R language basics, part 2 HUST Bioinformatics course series

Wei-Hua Chen (CC BY-NC 4.0)

02 August, 2021

section 1: TOC

前情提要

vector & matrix:

- declaration
- manipulation
- arithmetic
- transposition

vectorization

- every is a vector!!
- vectorization verses loop (will be explained later)
- advantages using vectorization

今次预报

- 1 data.frame, tibble
- read files from harddrive (IO)
- ∮ factors (初步)
- exercises & homework

section 2: data.frame and tibble

data.frame, outline

- what is a data.frame???
- how to make a data.frame
- how to add row(s)/col(s) to an existing data.frame how to combine two data.frames
- 4 how to manipulate a data.frame

2.1 what is a data.frame?

眼见为实:

```
library(tidyverse); ## 装入包
knitr::kable( head(mpg) ); ## 显示前几行数据
```

manufacturer	model	displ	year	cyl	trans	drv	cty	hwy	fl	class
audi	a4	1.8	1999	4	auto(I5)	f	18	29	р	compact
audi	a4	1.8	1999	4	manual(m5)	f	21	29	р	compact
audi	a4	2.0	2008	4	manual(m6)	f	20	31	р	compact
audi	a4	2.0	2008	4	auto(av)	f	21	30	p p	compact
audi	a4	2.8	1999	6	auto(l5)	f	16	26	p p	compact
audi	a4	2.8	1999	6	manual(m5)	f	18	26	p	compact

注意 head() tail() 的用法和参数

head 和 tail 的用法

```
nrow(mpg); ## total number of rows
```

[1] 234

```
knitr::kable( head(mpg, n=3)); ## 显示前 3 行数据
```

manufacturer	model	displ	year	cyl	trans	drv	cty	hwy	fl	class
audi audi audi	a4 a4 a4	1.8 1.8 2.0	1999 1999 2008	4		f f f	18 21 20	29 29 31	p p p	compact compact compact

```
knitr::kable( tail(mpg, n=3)); ## 显示最后 3 行数据
```

manufacturer	model	displ	year	cyl	trans	drv	cty	hwy	fl	class
volkswagen	passat	2.8	1999	6	auto(I5)	f	16	26	р	midsize
volkswagen	passat	2.8	1999	6	manual(m5)	f	18	26	p	midsize
volkswagen	passat	3.6	2008	6	auto(s6)	f	17	26	p	midsize

data.frame 的组成与常用函数

组成

- 二维表格
- 由不同列组成;每列是一个 vector,不同列的数据类型可以不同,但 一列只包括一种数据类型 (int, num, chr ...)
- 各列的长度相同

常用 functions

- nrow();
- ncol();
- dim();
- ..

structure of data.frame: str 函数

```
str( mpg );
## tibble [234 x 11] (S3: tbl df/tbl/data.frame)
   $ manufacturer: chr [1:234] "audi" "audi" "audi" "audi" ...
   $ model
                 : chr [1:234] "a4" "a4" "a4" "a4" ...
## $ displ
                 : num [1:234] 1.8 1.8 2 2 2.8 2.8 3.1 1.8 1.8 2 ...
                 : int [1:234] 1999 1999 2008 2008 1999 1999 2008 1999 1999 2008 ...
## $ year
## $ cvl
                 : int [1:234] 4 4 4 4 6 6 6 4 4 4 ...
                 : chr [1:234] "auto(15)" "manual(m5)" "manual(m6)" "auto(av)" ...
## $ trans
                 : chr [1:234] "f" "f" "f" "f" ...
   $ drv
   $ ctv
                 : int [1:234] 18 21 20 21 16 18 18 18 16 20 ...
                 : int [1:234] 29 29 31 30 26 26 27 26 25 28 ...
   $ hwy
                 : chr [1:234] "p" "p" "p" "p" ...
   $ fl
   $ class
                 : chr [1:234] "compact" "compact" "compact" "compact" ...
```

注: Tibble class 是 data.frame 的升级版本;本课程将二者混用,以 tibble 为主。用?mpg 命令查看 mpg 各列的意义

2.2 make a new data.frame

使用 data.frame 函数创建新的 data.frame:

90 3 11 39 1 93 24 73 82 4

"A" "C" "A" "C" ...

```
## data.frame()
( dat2 <-
 data.frame( data = sample( 1:100, 10 ),
       group = sample( LETTERS[1:3], 10, replace = TRUE),
       data2 = 0.1)
);
     data group data2
       90
                  0.1
                 0.1
## 3
       11
                 0.1
## 4
       39
                 0.1
## 5
                 0.1
## 6
       93
                 0.1
## 7
       24
                 0.1
## 8
       73
                 0.1
## 9
       82
                 0.1
## 10
                   0.1
str(dat2);
## 'data frame':
                    10 obs. of 3 variables:
```

\$ data : int

\$ group: chr

イロト 不問 トイラト イラト

2.3 how to add row(s)/col(s) to an existing data.frame

先创建"表头",再填充

```
df2 <- data.frame( x = character(), y = integer(), z = double() , stringsAsFactors = FALSE );
##
df2 <- rbind( df2, data.frame( x = "a", y = 1L, z = 2.2 ) );
df2 <- rbind( df2, data.frame( x = "b", y = 2, z = 4.4 ) );
df2;</pre>
```

```
## x y z
## 1 a 1 2.2
## 2 b 2 4.4
```

注意

- 使用 rbind 函数
- 新的一行用 data.frame 定义,其 "表头" 需要与合并表相同

问题:

以下代码能顺利执行吗?

```
## 注意这里的 data.frame 会有多行 ...
df2 <- rbind( df2, data.frame( x = c("a","b","c"), y = 1L, z = 2.2 ));
```

data.frame, add column

用 cbind 函数增加列:column bind

```
m <- cbind(1, 1:7); ## 产生两列数据 7 行数据 ..
( m <- cbind(m, 8:14)); ## 增加一列 也有 7 行数据 ...
```

```
## [1,] 1 1 8
## [2,] 1 2 9
## [3,] 1 3 10
## [4,] 1 4 11
## [5,] 1 5 12
## [6,] 1 6 13
## [7,] 1 7 14
```

[,1] [,2] [,3]

data.frame, add column, cont.

自行练习,回答代码中的问题:

```
## 1. 生成一个 10 行 2 列的 data.frame
df3 <- data.frame( data = 1:10, group = c("A","B"));

## 2. 增加一列, 其长度是 1, 可以吗?
cbind(df3, newcol = 1);

## 3. 增加一列, 其长度是 10, 可以吗?
cbind(df3, newcol = 1:10);

## 4. 增加一列, 其长度是 2, 可以吗?
cbind(df3, newcol = 1:2);

## 5. 增加一列, 其长度是 3, 可以吗?
cbind(df3, newcol = 1:3);
```

data.frame, 以列方式合并两个 data.frame

同样使用 cbind

```
df4 \leftarrow data.frame(data = 1:10, group = c("A", "B"));
df5 <- data.frame( length = sample(1:100, 10), width = sample(1:100, 10) );
## --
head( cbind( df4, df5 ) ):
    data group length width
## 1
                   36
                         76
## 2
       2
               71
                         88
## 3
       3 A 96
       4 B 74 79
## 4
## 5
                   32
                        86
## 6
                         26
## 如果 一个 df 的行数少于另一处怎么办?
df6 \leftarrow data.frame(length = sample(1:100, 5), width = sample(1:100, 5));
head( cbind( df4, df6 ) ):
    data group length width
## 1
                   71
                         80
             B 56
```

A 100

55

65

62

20

3

4

3

4

5

2.4 how to manipulate a data.frame

自行尝试以下操作

```
## 取行:
df4[ 1:2, ];
## 取列
df4[, 2]
## 取行, 重新排序
df4[c(2,3,1),]
## 取列, 重新排序
df4[, c(2,1)]
## 替换一行:
df4[1, ] <- data.frame( data = 100, group = "A" );
## 替换一列:
df4[, "data"] <- sample( 1:100, 5 );
```

tibble, outline

- 6 how to make a tibble
- how to add row(s)/col(s) to an existing tibble how to combine two tibble
- how to manipulate a tibble

2.5 make a new tibble

\FontSmall

```
```r
library(tibble); ## 或 library(tidiverse);
用 tibble 函数创建, 用法和 data.frame() 相似
(dat <-
 tibble (data = sample (1:100, 10),
 group = sample(LETTERS[1:3], 10, replace = TRUE),
 data2 = 0.1)
);
A tibble: 10 \times 3
##
 data group data2
##
 <int> <chr> <dbl>
 0.1
##
 29 B
```

# str( dat )

str(dat);

## 查看得到的数据结构

```
tibble [10 x 3] (S3: tbl_df/tbl/data.frame)
$ data : int [1:10] 29 21 25 36 69 41 88 30 46 39
$ group: chr [1:10] "B" "A" "B" "C" ...
$ data2: num [1:10] 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1
```

# 创建 tibble 的另一种方式 (by row)

```
A tibble: 2 x 3
x y z
<chr> <dbl> <dbl> dbl> ## 1 a 2 3.6
2 b 1 8.5
```

# 2.6 how to add row(s)/col(s) to an existing tibble

```
新 tibble, with defined columns ... 创建表头
tb <- tibble(x = character(), y = integer(), z = double());
dim(tb);

[1] 0 3

增加行 ...
tb <- add_row(tb, x = "a", y = 2, z = 3.6);
tb <- add_row(tb, x = "b", y = 1, z = 8.5);

显示
tb;
```

```
A tibble: 2 x 3
x y z
<chr> <dbl> <dbl> <dbl> ## 1 a 2 3.6
2 b 1 8.5
```

# tibble, add\_row 插入时指定行号

```
生成一个 tibble
df <- tibble(x = 1:3, y = 3:1);
在第二行之前插入
df <- add_row(df, x = 4, y = 0, .before = 2);
df;
```

```
A tibble: 4 x 2
x y
<dbl> <dbl> 1 3
2 4 0
3 2 2
4 3 1
```

# tibble, add\_row 插入多行, 插入另一个 tibble??

```
插入多行
df <- add_row(df, x = 4:5, y = 0:-1);

插入另一个 tibble (与另一个 tibble 合并) ???
df2 <- tibble(x = as.double(200:202), y = as.double(1000:1002));
df3 <- add_row(df, df2); ## 不能运行 ...
```

# tibble, 合并多个 tibble

-1

1001

## 7

## 8

## 9

200 1000

201

202 1002

## tibble, add column

```
A tibble: 2 x 6
x y z a b c
<chr> <dbl> <dbl> <dbl> <chr> <chr> = 1 a 2 3.6 98 A CHEN
2 b 1 8.5 98 B WANG
```

## tibble, 按列合并两个 tibble?

#### 练习:

- 尝试用 add\_column 合并两个 tibble
- ② 使用 bind\_cols 合并两个 tibble

# 2.7 how to manipulate a tibble

### 自行练习以熟悉以下操作:

```
取得行
tb3[c(1,2),];
取得列,接顺序取列
tb3[,c("z", "y")];
替换列
tb3[["z"]] <- c(4.6, 5.5);
替换行
tb3[1,] <- tibble(x = "d", y = 20, z = 46, a = 10, b = "C", c = "LILI");
```

# 2.8 tibble 与 data.frame 之间相互转换

```
library(tibble)
head(as_tibble(iris));
```

```
A tibble: 6 x 5
 Sepal.Length Sepal.Width Petal.Length Petal.Width Species
 <dbl>
##
 <dbl>
 <dbl>
 <dbl> <fct>
1
 5.1
 3.5
 1.4
 0.2 setosa
 4.9
2
 3
 1.4
 0.2 setosa
3
 4.7
 3.2
 1.3
 0.2 setosa
 4.6
 3.1
 1.5
 0.2 setosa
 3.6
5
 1.4
 0.2 setosa
6
 5.4
 3.9
 1.7
 0.4 setosa
```

note: iris data set gives the measurements in centimeters of the variables sepal length and width and petal length and width, respectively, for 50 flowers from each of 3 species of iris (鸢尾属植物). The species are Iris setosa, versicolor, and virginica.

## tibble to dataframe

```
library(tibble)
as.data.frame(head(as_tibble(iris));
```

```
Sepal.Length Sepal.Width Petal.Length Petal.Width Species
1
 5.1
 3.5
 1.4
 0.2
 setosa
2
 4.9
 3.0
 1.4
 0.2 setosa
3
 4.7
 3.2
 1.3
 0.2 setosa
 4.6
 3.1
 1.5
4
 0.2 setosa
5
 5.0
 3.6
 1.4
 0.2 setosa
6
 5.4
 3.9
 1.7
 0.4 setosa
```

## 2.9 differences between tibble and data.frame

#### tibble evaluates columns sequentially

```
rm(x,v); ## 删除可能存在的 x , y
tibble(x = 1:5, y = x ^ 2); ## 可以用 tibble 这样做
A tibble: 5 x 2
 <int> <dbl>
1
4 4 16
5 5 25
练习:
data.frame(x = 1:5, v = x^2): ## 但 data.frame 不行
Error in data.frame(x = 1:5, y = x^2): object 'x' not found
```

## data.frame 在取 subset 操作时,会造成困扰

```
df1 \leftarrow data.frame(x = 1:3, y = 3:1);
class(df1[, 1:2]);
[1] "data.frame"
subset 操作: 取一列, 期待得到一个 data.frame ()
class(df1[, 1]); ## 结果得到一个 vector ...
[1] "integer"
而 tibble 则不会
df2 \leftarrow tibble(x = 1:3, v = 3:1):
class(df2[, 1]); ## 永远都是 tibble
[1] "tbl df"
 "tbl"
 "data.frame"
```

#### tibble 可以进行可控的数据类型转换:

```
class(df2[[1]]); ## 取一列, 转换为 vector

[1] "integer"

class(df2$x); ## 用 [[]] 或 $ 都可以哦

[1] "integer"
```

```
recycling
data.frame(a = 1:6, b = LETTERS[1:2]): ## data.frame 可以!!!
2 2 B
3 3 A
4 4 B
5 5 A
6 6 B
tibble(a = 1:6, b = LETTERS[1:2]): ## 但 tibble 不行!!!
Error: Tibble columns must have compatible sizes.
* Size 6: Existing data.
* Size 2: Column `b`.
i Only values of size one are recycled.
注意 tibble 的 recycling 仅限于长度为 1 或等长;而 data.frame 则为整除即
可。
```

# practises for recycling

```
tibble(a = 1, b = 1:3);
A tibble: 3 x 2
 <dbl> <int>
2 1
3 1
tibble(a = 1:3, b = 1);
A tibble: 3 x 2
 а
 <int> <dbl>
1
tibble(a = 1:3, c = 1:2);
Error: Tibble columns must have compatible sizes.
```

## \* Size 3: Existing data.
## \* Size 2: Column `c`.

## i Only values of size one are recycled.

### data.frame will do partial matching

```
df <- data.frame(abc = 1)
df$ab; ## unwanted result ...

[1] 1

-- but tibble will never do it;
df2 <- tibble(abc = 1)
df2$a; ## produce a warning and return NULL

Warning: Unknown or uninitialised column: `a`.</pre>
NULL
```

### 2.10 data.frame 和 tibble 的高级使用技巧

#### attach 和 detach

```
head(iris, n = 3):
 Sepal.Length Sepal.Width Petal.Length Petal.Width Species
 5.1
 3.5
 1.4
 0.2 setosa
 4.9
 3.0 1.4 0.2 setosa
2
3
 4.7
 3.2
 1.3
 0.2 setosa
head(iris$Sepal.Length , n = 10); ## 用 $ 操作符取得一列 ...
 [1] 5.1 4.9 4.7 4.6 5.0 5.4 4.6 5.0 4.4 4.9
attach(iris):
head(Sepal.Length , n = 10); ## 直接用列名获取数据;
```

detach(iris): ## 取消 attach 操作 --

[1] 5.1 4.9 4.7 4.6 5.0 5.4 4.6 5.0 4.4 4.9

# with 函数

```
with(iris, head(Sepal.Length, n = 10)); ## 用 with 也可以实现
```

```
[1] 5.1 4.9 4.7 4.6 5.0 5.4 4.6 5.0 4.4 4.9
```

## within 函数

### 也可以用 within 对多列数据进行修改

```
head(airquality , n = 3);
 Ozone Solar.R Wind Temp Month Day
1
 41
 190 7.4
 67
2
 36 118 8.0
 72 5 2
3
 12
 149 12.6
 74
aq <- within(airquality, {
 # Notice that multiple vars can be changed
 10zone <- log(Ozone)
 Month <- factor(month.abb[Month])</pre>
 cTemp <- round((Temp - 32) * 5/9, 1) # From Fahrenheit to Celsius
 S.cT <- Solar.R / cTemp # using the newly created variable
 rm(Day, Temp) ## 删除特定列 ...
});
head(aq, n = 3);
```

41

12

## 1

## 2

## 3

Ozone Solar.R Wind Month

36 118 8.0

190 7.4

149 12.6

S.cT cTemp 10zone

May 9.793814 19.4 3.713572

May 5.315315 22.2 3.583519

May 6.394850 23.3 2.484907

section 3: file IO: read a file into tibble & write tibble to a file

### read from files

### 使用 functions from the readr package

```
readr is part of tidyverse
library(tidyverse); ## or alternatively
library(readr);
```

#### available functions

- read\_csv(): comma separated (CSV) files
- read\_tsv(): tab separated files
- read\_delim(): general delimited files
- read\_fwf(): fixed width files
- read\_table(): tabular files where columns are separated by white-space.
- read\_log(): web log files

### read a file into tibble

```
myiris <- read_csv("data/talk03/iris.csv");

##

-- Column specification ------
cols(
Sepal.Length = col_double(),
Sepal.Width = col_double(),
Petal.Length = col_double(),
Petal.Width = col_double(),
Species = col_character()
)</pre>
```

注意输出的 columns 定义

## read with predifined column types

```
myiris2 <- read_csv("data/talk03/iris.csv", col_types = cols(
 Sepal.Length = col_double(),
 Sepal.Width = col_double(),
 Petal.Length = col_double(),
 Petal.Width = col_double(),
 Species = col_character()
));</pre>
```

### how to read from other formats??

#### try the following packages for other formats

- haven SPSS, Stata, and SAS files
- readxl excel files (.xls and .xlsx)
- DBI databases
- jsonlite json
- xml2 XML
- httr Web APIs
- rvest HTML (Web Scraping)

### write to files

#### use the following functions to write object(s) to external files

- Comma delimited file: write\_csv(x, path, na = "NA", append = FALSE, col\_names = !append)
- File with arbitrary delimiter: write\_delim(x, path, delim = " ", na = "NA", append = FALSE, col\_names = !append)
- CSV for excel: write\_excel\_csv(x, path, na = "NA", append = FALSE, col\_names = !append)
- String to file: write\_file(x, path, append = FALSE)
- String vector to file, one element per line: write\_lines(x,path, na = "NA", append = FALSE)
- Object to RDS file: write\_rds(x, path, compress = c("none", "gz", "bz2", "xz"), ...)
- Tab delimited files: write\_tsv(x, path, na = "NA", append = FALSE, col\_names = !append)

# 练习

```
write iris to outfiles of various formats
write_csv(iris, "iris.csv");
write_tsv(iris, "iris.tsv", quote_escape = "none");
```

check readr cheatsheet (please Google).

# section 4: 练习 & 作业

### 练习 & 作业

- Exercises and homework 目录下 talk03-homework.Rmd 文件;
- 完成时间: 见钉群的要求

### 小结

#### 今次提要

- data.frame, tibble
- ② 定义、区别、转化
- read files from harddrive (IO)

#### 下次预告

- factor: R 另一个超级重要且难以上手的概念
- 基础和进阶绘图 (配合 factor 讲解)

#### important

all codes are available at Github: https://github.com/evolgeniusteam/R-for-bioinformatics