(x,y)
plot(x,y,col="red")

many functions have additional parameters
boxplot(x,y,col="red")
boxplot(x,y,col=c("hotpink", "yellow"))

boxplot(x,y,col=c("hotpink", "yellow"),main="Lec2")

can use the ? sign to find out more about function ?boxplot

Running out of functions to use?

Use Packages

- R consists of a core and additional packages.
- Collections of R functions, data, and compiled code
- Well-defined format that ensures easy installation, a basic standard of documentation, and enhances portability and reliability

Install R packages

- An R **package** is a collection of functions, data, and documentation that extends the capabilities of base R.
- Using packages is key to the successful use of R.
- Understanding **tidyverse** is highly recommended.

install
install.packages("tidyverse")

#after it's installed, you can initiate by using **library library**(tidyverse)

http://r4ds.had.co.nz/introduction.html#rstudio

Tidyverse package (much better/easier functions)

Tidyverse

Packages Articles Learn Help Contribute

R packages for data science

The tidyverse is an opinionated **collection of R packages** designed for data science. All packages share an underlying design philosophy, grammar, and data structures.

Install the complete tidyverse with:

install.packages("tidyverse")

Communicate: R markdown in Rstudio

Tidyverse package (much better/easier functions)

Program

dplyr package

- Pick observations by their values (filter()).
- Reorder the rows (arrange()).
- Pick variables by their names (select()).
- Create new variables with functions of existing variables (mutate()).
- Collapse many values down to a single summary (summarise()).

filter

filter() allows you to subset observations based on their values. The first argument is the name of the data frame. The second and subsequent arguments are the expressions that filter the data frame. For example, we can select all flights on January 1st with:

```
filter(flights, month == 1, day == 1)
jan1 <- filter(flights, month == 1, day == 1)
filter(flights, month = 1)
filter(flights, month == 11 | month == 12)
nov_dec <- filter(flights, month %in% c(11, 12))</pre>
```


arrange

arrange() works similarly to filter() except that instead of selecting rows, it changes their order. It takes a data frame and a set of column names (or more complicated expressions) to order by. If you provide more than one column name, each additional column will be used to break ties in the values of preceding columns:

arrange(flights, desc(dep_delay))

arrange(flights, dep_delay)

select

Besides selecting sets of existing columns, it's often useful to add new columns that are functions of existing columns. That's the job of mutate().

select(flights, year, month, day)

Select all columns between year and day (inclusive) **select**(flights, year:day)

select(flights, -(year:day))

mutate

select(flights, year, month, day)

Select all columns between year and day (inclusive) **select**(flights, year:day)

select(flights, -(year:day))

mutate()

Besides selecting sets of existing columns, it's often useful to add new columns that are functions of existing columns. That's the job of mutate().

```
flights_sml <- select(flights,
  year:day,
  ends_with("delay"),
  distance,
  air_time
)
mutate(flights_sml,
  gain = dep_delay - arr_delay,
  speed = distance / air_time * 60
```


transmute()

If you only want to keep the new variables, use transmute() :

transmute(flights, gain = dep_delay - arr_delay, hours = air_time / 60, gain_per_hour = gain / hours)

summarise() and group_by

by_day <- group_by(flights, year, month, day)
summarise(by_day, delay = mean(dep_delay, na.rm = TRUE))</pre>

```
by_dest <- group_by(flights, dest)
delay <- summarise(by_dest,
count = n(),
dist = mean(distance, na.rm = TRUE),
delay = mean(arr_delay, na.rm = TRUE) )
delay <- filter(delay, count > 20, dest != "HNL")
```


Combine functions into a pipe

```
delays <- flights %>%
    group_by(dest) %>%
    summarise( count = n(),
        dist = mean(distance, na.rm = TRUE),
        delay = mean(arr_delay, na.rm = TRUE) ) %>%
    filter(count > 20, dest != "HNL")
```

Data wrangling

Data wrangling is very important: without it you can't work with your own data!

Program

Tibble

- work with "tibbles" instead of R's traditional data.frame. Tibbles are data frames, but they tweak some older behaviours to make life a little easier.
- R is an old language, and some things that were useful 10 or 20 years ago now get in your way. It's difficult to change base R without breaking existing code, so most innovation occurs in packages.

as_tibble(iris)

#> #	A tibble: 150	0 x 5			
#>	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
#>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<fct></fct>
#> 1	5.1	3.5	1.4	0.2	setosa
#> 2	4.9	3	1.4	0.2	setosa
#> 3	4.7	3.2	1.3	0.2	setosa
#> 4	4.6	3.1	1.5	0.2	setosa
#> 5	5	3.6	1.4	0.2	setosa
#> 6	5.4	3.9	1.7	0.4	setosa
#> #	with 144 mc	ore rows			

Tibble vs. data.frame

- Tibbles have a refined print method that shows only the first 10 rows, and all the columns that fit on screen. This makes it much easier to work with large data. In addition to its name, each column reports its type
- So far all the tools you've learned have worked with complete data frames. If you want to pull out a single variable, you need some new tools, \$ and [[]. [[can extract by name or position; \$ only extracts by name but is a little less typing.

Tidy data (perhaps the most important part of tutorial)

tidyr package

"Happy families are all alike; every unhappy family is unhappy in its own way." — Leo Tolstoy

"Tidy datasets are all alike, but every messy dataset is messy in its own way." — Hadley Wickham

Dataset example; which is preferred?

#> # A tibble: 6 x 4

#>		country	year	cases	population
#>		<chr></chr>	<int></int>	<int></int>	<int></int>
#>	1	Afghanistan	1999	745	19987071
#>	2	Afghanistan	2000	2666	20595360
#>	3	Brazil	1999	37737	172006362
#>	4	Brazil	2000	80488	174504898
#>	5	China	1999	212258	1272915272
#>	6	China	2000	213766	1280428583

#> # A tibble: 12 x 4

#>	country	year	type	count				
#>	<chr></chr>	<int></int>	<chr></chr>	<int></int>				
#> 1	Afghanistan	1999	cases	745				
#> 2	Afghanistan	1999	population	19987071				
#> 3	Afghanistan	2000	cases	2666				
#> 4	Afghanistan	2000	population	20595360				
#> 5	Brazil	1999	cases	37737				
#> 6	Brazil	1999	population	172006362				
#> # with 6 more rows								

table1 table2

table3

#spread across two tables table4a table4b

Definition of tidy dataset

Each variable must have its own column.
 Each observation must have its own row.
 Each value must have its own cell.

table1 is tidy. It's the only representation where each column is a variable.

1. There's a general advantage to picking one consistent way of storing data. If you have a consistent data structure, it's easier to learn the tools that work with it because they have an underlying uniformity.

2. There's a specific advantage to placing variables in columns because it allows R's vectorised nature to shine. As you learned in <u>mutate</u> and <u>summary functions</u>, most built-in R functions work with vectors of values. That makes transforming tidy data feel particularly natural.

Most data that you will encounter will be untidy.

There are two main reasons:

- Most people aren't familiar with the principles of tidy data, and it's hard to derive them yourself unless you spend a *lot* of time working with data.
- Data is often organised to facilitate some use other than analysis. For example, data is often organised to make entry as easy as possible.

This means for most real analyses, you'll need to do some tidying.

- first step is always to figure out what the variables and observations are. Sometimes this is easy; other times you'll need to consult with the people who originally generated the data.
- second step is to resolve one of two common problems:
 - One variable might be spread across multiple columns.
 - One observation might be scattered across multiple rows.

A common problem is a dataset where some of the column names are not names of variables, but values of a variable. Take table4a : the column names 1999 and 2000 represent values of the year variable, the values in the 1999 and 2000 columns represent values of the cases variable, and each row represents two observations, not one.

table4a							
<pre>#> # A tibble: 3</pre>	x 3						
<pre>#> country</pre>	`1999`	`2000`					
#> * <chr></chr>	<int></int>	<int></int>					
<pre>#> 1 Afghanistan</pre>	745	2666					
#> 2 Brazil	37737	80488					
#> 3 China	212258	213766					

table4a

To tidy a dataset like this, we need to **pivot** the offending columns into a new pair of variables. To describe that operation we need three parameters:

- The set of columns whose names are values, not variables. In this example, those are the columns 1999 and 2000.
- The name of the variable to move the column names to. Here it is year .
- The name of the variable to move the column values to. Here it's cases .

Pivoting table4 into a longer, tidy form.


```
table4a %>%

pivot_longer(c(`1999`, `2000`), names_to = "year", values_to = "cases")
```

pivot_wider() is the opposite of pivot_longer(). You use it when an observation is scattered across multiple rows. For example, take table2 : an observation is a country in a year, but each observation is spread across two rows.

#> # A tibble: 12 x 4									
<pre>#> country</pre>	year	type	count						
#> <chr></chr>	<int></int>	<chr></chr>	<int></int>						
<pre>#> 1 Afghanistan</pre>	1999	cases	745						
<pre>#> 2 Afghanistan</pre>	1999	population	19987071						
<pre>#> 3 Afghanistan</pre>	2000	cases	2666						
<pre>#> 4 Afghanistan</pre>	2000	population	20595360						
#> 5 Brazil	1999	cases	37737						
#> 6 Brazil	1999	population	172006362						
#> # with 6 mor	#> # with 6 more rows								

table2

To tidy this up, we first analyse the representation in similar way to pivot_longer(). This time, however, we only need two parameters:

- The column to take variable names from. Here, it's type .
- The column to take values from. Here it's count .

table2 %>%

pivot_wider(names_from = type, values_from = count)

country	year	key	value
Afghanistan	1999	cases	745
Afghanistan	1999	population	19987071
Afghanistan	2000	cases	2666
Afghanistan	2000	population	20595360
Brazil	1999	cases	37737
Brazil	1999	population	172006362
Brazil	2000	cases	80488
Brazil	2000	population	174504898
China	1999	cases	212258
China	1999	population	1272915272
China	2000	cases	213766
China	2000	population	1280428583
	ta	able2	

More functions in tidyr

separate(rate, into = c("cases", "population"), sep = "/")

table5 %>%

unite(new, century, year, sep = "")

					$\overline{\ }$					
country	vear	rate	co	ountry	vear	cases	population	country	vear	rate
Afghanistan	1999	745 / 19987071	Afgl	ghanistan	1999	745	19987071	Afghanistan	19 99	745 / 19987071
Afghanistan	2000	2666 / 20595360	Afgl	ghanistan	2000	2666	20595360	Afghanistan	20 00	2666 / 20595360
Brazil	1999	37737 / 172006362	Bra	azil	1999	37737	172006362	Brazil	19 99	37737 / 172006362
Brazil	2000	80488 / 174504898	Bra	azil	2000	80488	174504898	Brazil	20 00	80488 / 174504898
China	1999	212258 / 1272915272	Chi	nina	1999	212258	1272915272	China	19 99	212258 / 1272915272
China	2000	213766 / 1280428583	Chi	nina	2000	213766	1280428583	China	20 00	213766 / 1280428583

table3

table6

Relational data

 It's rare that a data analysis involves only a single table of data. Typically you have many tables of data, and you must combine them to answer the questions that you're interested in. Collectively, multiple tables of data are called **relational data** because it is the relations, not just the individual datasets, that are important.

To work with relational data you need verbs that work with pairs of tables. There are three families of verbs designed to work with relational data:

•Mutating joins, which add new variables to one data frame from matching observations in another.

•Filtering joins, which filter observations from one data frame based on whether or not they match an observation in the other table.

•Set operations, which treat observations as if they were set elements.

Mutating joins

https://rstudio.com/wp-content/uploads/2015/02/datawrangling-cheatsheet.pdf

Filtering joins; semi_join and anti_join

Filtering joins keep cases from the left data table (i.e. the X-data) and use the right data (i.e. the Y-data) as filter.

semi_join(data1, data2, by = "ID")
anti_join(data1, data2, by = "ID")

R for Data Science

https://statisticsglobe.com/r-dplyr-join-inner-left-right-fullsemi-anti

Visualisation

"The simple graph has brought more information to the data analyst's mind than any other device." — John Tukey

Examples I - amplicon

Q: Is the relative abundance of OTUn associated with abiotic factors?

ΟΤυ	Site1	Site2	Site3	Site	pН	metadata2	metadata3
OTU2	4	10	3	Site1	3	1	4
OTU4	8	15	1	Site2	5	2	5
				Site3	7	2	6

Q: Is the relative abundance of OTUn associated with particular trait?

OTU	Species	Trait2	Trait3
OTU2	Bacteria	Pathogen	44
OTU4	Fungus	free-living	32

Examples II – genome features

Program1 output

Chromosome	Region start	Region end	Gene density
Chrl	1	1000	30
Chrl	1001	2000	40
Chrl	2001	3000	3

Program2 output

Chromosome	Region start	Region end	TE density
Chrl	1	1000	3
Chrl	1001	2000	1
Chrl	2001	3000	60

#Ideal table?

Chromosome	Midpoint	Gene density	TE density	GC content
Chrl	500	30	3	30
Chrl	1500	40	1	35
Chrl	2500	3	60	40

Program3 output

Chromosome	Region start	Region end	GC content
Chrl	1	1000	30
Chrl	1001	2000	35
Chrl	2001	3000	40

A tibble: 150 x 5

Sepal.Length Sepal.Width Petal.Length Petal.Width Species <db1> <db1> <db1> <dbl> <fct> 5.1 3.5 0.2 setosa 1.4 1 2 3 0.2 setosa 4.9 1.4 3 3.2 4.7 1.3 0.2 setosa 4 4.6 0.2 setosa 3.1 1.5 5 5 3.6 0.2 setosa 1.4 3.9 6 5.4 1.7 0.4 setosa 7 4.6 3.4 1.4 0.3 setosa 8 5 3.4 1.5 0.2 setosa 9 4.4 2.9 1.4 0.2 setosa 10 4.9 3.1 1.5 0.1 setosa

... with 140 more rows

ggplot(tb, aes(x = Sepal.Length, y = Sepal.Width)) +
geom_point()

aes : Aesthetic mappings describe how variables in the data are mapped to visual properties (aesthetics) of geoms ggplot(tb) +
geom_point(aes(x = Sepal.Length, y = Sepal.Width))

ggplot(tb, aes(x = Sepal.Length, y = Sepal.Width)) +
geom_point(aes(color=Species))

ggplot(tb, aes(x = Sepal.Length, y = Sepal.Width)) +
geom_point(aes(color=Species, shape=Species))

7

Sepal.Length

6

ggplot(tb, aes(x = Sepal.Length, y = Sepal.Width)) +
geom_point(aes(color=Species))

ggplot(tb, aes(x = Sepal.Length, y = Sepal.Width)) +
geom_point(aes(color=Species, shape=Species))

7

Sepal.Length

6

p <- ggplot(tb, aes(x = Sepal.Length, y = Sepal.Width, color=Species)) +
geom_point(aes(shape=Species))</pre>

p + geom_smooth(method="lm")

facet

rows p + geom_smooth(method="loess") + facet_grid(. ~ Species)

along columns
p + geom_smooth(method="loess") +
facet_grid(Species ~ .)

More ggplot functions and extensions

https://exts.ggplot2.tidyverse.org/gallery/

http://r-statistics.co/Top50-Ggplot2-Visualizations-MasterList-R-Code.html

Top 50 ggplot2 Visualizations - The Master List (With Full R Code)

What type of visualization to use for what sort of problem? This tutorial helps you choose the right type of chart for your specific objectives and how to implement it in R using ggplot2.

Exercise – iris

library(tidyverse)
tb <- as_tibble(iris)</pre>

Try to plot boxplot of Sepal.Width categorized by species
hint: use geom_boxplot and ?geom_boxplot to find usage

add colour to each boxplot
hint: use fill

plot all four lengths in multiple boxes categorized by species
hint: think about tidy data (long and wide?)
final plot

Can you make it better?
title?
a different theme?

Exercise – starwar 😳

library("tidyverse") starwars **glimpse**(starwars)

some data exploration
plot height vs mass using ggplot and geom_point
who's the heaviest? ; add color by sex to categorise this character quickly
alternatively, facet_grid?

average height by species?
hint: group_by and summarise
hint2: use mean(height, na.rm = TRUE) to deal with na figures

which species is the shortest?
hint: arrange

visualize numbers of characters based on sex
this is categorical data ; use geom_bar

for each bar, can you further split them into hair_color?

what about proportions? (final plot)

why NA in hair_color in the hermaphroditic category? # Note: this is purely for star wars fans

Final plot

Good References

OpenIntro Statistics *** great book about statistics

<u>https://www.openintro.org/</u>

R statistics

- http://r-statistics.co/
- # If you want to practice more:
- <u>https://www.datacamp.com/onboarding/learn?technology=r</u>
- <u>https://www.coursera.org/specializations/data-science-foundations-r</u>