R for bioinformatics, data visualisation HUST Bioinformatics course series

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section 1: TOC



前情提要

iterations 与并行计算

- for loop
- apply functions
- dplyr 的本质是遍历
- map functions in purrr package
- 遍历与并行计算

相关包

- purrr
- parallel
- foreach
- iterators

ggplot2 basics

本次提要

part 2: ggplot2 进阶

- ① 如何在一张图中画多个 panel?
- ② 如何写公式
- 3 ggplot2 的核心是先计算,再做图
- themes and legends

ggplot2 进阶 1: 如何在一张图中画多个 panel?

ggplot2 进阶 1: 如何在一张图中画多个 panel?

key requirements for multi-panel plots

- order / position
- labeling
- layout

combine multiple plots

Useful packages:

- gridExtra
- cowplot
- grid
- lattice

install or load packages

```
if (!require("gridExtra")){
   install.packages("gridExtra");
}
if (!require("cowplot")){
   install.packages("cowplot");
}
library( cowplot );
library( gridExtra );
```

arranging multiple graphs using cowplot

cowplot:

- plot_grid
- ggdraw + draw_plot

prepare four panels

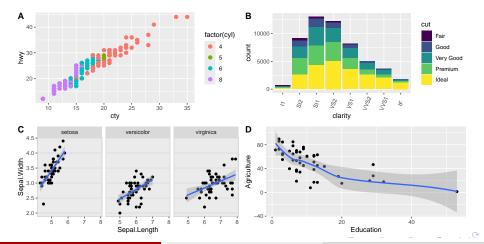
```
library(tidyverse);
plot.hwy <- ggplot(mpg, aes(x = cty, y = hwy, colour = factor(cyl)))+
geom_point(size=2.5)

# Bar plot

plot.dose <- ggplot(diamonds, aes(clarity, fill = cut)) +
geom_bar() +
theme(axis.text.x = element_text(angle=70, vjust=0.5))

plot.iris <- ggplot(iris, aes(Sepal.Length, Sepal.Width)) +
geom_point() + facet_grid(. - Species) + stat_smooth(method = "lm") +
background_grid(major = 'y', minor = "none") + # add thin horizontal lines
panel_border();
plot.swiss <- swiss %>% ggplot(aes(Education, Agriculture)) +
geom_point() + geom_smooth();
```

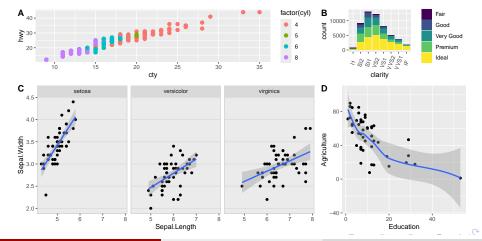
Combine four plots using plot_grid



plot_grid parameters

```
plot_grid(
  . . . ,
 plotlist = NULL,
  align = c("none", "h", "v", "hv"),
  axis = c("none", "l", "r", "t", "b", "lr", "tb", "tblr"),
 nrow = NULL.
 ncol = NULL.
 rel widths = 1, ## 相对宽度
 rel_heights = 1, ## 相对高度
 labels = NULL.
  label size = 14,
  label fontfamily = NULL,
  label fontface = "bold",
  label colour = NULL,
 label x = 0.
 label y = 1.
 hjust = -0.5,
  viust = 1.5.
  scale = 1,
  greedy = TRUE,
 byrow = TRUE,
  cols = NULL.
 rows = NULL.
```

调整相对大小



more complex layout using draw_plot

```
plot <-
    ggdraw() +
    draw_plot(plot.iris, x=0, y=.5, width=1, height=.5) +
    draw_plot(plot.hwy, 0, 0, .5, .5) +
    draw_plot(plot.dose, .5, 0, .5, .5) +
    draw_plot_label(c("A", "B", "C"), c(0, 0, 0.5), c(1, 0.5, 0.5), size = 15);</pre>
```

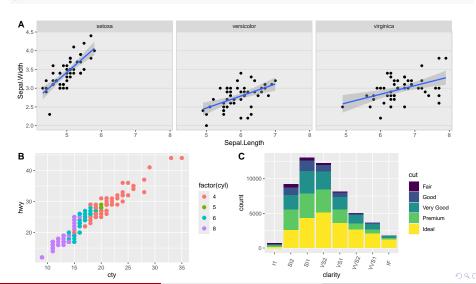
'geom smooth()' using formula = 'y ~ x'

```
draw_plot(plot, x = 0, y = 0, width = 1, height = 1) 详解:
```

- plot: the plot to place (ggplot2 or a gtable)
- x: The x location of the lower left corner of the plot.
- y: The y location of the lower left corner of the plot.
- width, height: the width and the height of the plot

draw_plot results

plot



draw_plot_label parameters

Use draw_plot_label to add the labels

```
draw_plot_label(c("A", "B", "C"), c(0, 0, 0.5), c(1, 0.5, 0.5), size = 15);

draw_plot_label(
    label,
    x = 0,
    y = 1,
    hjust = -0.5,
    vjust = 1.5,
    size = 16,
    fontface = "bold",
    family = NULL,
    color = NULL,
    colour,
    ...
)
```

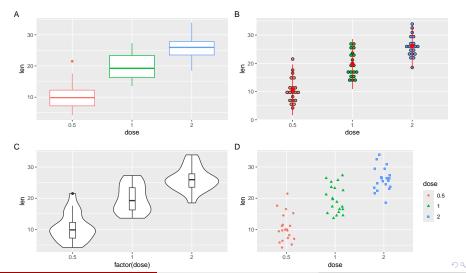
use gridExtra::grid.arrange

Create four plots, again

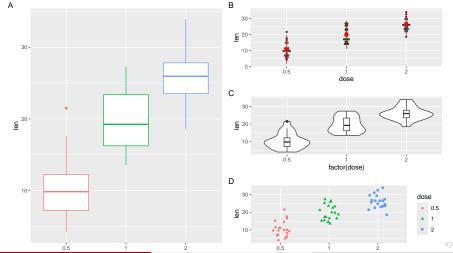
```
library(ggplot2); library("gridExtra");
df <- ToothGrowth
df$dose <- as.factor(df$dose)
bp <- ggplot(df, aes(x=dose, v=len, color=dose)) +</pre>
  geom boxplot() +
  theme(legend.position = "none") + labs( tag = "A");
dp <- ggplot(df, aes(x=dose, v=len, fill=dose)) +</pre>
  geom dotplot(binaxis='v', stackdir='center')+
  stat summary(fun.data=mean sdl. mult=1.
                 geom="pointrange", color="red")+
   theme(legend.position = "none") + labs( tag = "B")
vp <- ggplot(df, aes(x=factor(dose), v=len)) +</pre>
  geom violin()+
  geom boxplot(width=0.1) + labs( tag = "C")
sc <- ggplot(df, aes(x=dose, y=len, color=dose, shape=dose)) +</pre>
  geom jitter(position=position jitter(0.2))+
  theme(legend.position = "none") +
 theme grav() + labs( tag = "D")
```

use gridExtra::grid.arrange

grid.arrange(bp, dp, vp, sc, ncol=2, nrow =2);



use layout_matrix parameter in grid.arrange



explain layout_matrix

How the layout look like??

```
cbind(c(1,1,1), c(2,3,4));
```

```
## [,1] [,2]
## [1,] 1 2
## [2,] 1 3
## [3,] 1 4
```

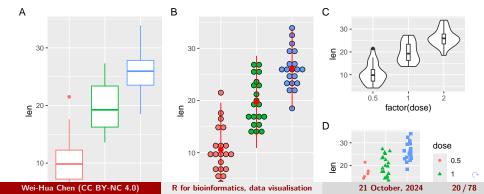
make a different layout???

three columns, A and B take the first two, C and D take the third one.

```
( laymat = cbind(c(1,1), c(2,2), c(3,4)) );
```

```
## [,1] [,2] [,3]
## [1,] 1 2 3
## [2,] 1 2 4
```

```
grid.arrange(bp, dp, vp, sc, ncol = 3, layout_matrix = laymat);
```



Add a common legend for multiple ggplot2 graphs

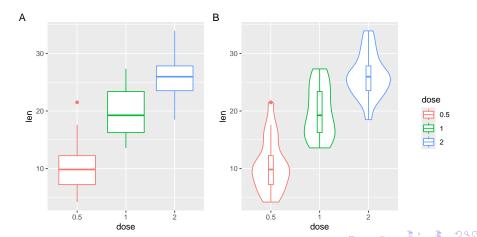
Prepare a function to extract legend from a plot. Note the legend should exist.

```
library(gridExtra)
get_legend<-function(myggplot){
  tmp <- ggplot_gtable(ggplot_build(myggplot))
  leg <- which(sapply(tmp%grobs, function(x) x*name) == "guide-box")
  legend <- tmp%grobs[[leg]]
  return(legend)
}</pre>
```

Prepare the graphs and a legend

```
## 1. Create a box plot WITH legend
bp <- ggplot(df, aes(x=dose, y=len, color=dose)) +
  geom_boxplot() + labs(tag = "A");
## 2. Create a violin plot WITHOUT legend
vp <- ggplot(df, aes(x=dose, y=len, color=dose)) +
  geom_violin()+ geom_boxplot(width=0.1) + labs( tag = "B") +
  theme(legend.position="none") ## no legend
## 3. extract the legend from the first plot
legend <- get_legend(bp);
## 4. remove the legend from the first plot
bp2 <- bp + theme(legend.position="none");</pre>
```

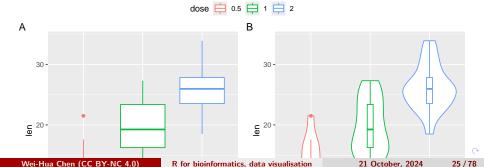
plot the common legned to the right



issue

缺点: legend 看起来属于 B, 而不是共同的。

fix: place the legend at top and align to the center



Explain

```
## [,1] [,2]
## [1,] 1 1
## [2,] 2 3
```

rbind(c(1,1), c(2,3));

- legend takes the first row, and has a height of 0.2
- the other two graphs take the second row and has a height of 2.5

Practise on your own

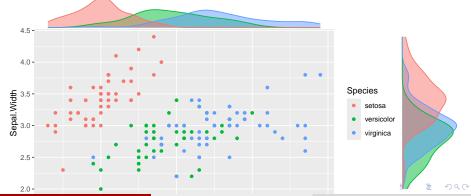
To place the legend at:

- the bottom, centered at the middle
- top-left
- top-right
- bottom-left
- bottom-right

ggExtra - Add marginal histograms to ggplot2

```
please install the package if not exists ...
install.packages("ggExtra")

library(ggExtra);
piris <- ggplot(iris, aes(Sepal.Length, Sepal.Width, colour = Species)) +
    geom_point()
ggMarginal(piris, groupColour = TRUE, groupFill = TRUE)</pre>
```



也可自己写代码实现

```
piris <- ggplot(iris, aes(Sepal.Length, Sepal.Width, colour = Species)) +
  geom point() + theme(legend.position=c(0,1), legend.justification=c(0,1))
## Warning: A numeric `legend.position` argument in `theme()` was deprecated in ggplot2
## 3.5.0.
## i Please use the `legend.position.inside` argument of `theme()` instead.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last lifecycle warnings()` to see where this warning was
## generated.
xdensity <- ggplot(iris, aes(Sepal.Length, fill = Species)) +</pre>
  geom density(alpha=.5) + theme(legend.position = "none")
ydensity <- ggplot(iris, aes(Sepal.Width, fill=Species)) +</pre>
  geom density(alpha=.5) + theme(legend.position = "none") + coord flip()
grid.arrange(xdensity, NULL, piris, ydensity,
        ncol=2, nrow=2, widths=c(4, 1.4), heights=c(1.4, 4):
0.8 -
0.4 -
0.0 -
                                   Sepal.Length
  4.5 -
                                                                             4.5 -
     Species
         versicolor
                                                                           £ 3.5
€ 3.5 -
         virginica
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                                   R for bioinformatics, data visualisation
                                                                            21 October, 2024
                                                                                                 29 / 78
```

Extended reading

Other ggplot2 extensions

See the gallery at https://exts.ggplot2.tidyverse.org/gallery/. Or Google ggplot2 extensions gallery.

Explore the grid package

- create graphical objects (grobs)
- arrange multiple grobs using arrangeGrob function

Explore the gridExtra package

- plot table
- ..

complex layout 小结

Essentials for combining multiple graphs in one:

- ordering
- layout

cowplot

- plot_grid
- draw_plot

gridExtra

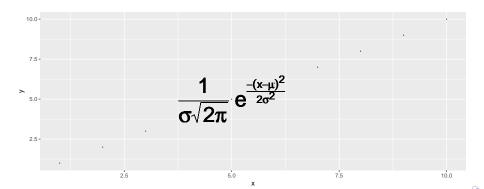
grid.arrange

ggplot2 进阶 2: 如何写公式?

two kinds of equations

- expression w/o variable substitution
- expression w/ variable substitution

the 1st kind equations (expression)



公式中的写法之代数符号

分类	R 的表达式	显示结果
代数符号	expression(x + y)	x + y
	expression(x - y)	x-y
	expression(x * y)	xy
	expression(x / y)	x/y
	expression(x %+-% y)	$x \pm y$
	expression(x %/% y)	$x \div y$
	expression(x %*% y)	$x \times y$
	expression(x %.% y)	$x \cdot y$
	expression(x[i])	x_i
	expression(x^2)	x^2
	expression(sqrt(x))	\sqrt{x}
	expression(sqrt(x,y))	∜x
	expression(list(x,yz))	x, y, z

... 更多,不在这里介绍了。

希腊字符

代码

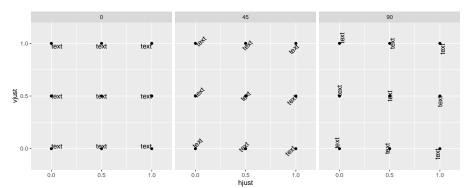
希腊字符, cont.

4- Q alpha	႘ beta	y gamma	delta	E epsilon	zela
3. n eta	theta	1 iota	K kappa	lambda	$\underset{mu}{\mu}$
2- V	چ ×	O omicron	$\pi_{_{pi}}$	ρ mo	O sigma
1- T	ູນ upsilon	ф phi	χ chi	Ψ psi	⊕ omega

х

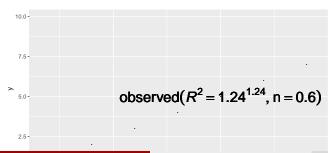
hjust 和 vjust

geom_text(aes(angle, hjust, vjust)) 三参数详解



2. 有变量代入值的公式

举例 1:



有代入变量值的公式举例 2:

使用 paste 和 substitute:

```
x_mean <- 1.5;
x_sd <- 1.2;

# 表达式
ex <- substitute(
    paste(X[i], " ~ N(", mu, "=", m, ", ", sigma^2, "=", s2, ")"),
    list(m = x_mean, s2 = x_sd^2)
);

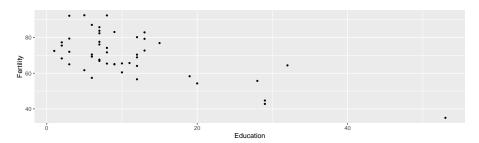
# histogram
ggplot( data.frame( x = rnorm(100, x_mean, x_sd) ), aes( x ) ) +
    geom_histogram( binwidth=0.5 ) +
    ggtitle(ex); ## 为什么不需要 parse = TURE ????</pre>
```



详解

示例:显示两组数据间的相关性

```
## 作图
ggplot( swiss, aes( x = Education, y = Fertility ) ) +
geom_point( shape = 20 );
```

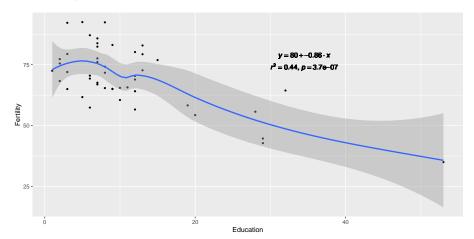


```
## 分析
with( swiss, cor.test( Education, Fertility )$estimate );
```

```
## cor
## -0.6637889
```

在图中加入公式和统计信息

先展示一下结果



公式详解

$$y = 80 + -0.86 \cdot x$$

$$r^2 = 0.44, p = 3.7e - 0.7$$
paste('italic(r)'^2, "=", r2, ", ", italic(p)==pvalue, sep = ""))

Figure 1: equation explained!

公式详解, cont.

以下代码实现两个任务:

- 将两个公式上下放置 atop (<equation_1> , <equation_2>);
- ② 将公式中的某些值替换为数值 substitute(<equation>, list(...))

完整代码

```
## 计算 ...
m = lm(Fertility ~ Education. swiss):
c = cor.test( swiss$Fertility, swiss$Education );
## 牛成公式
eq <- substitute( atop( paste( italic(y), " = ", a + b %.% italic(x), sep = ""),
                       paste( italic(r)^2, " = ", r2, ", ", italic(p)==pvalue, sep = "" ) ),
                     list(a = as.vector(format(coef(m)[1], digits = 2)).
                          b = as.vector( format(coef(m)[2], digits = 2)),
                          r2 = as.vector(format(summary(m)$r.squared, digits = 2)),
                          pvalue = as.vector(format(c$p.value, digits = 2)))
   );
## 用 as.expression 对公式进行转化 !!!!
eq <- as.character(as.expression(eq)):
## 作图, 三个图层; 特别是 geom text 使用自己的 data 和 aes ...
ggplot(swiss, aes( x = Education, y = Fertility ) ) +
       geom_point( shape = 20 ) +
       geom smooth( se = T ) + ## smooth line ...
       geom text( data = NULL.
                  aes(x = 30, y = 80, label= eq, hjust = 0, vjust = 1), ## hjust, vjust ???
                  size = 4, parse = TRUE, inherit.aes=FALSE); ## 注意: parse = TRUE !!!
```

equation 的其它写法(更复杂难懂)

```
## 计算 ...
m = lm(Fertility ~ Education, swiss);
c = cor.test( swiss$Fertility, swiss$Education );
## 牛成公式
eq <- substitute( atop( italic(y) == a + b %.% italic(x),
                           italic(r)^2 = r2*, = italic(p) = pvalue),
                     list(a = as.vector(format(coef(m)[1], digits = 2)).
                          b = as.vector( format(coef(m)[2], digits = 2)),
                          r2 = as.vector(format(summary(m)$r.squared, digits = 2)),
                          pvalue = as.vector( format( c$p.value , digits = 2) ) )
   ):
## 用 as.expression 对公式进行转化 !!!!
eq <- as.character(as.expression(eq)):
## 作图, 三个图层; 特别是 geom_text 使用自己的 data 和 aes ...
ggplot(swiss, aes( x = Education, y = Fertility ) ) +
       geom point( shape = 20 ) +
       geom smooth( se = T ) + ## smooth line ...
       geom text( data = NULL,
                  aes(x = 30, y = 80, label= eq, hjust = 0, vjust = 1), ## hjust, vjust ???
                  size = 4, parse = TRUE, inherit.aes=FALSE); ## 注意: parse = TRUE !!!
```

公式详解

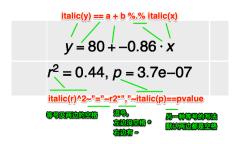


Figure 2: equation explained!

注

● 引号两边必须有 * 或 ~ 字符, ~ 表示空格, * 表示什么都没有。~~ 表示两个空格。如果公式中需要~字符怎么办??见下面"公式示 例 3"。

公式小结

- 表达式
- 罗马字符
- 代入变量

ggplot2 进阶 3: 核心在于先计算再做图

举例说明

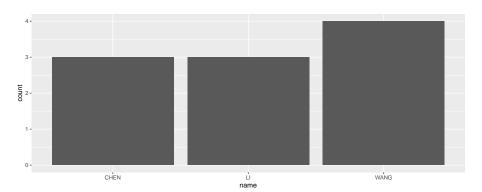
先看数据 (来自 talk05):

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

geom_bar

任务: 画出每位学生及格的课程数

```
ggplot( grades2 %>% filter( grade >= 60 ), aes( name ) ) +
  geom_bar();
```



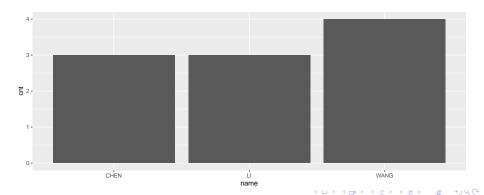
为什么会这样呢?因为 geom_bar(stat = "count")的默认参数是 count

即数一下每个 factor 的出现次数。

geom_bar , cont.

以上命令,实际上等于:

```
## 先做统计
cnt <- grades2 %>% group_by( name ) %>% summarise( cnt = sum( grade >= 60 ) );
ggplot( cnt, aes( x = name, y = cnt ) ) +
   geom_bar( stat = "identity" );
```



default stat behaviors (默认计算方法)

- geom_bar : count
- geom_boxplot : boxplot
- geom_count : sum
- geom_density : density
- geom_histogram : bin
- geom_quantile : quantile ...

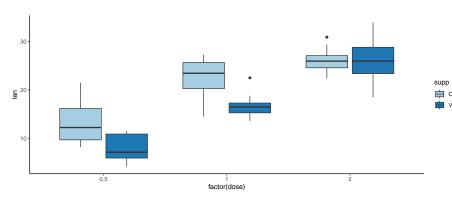
ggplot2 进阶 4: themes and legends

改变 theme()

theme 调整包括 theme() 函数,用于调整各个 elements

和 theme_xxx()函数,直接使用已经定制好的内容;

```
ggplot(ToothGrowth, aes(x=factor( dose ), y=len, fill=supp)) +
  geom_boxplot() + scale_fill_brewer( palette = "Paired" ) + theme_classic();
```



ggplot2 中的主题

- theme_gray:系统默认主题
- theme_bw , theme_linedraw, theme_light, theme_dark, theme_minimal , theme_classic, theme_void()

see here for a complete list:

https://ggplot2.tidyverse.org/reference/ggtheme.html

theme() 函数

除了 theme_ 用于调整整体视觉效果外,ggplot2 还提供了 theme() 函数用于细调。

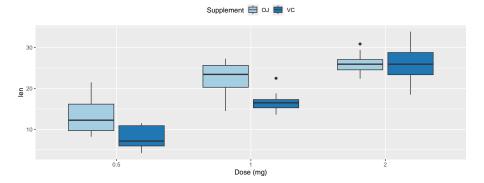
- line, rect, text, title: 整体框架
- axis.<compoment>: 调整坐标轴
- legend.<parameter>: 调整图例
- plot.<>:控制 title, subtitle 等细节
- panel.<...>: 调整 facet 情况下的 panel (facet 下面会介绍)
- strip.<...>: 调整 facet 的标题细节 …

更多详见:

官方: https://ggplot2.tidyverse.org/reference/theme.html

legend 细调

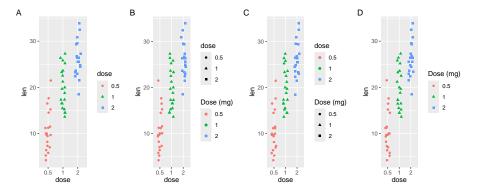
```
ggplot(ToothGrowth, aes(x=factor( dose ), y=len, fill=supp)) +
  geom_boxplot() + scale_fill_brewer( palette = "Paired" ) +
  labs( fill = "Supplement", x = "Dose (mg)" ) +
  theme( legend.position = "top" )
```



labs() function: Modify axis, legend, and plot labels

```
labs(
...,
x = "<x label>",
y = "cy label>",
colour = "<legend title>", # 与 aes 里的 colour 配合使用
fill = "<legend title>", # 与 aes 里的 fill 配合使用
shape = "<legend title>", # 与 aes 里的 shape 配合使用
title = waiver(),
subtitle = waiver(),
caption = waiver(),
tag = waiver(),
alt = waiver(),
alt_insight = waiver()
)
```

labs() with examples



ggplot2 进阶 5: stacked bars 及其它

stacked bars

应用场景: 宏基因组多样本物种丰度图

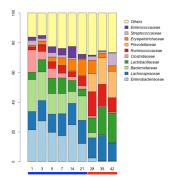


Figure 3: Microbiome 3, 28 2015

stacked bars, cont.

load data

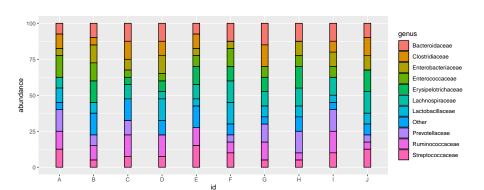
```
## Rows: 110 Columns: 3
## -- Column specification -------
## Delimiter: "\t"
## chr (2): id, genus
## dbl (1): abundance
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.
head( speabu );
```

```
id
                              abundance
##
           genus
    <chr> <chr>
                                  <dh1>
## 1 A
           Enterobacteriaceae
## 2 A
          Lachnospiraceae
                                 7.5
## 3 A
          Bacteroidaceae
                                  7.5
## 4 A
         Lactobacillaceae
                                  10
## 5 A
          Clostridiaceae
                                  10
## 6 A
                                  12.5
           Ruminococcaceae
```

A tibble: 6 x 3

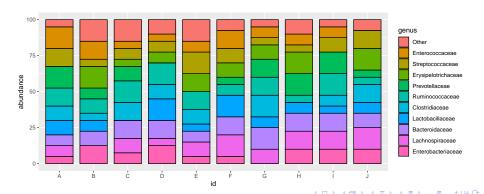
stacked bars, cont.

```
ggplot( speabu, aes( x = id, y = abundance, fill = genus ) ) +
  geom_bar( stat = "identity", position = "stack", color = "black", width = 0.2 );
```



指定 Genus 展示顺序

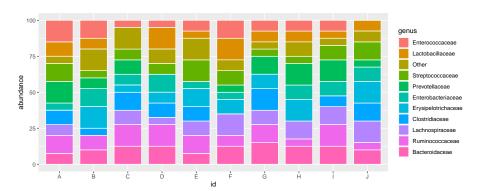
factor 的操纵详见第 4 章。



按丰度排序

按丰度中值大小排序

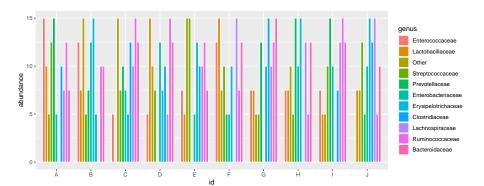
```
speabu$genus <- reorder( speabu$genus, speabu$abundance, median );
ggplot( speabu, aes( x = id, y = abundance, fill = genus ) ) +
   geom_bar( stat = "identity", position = "stack", color = "white", width = 0.8 );</pre>
```



position = "stack" 又是什么??

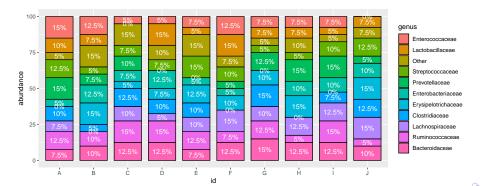
position = "dodge" : plot bars next to each other ...

```
ggplot( speabu, aes( x = id, y = abundance, fill = genus ) ) +
  geom_bar( stat = "identity", position = "dodge", color = "white", width = 0.8 );
```



显示数值 ...

```
## 先计算显示位置
speabu <- speabu %>% arrange(id, desc(factor(genus))) %>%
 group by (id) %>% mutate( vpos = cumsum( abundance ) - abundance / 2):
## 画图
ggplot( speabu, aes( x = id, y = abundance, fill = genus ) ) +
 geom_bar( stat = "identity", position = "stack", color = "black", width = 0.8 ) +
 geom text( aes( y = ypos, label = paste( abundance, "%", sep = "" ) ), color = "white" );
```

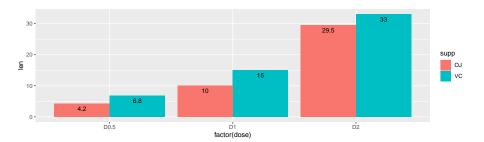


显示数值 ..., cont.

要点

- 使用 ddplyr 的 cumsum() 函数 ...
- 计算位置: 当前累加值 自身值/2, 使数字显示在当前值的中间
- 累加前,要对数据按 factors 进行排序;通过 arrange 函数实现;

在 position = "dodge" 的情况下添加 label



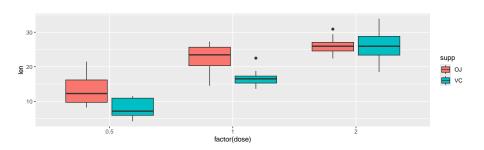
position 的其它取值

除了 "dodge", "stack" 之外, position 还可以:

- position = position_stack(reverse = TRUE)
- position = position_dodge(reverse = TRUE)
- position = position_identity()
- position = position_jitter(): jitter points to avoid overplotting ...
- position = position_nudge(): is generally useful for adjusting the position of items on discrete scales by a small amount

不同的图层有不同默认值

```
ggplot(ToothGrowth, aes(x=factor( dose ), y=len, fill=supp)) +
    geom_boxplot()
```



geom_boxplot(): 默认为 dodge

more to read

ggplot2 的在线书

https://ggplot2-book.org/themes

Exercise and home work

总结,本节内容

ggplot2 基础

- 优缺点
- 用法
- 基本组成

ggplot2 进阶

- 颜色和色板
- 复杂 layout 的实现
- 公式
- ggplot2 的数据统计逻辑

更多阅读

 Ggplot2: Elegant Graphics for Data Analysis, Book by Hadley Wickham

写在后面

- ① ggplot2 博大精深,需要一门课去讲
- ② 上手容易,精通难
- ◎ 太多记忆点
- 本节内容只涉及了基础中的基础,更多内容,包括进阶技巧和生信相关的扩展包,更多的需要同学们自行探索
- 遇到不会的图, 先百度/Google, 找包和代码

下次预告

data summary and modeling



作业

- Exercises and homework 目录下 talk09-homework.Rmd 文件;
- 完成时间: 见钉群的要求