

Trinity College Dublin Coláiste na Tríonóide, Baile Átha Cliath The University of Dublin



Introduction to R, Github and Gitlab

27/11/2018

Pierpaolo Maisano Delser

mail: maisanop@tcd.ie ; pm604@cam.ac.uk

Outline:

- Why R? What can R do?
- Basic commands and operations
- Data analysis in R
- Github and Gitlab

Outline:

- Why R? What can R do?
- Basic commands and operations
- Data analysis in R
- Github and Gitlab

- R is a language and environment for statistical computing and graphics;
- It is open source and free software package;
- Lots of resources, packages and support

. . . nwon0008 — R — 80×24 Last login: Thu Oct 5 11:06:23 on ttys001 MU00105304X:~ nwon0008\$ R R version 3.4.1 (2017-06-30) -- "Single Candle" Copyright (C) 2017 The R Foundation for Statistical Computing Platform: x86_64-apple-darwin15.6.0 (64-bit) R is free software and comes with ABSOLUTELY NO WARRANTY. You are welcome to redistribute it under certain conditions. Type 'license()' or 'licence()' for distribution details. Natural language support but running in an English locale R is a collaborative project with many contributors. Type 'contributors()' for more information and 'citation()' on how to cite R or R packages in publications. Type 'demo()' for some demos, 'help()' for on-line help, or 'help.start()' for an HTML browser interface to help. Type 'q()' to quit R. > []



R vs Excel



- Dragging and updating formula;
- Spreadsheets can get really big and confusing;
- Lack of quick way to get a summary of the data;

Ziemann et al. Genome Biology (2016) 17:177 DOI 10.1186/s13059-016-1044-7

COMMENT

Gene name errors are widespread in the scientific literature

Mark Ziemann¹, Yotam Eren^{1,2} and Assam El-Osta^{1,3*}

Abstract

The spreadsheet software Microsoft Excel, when used with default settings, is known to convert gene names to dates and floating-point numbers. A programmatic scan of leading genomics journals reveals that approximately one-fifth of papers with supplementary Excel gene lists contain erroneous gene name conversions.

Keywords: Microsoft Excel, Gene symbol, Supplementary data

Abbreviations: GEO, Gene Expression Omnibus; JIF, journal impact factor frequently reused. Our aim here is to raise awareness of the problem.

We downloaded and screened supplementary files from 18 journals published between 2005 and 2015 using a suite of shell scripts. Excel files (.xls and.xlsx suffixes) were converted to tabular separated files (tsv) with ssconvert (v1.12.9). Each sheet within the Excel file was converted to a separate tsv file. Each column of data in the tsv file was screened for the presence of gene symbols. If the first 20 rows of a column contained five or more gene symbols, then it was suspected to be a list of gene symbols, and then a regular expression (regex) search of the entire column was applied to identify gene symbol errors. Official gene symbols from Ensembl version 82, accessed November 2015, were obtained for Archidencia theliana. Converbenditic elegene. Descent

Genome Biology

Open Access

CrossMark

R vs Excel

- Point-and-click software is not time efficient;
- Automating tasks will pay off within the time frame of a PhD and thereafter



R is more efficient

R vs Excel

• **Reproducibility:** there is an increasing expectation that material, data and analysis details are provided alongside the research, this is easier when analyses are script based.

Flexibility:

- Read different file formats;
- Compute analysis;
- Generate graphs and plots;
- Summary of your data;
- R works on vector, matrix and dataframe;
- Generate reports;













- Fast and free
- Statistical researchers provide their methods as R packages
- Good graphics (MATLAB and python)
- Active user community (great support)
- Excellent data analysis;
- Forces you to think about your analysis
- Functions can be integrated in R packages

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Disadvantages:

- "Not user friendly at start steep learning curve, minimal GUI"
- Easy to make mistakes and not know.
- Working with large datasets is limited by RAM

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• Functions can be integrated in R packages

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t<-read.table("/home/pier/data/input_stat")</pre>

dim(t) #number of columns and rows

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```
t<-read.table("/home/pier/data/input stat")</pre>
dim(t) #number of columns and rows
#I want to calculate the sum of each column
and if it is > 10, print out "column X has
sum greater than 10"
for (i in 1:ncol(t)) {
      f < -sum(t[,i])
      if (f>10) {
            print (paste("Column ", i, "
has a sum greater than 10'', sep=""))
      else {
}
```

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```
sum 10 <- function(table) {</pre>
for (i in 1:ncol(table)) {
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      if (f>10) {
             print
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        }
        else {
        }
    }
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sum 10(t)

• Active user community (great support)

R packages for:

- Statistical analysis;
- Plotting;
- Graphs;

...

- Managing calendar dates;
- Selecting colour palette;
- Machine learning;
- Population genetics;



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EuroBioC 2018

The European Bioconductor meeting is on December 6 and 7, 2018, at the Technical University of Munich, Germany. The meeting is for biologists, bioinformaticians, statisticians, programmers and software engineers. The meeting aims to foster the exchange of technical expertise while keeping contributors up to speed with the latest developments in *Bioconductor*.

About Bioconductor

Bioconductor provides tools for the analysis and comprehension of highthroughput genomic data. Bioconductor uses the R statistical programming language, and is open source and open development. It has two releases each year, <u>1560</u> <u>software packages</u>, and an active user community. Bioconductor is also available as an <u>AMI</u> (Amazon Machine Image) and a series of <u>Docker</u> images.

Nowo



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Variables:

- Alphanumeric symbols, plus "." and "_" are allowed;
- Variables are case sensitive, so "T" is different from "t";

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Assignment "<-":

- t<-3, T<-5, X.1<-9;
- In 2001, the "=" assignment was introduced for compatibility with other languages;

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- Variables are case sensitive, so "T" is different from "t";

Assignment "<-":

- t<-3, T<-5, X.1<-9;
- In 2001, the "=" assignment was introduced for compatibility with other languages;

> t<-3

> k<-"hello"

> a<-1.435275289

Arithmetic operators:

- Addition: +
- Subtraction: -
- Division: /
- Multiplication: *
- Exponentiation: ^
- We can use R as a calculator:

> (3+2)^2
[1] 25
> (7-5)/2
[1] 1
> 1*2*3*4

[1] 24

Data type:

• Numeric, character and logical

- > t<-2.356 #numeric variable</pre>
- > t<-"hello" #character variable</pre>
- > t<-TRUE; f<-FALSE #logical variables

- **Vector**: an ordered collection of data;
- Matrix: two-dimensional generalisations of vectors
- Array: multi-dimensional generalisations of vectors

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```
> t<-c(3, 5.6748, 67, 5) #numeric vector
> t<-c(1, 1:3, c(5, 8), 13)
[1] 1 1 2 3 5 8 13
> t<-c("hello", "how", "are", "you", "?") #character vector</pre>
```

- **Vector**: an ordered collection of data;
- Matrix: two-dimensional generalisations of vectors
- Array: multi-dimensional generalisations of vectors

> t<-c(3, 5.6748, 67, 5) #numeric vector

> length(t) [1] 4

- Vector: an ordered collection of data;
- Matrix: two-dimensional generalisations of vectors
- Array: multi-dimensional generalisations of vectors

```
> matrix(c(1,2,3,4,5,6), ncol=2, nrow=3)
       [,1] [,2]
       [1,] 1 4
       [2,] 2 5
       [3,] 3 6
```

- **Vector**: an ordered collection of data;
- Matrix: two-dimensional generalisations of vectors
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```
> t<- matrix(c(1,2,3,4,5,6), ncol=2, nrow=3)
       [,1] [,2]
[1,] 1 4
[2,] 2 5
[3,] 3 6
> dim(t)
[1] 3 2
```

- **Vector**: an ordered collection of data;
- Matrix: two-dimensional generalisations of vectors
- Array: multi-dimensional generalisations of vectors

```
> matrix(c(1,2,3,4,5,6), ncol=2, nrow=3, dimnames=list(c("Variable_1",
"Variable 2", "Variable 3"), c("factor 1","factor 2")))
```

	factor_1	factor_2
Variable_1	1	4
Variable_2	2	5
Varibale_3	3	6

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```
> array(1:24,dim = c(4, 3, 2), dimnames = list(c("one", "two", "three",
"four"),c("apple", "orange", "pear"),
   c("land", "sea")))
, , land
    apple orange pear
              5 9
        1
one
two2610three3711
four 4
              8 12
, , sea
     apple orange pear
   13 17 21
one
   14 18 22
two
         19 23
    15
three
four 16
         20
               24
```

• **Data frame**: are matrix-like structure but the columns can be of different data types (i.e. numerical and character)

> data	a.frame(veight=c(1,23,4,56,32), gender=c("M","F","F","M","F"))
	weight	gender
1	1	Μ
2	23	F
3	4	F
4	56	Μ
5	32	F

Indexing and selecting:
• Vector:

```
> t<-c(3, 5.6748, 67, 5) #numeric vector
> length(t)
[1] 4
> t[3]
[1] 67
> t[c(2,4)]
[1] 5.6748 5
```

• Matrix:

```
> t<- matrix(c(1,2,3,4,5,6), ncol=2, nrow=3)</pre>
      [,1] [,2]
[1,] 1 4
[2,] 2 5
[3,] 3 6
> dim(t)
[1] 3 2
> t[1,] #row 1
[1] 1 4
> t[,2] #column 2
[1] 4 5 6
```

• Matrix:

```
> t<- matrix(c(1,2,3,4,5,6), ncol=2, nrow=3)
      [,1] [,2]
[1,] 1 4
[2,] 2 5
[3,] 3 6
> dim(t)
[1] 3 2
> t[3,2] #specific cell
[1] 6
```

• Matrix:

```
> t <- matrix(c(1,2,3,4,5,6), ncol=2, nrow=3, dimnames=list(c("Variable_1",
"Variable_2", "Variable_3"), c("factor_1","factor_2")))
```

```
factor_1 factor_2
Variable_1 1 4
Variable_2 2 5
Varibale_3 3 6
> t["Variable_3", "factor_2"]
[1] 6
```

```
> t <- array(1:24,dim = c(4, 3, 2), dimnames = list(c("one", "two",
"three", "four"),c("apple", "orange", "pear"),
   c("land", "sea")))
, , land
    apple orange pear
              5 9
   1
one
two2610three3711
four 4
              8 12
, , sea
    apple orange pear
one 13 17 21
two 14 18 22
         19 23
three 15
four 16
         20
               24
```

```
> t <- array(1:24,dim = c(4, 3, 2), dimnames = list(c("one", "two",
"three", "four"),c("apple", "orange", "pear"),
   c("land", "sea")))
, , land
     apple orange pear
               5 9
        1
one
two2610three3711
                                      > t[3, 1, 2]
                                      [1] 15
four 4
               8 12
                                      > t["two", "orange", "land"]
                                      [1] 6
, , sea
     apple orange pear
   13
          17 21
one
   14 18 22
two
          19 23
three
    15
four 16
          20
                24
```

Basic commands and operations

Deleting:

```
> t<-10:20 #vector
> t
 [1] 10 11 12 13 14 15 16 17 18 19 20
> t[-2] \#remove element in position number 2
 [1] 10 12 13 14 15 16 17 18 19 20
> t1<-t[-2]
> t1
[1] 10 12 13 14 15 16 17 18 19 20
```

Deleting:

```
> t<- matrix(c(1,2,3,4,5,6), ncol=3, nrow=2)</pre>
> t
    [,1] [,2] [,3]
[1,]135[2,]246
> t[-1,] #remove row1
[1] 2 4 6
> t[,-2] #remove col2
    [,1] [,2]
[1,] 1 5
[2,] 2 6
```

Commands/operations:

- paste text strings together;
- append element to vectors;
- operations between vectors and matrices (sum, difference);
- "apply" a specific rule/function to all columns/rows of a matrix;
- match specific elements;
- subset a vector or a matrix;
- ...and many more!!

Commands/operations:

- paste text strings together;
- append element to vectors;
- operations between vectors and matrices (sum, difference);
- "apply" a specific rule/function to all columns/rows of a matrix;
- match specific elements;
- subset a vector or a matrix;
- ...and many more!!
- "which" element satisfies a specific condition...

```
> t<-10:20 #vector
> t
[1] 10 11 12 13 14 15 16 17 18 19 20
> which(t>15)
[1] 7 8 9 10 11
> t[which(t>15)]
[1] 16 17 18 19 20
```

Syntax:

}

for (variable in sequence) {
 statements

Syntax:

```
for (variable in sequence) {
       statements
}
    > for (i in 1:10)
    + print(i)
    + }
    [1] 1
    [1]
         -2
    [1]
         3
    [1]
         4
    [1] 5
    [1]
         6
    [1]
    [1]
         8
         9
    [1]
         10
    [1]
```

```
> for (i in 1:10) {
+ print(paste("hello to our customer number ",
i, sep=""))
+ }
   "hello to our customer number 1"
[1]
   "hello to our customer number 2"
[1]
   "hello to our customer number 3"
[1]
    "hello to our customer number 4"
[1]
   "hello to our customer number 5"
[1]
    "hello to our customer number 6"
[1]
    "hello to our customer number 7"
[1]
   "hello to our customer number 8"
[1]
[1]
   "hello to our customer number 9"
   "hello to our customer number 10"
[1]
```

Comparison operators

equal: == not equal: != greater: > less than: < greater or equal: >= less than or equal: <=

Logical operators

and: & or: | not: !

Comparison operators

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Logical operators

and: & or: | not: !





- > x<--4 > if(x>0){
- + print("Positive number")
- + } else if (x==0) {
- + print("Zero")
- + } else {
- + print("Negative number")
- + }
- [1] "Negative number"

User-defined functions

```
myFunction <- function(arg1, arg2,..) {
    function_body
}</pre>
```

}

myFunction(arg1=..., arg2=...)

User-defined functions

}

```
myFunction <- function(arg1, arg2,..) {
    function_body</pre>
```

myFunction(arg1=..., arg2=...)

```
> myvar<-function(x) {</pre>
+ y < -sum((x-mean(x))^2)/(length(x)-1)
+ return(y)
+ }
> a < -rnorm(6)
> a
[1] -0.9379583 0.6599282 0.6204624
0.4395611 1.0989696 2.4148308
> var(a)
[1] 1.171392
> myvar(a)
[1] 1.171392
```

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- Why R? What can R do?
- Basic commands and operations
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- Descriptive Statistics
- Statistical Modeling
 - Regressions: Linear and Logistic;
 - Time Series;
 - ...
- Multivariate Functions
- Bayesian statistics
- Machine learning
- Inbuilt Packages, contributed packages

Basic statistical analysis

```
#generate random number form normal distribution
> x<-rnorm(10000,0,1)</pre>
```

```
#get a summary of the distribution
> summary(x)
Min. 1st Qu. Median Mean 3rd Qu. Max.
-3.55700 -0.66420 0.00822 0.00131 0.66440 3.90500
```

> boxplot(x, main="Box plot")



Basic statistical analysis

> hist(x, col="blue")



х

Basic statistical analysis

> qqnorm(x)



Theoretical Quantiles

Parallel boxplots

```
> set.seed(12345)
```

```
> weight<-
round(c(rnorm(10,0,1),rnorm(10,2,
1)),3)</pre>
```

```
> group<-rep(c("ctrl","case"),
each=10)</pre>
```

> mydata<-data.frame(weight,
group)</pre>

> plot(weight~group, mydata)

Parallel boxplots

> set.seed(12345)

> weight<round(c(rnorm(10,0,1),rnorm(10,2,
1)),3)</pre>

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We	eight gr	oup
1	0.586	ctrl
2	0.709	ctrl
3	-0.109	ctrl
4	-0.453	ctrl
5	0.606	ctrl
6	-1.818	ctrl
7	0.630	ctrl
8	-0.276	ctrl
9	-0.284	ctrl
10	-0.919	ctrl
11	1.884	case
12	3.817	case
13	2.371	case
14	2.520	case
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17	1.114	case
18	1.668	case
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Parallel boxplots



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```
T-test
```

```
> t.test(weight~group, mydata)
```

```
Welch Two Sample t-test
```

A t-test is a linear regression...

```
> summary(lm(weight~group, mydata))
Call:
lm(formula = weight ~ group, data = mydata)
Residuals:
   Min 10 Median 30 Max
-1.6852 -0.4560 0.0184 0.7238 1.5310
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 2.2860 0.2618 8.733 6.89e-08 ***
groupctrl -2.4188 0.3702 -6.534 3.85e-06 ***
Signif. codes: 0 `***' 0.001 `**' 0.01 `*' 0.05 `.' 0.1 `' 1
```

Residual standard error: 0.8278 on 18 degrees of freedom Multiple R-squared: 0.7034, Adjusted R-squared: 0.6869 F-statistic: 42.69 on 1 and 18 DF, p-value: 3.85e-06

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Parallel boxplots



weight group					
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2	0.709	ctrl			
3	-0.109	ctrl			
4	-0.453	ctrl			
5	0.606	ctrl			
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7	0.630	ctrl			
8	-0.276	ctrl			
9	-0.284	ctrl			
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11	1.884	case			
12	3.817	case			
13	2.371	case			
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15	1.249	case			
16	2.817	case			
17	1.114	case			
18	1.668	case			
19	3.121	case			
20	2.299	case			

- Logistic regression;
- Bayesian analysis (Bayer factor, library(BayesFactor);
- ANOVA;
- Approximate Bayesian Computation (ABC) framework;
- •

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• Github: "GitHub is a development platform inspired by the way you work. From open source to business, you can host and review code, manage projects, and build software alongside 31 million developers."

Coding











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EIG

Eigen tools by Nick Patterson and Alkes Price lab



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Thibaut Jombart thibautjombart

Lecturer in genetic analysis & outbreak response at Imperial College London. R geek. Muay Thai enthusiast. Vocalist of the grind/hardcore band The Brood.

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🎎 Imperial College London

Iondon, UK

➡ thibautjombart@gmail.com

1,198 contributions in the last year

Phylogenetic Methods for Multiple Gene Data

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- Gitlab: Github for companies, university group, enterprises
 - More interaction between users;
 - You can create different projects;
 - You can submit issues and assign them to different lab members;
 - You can use as lab notebook;
 - You can set up mile stones;
 - •

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Repository	#59 · opened 1 month ago by Robert Beyer	updated 1 month ago
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List Board	cell distance is hardcoaded, it shoudl be a paramater from the environment file #57 · opened 4 months ago by Andrea Manica New feature	🌻 🗪 1 updated 4 months ago
Labels Milestones	Add MD5 checksum for input files to output streams #52 · opened 4 months ago by Mario Krapp ② Version 1.0 <u>New feature</u>	🔹 🗪 1 updated 3 months ago
17 Merge Requests 0	rename variable names for consistency with input variables #50 · opened 4 months ago by Mario Krapp	s 🌚 🔿 2 updated 4 months ago
CI / CDOperations	Add Continuous Integration #42 · opened 5 months ago by Mario Krapp	🌒 🎈 🗪 1 updated 5 months ago
Registry	Add parameter values + input file names to output files (demography_output.nc, genealogy_trees.txt) #40 · opened 5 months ago by Robert Beyer	🕲 🗪 2 updated 3 months ago
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🎖 Snippets	#38 · opened 5 months ago by Eppie Jones New feature	updated 5 months ago
✓ Collapse sidebar	Find optimal number for genealogy trees to decrease overall runtime of MC sweep #37 · opened 5 months ago by Mario Krapp <u>New feature</u>	S 🏐 🗪 0 updated 5 months ago

• Github and gitlab...why???

- It helps to promote reproducible science;
- More transparent and clear specifically for data analysis;
- Working together (with other users) helps to improve and grow faster;

Conclusions:

- R is a flexible language for data analysis, summary, visualisation and modelling;
- R community is vast, lots of support and developers (R package);
- Sharing code, science reproducibility and help the scientific community to grow faster;