R for bioinformatics, data wrangler, part 1

HUST Bioinformatics course series for '16 class

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section 1: TOC

前情提要

1. IO, project management, working enviroment 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

- dplyr 、tidyr (超级强大的数据处理) part 1

section 2: data wrangler - dplyr

dplyr

what is `dplyr` ?

- the next iteration of plyr,
- focussing on only data frames.
- 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

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

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

Development version

```
# 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 = "" );
```

```
## Parsed with column specification:
## cols(
##   `Gene stable ID` = col_character(),
##   `Transcript stable ID` = col_character(),
##   `Protein stable ID` = col_character(),
##   `Transcript length (including UTRs and CDS)` = col_double(),
##   `Transcript type` = col_character(),
##   `Chromosome/scaffold name` = col_character()
## )
```

查看 mouse.tibble 的內容

```
table( mouse.tibble$`Transcript type` );
```

```
##
##           3prime_overlapping_ncRNA                        antisense
##                                  3                             4289
##      bidirectional_promoter_lncRNA                        IG_C_gene
##                                267                               21
##                    IG_C_pseudogene                        IG_D_gene
##                                  1                               19
##                    IG_D_pseudogene                        IG_J_gene
##                                  3                               14
##                         IG_LV_gene                     IG_pseudogene
##                                  4                                2
##                          IG_V_gene                    IG_V_pseudogene
##                                301                              155
##                            lincRNA                     macro_lncRNA
##                               8557                                2
##                             miRNA                        misc_RNA
##                               2265                              572
##                            Mt_rRNA                         Mt_tRNA
##                                  2                               22
##                     non_stop_decay       nonsense_mediated_decay
##                                 26                             6755
##              polymorphic_pseudogene         processed_pseudogene
##                                 94                             9425
##               processed_transcript               protein_coding
##                              15572                            58384
```

查看 mouse.tibble 的內容, cont.

```
table( mouse.tibble$`Chromosome/scaffold name`);
```

```
##
##                          1                          10
##                       8553                        6568
##                         11                          12
##                       8673                        5308
##                         13                          14
##                       5618                        5843
##                         15                          16
##                       5142                        4425
##                         17                          18
##                       5050                        2096
##                         19                           2
##                       2982                       10877
##                          3                           4
##                       6938                        7573
##                          5                           6
##                       8955                        7845
##                          7                           8
##                      12344                        6385
##                          9      CHR_CAST_EI_MMCHR11_CTG4
##                       8030                          14
##   CHR_CAST_EI_MMCHR11_CTG5             CHR_MG104_PATCH
##                         40                          17
##             CHR_MG117_PATCH             CHR_MG132_PATCH
##                         52                          29
```

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 ) );
```

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

这种显示格式通常被称为：**长数据格式**!! 又称为**数据扁平化**

数据扁平化的优点？

1. 便于用 dplyr 或 tapply 等进行计算；
2. 更灵活，用于保存稀疏数据

适合扁平化的数据举例

成绩单

```
library(RMySQL);
library(dplyr);

mysql.dbname = "r4ds_test";
dbCon <- dbConnect(MySQL(), user="r4ds", password="r4ds",
                   dbname=mysql.dbname );

grades <- dbGetQuery(dbCon, "SELECT * FROM grades_stats");

knitr::kable( head(grades, n=20) )
```

name	course	grade
Zhi Liu	Microbiology	100
Zhi Liu	English	50
Zhi Liu	Chinese	69
Weihua Chen	Microbiology	89
Weihua Chen	English	99
Weihua Chen	Bioinformatics	99
Kang Ning	Bioinformatics	100
Kang Ning	Chinese	20
Kang Ning	Chemistry	76

长数据与宽数据之间的转换

什么是宽数据？

```
dat2 <- dat %>% select( CHR, TYPE, `count` ) %>%  spread( TYPE, count  );
knitr::kable( head(dat2, n=10) );
```

CHR	lincRNA	miRNA	protein_coding
1	347	128	1200
10	398	91	1020
11	189	137	1640
12	327	146	644
13	428	97	831
14	281	71	901
15	215	94	781
16	176	76	661
17	114	73	1066
18	43	57	524

宽数据举例 2

```
grades2 <- grades %>% spread( course, grade );
knitr::kable( grades2 );
```

name	Bioinformatics	Chemistry	Chinese	English	Microbiology
Kang Ning	100	76	20	NA	NA
Weihua Chen	99	NA	NA	99	89
Zhi Liu	NA	NA	69	50	100

可以想像，如果以此为输入，用 R 计算每个人的平均成绩、不及格门数、总学分，将会是很繁琐的一件事（但对其它工具（如 Excel）可能会比较简单）

spread explained!

```
grades2 <- grades %>% spread( course, grade );
```

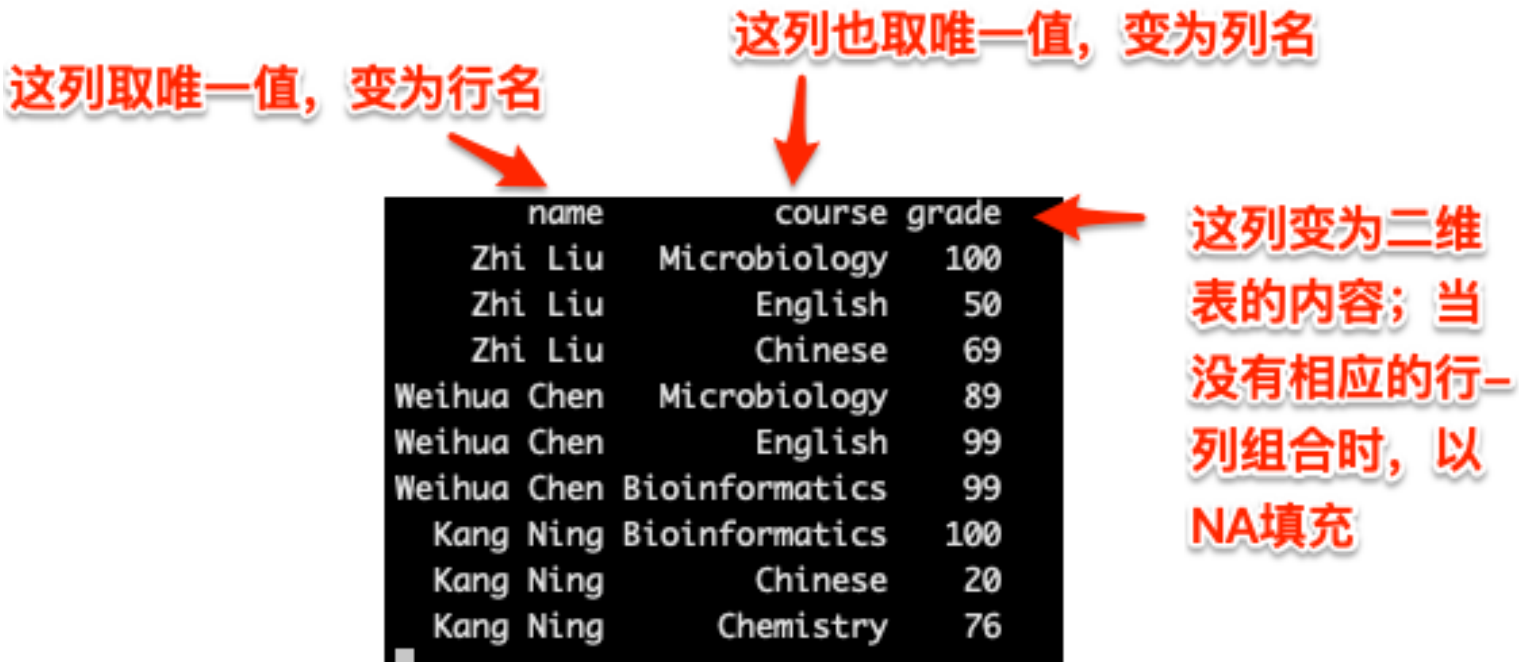


Figure 2: spread function explained

宽数据转为长数据

use gather() function in tidyr

```
grades_melted <- grades2 %>% gather( course, grade, -name ); ## 注意参数的使用 ~~
knitr::kable( head( grades_melted ) );
```

name	course	grade
Kang Ning	Bioinformatics	100
Weihua Chen	Bioinformatics	99
Zhi Liu	Bioinformatics	NA
Kang Ning	Chemistry	76
Weihua Chen	Chemistry	NA
Zhi Liu	Chemistry	NA

gather explained!

```
grades_melted <- grades2 %>% gather( course, grade, -name ); ## 注意参数的使用 ~~
```

-name: 此列保留

列名变为第一列，取名为 course

name	Bioinformatics	Chemistry	Chinese	English	Microbiology
Kang Ning	100	76	20	NA	NA
Weihua Chen	99	NA	NA	99	89
Zhi Liu	NA	NA	69	50	100

值变为第二列，取名为 grade

Figure 3: annotated gather function

有 NA 值怎么办？

```
grades_melted1 <- grades_melted[ !is.na(grades_melted$grade),  ];
grades_melted2 <- grades_melted[ complete.cases( grades_melted )  ,  ];

## -- 更好的方法 ~~
grades_melted <- grades2 %>% gather( course, grade, -name , na.rm = T );
```

宽长数据转换练习

用 spread 和 gather 对下面的数据 mini_iris 进行宽长转换:

```
( mini_iris <- iris[ c(1, 51, 101),  ] );
```

```
##     Sepal.Length Sepal.Width Petal.Length Petal.Width    Species
## 1            5.1         3.5          1.4         0.2     setosa
## 51           7.0         3.2          4.7         1.4 versicolor
## 101          6.3         3.3          6.0         2.5  virginica
```

iris 是鸢尾属一些物种花瓣的量表

宽长数据转换练习，cont.

```
## -- 注意: 第一、二个参数可以自行命名，分别对应原始数据中的 column names 及 values ...
mini_iris.melted <- mini_iris %>% gather( type, dat, -Species );
knitr::kable( mini_iris.melted  );
```

Species	type	dat
setosa	Sepal.Length	5.1
versicolor	Sepal.Length	7.0
virginica	Sepal.Length	6.3
setosa	Sepal.Width	3.5
versicolor	Sepal.Width	3.2
virginica	Sepal.Width	3.3
setosa	Petal.Length	1.4
versicolor	Petal.Length	4.7
virginica	Petal.Length	6.0
setosa	Petal.Width	0.2
versicolor	Petal.Width	1.4
virginica	Petal.Width	2.5

比较复杂的例子

```
grades2 <- read_delim( file = "data/talk05/grades2.txt", delim = "\t",
                       quote = "", col_names = T);
knitr::kable( grades2 );
```

name	class	course	grade
CHEN	1	bioinformatics	90
CHEN	1	chemistry	92
CHEN	2	chinese	35
CHEN	3	german	62
LI	1	bioinformatics	44
LI	2	chinese	68
LI	3	microbiology	95
LI	3	japanese	90
WANG	1	bioinformatics	35
WANG	1	chemistry	76
WANG	1	mathmatics	82
WANG	3	german	100
WANG	3	spanish	78

怎么用 spread 把它变为以下的格式？

```
## # A tibble: 8 x 10
##   name  class bioinformatics chemistry chinese german japanese mathmatics
##   <chr> <dbl>          <dbl>     <dbl>   <dbl>  <dbl>    <dbl>       <dbl>
## 1 CHEN      1             90        92      NA     NA       NA          NA
## 2 CHEN      2             NA        NA      35     NA       NA          NA
## 3 CHEN      3             NA        NA      NA     62       NA          NA
## 4 LI        1             44        NA      NA     NA       NA          NA
## 5 LI        2             NA        NA      68     NA       NA          NA
## 6 LI        3             NA        NA      NA     NA       90          NA
## 7 WANG      1             35        76      NA     NA       NA          82
## 8 WANG      3             NA        NA      NA    100       NA          NA
## # ... with 2 more variables: microbiology <dbl>, spanish <dbl>
```

又怎么把它变回来 ???

dplyr cont. 用结果做图

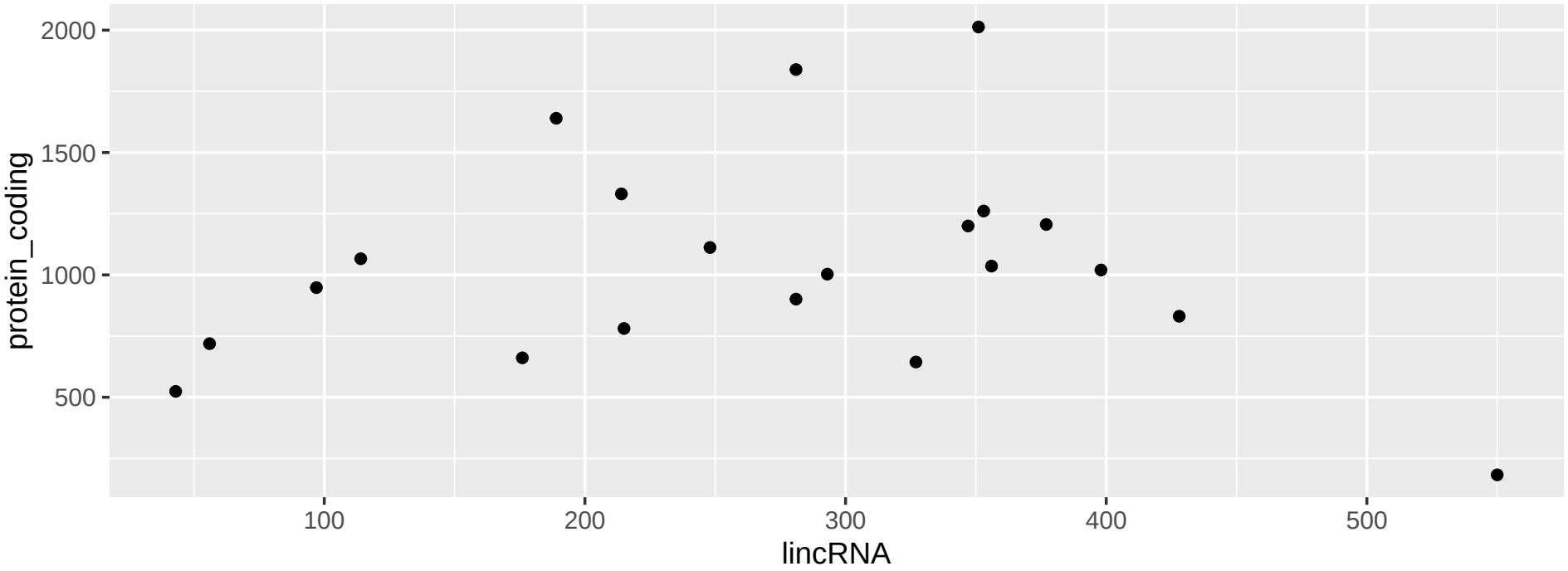
再看一下数据:

```
dat2;
```

```
## # A tibble: 21 x 4
## # Groups:   CHR [21]
##    CHR   lincRNA miRNA protein_coding
##    <chr>   <int> <int>          <int>
##  1 1         347   128           1200
##  2 10        398    91           1020
##  3 11        189   137           1640
##  4 12        327   146            644
##  5 13        428    97            831
##  6 14        281    71            901
##  7 15        215    94            781
##  8 16        176    76            661
##  9 17        114    73           1066
## 10 18         43    57            524
## # ... with 11 more rows
```

dat2 散点图

```
ggplot( dat2, aes( x = lincRNA, y = protein_coding ) ) +
  geom_point( na.rm = T);
```



dplyr 常用函数示例

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           60              89      52             63
## 2 Mm Hu         Student           68              90      59             84
## 3 John Doe      Teacher           93              87      58             77
## 4 Jane Doe      Student           77              80      85             81
## 5 Warren Buffet Entrepreneur      92              84      60             41
## 6 Elon Musk     Entrepreneur      81              86      71             47
## 7 Jack Ma       Entrepreneur      98              83      55             60
```

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 );

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

```
## # A tibble: 7 x 4
## # Groups:   Name [7]
##   Name          Occupation   avg_grades courses_count
##   <chr>         <chr>             <dbl>          <int>
## 1 Jane Doe      Student            80.8              4
## 2 John Doe      Teacher            78.8              4
## 3 Mm Hu         Student            75.2              4
## 4 Jack Ma       Entrepreneur       74                4
## 5 Elon Musk     Entrepreneur       71.2              4
## 6 Warren Buffet Entrepreneur       69.2              4
## 7 Weihua Chen   Teacher            66                4
```

use gather & dplyr functions

问题：每个人的最强科目是什么 ??

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

```
## # A tibble: 7 x 4
##   Name          avg_grades best_course     best_grade
##   <chr>              <dbl> <chr>                <int>
## 1 Jane Doe            80.8 Biology                 85
## 2 John Doe            78.8 English                 93
## 3 Mm Hu               75.2 ComputerScience         90
## 4 Jack Ma             74   English                 98
## 5 Elon Musk           71.2 ComputerScience         86
## 6 Warren Buffet       69.2 English                 92
## 7 Weihua Chen         66   ComputerScience         89
```

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 4: dplyr::summarise 可用的操作

练习 & 作业

问题：

1. 每个人最差的学科和成绩分别是什么？
2. 哪个职业的平均成绩最好？
3. 每个职业的最佳学科分别是什么（按平均分排序）???

上交：

1. 产生的数据（导出为 tsv 格式）
2. 分析结果（copy & paste 到单独的文本文件里）
3. 完整的可独立运行的代码

更多练习，使用 starwars tibble

```
head(starwars);
```

```
## # A tibble: 6 x 13
##   name  height  mass hair_color skin_color eye_color birth_year gender
##   <chr>  <int> <dbl> <chr>      <chr>      <chr>           <dbl> <chr>
## 1 Luke~    172    77 blond      fair       blue             19   male
## 2 C-3PO    167    75 <NA>       gold       yellow          112   <NA>
## 3 R2-D2     96    32 <NA>       white, bl~ red              33   <NA>
## 4 Dart~    202   136 none       white      yellow           41.9 male
## 5 Leia~    150    49 brown      light      brown            19   female
## 6 Owen~    178   120 brown, gr~ light      blue             52   male
## # ... with 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

而 dplyr::summarise 则会使列数减少（通常与 group_by 联合使用）

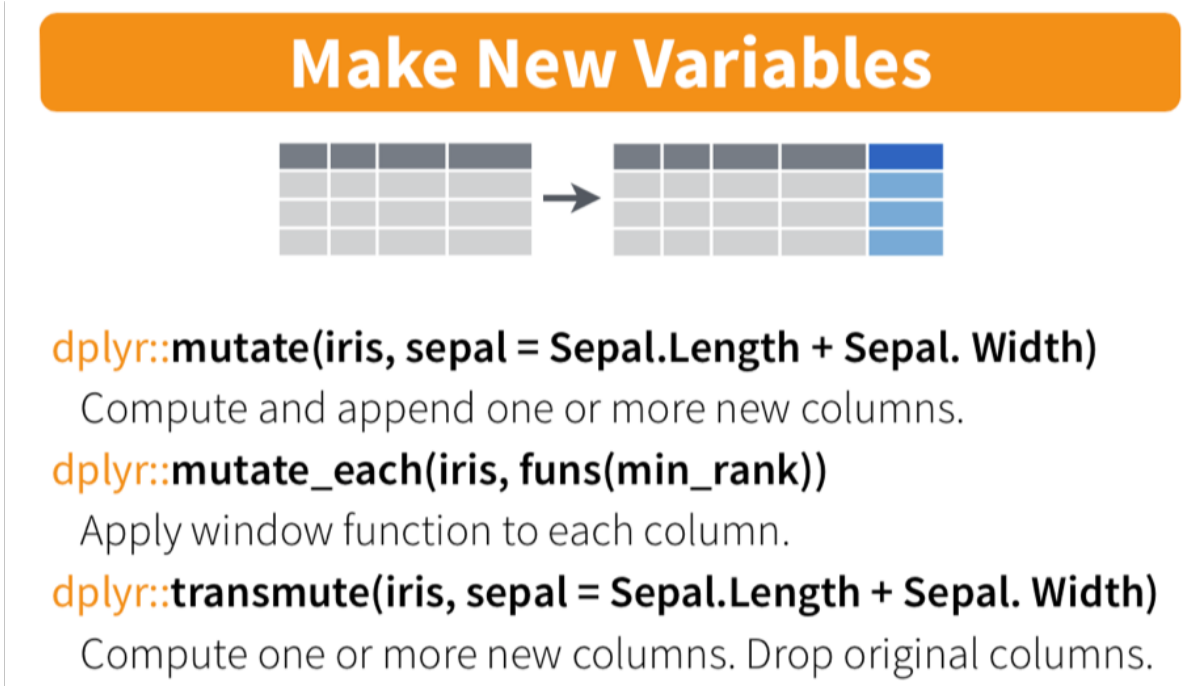


Figure 5: dplyr::mutate

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

```
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.

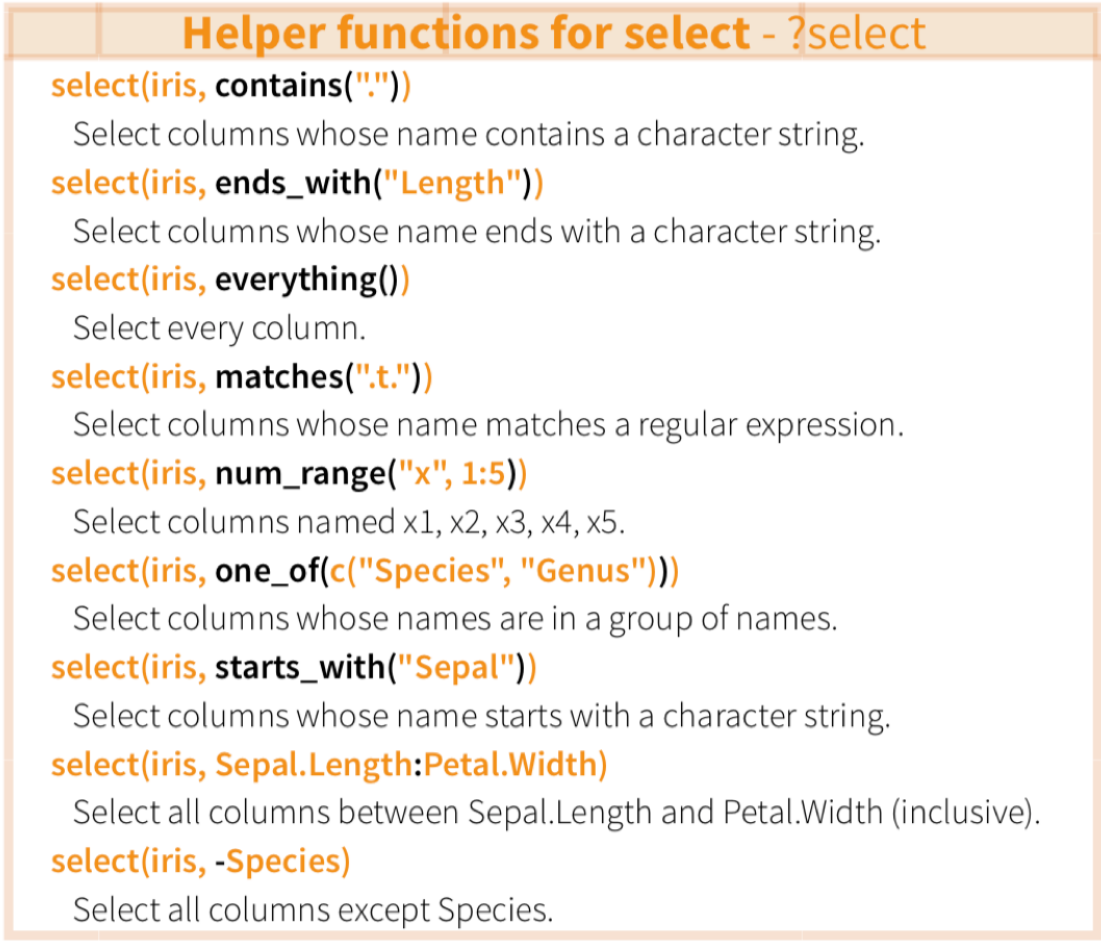


Figure 6: dplyr::select 支持的操作

dplyr::filter - 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      male   Human
## 2 Anakin Skywalker blond      fair       blue      male   Human
## 3 Finis Valorum    blond      fair       blue      male   Human
```

dplyr 中其它取行的操作

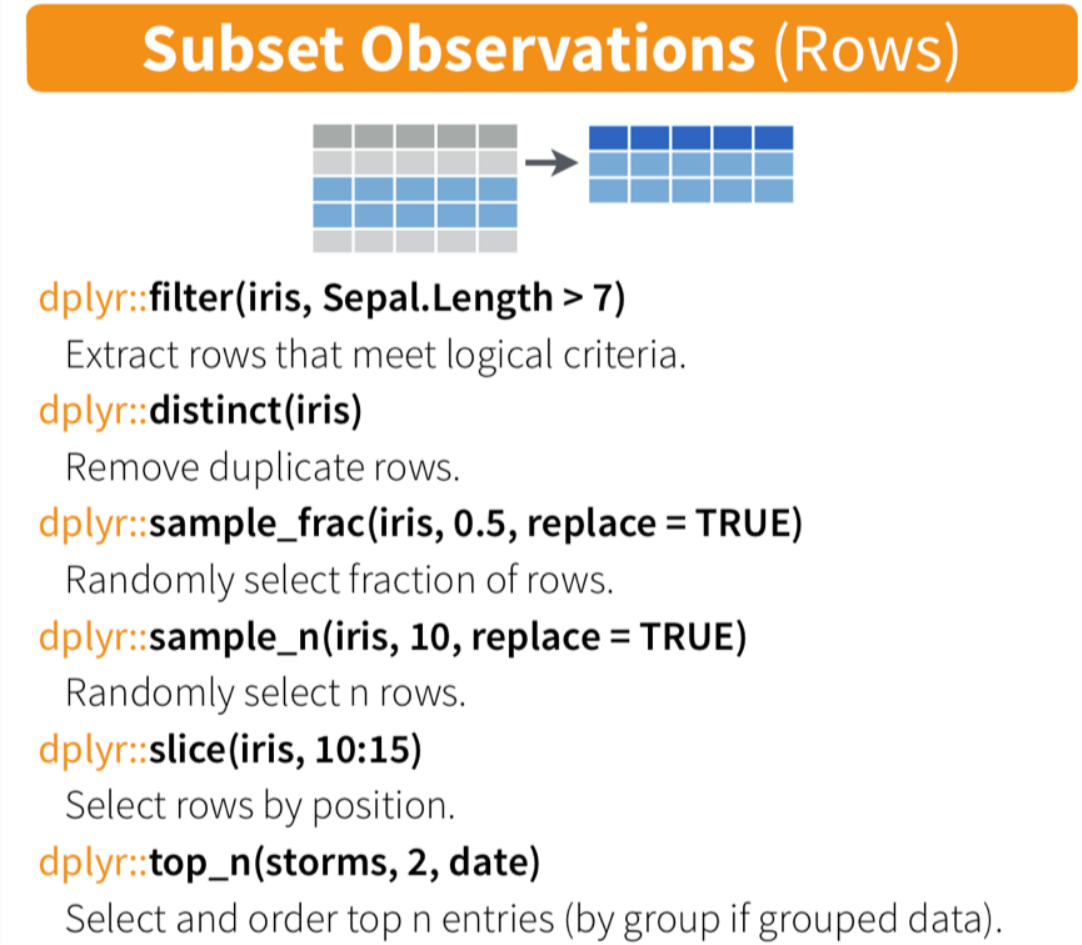


Figure 7: dplyr 与行相关的操作

tidyr::separate

https://r4ds.had.co.nz/tidy-data.html

tidyr::unite

https://r4ds.had.co.nz/tidy-data.html

section 3：练习与作业

more to read

https://www.dataschool.io/dplyr-tutorial-for-faster-data-manipulation-in-r/
https://pages.rstudio.net/Webinar-Series-Recording-Essential-Tools-for-R.html
https://github.com/tidyverse/dplyr http://genomicsclass.github.io/book/pages/dplyr_tutorial.html
http://stat545.com/block009_dplyr-intro.html https://cran.r-project.org/web/packages/dplyr/vignettes/dplyr.html

练习

1. let's get started with dplyr
2. dplyr: more smooth data exploration
3. some more exercise
4. dplyr: 50 examples; 包含了许多本章并未讲到的内容

作业

1. 前半部分提到的作业
2. 使用 mouse.tibble 数据，统计：

   - 每个染色体上每种基因类型的数量、平均长度、最大和最小长度，挑出最长和最短的基因
   - 去掉含有 500 以下基因的染色体，按染色体、数量高 -> 低进行排序

要求上交：

1. 完整能运行的代码，
2. 保存至文本文件的输出结果

下次提要

dplyr, tidyr 和 forcats 的更多功能与生信操作实例