R for bioinformatics, data wrangler, part 1

HUST Bioinformatics course series

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section 1: TOC

前情提要

1. IO, project management, working environment management
2. factors: R 中最重要的概念之一

- factors 基本概念
- factors 操作
- factors 在做图中的使用
- ggplot2 和 dplyr 初步

今次提要

- pipe
- dplyr 、tidyr (超级强大的数据处理) part 1

section 2: pipe

什么是 pipe ？

- pipe 就是 %>%
- it comes from the `magrittr` package by **Stefan Milton Bache**
- Packages in the tidyverse load %>% for you automatically, so you don't usually load magrittr explicitly.
- 实质是中间值的传递

示例：

```r
## 比如：这段代码可以合并为：
library(tidyverse); ## 装入包
library(magrittr);
a <- subset( swiss, Fertility > 20 );
cor.test(a$Fertility, a$Education);
```

```
##
##  Pearson's product-moment correlation
##
## data:  a$Fertility and a$Education
## t = -5.9536, df = 45, p-value = 3.659e-07
## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
##  -0.7987075 -0.4653206
## sample estimates:
```

pipe 版本

```
## -- 新代码 ...
swiss %>%
  subset(., Fertility > 20) %$%
  cor.test( Education , Fertility );
```

```
##
##  Pearson's product-moment correlation
##
## data:  Education and Fertility
## t = -5.9536, df = 45, p-value = 3.659e-07
## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
##  -0.7987075 -0.4653206
## sample estimates:
##        cor
## -0.6637889
```

是否所有函数都支持 pipe ？

是的。

通常需要用 . 指代传递来的数据，并以参数的形式赋予下游函数:

```
swiss %>% do( head(.,  n = 4 ) );
```

```
##              Fertility Agriculture Examination Education Catholic
## Courtelary        80.2        17.0          15        12     9.96
## Delemont          83.1        45.1           6         9    84.84
## Franches-Mnt      92.5        39.7           5         5    93.40
## Moutier           85.8        36.5          12         7    33.77
##              Infant.Mortality
## Courtelary               22.2
## Delemont                 22.2
## Franches-Mnt             20.2
## Moutier                  20.3
```

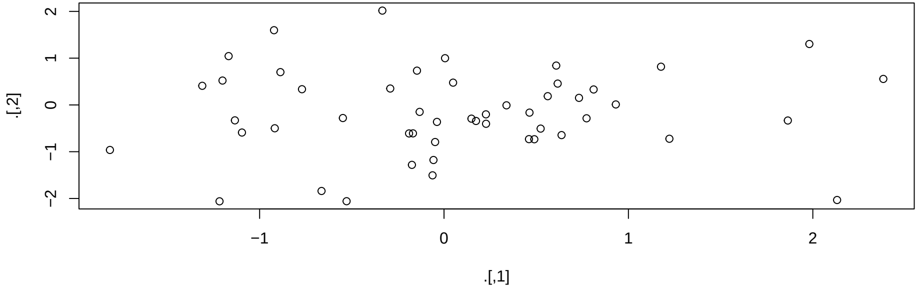
```
## 也可以写为
swiss %>% head(.,  n = 4 );
```

```
##              Fertility Agriculture Examination Education Catholic
## Courtelary        80.2        17.0          15        12     9.96
## Delemont          83.1        45.1           6         9    84.84
## Franches-Mnt      92.5        39.7           5         5    93.40
## Moutier           85.8        36.5          12         7    33.77
##              Infant.Mortality
```

其它形式的 pipe

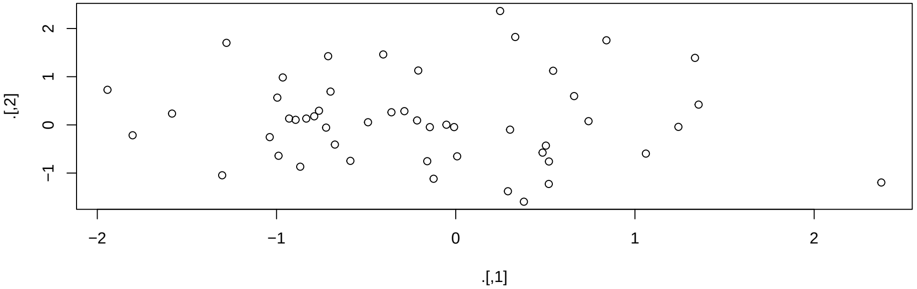
%T>% ：返回上游的值（???）

```
## 示例：res1 是空值 ...
res1 <-
  rnorm(100) %>%
    matrix(ncol = 2) %>%
    plot();
```



%T>%: 返回上游值 (left-side values)

```r
## 示例: res2 是 matrix() 内容 ...
res2 <-
  rnorm(100) %>%
    matrix(ncol = 2) %T>%
    plot();
```



%T>%: 返回上游值 (left-side values), cont.

```r
head(res2);
```

```
##            [,1]       [,2]
## [1,] -0.9955958  0.5655098
## [2,] -0.3588513  0.2618761
## [3,]  0.3802336 -1.5943304
## [4,] -0.6742937 -0.4085359
## [5,]  0.5434302  1.1228771
## [6,] -0.1590719 -0.7534904
```

%$% : attach ???

```
attach( mtcars ); ## note the warning message ...
```

```
## The following object is masked from package:ggplot2:
##
##     mpg
```

```
cor.test( cyl, mpg ); ## 汽缸数与燃油效率
```

```
##
##  Pearson's product-moment correlation
##
## data:  cyl and mpg
## t = -8.9197, df = 30, p-value = 6.113e-10
## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
##  -0.9257694 -0.7163171
## sample estimates:
##       cor
## -0.852162
```

%$% : attach ??? , cont.

```r
detach( mtcars );
with( mtcars, cor.test( cyl, mpg ) );
```

```
##
##  Pearson's product-moment correlation
##
## data:  cyl and mpg
## t = -8.9197, df = 30, p-value = 6.113e-10
## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
##  -0.9257694 -0.7163171
## sample estimates:
##       cor
## -0.852162
```

%$% : attach ??? , cont.

```r
mtcars %$%
  cor.test( cyl, mpg );
```

```
##
##  Pearson's product-moment correlation
##
## data:  cyl and mpg
## t = -8.9197, df = 30, p-value = 6.113e-10
## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
##  -0.9257694 -0.7163171
## sample estimates:
##       cor
## -0.852162
```

其它 pipe 及注意事项

```r
## 双向 pipe
mtcars %<>% transform(cyl = cyl * 2);
```

注

- pipe 的使用可以使思路更清晰
- 因此，尽量使用 %>% （方向明确），而不使用其它方向不明确的 pipe

section 3: data wrangler - dplyr

dplyr

what is `dplyr` ?

- the next iteration of plyr,
- focusing on only data frames (also tibble),
- row-based manipulation,
- dplyr is faster and has a more consistent API.

Figure 1: dplyr logo

dplyr, overview

dplyr provides a consistent set of verbs that help you **solve the most common data manipulation challenges**:

- select() 选择列，根据列名规则
- filter() 按规则过滤行
- mutate() 增加新列，从其它列计算而得（不改变行数）
- summarise() 将多个值转换为单个值（通过 mean, median, sd 等操作），生成新列（总行数减少，通常与 `group_by` 配合使用）
- arrange() 对行进行排序

dplyr 安装

```r
# The easiest way to get dplyr is to install the whole tidyverse:
install.packages("tidyverse")

# Alternatively, install just dplyr:
install.packages("dplyr")
```

Development version

```r
# install.packages("devtools")
devtools::install_github("tidyverse/dplyr")
```

Get the cheatsheet at here

an example of dplyr

get the data ready

```
mouse.tibble <- read_delim( file = "data/talk04/mouse_genes_biomart_sep2018.txt",
                            delim = "\t", quote = "" );
```

```
## Rows: 138532 Columns: 6
## -- Column specification --------------------------------------------------------
## Delimiter: "\t"
## chr (5): Gene stable ID, Transcript stable ID, Protein stable ID, Transcript...
## dbl (1): Transcript length (including UTRs and CDS)
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

查看 mouse.tibble 的内容

```
( ttype.stats <- mouse.tibble %>% count( `Transcript type` ) %>% arrange(-n) );
```

```
## # A tibble: 48 x 2
##    `Transcript type`            n
##    <chr>                    <int>
##  1 protein_coding           58384
##  2 retained_intron          21021
##  3 processed_transcript     15572
##  4 processed_pseudogene      9425
##  5 lincRNA                   8557
##  6 nonsense_mediated_decay   6755
##  7 antisense                 4289
##  8 TEC                       3265
##  9 unprocessed_pseudogene    2650
## 10 miRNA                     2265
## # i 38 more rows
```

查看 mouse.tibble 的内容，cont.

```
( chr.stats <- mouse.tibble %>% count( `Chromosome/scaffold name` ) %>% arrange(-n) );
```

```
## # A tibble: 117 x 2
##    `Chromosome/scaffold name`     n
##    <chr>                      <int>
##  1 7                          12344
##  2 2                          10877
##  3 5                           8955
##  4 11                          8673
##  5 1                           8553
##  6 9                           8030
##  7 6                           7845
##  8 4                           7573
##  9 3                           6938
## 10 10                          6568
## # i 107 more rows
```

分析任务

1. 将染色体限制在常染色体和 XY 上（去掉未组装的小片段）；处理行
2. 将基因类型限制在 protein_coding, miRNA 和 lincRNA 这三种；处理行
3. 统计每条染色体上不同类型基因（protein_coding, miRNA, lincRNA）的数量
4. 按染色体（正）、基因数量（倒）进行排序

用 dplyr 实现

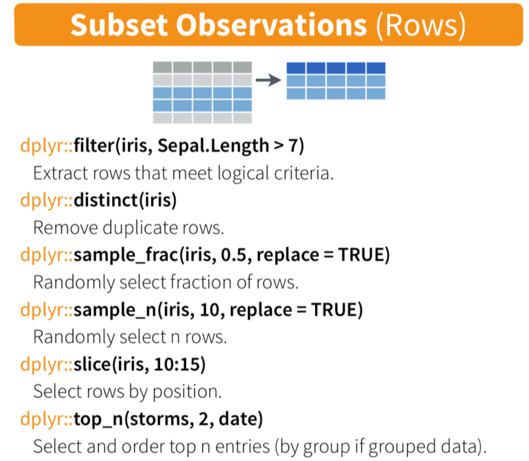
```
dat <- mouse.tibble %>%
  ## 1.

  filter( `Chromosome/scaffold name` %in% c( 1:19, "X", "Y" )    ) %>%

  ## 2.
  filter( `Transcript type` %in% c( "protein_coding", "miRNA", "lincRNA" ) ) %>%

  ## change column name ...
  select( CHR = `Chromosome/scaffold name`, TYPE = `Transcript type`,
          GENE_ID = `Gene stable ID`,
          GENE_LEN =  `Transcript length (including UTRs and CDS)`  ) %>%

  ## 3.
  group_by( CHR, TYPE ) %>%
  summarise( count = n_distinct( GENE_ID ), mean_len = mean( GENE_LEN ) ) %>%

  ## 4.
  arrange(  CHR  , desc( count ) );
```

```
## `summarise()` has grouped output by 'CHR'. You can override using the `.groups`
## argument.
```

检查运行结果

CHR	TYPE	count	mean_len
1	protein_coding	1200	2699.59009
1	lincRNA	347	1206.76149
1	miRNA	128	97.97656
10	protein_coding	1020	2408.16454
10	lincRNA	398	1220.35543
10	miRNA	91	89.87912
11	protein_coding	1640	2431.87666
11	lincRNA	189	1134.49174
11	miRNA	137	87.48905
12	protein_coding	644	2523.94822
12	lincRNA	327	1277.14979
12	miRNA	146	86.24658
13	protein_coding	831	2380.41499
13	lincRNA	428	1251.04552
13	miRNA	97	105.52577

dplyr 中其它取行的操作



Subset Observations (Rows)

dplyr::**filter(iris, Sepal.Length > 7)**
Extract rows that meet logical criteria.

dplyr::**distinct(iris)**
Remove duplicate rows.

dplyr::**sample_frac(iris, 0.5, replace = TRUE)**
Randomly select fraction of rows.

dplyr::**sample_n(iris, 10, replace = TRUE)**
Randomly select n rows.

dplyr::**slice(iris, 10:15)**
Select rows by position.

dplyr::**top_n(storms, 2, date)**
Select and order top n entries (by group if grouped data).

Figure 2: dplyr 与行相关的操作

课堂练习：使用常用函数解决问题

先创建一个新 tibble

```
grades <- tibble( "Name" = c("Weihua Chen", "Mm Hu", "John Doe", "Jane Doe",
                             "Warren Buffet", "Elon Musk", "Jack Ma"),
                  "Occupation" = c("Teacher", "Student", "Teacher", "Student",
                                   rep( "Entrepreneur", 3 ) ),
                  "English" = sample( 60:100, 7 ),
                  "ComputerScience" = sample(80:90, 7),
                  "Biology" = sample( 50:100, 7),
                  "Bioinformatics" = sample( 40:90, 7)
                  );
grades;
```

```
## # A tibble: 7 x 6
##   Name          Occupation   English ComputerScience Biology Bioinformatics
##   <chr>         <chr>          <int>           <int>   <int>          <int>
## 1 Weihua Chen   Teacher           65              80      95             42
## 2 Mm Hu         Student           63              83      99             51
## 3 John Doe      Teacher           94              82      82             86
## 4 Jane Doe      Student           81              89      65             57
## 5 Warren Buffet Entrepreneur      85              85     100             52
## 6 Elon Musk     Entrepreneur      75              81      83             82
## 7 Jack Ma       Entrepreneur      87              87      66             49
```

use gather & dplyr functions

Question: 1. 每个人平均成绩是多少？2. 哪个人的平均成绩最高？

```
grades.melted <- grades %>%
  gather( course, grade, -Name, -Occupation, na.rm = T );

## 检查数据 ...
knitr::kable( head(grades.melted) );
```

Name	Occupation	course	grade
Weihua Chen	Teacher	English	65
Mm Hu	Student	English	63
John Doe	Teacher	English	94
Jane Doe	Student	English	81
Warren Buffet	Entrepreneur	English	85
Elon Musk	Entrepreneur	English	75

成绩分析，cont

```
grades.melted %>%
  group_by(Name, Occupation) %>%
  summarise( avg_grades = mean( grade ), courses_count = n() ) %>%
  arrange( -avg_grades );
```

```
## `summarise()` has grouped output by 'Name'. You can override using the
## `.groups` argument.

## # A tibble: 7 x 4
## # Groups:   Name [7]
##   Name          Occupation   avg_grades courses_count
##   <chr>         <chr>             <dbl>         <int>
## 1 John Doe      Teacher            86               4
## 2 Warren Buffet Entrepreneur       80.5             4
## 3 Elon Musk     Entrepreneur       80.2             4
## 4 Mm Hu         Student            74               4
## 5 Jane Doe      Student            73               4
## 6 Jack Ma       Entrepreneur       72.2             4
## 7 Weihua Chen   Teacher            70.5             4
```

```
## 显示最终结果
knitr::kable( head( grades.melted ) );
```

Name	Occupation	course	grade
Weihua Chen	Teacher	English	65

use gather & dplyr functions

问题： 每个人的最强科目是什么 ??

```
## 步骤 1: 排序:
grades.melted2 <-
  grades.melted %>%
  arrange( Name, -grade );

knitr::kable( head(grades.melted2) );
```

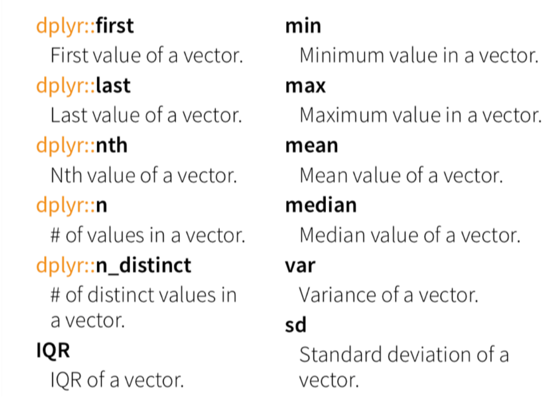
Name	Occupation	course	grade
Elon Musk	Entrepreneur	Biology	83
Elon Musk	Entrepreneur	Bioinformatics	82
Elon Musk	Entrepreneur	ComputerScience	81
Elon Musk	Entrepreneur	English	75
Jack Ma	Entrepreneur	English	87
Jack Ma	Entrepreneur	ComputerScience	87

最强科目问题，cont.

```
grades.melted2 %>%
  group_by(Name) %>%
  summarise( best_course = first( course ),
             best_grade = first( grade ),
             avg_grades = mean( grade ) ) %>%
  arrange( -avg_grades );
```

```
## # A tibble: 7 x 4
##   Name          best_course     best_grade avg_grades
##   <chr>         <chr>                <int>      <dbl>
## 1 John Doe      English                 94       86
## 2 Warren Buffet Biology                100       80.5
## 3 Elon Musk     Biology                 83       80.2
## 4 Mm Hu         Biology                 99       74
## 5 Jane Doe      ComputerScience         89       73
## 6 Jack Ma       English                 87       72.2
## 7 Weihua Chen   Biology                 95       70.5
```

dplyr::summarise 的其它操作



dplyr::**first**	First value of a vector.
dplyr::**last**	Last value of a vector.
dplyr::**nth**	Nth value of a vector.
dplyr::**n**	# of values in a vector.
dplyr::**n_distinct**	# of distinct values in a vector.
IQR	IQR of a vector.
min	Minimum value in a vector.
max	Maximum value in a vector.
mean	Mean value of a vector.
median	Median value of a vector.
var	Variance of a vector.
sd	Standard deviation of a vector.

Figure 3: dplyr::summarise 可用的操作

练习考察

问题 1： 每个人的最差科目是什么 ??

** 列的使用！ **，以 starwars tibble 为例

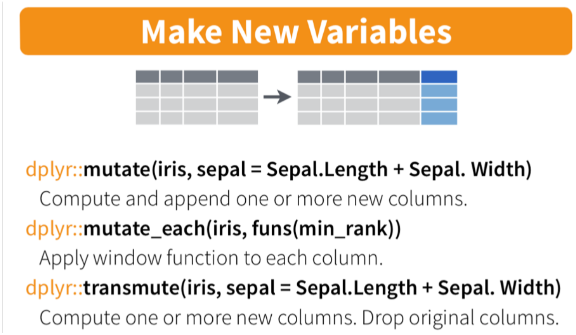
```r
head(starwars);
```

```
## # A tibble: 6 x 14
##   name      height  mass hair_color skin_color eye_color birth_year sex   gender
##   <chr>      <int> <dbl> <chr>      <chr>      <chr>          <dbl> <chr> <chr>
## 1 Luke Sky~    172    77 blond      fair       blue            19   male  mascu~
## 2 C-3PO        167    75 <NA>       gold       yellow         112   none  mascu~
## 3 R2-D2         96    32 <NA>       white, bl~ red             33   none  mascu~
## 4 Darth Va~    202   136 none       white      yellow          41.9 male  mascu~
## 5 Leia Org~    150    49 brown      light      brown           19   fema~ femin~
## 6 Owen Lars    178   120 brown, gr~ light      blue            52   male  mascu~
## # i 5 more variables: homeworld <chr>, species <chr>, films <list>,
## #   vehicles <list>, starships <list>
```

note 包含 87 行 13 列，星战部分人物的信息，包括身高、体重、肤色等

用 ?starwars 获取更多帮助

dplyr::mutate - 产生新列，不改变行数


Make New Variables

dplyr::mutate(iris, sepal = Sepal.Length + Sepal. Width)
Compute and append one or more new columns.
dplyr::mutate_each(iris, funs(min_rank))
Apply window function to each column.
dplyr::transmute(iris, sepal = Sepal.Length + Sepal. Width)
Compute one or more new columns. Drop original columns.

Figure 4: dplyr::mutate

另见下页的例子

dplyr::select - 取列

目标：

- 取出相关列，用于计算人物的 BMI

```
stats <-
  starwars %>%
  select( name, height, mass ) %>%
  mutate( bmi = mass / ( (height / 100 ) ^ 2 ) ) ;

head(stats);
```

```
## # A tibble: 6 x 4
##   name           height  mass   bmi
##   <chr>           <int> <dbl> <dbl>
## 1 Luke Skywalker    172    77  26.0
## 2 C-3PO             167    75  26.9
## 3 R2-D2              96    32  34.7
## 4 Darth Vader       202   136  33.3
## 5 Leia Organa       150    49  21.8
## 6 Owen Lars         178   120  37.9
```

dplyr::select - 取列, cont.

由于 name, height 和 mass 正好是相邻列，可以用 name:mass 获取：

```
stats <-
  starwars %>%
  select( name:mass ) %>%
  mutate( bmi = mass / ( (height / 100 ) ^ 2 ) ) ;

head(stats);
```

```
## # A tibble: 6 x 4
##   name           height  mass   bmi
##   <chr>           <int> <dbl> <dbl>
## 1 Luke Skywalker    172    77  26.0
## 2 C-3PO             167    75  26.9
## 3 R2-D2              96    32  34.7
## 4 Darth Vader       202   136  33.3
## 5 Leia Organa       150    49  21.8
## 6 Owen Lars         178   120  37.9
```

dplyr::select - 取列，cont.

获取与颜色相关的列：hair_color, skin_color, eye_color

```r
stats2 <- starwars %>%
  select( name, ends_with("color") );

head(stats2);
```

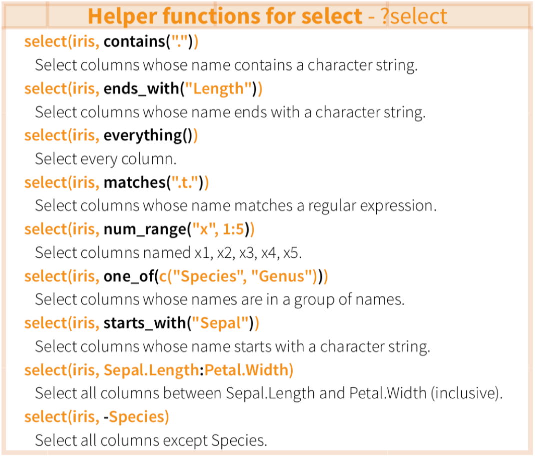
```
## # A tibble: 6 x 4
##   name           hair_color  skin_color  eye_color
##   <chr>          <chr>       <chr>       <chr>
## 1 Luke Skywalker blond       fair        blue
## 2 C-3PO          <NA>        gold        yellow
## 3 R2-D2          <NA>        white, blue red
## 4 Darth Vader    none        white       yellow
## 5 Leia Organa    brown       light       brown
## 6 Owen Lars      brown, grey light       blue
```

dplyr::select - 去除列，cont.

请自行检查以下操作的结果

```
head( starwars %>% select( -hair_color, -eye_color )  );
```

dplyr::select - 其它操作，cont.



Helper functions for select - ?select

select(iris, contains("."))
Select columns whose name contains a character string.

select(iris, ends_with("Length"))
Select columns whose name ends with a character string.

select(iris, everything())
Select every column.

select(iris, matches(".t."))
Select columns whose name matches a regular expression.

select(iris, num_range("x", 1:5))
Select columns named x1, x2, x3, x4, x5.

select(iris, one_of(c("Species", "Genus")))
Select columns whose names are in a group of names.

select(iris, starts_with("Sepal"))
Select columns whose name starts with a character string.

select(iris, Sepal.Length:Petal.Width)
Select all columns between Sepal.Length and Petal.Width (inclusive).

select(iris, -Species)
Select all columns except Species.

Figure 5: dplyr::select 支持的操作

同时对行列进行操作

任务：从星战中挑选**金发碧眼**的人物

```
starwars %>% select( name, ends_with("color"), gender, species ) %>%
  filter( hair_color == "blond" & eye_color == "blue" );
```

```
## # A tibble: 3 x 6
##   name             hair_color skin_color eye_color gender    species
##   <chr>            <chr>      <chr>      <chr>     <chr>     <chr>
## 1 Luke Skywalker   blond      fair       blue      masculine Human
## 2 Anakin Skywalker blond      fair       blue      masculine Human
## 3 Finis Valorum    blond      fair       blue      masculine Human
```

练习考察

问题 2：从 starwars 中选出 $18 < \text{bmi} < 25$ 的人物，统计他们的 homeworld 分布情况

提示：1. 需计算 bmi；2. 用 count 函数计算 homeworld 的分布

section 4：练习与作业

练习 & 作业

- `Exercises and homework` 目录下 `talk05-homework.Rmd` 文件;
- 完成时间: 见钉群的要求

小结

今次提要

- pipe
- dplyr 、tidyr (超级强大的数据处理) part 1

下次预告

- 长宽数据转换
- dplyr, tidyr 和 forcats 的更多功能与生信操作实例

important

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