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

本次提要

- basic plot functions
- basic ggplot2
- special letters
- equations
- advanced ggplot2

section 2: basic plot functions using R

R basic plot functions

过去几节课我们已经使用了 R basic plot 和 ggplot2 的一些绘画功能，比如讲 factor 时。今次我们进行系统的介绍。

基础做图由 `plot` 提供。先看示例。这里我们使用系统自带的 `swiss` 数据，它包含了 47 个法语地区的一些社会经济指标。

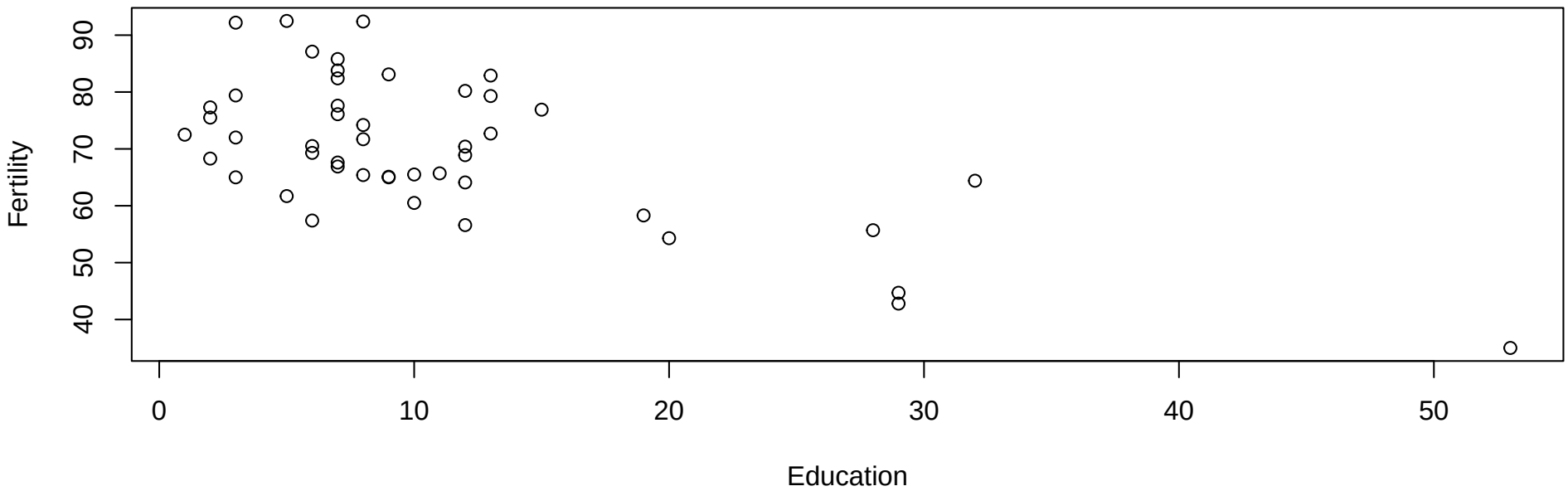
```
head(swiss);
```

```
##              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
## Neuveville        76.9        43.5          17        15     5.16
## Porrentruy        76.1        35.3           9         7    90.57
##              Infant.Mortality
## Courtelary               22.2
## Delemont                 22.2
## Franches-Mnt             20.2
## Moutier                  20.3
## Neuveville               20.6
## Porrentruy               26.6
```

散点图（dot plot）

我们看一下教育与生育率的关系：

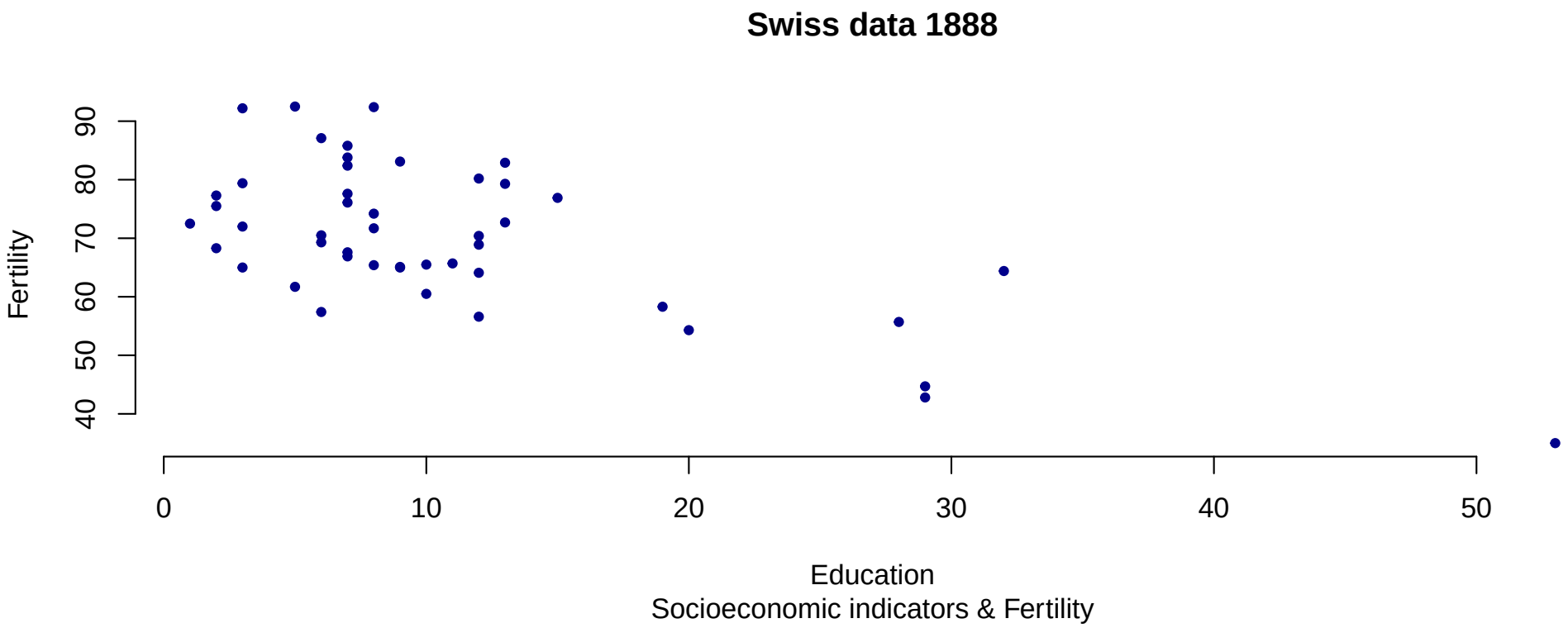
```
with( swiss, plot( Education, Fertility ) );
```



注意 `with` 的作用是什么 ??

plot 的参数初探：先看示例

```
with( swiss, plot(Education, Fertility, type = "p", main = "Swiss data 1888",
                  sub = "Socioeconomic indicators & Fertility",
                  xlab = "Education", ylab = "Fertility", col = "darkblue",
                  xlim = range( Education ), ylim = range( Fertility ),
                  pch = 20, frame.plot = F) );
```



plot 参数，an annotated example

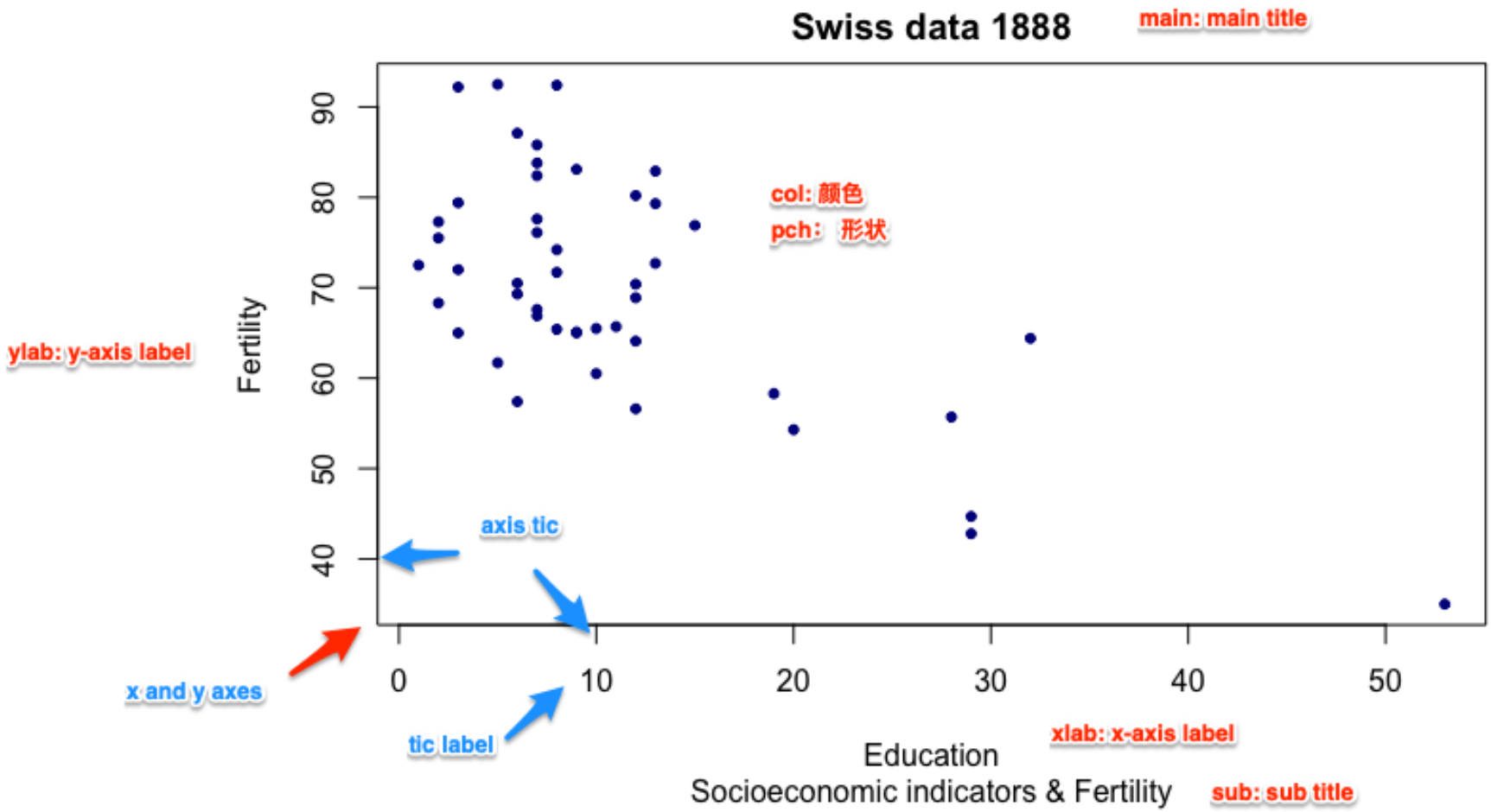
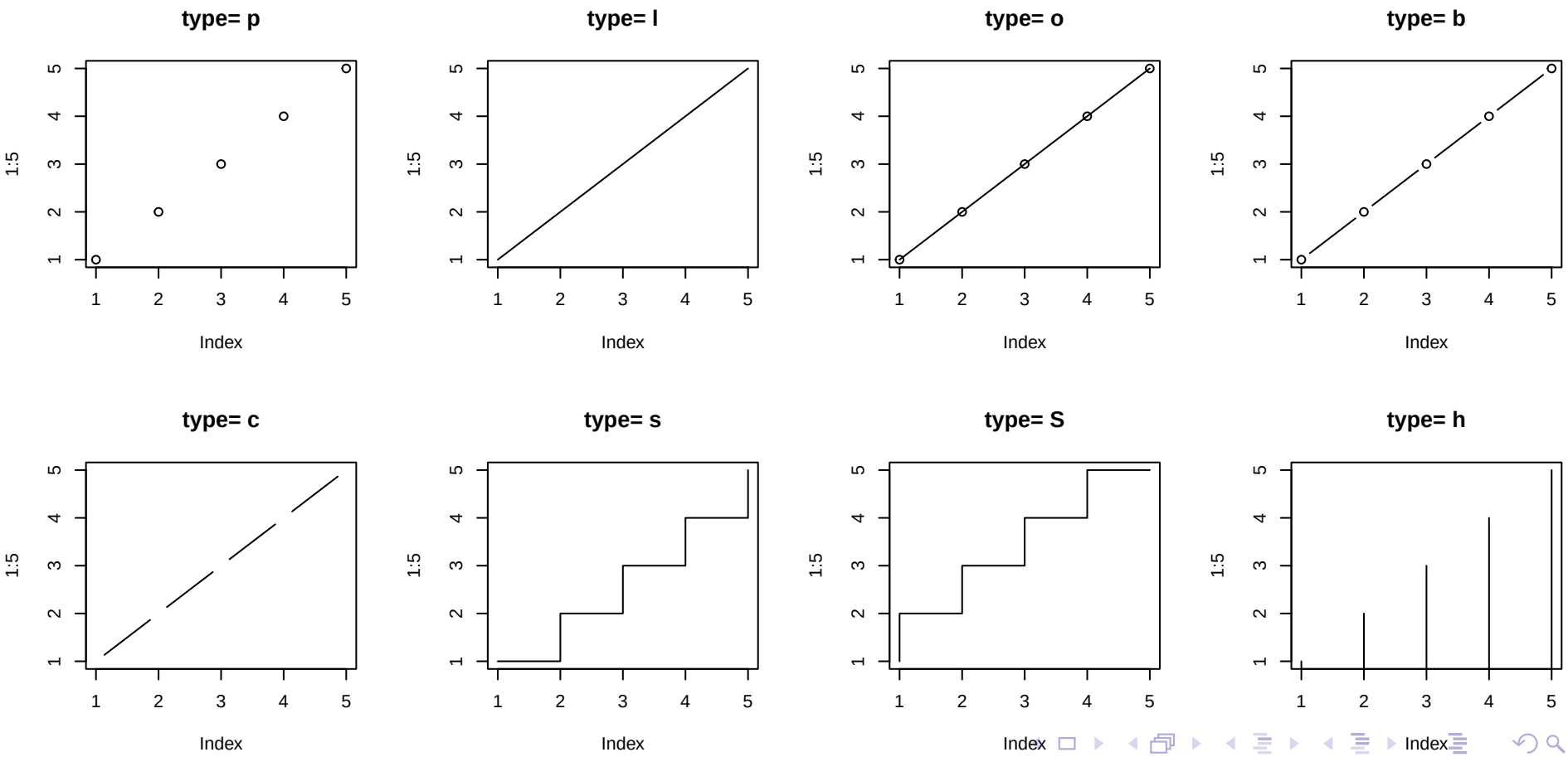


Figure 1: an annotated example

plot 支持的画图类型，参数 p = '?' 的取值

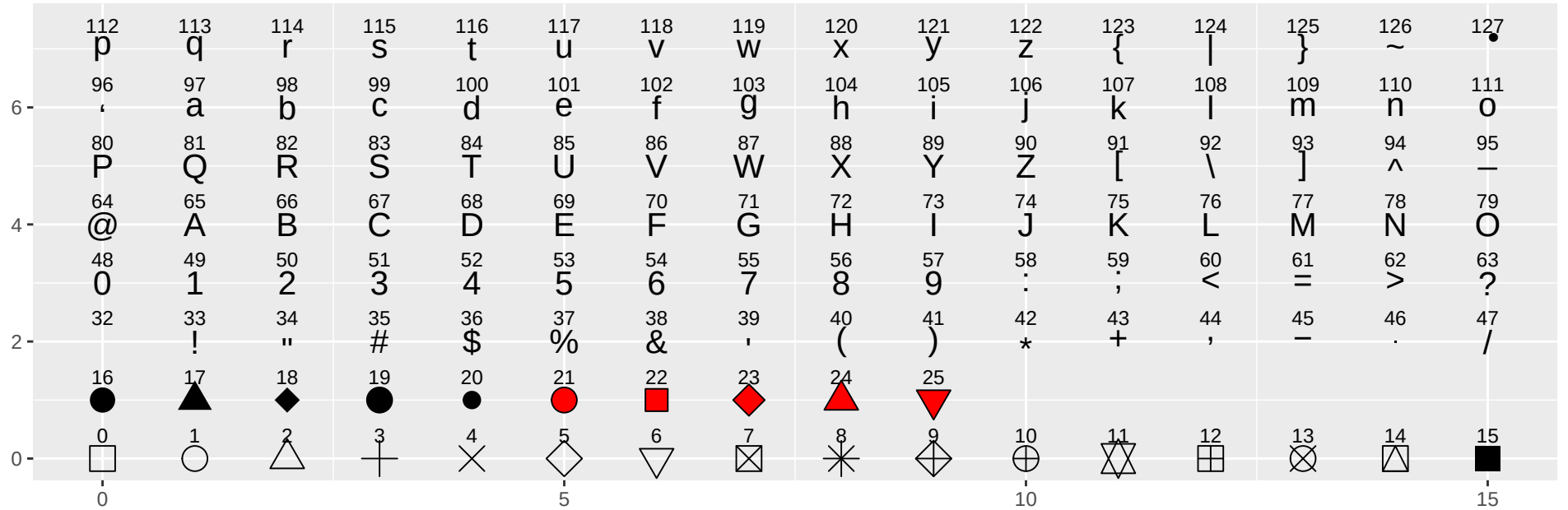
```
par( mfrow = c(2,4) ); ### 在一张图上画 2 x 4 个 panel
opts <- c( "p", "l", "o", "b", "c", "s", "S", "h" );
for( o in opts ){
  plot(1:5, type = o, main = paste( "type=", o ) );
}
```



pch 是什么？

决定了数据点的形状，注意它的取值范围

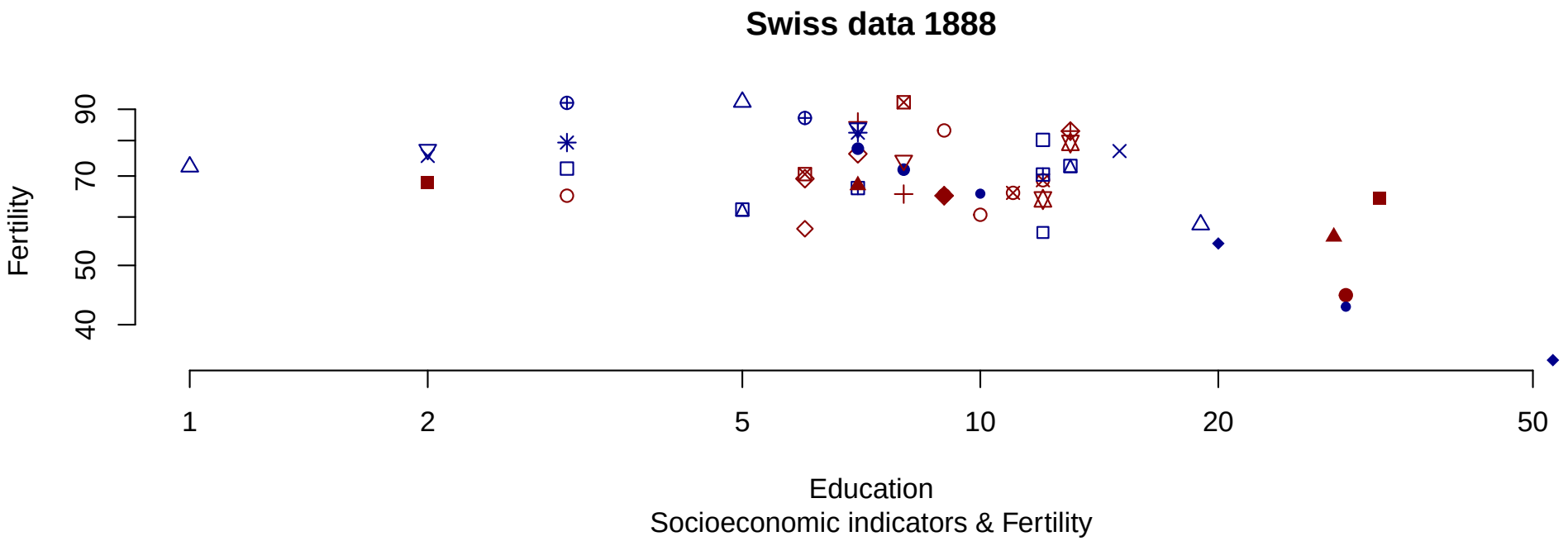
```
library(tidyverse);
ggplot( data.frame( p = c(0:25, 32:127) ) ) +
  scale_y_continuous( name = "" ) + scale_x_continuous( name = "" ) +
  scale_shape_identity() +
  geom_point( aes( x = p%%16, y = p%/%16, shape = p ), size = 5, fill = "red" ) +
  geom_text( aes( x = p %% 16, y = p%/%16 + 0.4, label = p  ), size = 3 );
```



log transform aexes

plot 还有一些其它有用的参数，详见：? plot.default

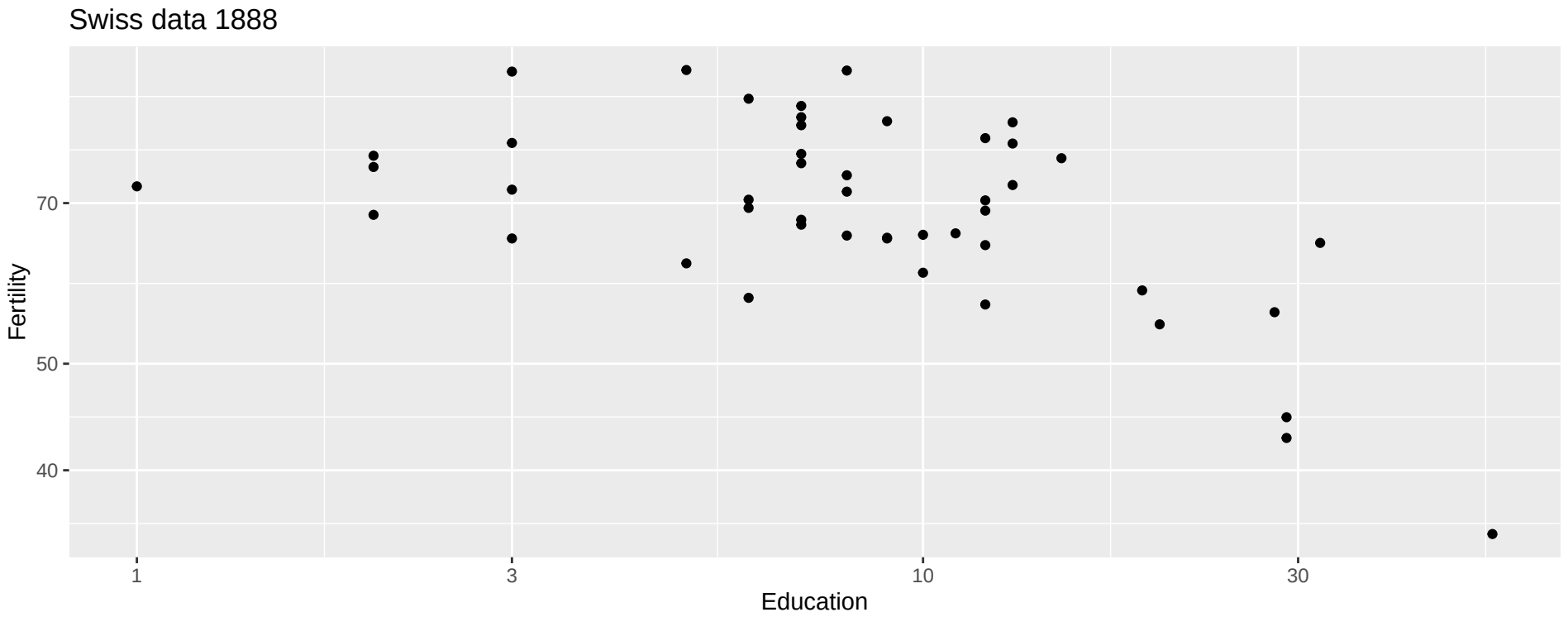
```
with( swiss, plot(Education, Fertility, type = "p", main = "Swiss data 1888",
                  sub = "Socioeconomic indicators & Fertility",
                  xlab = "Education", ylab = "Fertility", col = c("darkblue", "darkred"),
                  xlim = range( Education ), ylim = range( Fertility ),
                  pch = 0:25, frame.plot = F, log = "xy") );
```




```
## 注：也可以用 log='x' 或 log='y' 只对一个 axis 进行 log 处理
```

ggplot 版本

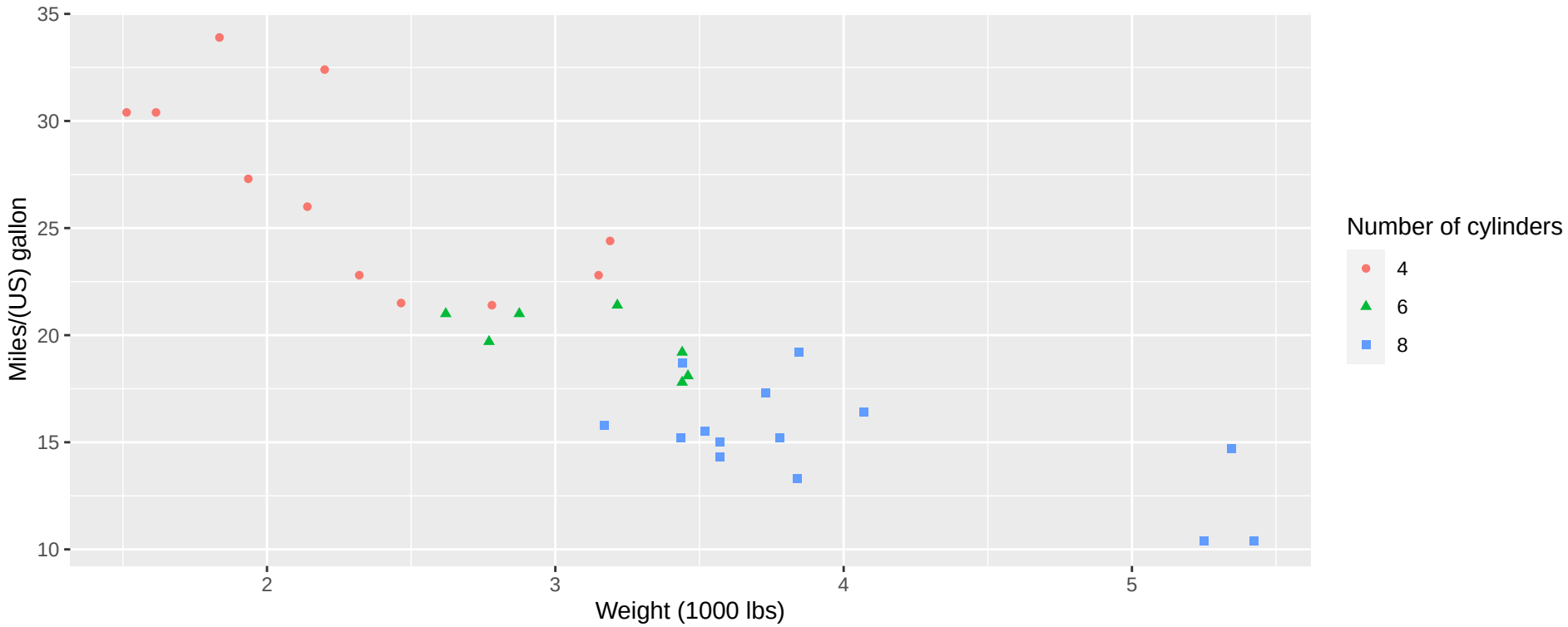
```
ggplot( swiss, aes( x = Education, y = Fertility ) ) +
  geom_point(  ) + scale_x_log10() + scale_y_log10() +
  xlab( "Education" ) + ylab( "Fertility" ) +
  ggtitle( "Swiss data 1888" );
```



ggplot 更多散点示例

以 mtcars 为例

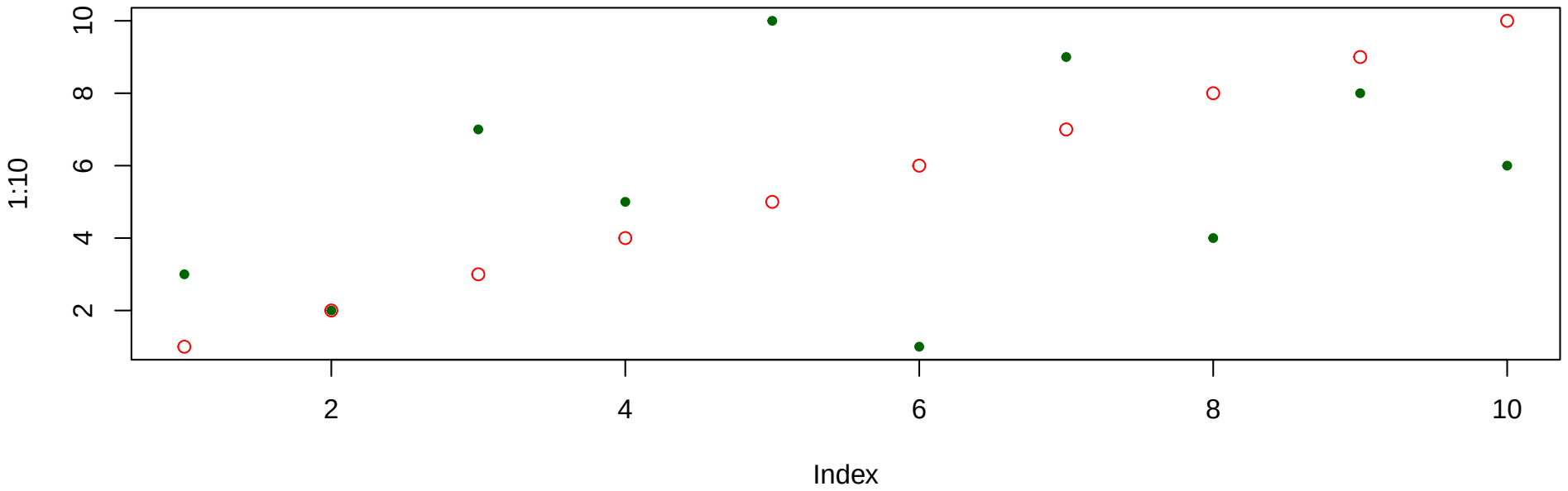
```
ggplot( mtcars, aes( x = wt, y = mpg, colour = factor( cyl ), shape = factor(cyl) ) ) +
  geom_point() + xlab( "Weight (1000 lbs)" ) + ylab( "Miles/(US) gallon" ) +
  labs( colour = "Number of cylinders", shape = "Number of cylinders" ) ;
```



plot: high-level vs. low-level plots

- **high level**: plotting functions create a new plot on the graphics device
- **low level**: plotting functions add more information to an existing plot

```
plot( 1:10, col = "red" ); ## high level
points( sample(1:10, 10), col = "darkgreen", pch = 20 ); ## low level
```



low level plots 列表

- points : 点图
- lines : 线图
- abline : 直线
- polygon : 多边形
- legend : 图例
- title : 标题
- axis : 轴 ...

high level plots 列表

- `plot`：通用画图函数
- `pairs`
- `coplot`
- `qqnorm`
- `hist`
- `dotchart`
- `image`
- `contour` ...

注：可以用 `add = TRUE` 参数（如果可用）将 high level 函数强制转换为 low level

图形相关参数（系统函数）

par() 函数：显示或修改当前**图形设备**的参数。用以下命令查看支持的内容：

```
par( c( "mar", "bg" ) ); ## 显示指定参数的值
```

```
## $mar
## [1] 5.1 4.1 4.1 2.1
##
## $bg
## [1] "transparent"
```

```
## 显示所有参数
par();
```

```
## $xlog
## [1] FALSE
##
## $ylog
## [1] FALSE
##
## $adj
## [1] 0.5
##
## $ann
## [1] TRUE
```

调整 par() 参数前请备份

par() 用于指定全局参数，因此在改变前尽量备份

```
oldpar <- par(); ## 备份

do some changes here ...

## 恢复
par( oldpar );
```

常用图形参数及调整：margin

图形边距（figure margins ）

```
par( mar = c( 5.1, 4.1, 4.1, 2.1 )); ## 设置新 martin
```

分别指定下 -> 左 -> 上 -> 右的边距，即从下面开始，顺时针移动。

单位是：text lines

或：

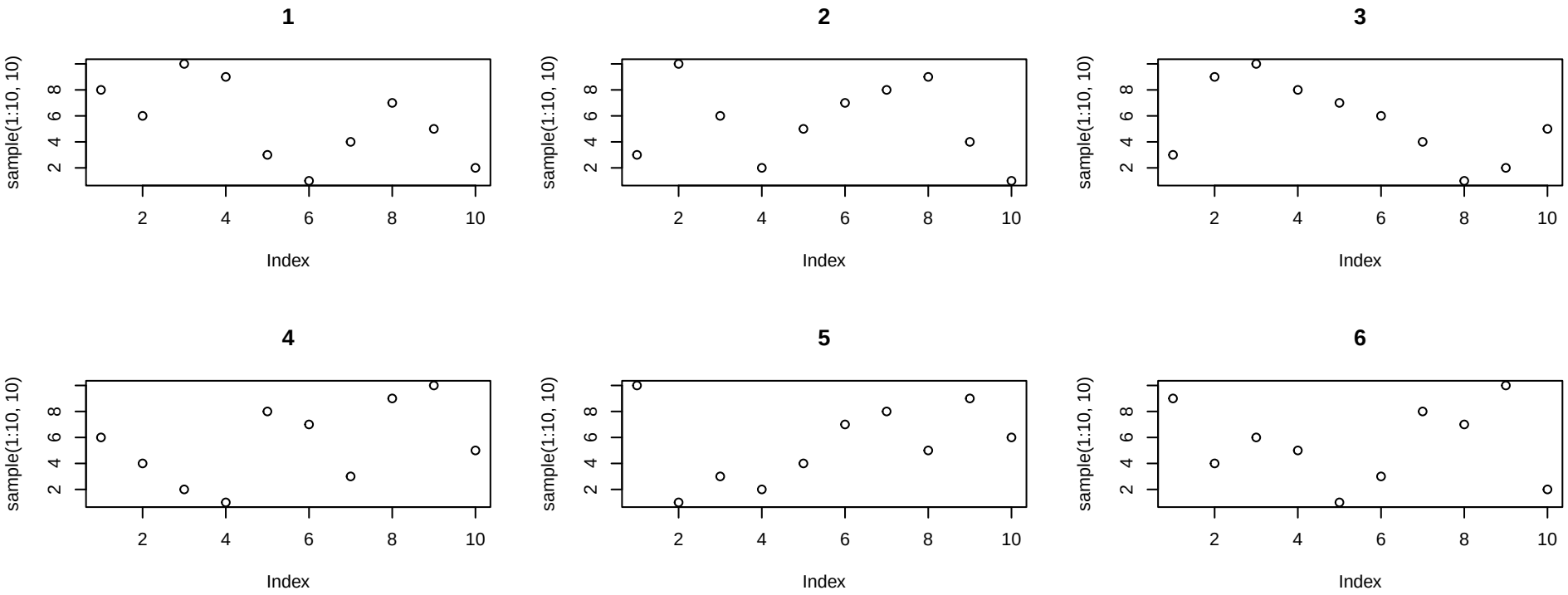
```
par( mai = c( 5.1, 4.1, 4.1, 2.1 )); ## 设置新 martin
```

单位是：inch

常用图形参数及调整：多 panel

画 2x3 共 6 个 panel，从左到右。(2 行 3 列)

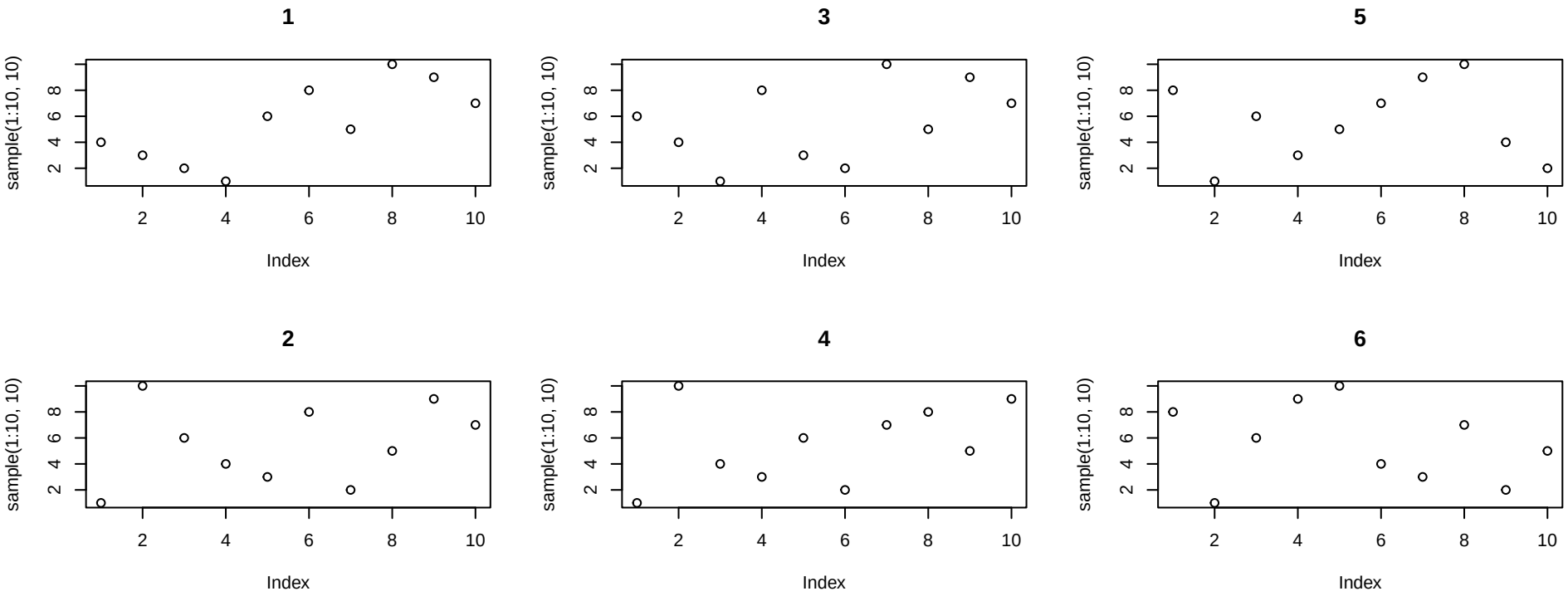
```
par( mfrow=c(2,3) );
for( i in 1:6 )
  plot( sample( 1:10, 10 ), main = i );
```



常用图形参数及调整：多 panel，cont.

画 2x3 共 6 个 panel，从上到下。(2 行 3 列)

```
par( mfcol=c(2,3) );
for( i in 1:6 )
  plot( sample( 1:10, 10 ), main = i );
```



重要概念：图形设备

图形设备是指图形输出的设备，可以将**图形设备**理解为**保存格式**。

默认设备是：

- X11()：*nix
- windows()：windows
- quartz()：OS X

图形显示在**显示器**上。

图形设备：cont.

常用其它设备有：

- pdf()
- png()
- jpeg()

分别对应输出文件格式。

常用图形设备：pdf()

使用方法如下：

```
pdf( file = "/path/to/dir/<file_name>.pdf", height = 5, width = 5 ); ## 创建一个新设备/ pdf 文件
plot(1:10); ## 作图;
dev.off(); ## 关闭设备
```

说明

1. 默认文件名为 Rplots.pdf ，
2. dev.off() 必须关闭。关闭后，返回到最近使用的图形设备
3. height 和 width 参数的单位是 inch
4. 如果运行多个 high level 作图命令，则会产生多页 pdf

请尽量使用 pdf 作为文件输出格式

1. 生信图片大多是点线图，适合保存为矢量格式（如 pdf, ps 等）;
2. 矢量图可无限放大而不失真（变成像素）;
3. 可由 Adobe Illustrator 等矢量图软件进行编辑

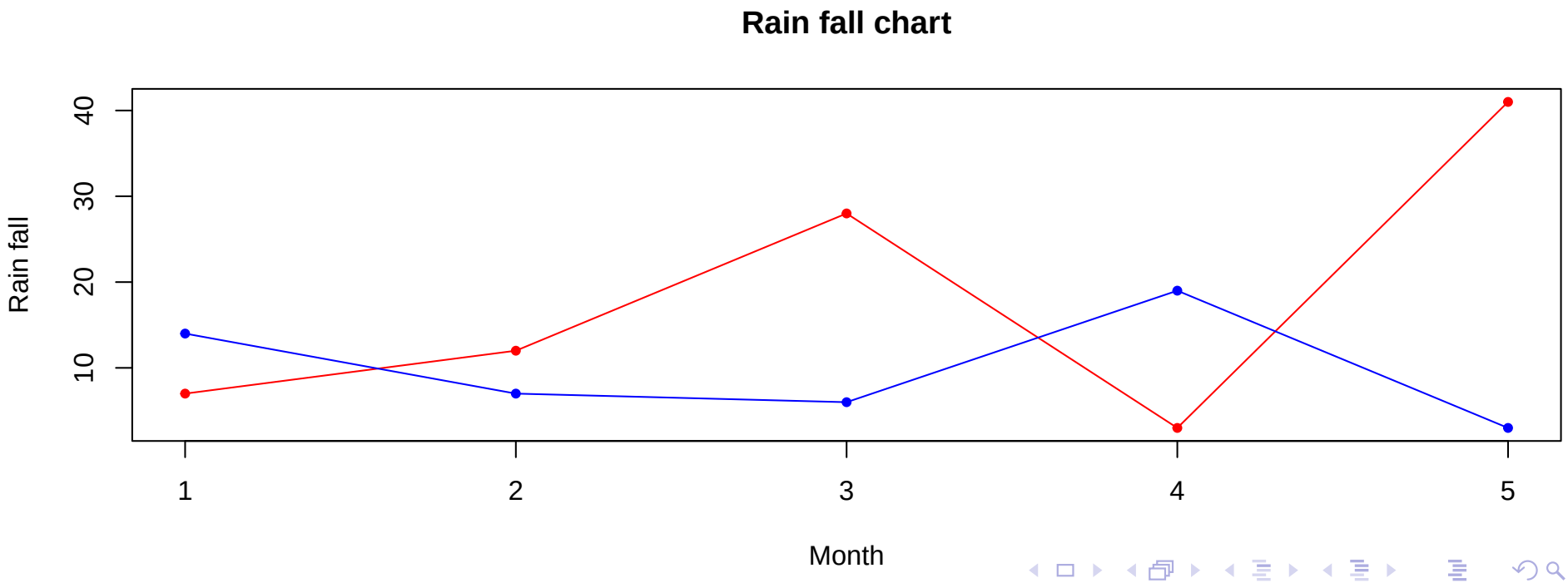
section 3: ggplot2 基础

为什么要使用 ggplot2 ？ 从一个简单示例开始

假设画两条线：

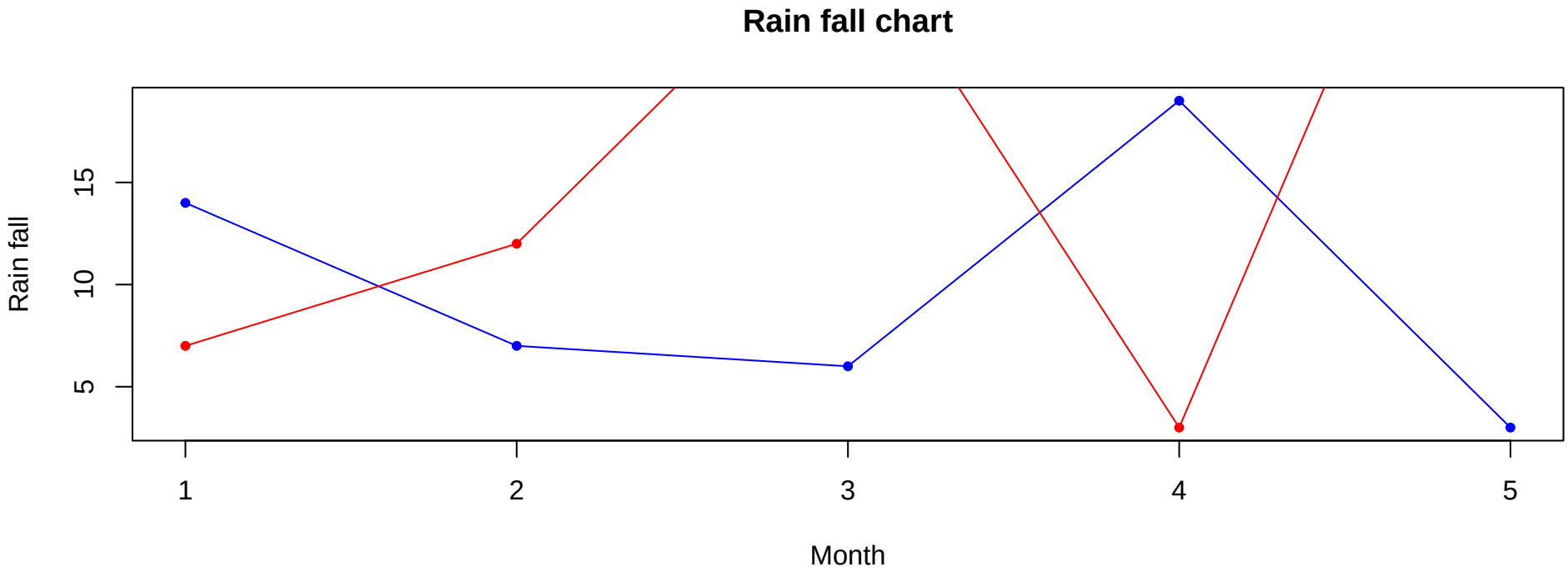
```
year1 <- c(7, 12, 28, 3, 41);
year2 <- c(14, 7, 6, 19, 3);

plot( year1, type = "o", pch = 20, col = "red", xlab = "Month", ylab = "Rain fall",
      main = "Rain fall chart");
lines( year2, type = "o", pch = 20, col = "blue");
```



如果改变画线的顺序？

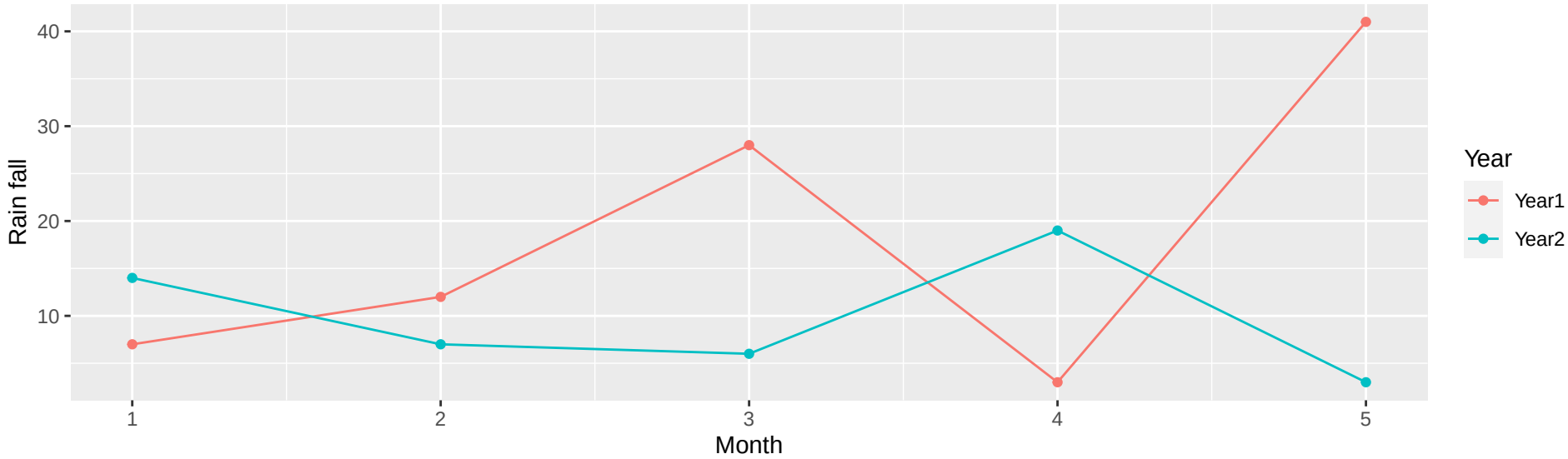
```
plot( year2, type = "o", pch = 20, col = "blue", xlab = "Month", ylab = "Rain fall",
      main = "Rain fall chart");
lines( year1, type = "o", pch = 20, col = "red");
```



ggplot2 的方法

```
df <- rbind( tibble( month = 1:length( year1 ), value = year1, cat = "Year1" ),
             tibble( month = 1:length( year2 ), value = year2, cat = "Year2 ") );

plot1 <-  ## 将图保存在变量中;
  ggplot( df, aes( x = month, y = value, colour = cat) ) +
  geom_line() + geom_point() +
  xlab( "Month" ) + ylab( "Rain fall" ) +
  labs( colour = "Year");
plot1;  ## 画图
```



ggplot2 基础概念详解

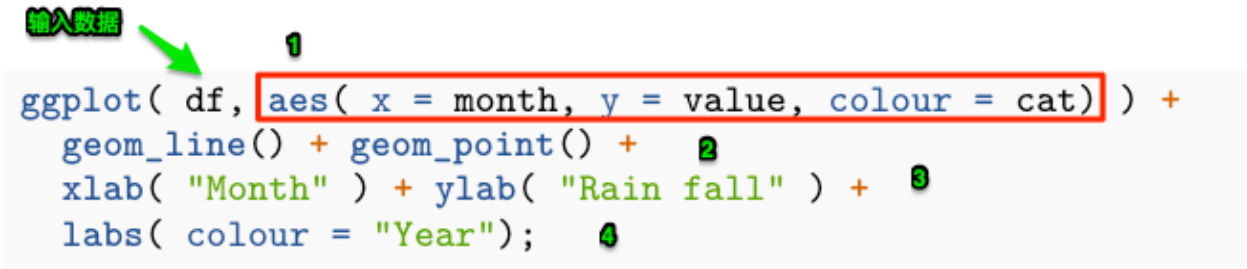


Figure 2: ggplot2 参数简介

1. aes (aesthetics) 美学：控制全局参数，包括：x,y 轴使用的数据，颜色 (colour, fill) ，形状 (shape)，大小 (size)，分组 (group) 等等；
2. 图层：geom_<layer_name> ；每张图可有多个图层（此处有两个）；图层可使用全局数据 (df) 和参数 (aes)，也可以使用自己的 aes 和数据；3-4. 其它参数

ggplot2 优缺点

ggplot2 优点：

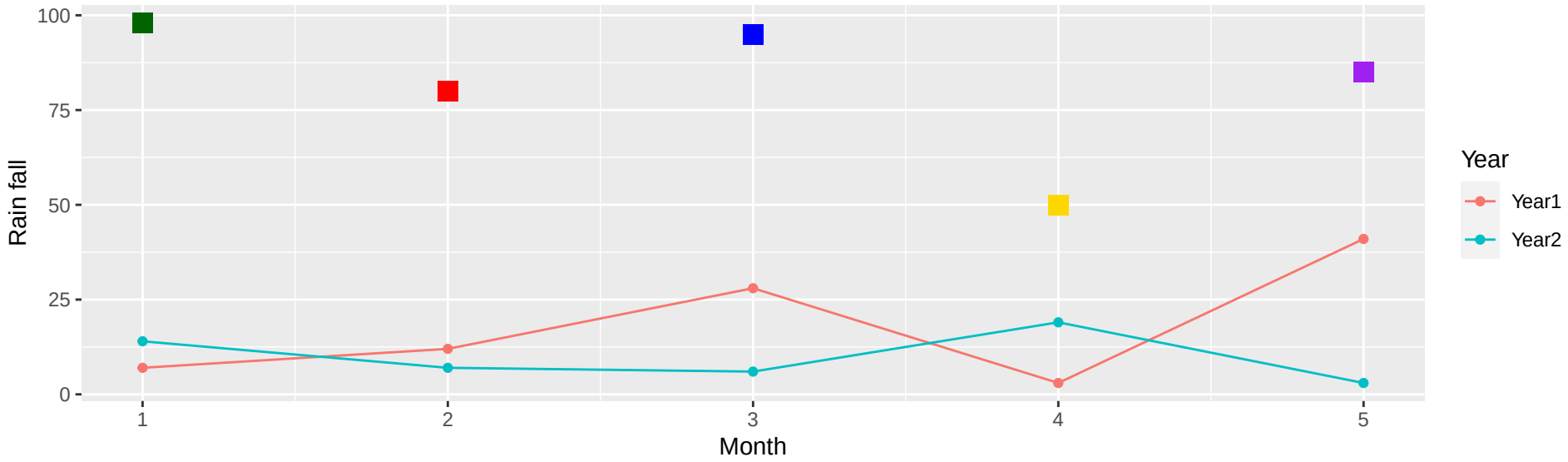
1. 强大又专业
2. 复杂又好看
3. canvas 大小，坐标会根据数据、图层自动调整，让用户专注于作图本身；

缺点：

太难学！

图层使用自己的数据，示例

```
plot1 +
  geom_point( data = data.frame( x2 = 1:5, y2 = sample(30:100, 5) ),  ## 注意： data = 是必须的
          aes( x = x2, y = y2 ),  ## 使用自己的 aes ...
          colour =  c("darkgreen", "red", "blue", "gold", "purple") , shape = 15, size = 4 )
```



要点

1. 如上所见，xy -axes 会随数据自动调整
2. ggplot2 作图结果可以保存在变量中，并可累加更多图层
3. 图层使用自己的数据时，需要用 data = 指定；而全局数据则不用 ggplot(data.frame(...))

aes( ) 内部和外部的 coulor, size, shape 参数有何区别？

在内部时，colour = < 列名 > 或 colour = factor(< 列名 >)，其真实结果是取的 factor，然后按顺序为每个 factor **自动指定一个颜色**。默认**颜色顺序为**：

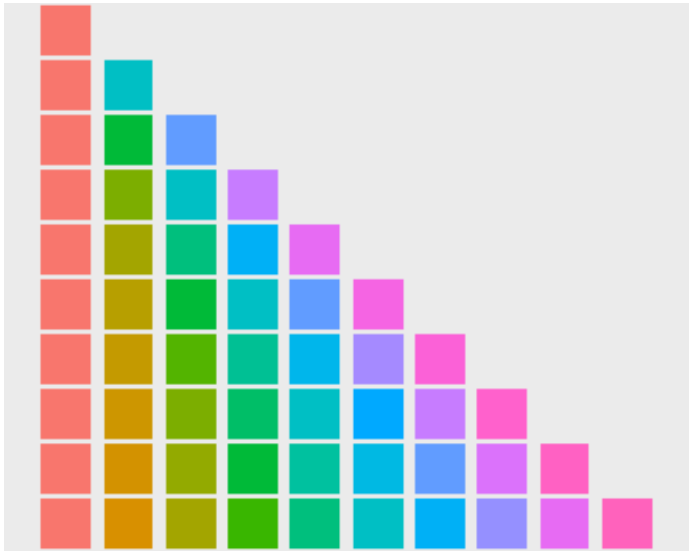
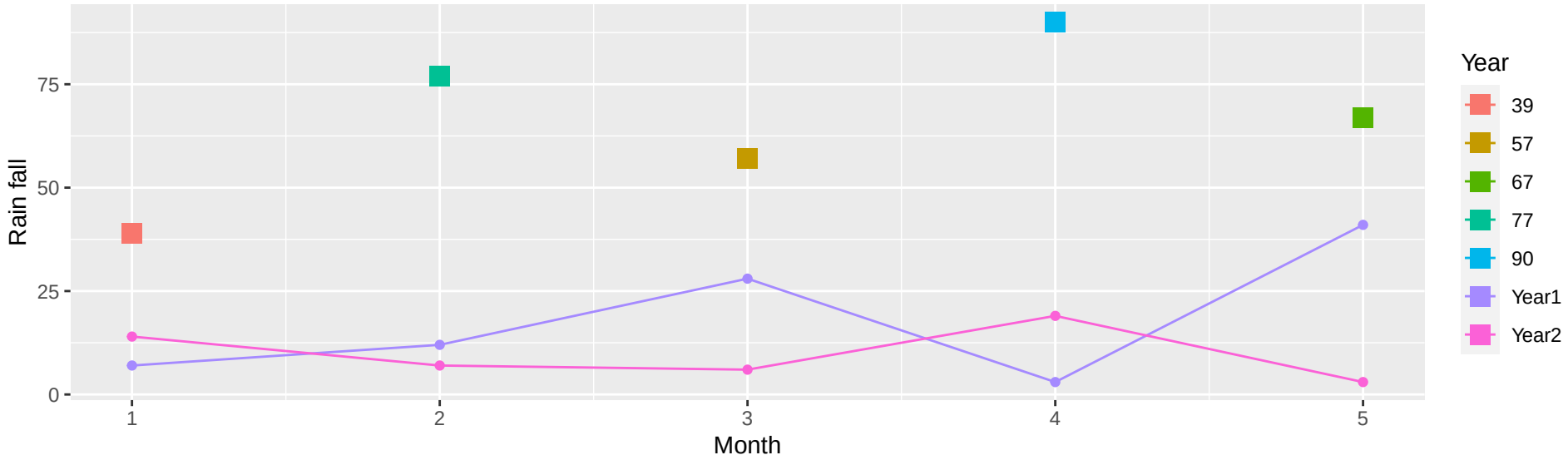


Figure 3: default discrete colour palette

color 举例

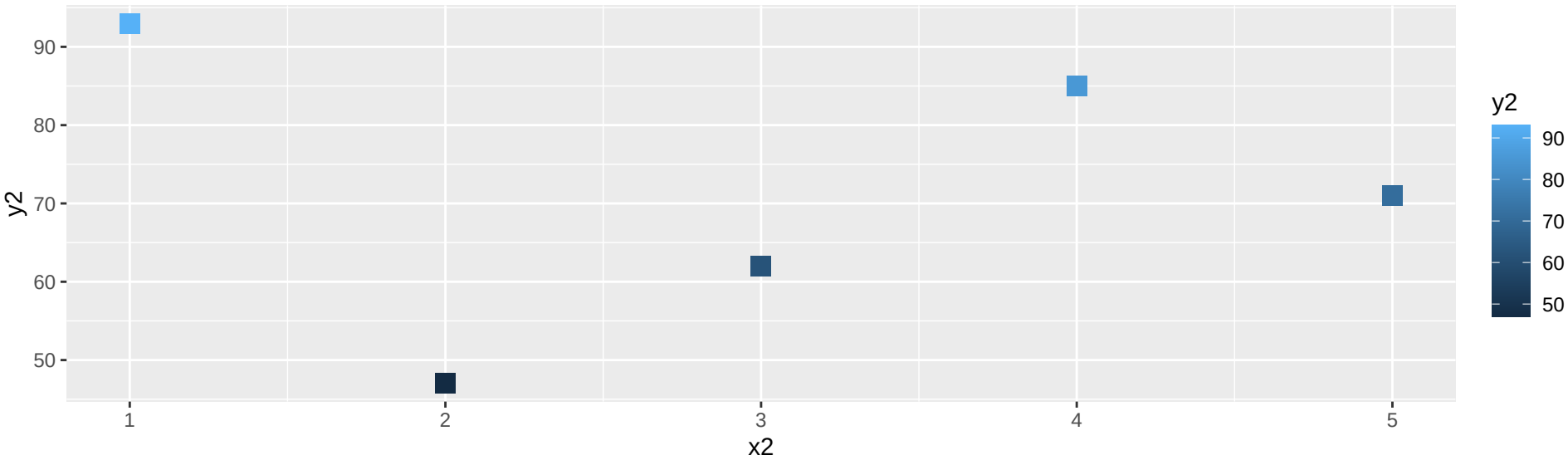
```
plot1 +
  geom_point( data = data.frame( x2 = 1:5, y2 = sample(30:100, 5) ),  ## 注意： data = 是必须的
              aes( x = x2, y = y2 , colour = factor( y2 ) ),  ## colour 在 aes 内部
              shape = 15, size = 4 )
```



共有 7 个颜色；注意与上页图的第 7 行对应一下！

当 colour = < 数字列 > , 则显示 color gradient

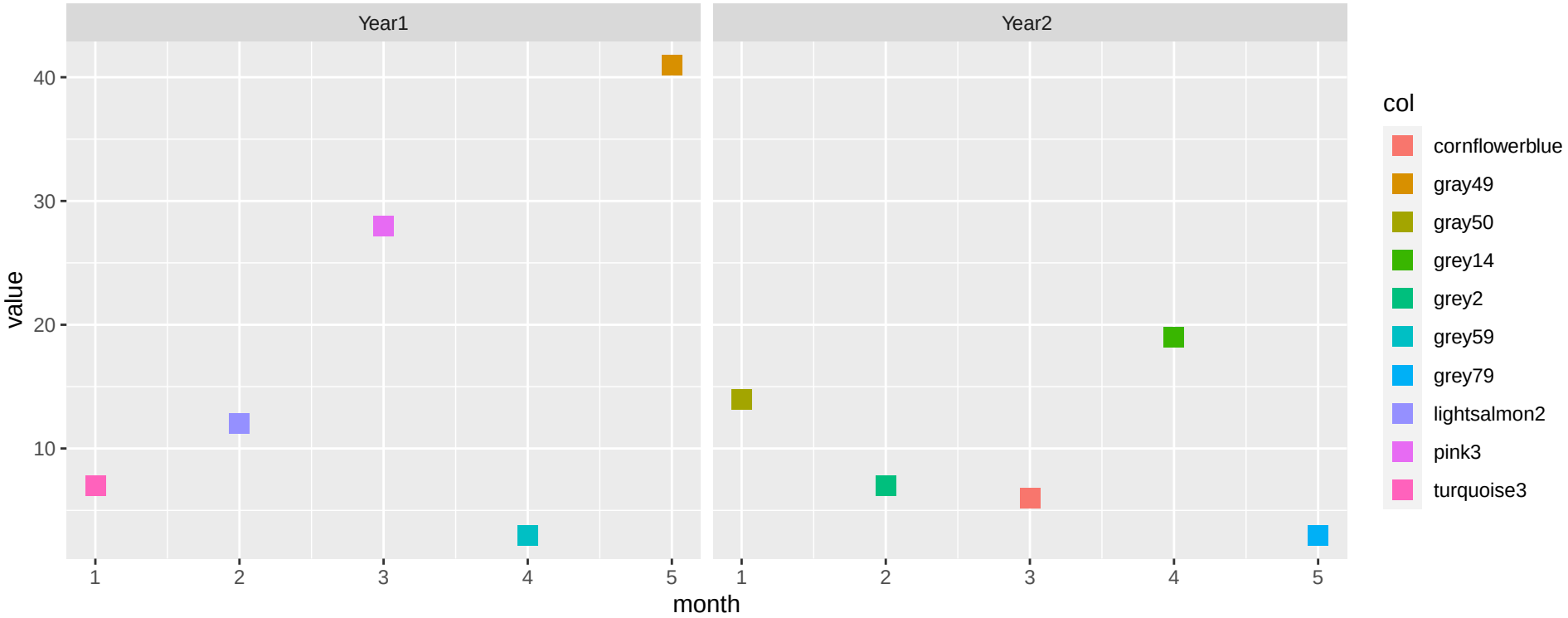
```
ggplot( data = data.frame( x2 = 1:5, y2 = sample(30:100, 5) ),
        aes( x = x2, y = y2 , colour = y2 ) ) +
  geom_point( shape = 15, size = 4 )
```



注意 discrete color (上页图) 和 continous color (or color gradient) 的默认画板 (color palette) 是不一样的!

更改画板，使用指定的颜色（不作为 factor 使用）

```
df$col <- sample( colours(), 10 ); ## 现有我们有颜色了!
ggplot(df, aes( x = month, y = value, colour = col ) ) +
  geom_point( size = 4, shape = 15 ) + facet_grid( ~ cat );
```

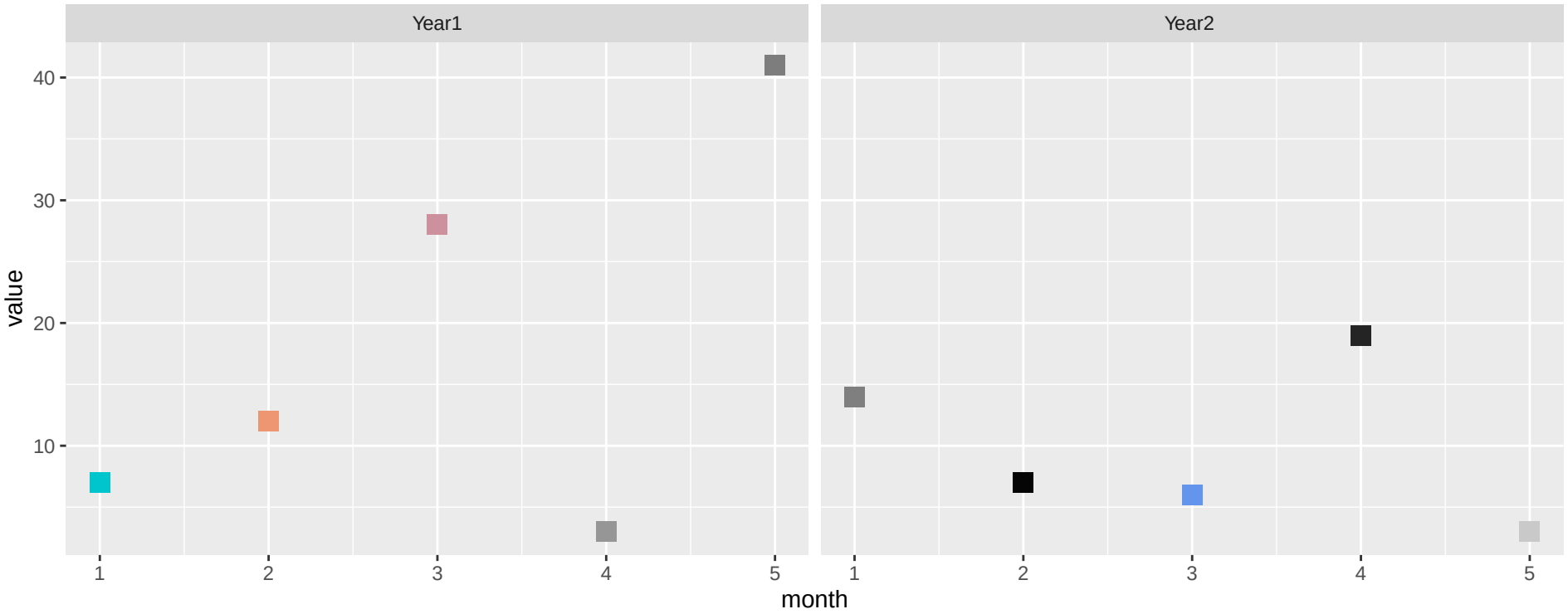


** 注 ** 默认情况下，col （颜色）列是作为 factor 使用。

更改画板，使用指定的颜色（不作为 factor 使用），cont.

解决方案：scale_color_identity

```
ggplot(df, aes( x = month, y = value, colour = col ) ) +
  geom_point( size = 4, shape = 15 ) + facet_grid( ~ cat ) +  ##  facet_grid 又是什么 ??
  scale_color_identity(); ## magic !!
```



图层简介

- geom_point，geom_line: 点线图，用于揭示两组数据间的关系；
- geom_smooth：常与 geom_point 联合使用，揭示数据走势
- geom_bar：bar 图
- geom_boxplot：箱线图，用于比较 N 组数据，揭示区别
- geom_path：与 geom_line 相似，但也可以画其它复杂图形
- geom_histogram, “ geom_density “‘：数据的分布，也可用于多组间的比较
- 其它十余种，请见 “ggplot2：elegant graphics for data analysis” 一书!!

section 4: ggplot2 作图的四个基本组成部分

ggplot2 的四个基本组成

1. 图层（layers）
   - geom_< 图层名 >
2. scale：控制数据至美学属性的 mapping
   - scale_< 属性 mapping 方式 >，e.g. scale_color_identity()

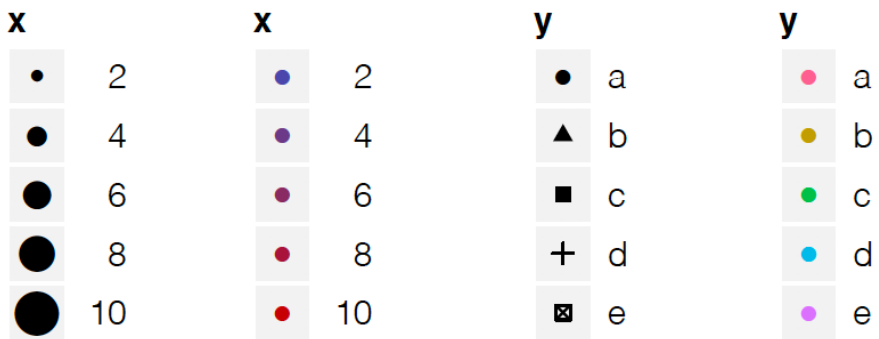


Figure 4: 数据的 4 种 scale 方法

ggplot2 的 scale

- `scale_color_...`
- `scale_shape_...`
- `scale_size_...`
- `scale_fill_...`

与坐标系统联动的函数

- `scale_x_log()`
- `scale_y_log()`

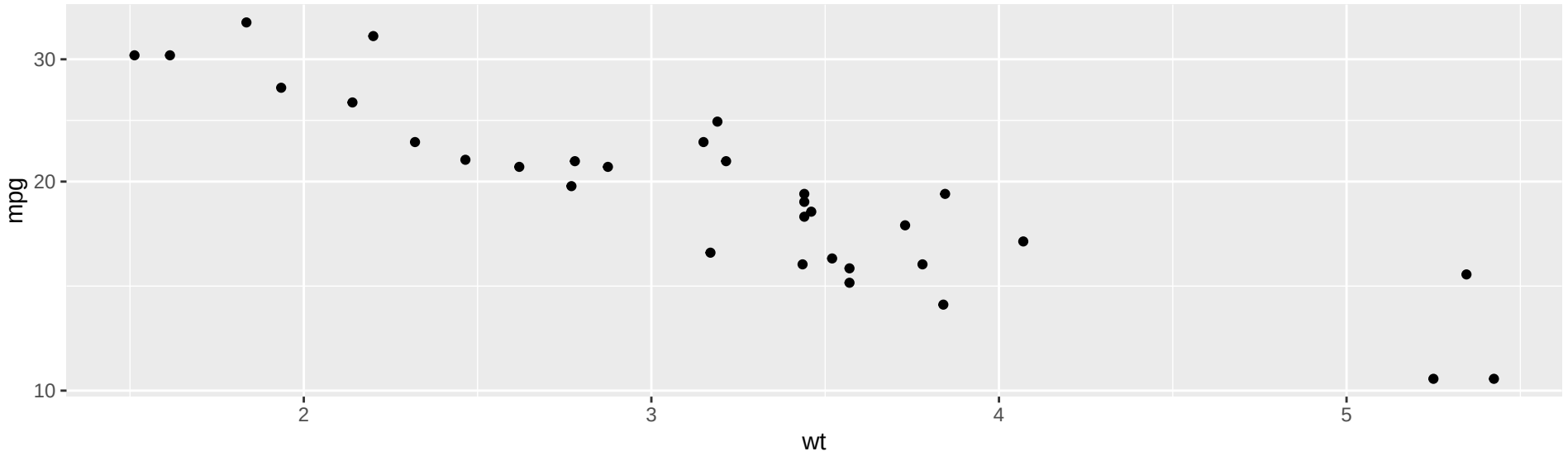
更多内容可以见《ggplot2: elegant graphics for data analysis》一书的第 6 章。

ggplot2 要素 3：坐标系统

- 正常
- log-transform

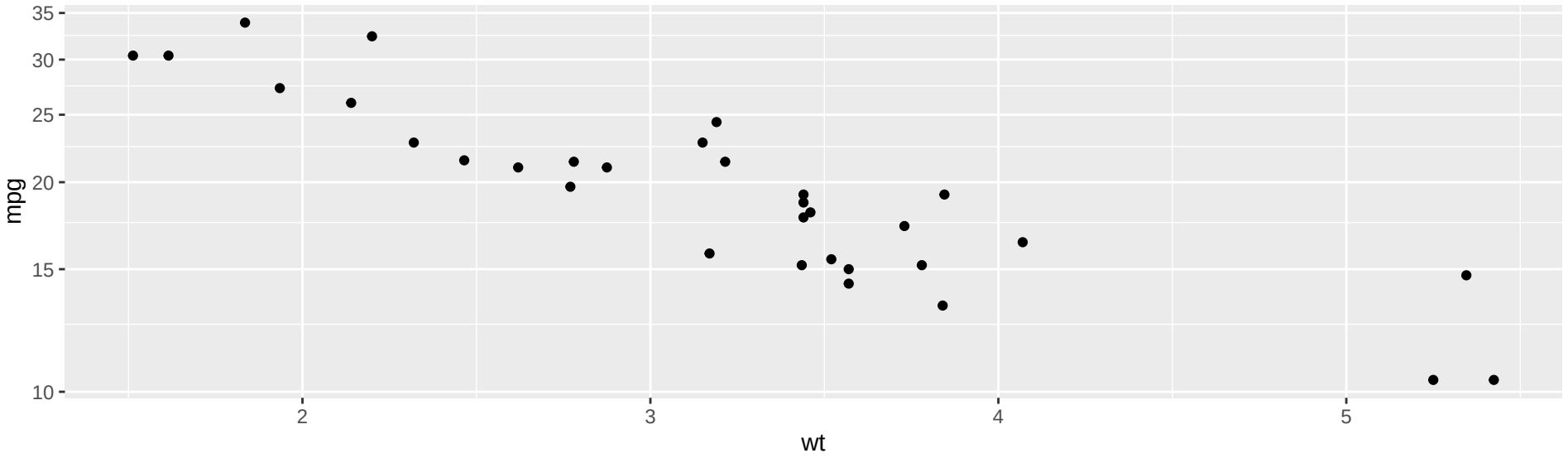
示例：

```
ggplot(mtcars, aes( wt , mpg)) + geom_point() +
  scale_y_log10()
```



ggplot2 要素 3：坐标系统，cont.

```
ggplot(mtcars, aes( wt , mpg)) + geom_point() +
  coord_trans( y = "log10" );
```



* limx, limy: 限制xy的显示范围

ggplot2要素3： 坐标系统，cont.

其它函数

* ```coord_flip()``` : x，y轴互换；竖bar变横bar;
* ```coord_polar()``` :

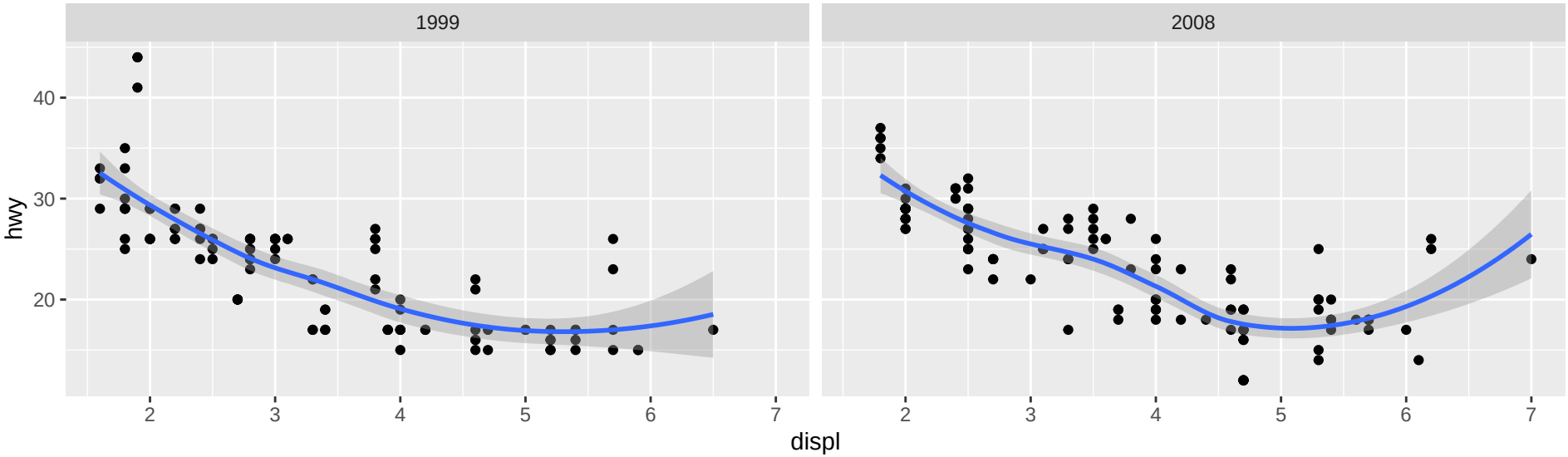
ggplot2 要素 3：坐标系统，cont.

```
plot1 + coord_polar();
```

ggplot2 要素 4：faceting ...

```
qplot(displ, hwy, data=mpg, facets = . ~ year) + geom_smooth();
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```

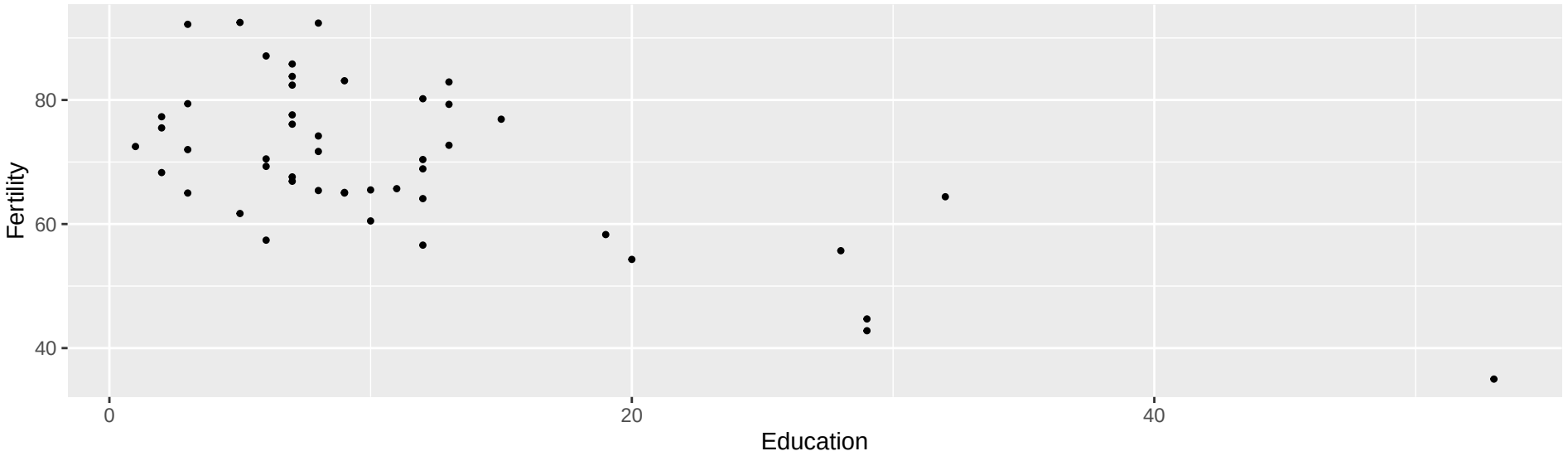


section 5: ggplot2 进阶 1

散点图的进一步分析

显示两组数据间的相关性：

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

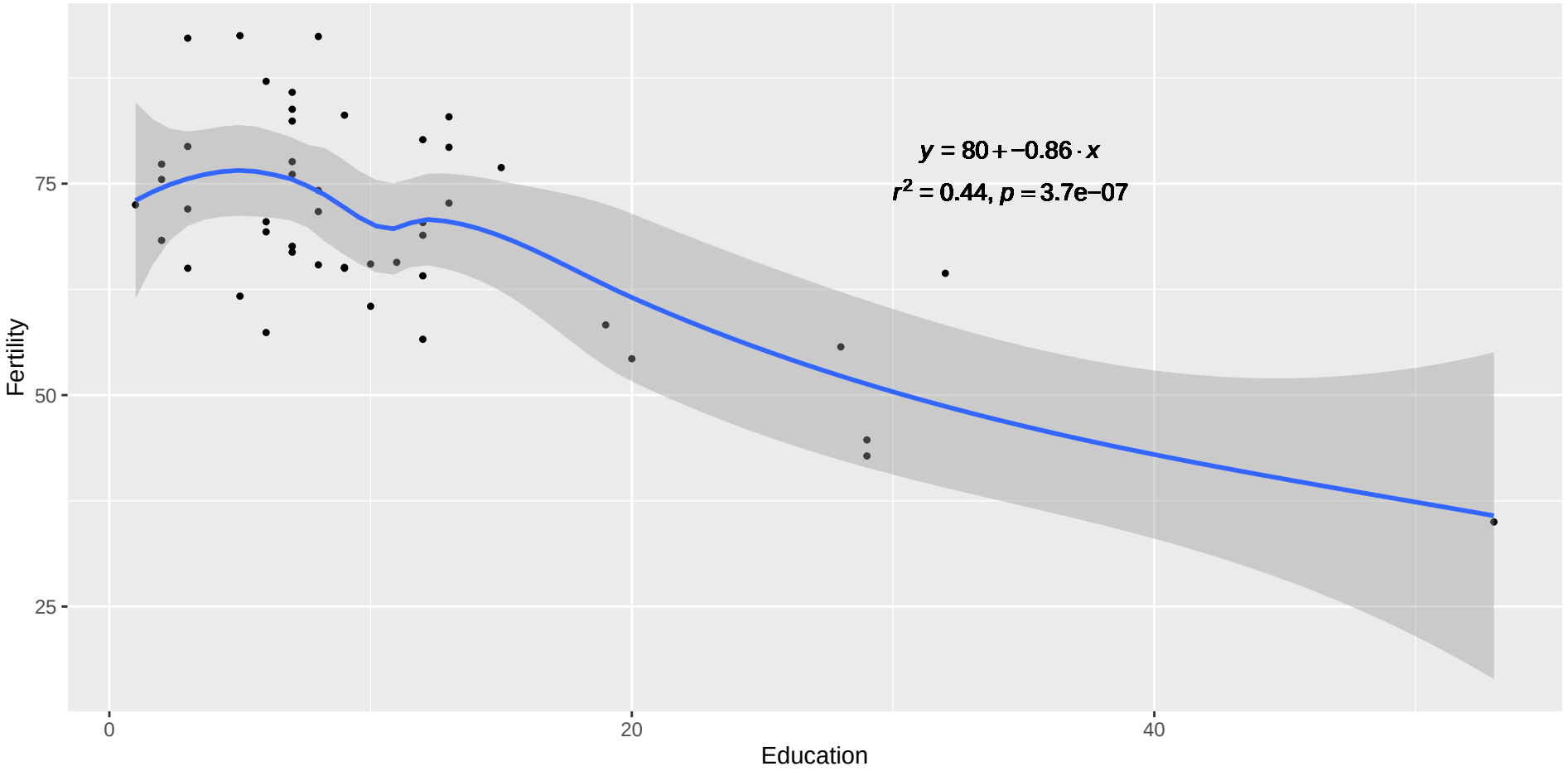



```
## 分析
with( swiss, cor.test( Education, Fertility  )$estimate );
```

```
##        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

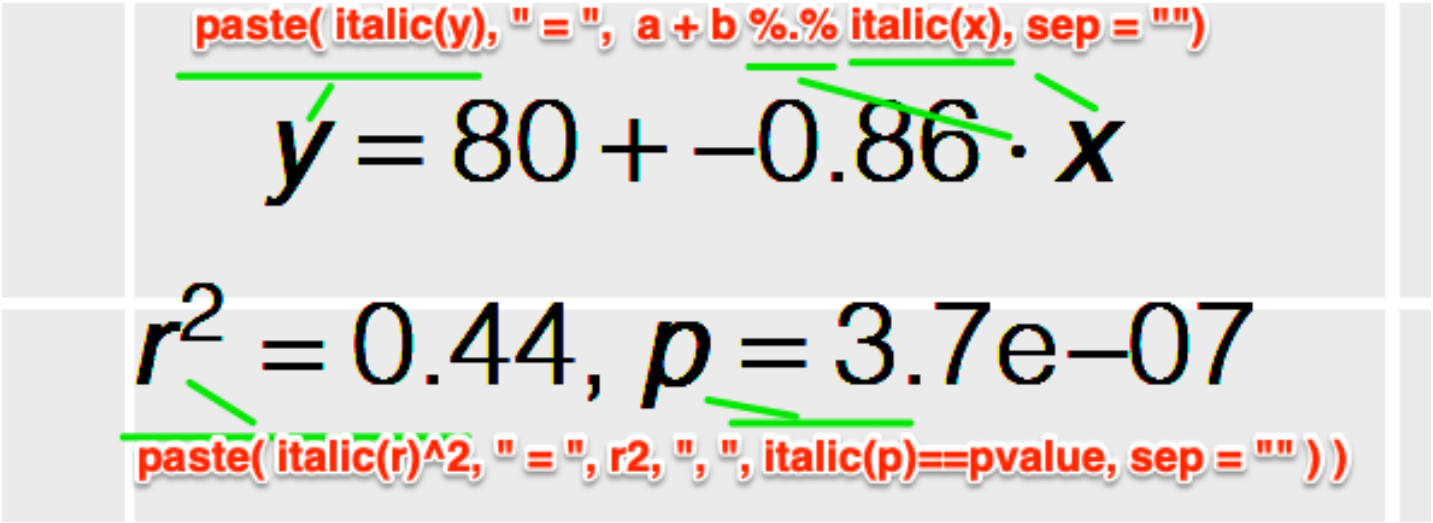


Figure 5: equation explained!

公式详解，cont.

以下代码实现两个任务：

1. 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(...))

```
## 计算 ...
m = lm(Fertility ~ Education, swiss);
c = cor.test( swiss$Fertility, swiss$Education );

## 生成公式
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));
```

完整代码

```
## 计算 ...
m = lm(Fertility ~ Education, swiss);
c = cor.test( swiss$Fertility, swiss$Education );

## 生成公式
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 );

## 生成公式
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

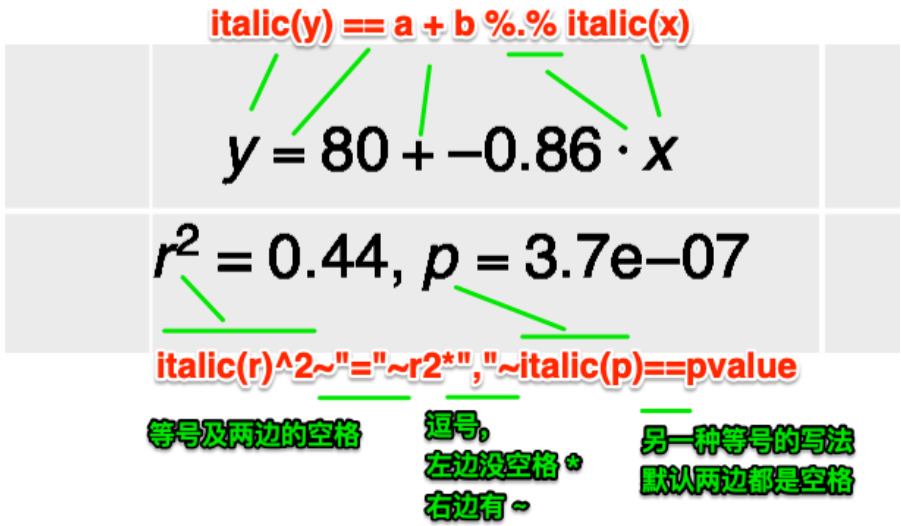


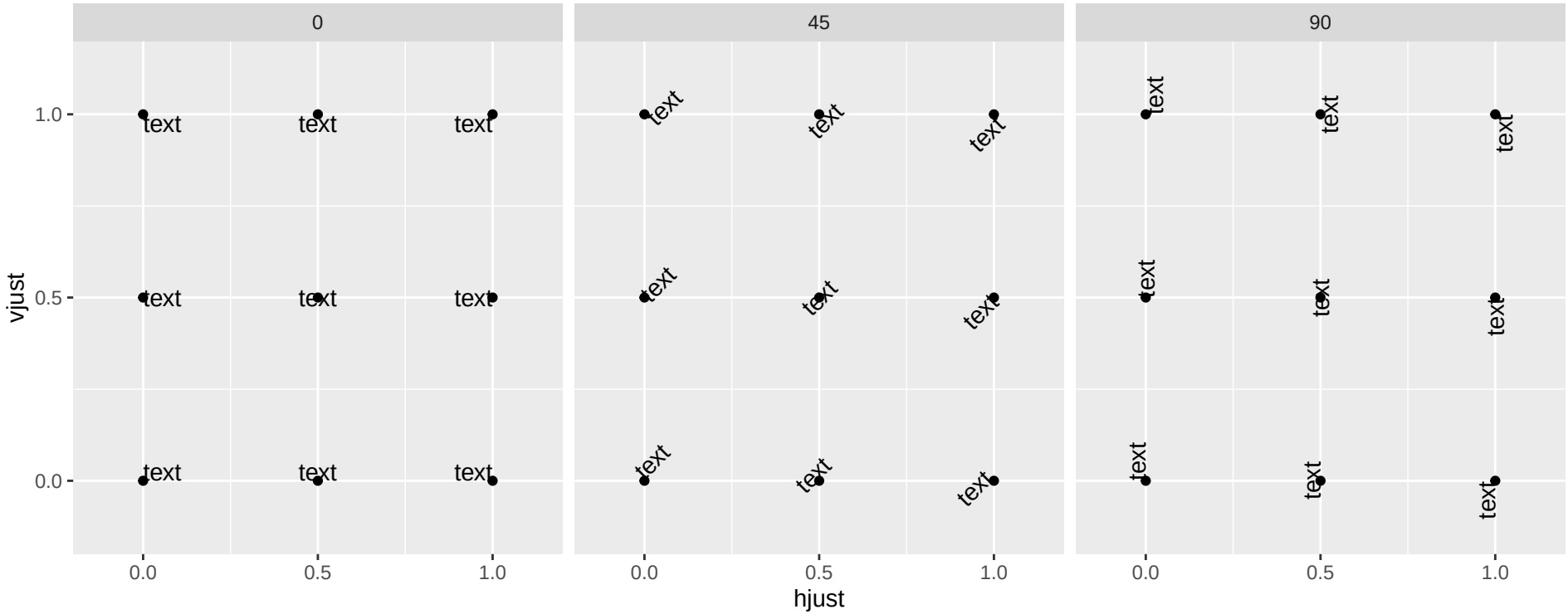
Figure 6: equation explained!

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”。

hjust 和 vjust

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



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))`	$\sqrt[y]{x}$
	`expression(list(x,yz))`	x, y, z

公式, cont.

分类	R 的表达式	显示结果
变量间的关系符号	`expression(x==y)`	$x = y$
	`expression(x!=y)`	$x \neq y$
	`expression(x<=y)`	$x \leqslant y$
	`expression(x>=y)`	$x \geqslant y$
	`expression(x %~~% y)`	$x \approx y$
	`expression(x %=~% y)`	$x \cong y$
	`expression(x %==% y)`	$x \equiv y$
	`expression(x %prop% y)`	$x \propto y$
	`expression(x %~% y)`	$x \sim y$
列表符号	`expression( list(x[1], ..., x[n] )`	$x_1, \ldots, x_n$
	`expression( list(x[1]+...+x[n]) )`	$x_1 + \ldots + x_n$

公式, cont.

分类	R 的表达式	显示结果
数组之间关系的符号	`expression( x %subset% y )`	$x \subset y$
	`expression( x %subseteq% y )`	$x \subseteq y$
	`expression( x %supset% y )`	$x \supset y$
	`expression( x %supseteq% y )`	$x \supseteq y$
	`expression( x %notsubset% y )`	$x \not\subset y$
	`expression( x %in% y )`	$x \in y$
注音符号	`expression( hat(x) )`	$\hat{x}$
	`expression( tilde(x) )`	$\tilde{x}$
	`expression( bar(xy) )`	$\bar{xy}$
	`expression( widehat(xy) )`	$\widehat{xy}$
	`expression( widetilde(x) )`	$\widetilde{xy}$

公式，cont.

分类	R 的表达式	显示结果
各种箭头	`expression( x %<->% y )`	$x \leftrightarrow y$
	`expression( x %->% y )`	$x \rightarrow y$
	`expression( x %<-% y )`	$x \leftarrow y$
	`expression( x %up% y )`	$x \uparrow y$
	`expression( x %down% y )`	$x \downarrow y$
	`expression( x %<=>% y )`	$x \Leftrightarrow y$
	`expression( x %=>% y )`	$x \Rightarrow y$
	`expression( x %<=% y )`	$x \Leftarrow y$
	`expression( x %dblup% y )`	$x \Uparrow y$
	`expression( x %dbldown% y )`	$x \Downarrow y$

公式, cont.

分类	R 的表达式	显示结果
特殊符号	`expression( infinity )`	∞
	`expression( 32 * degree )`	32°
	`expression( 60 * minute )`	$60'$
	`expression( 30 * second )`	$30''$
空白	`expression( x ~~ y )`	$x\ y$
	`expression( x + phantom() + y )`	$x + \ + y$
分式	`expression( frac(x,y) )`	$\frac{x}{y}$
	`expression( over(x,y) )`	$x + \frac{1}{\frac{x}{y}}$
	`expression( atop(x,y ) )`	

公式, cont.

分类	R 的表达式	显示结果
大型操作符	`expression( sum(x[i], i = 1, n ) )`	$\sum_1^n x_i$
	`expression( prod(plain(P)(X==x),x ) )`	$\prod_x P(X = x)$
	`expression( integral( f(x) * dx, a,b ) )`	$\int_a^b f(x)dx$
	`expression( union(A[i], i==1,n) )`	$\bigcup_{i=1}^n A_i$
	`expression( intersect(A[i], i==1, n) )`	$\bigcap_{i=1}^n A_i$
	`expression( lim(f(x), x %->% 0) )`	$\lim_{x \to 0} f(x)$
	`expression( min(g(x), x >= 0) )`	$\min_{x \geqslant 0} g(x)$
分组	`expression( group("(", list(a, b), "]") )`	$(a, b]$
	`expression( bgroup("(", atop(x, y), ")") )`	$\binom{x}{y}$
	`expression( group(lceil, x, rceil) )`	$\lceil x \rceil$
	`expression( group(lfloor, x, rfloor) )`	$\lfloor x \rfloor$

希腊字符

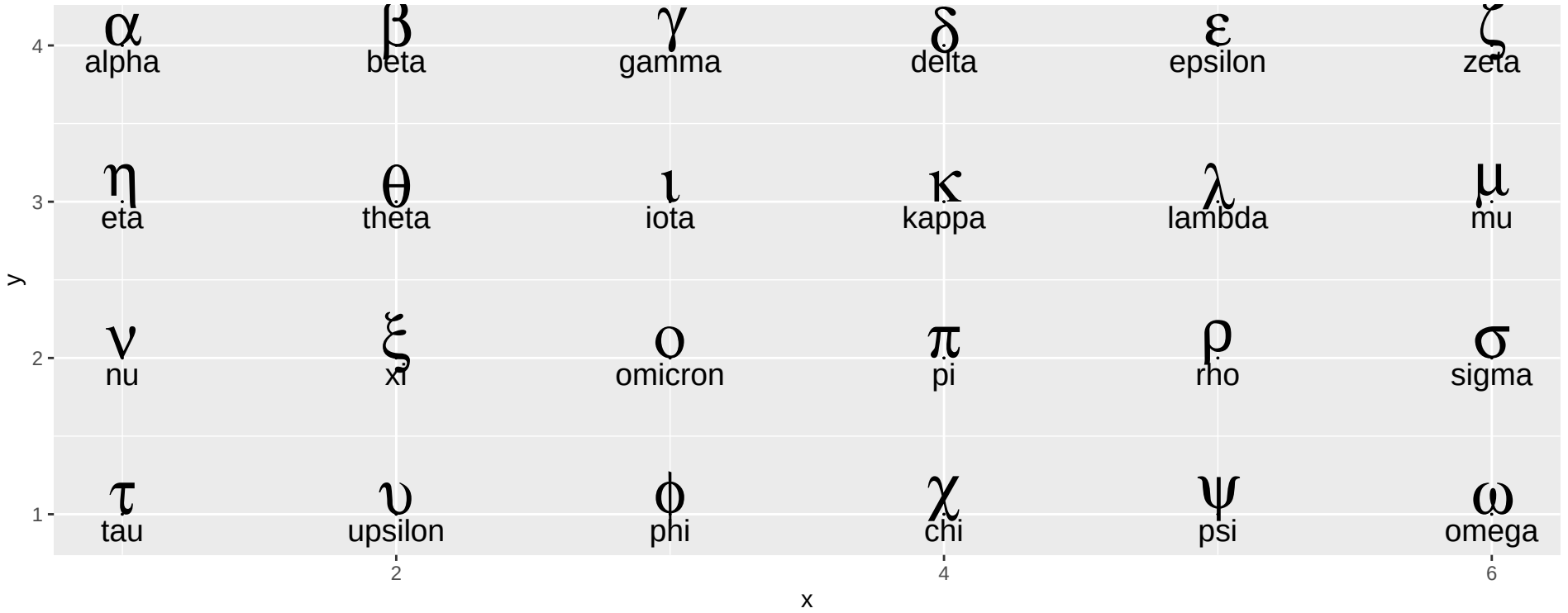
代码

```
greeks <- c("Alpha", "Beta", "Gamma", "Delta", "Epsilon", "Zeta",
            "Eta", "Theta", "Iota", "Kappa", "Lambda", "Mu",
            "Nu", "Xi", "Omicron", "Pi", "Rho", "Sigma",
            "Tau", "Upsilon", "Phi", "Chi", "Psi", "Omega");

dat <- data.frame( x = rep( 1:6, 4 ), y = rep( 4:1, each = 6), greek = greeks );

plot2 <-
  ggplot( dat, aes(x=x,y=y) ) + geom_point(size = 0) +
    # 画希腊字符，注意下面两行代码的区别
    geom_text( aes( x, y + 0.1, label = tolower( greek ) ), size = 10, parse = T ) +
    geom_text( aes( x, y - 0.1, label = tolower( greek ) ), size = 5  );
```

希腊字符，cont.

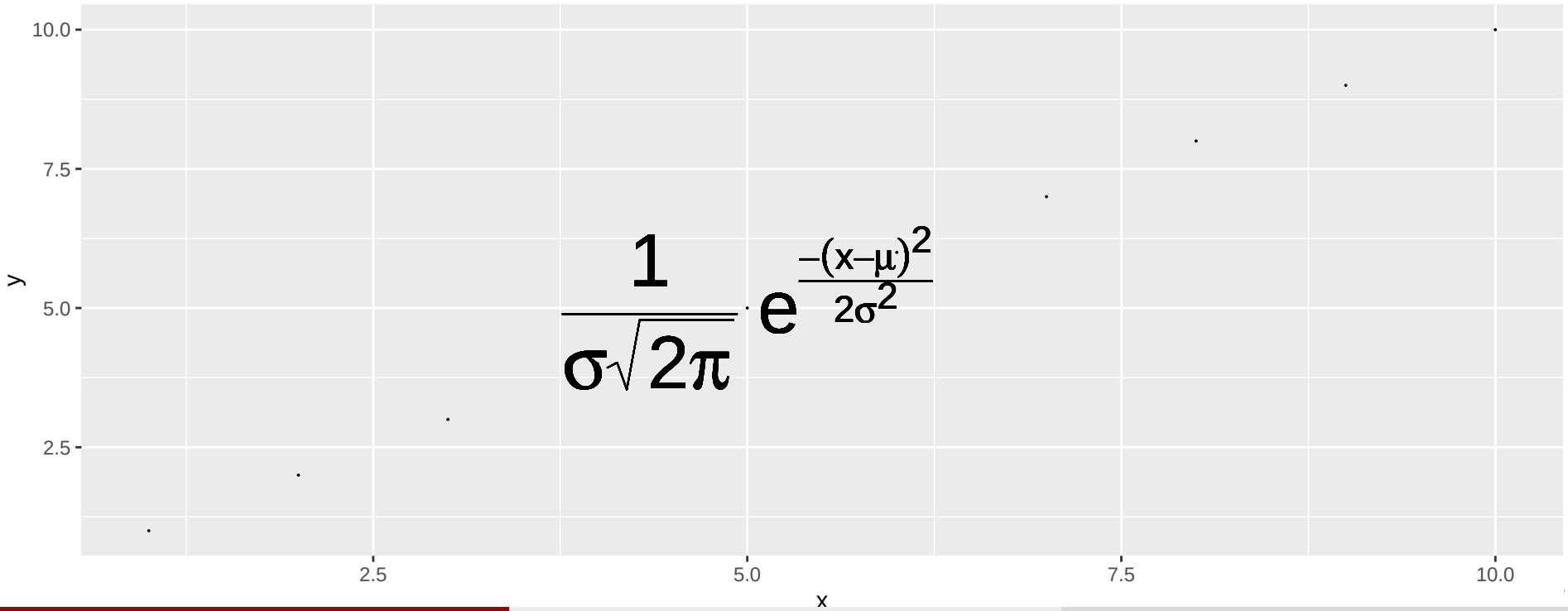

α
alpha
β
beta
γ
gamma
δ
delta
ε
epsilon
ζ
zeta
η
eta
θ
theta
ι
iota
κ
kappa
λ
lambda
μ
mu
ν
nu
ξ
xi
ο
omicron
π
pi
ρ
rho
σ
sigma
τ
tau
υ
upsilon
ϕ
phi
χ
chi
ψ
psi
ω
omega
y
x
4
3
2
1
2
4
6

公式示例

注写公式的方式很多

```
eq <- expression(paste(frac(1, sigma*sqrt(2*pi)), " ",
                       plain(e)^{frac(-(x-mu)^2, 2*sigma^2)}));

ggplot( data.frame(x=1:10, y=1:10), aes( x,y ) ) +
    geom_point( size = 0 ) +
    geom_text(data = NULL, x = 5, y = 5, size = 12,
              label = as.character(eq), parse = TRUE );
```



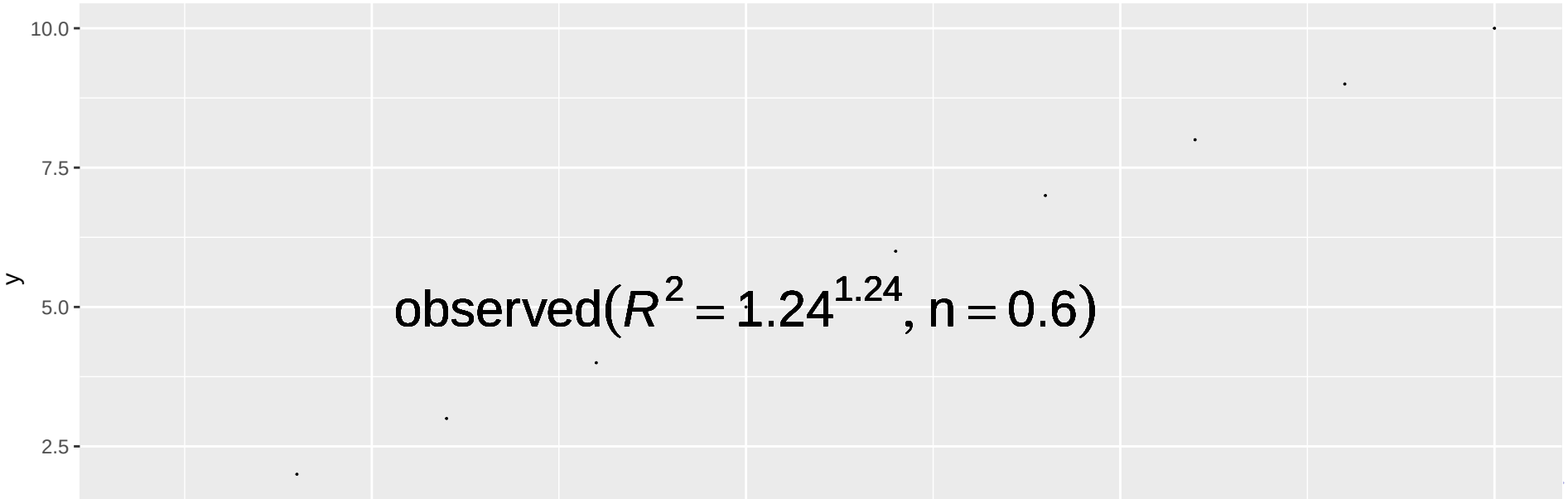
公式示例 2

另一种代入变量值的方法：

```
x <- 1.24;
y <- 0.6;

ex <- bquote(.(parse(text=paste( "observed (", "italic(R)^2==",
                                 x,  "^bold(", x, "), n == ", y, ")",
                                 sep = "  " ))) );

ggplot( data.frame(x=1:10, y=1:10), aes( x,y ) ) + geom_point( size = 0 ) +
    geom_text(data = NULL, x = 5, y = 5, size = 8,
              label = as.character(ex), parse = TRUE );
```



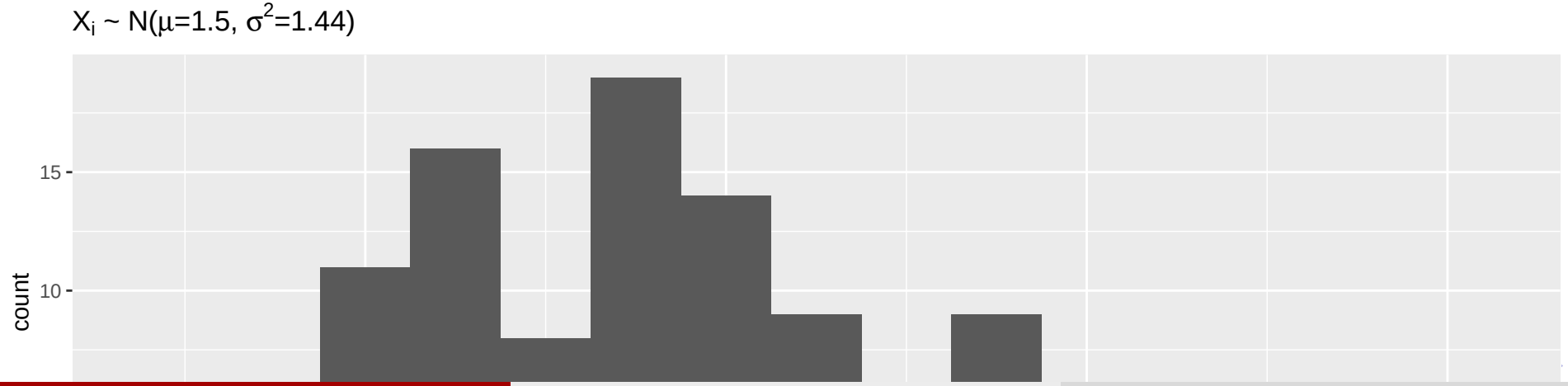
公式示例 3

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 ????
```



section 6: ggplot2 进阶 2

ggplot2 的核心在于先计算再做图

先看数据（来自 talk05）：

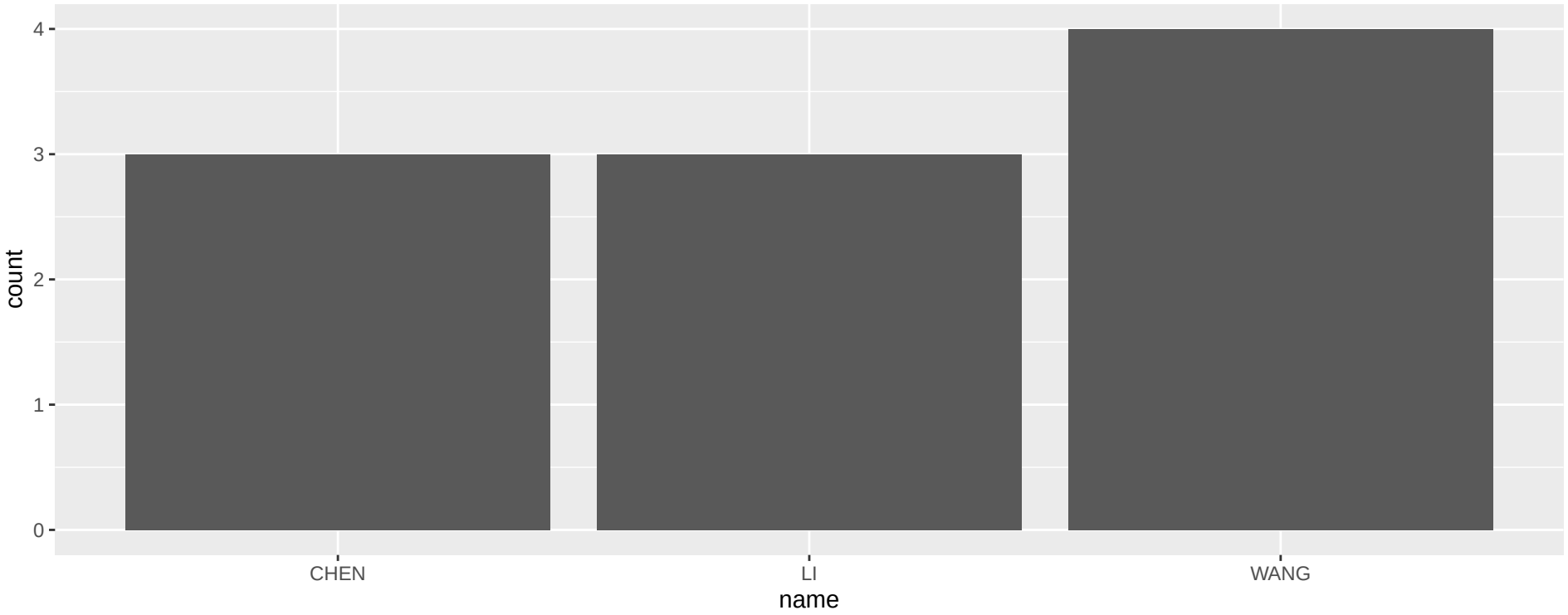
```
grades2 <- read_delim( file = "data/talk05/grades2.txt", delim = "\t",
                       quote = "", col_names = T);
knitr::kable( grades2 );
```

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

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();
```

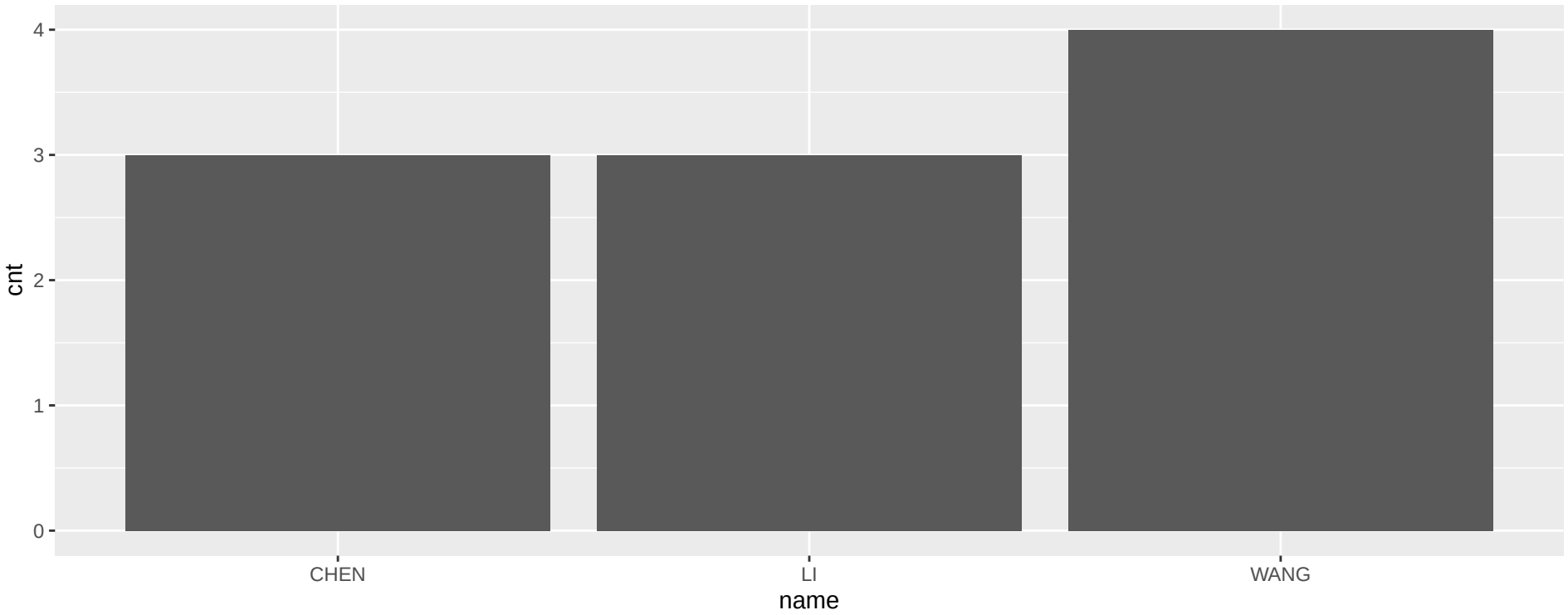


为什么会这样呢？因为 geom_bar(stat = "count") 的默认参数是 count，即数一下每个 factor 的出现次数。

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 ...

stacked bars

应用场景：宏基因组多样本物种丰度图

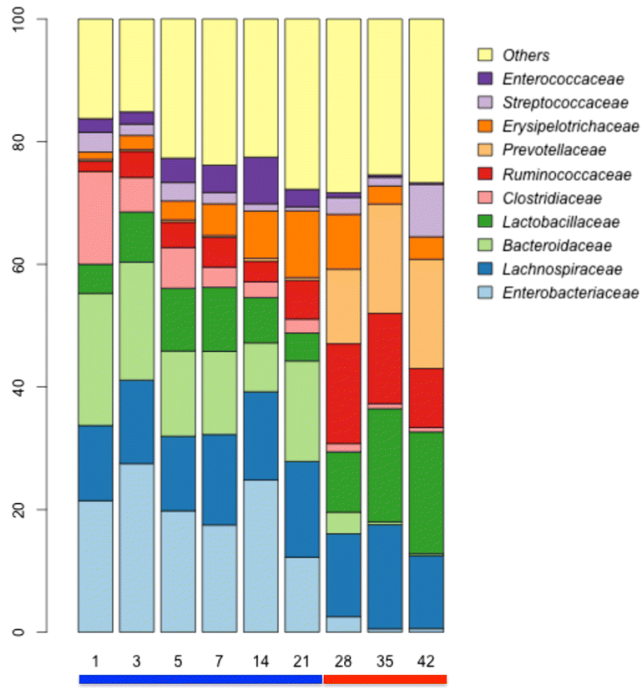


Figure 7: Microbiome 3, 28 2015

stacked bars , cont.

load data

```
speabu <-read_tsv( file = "data/talk09/mock_species_abundance.txt"  );
```

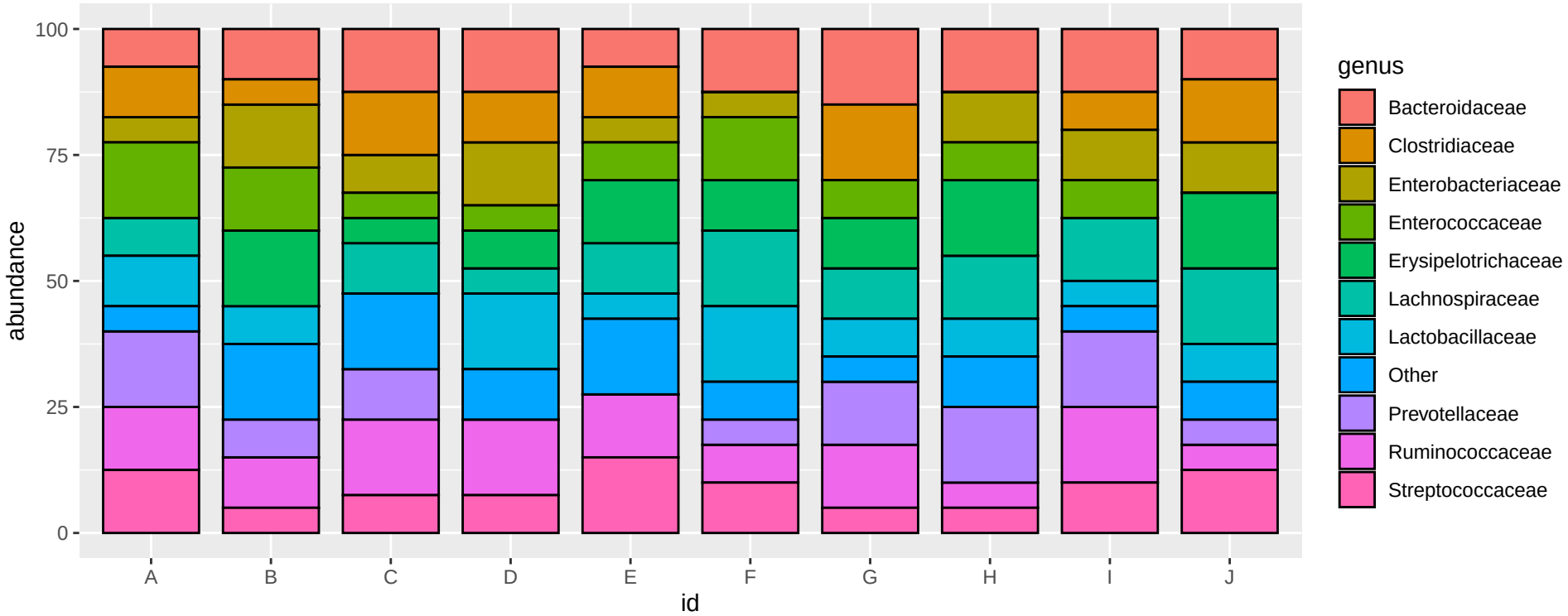
```
##
## -- Column specification --------------------------------------------------------
## cols(
##   id = col_character(),
##   genus = col_character(),
##   abundance = col_double()
## )
```

```
head( speabu );
```

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

stacked bars , cont.

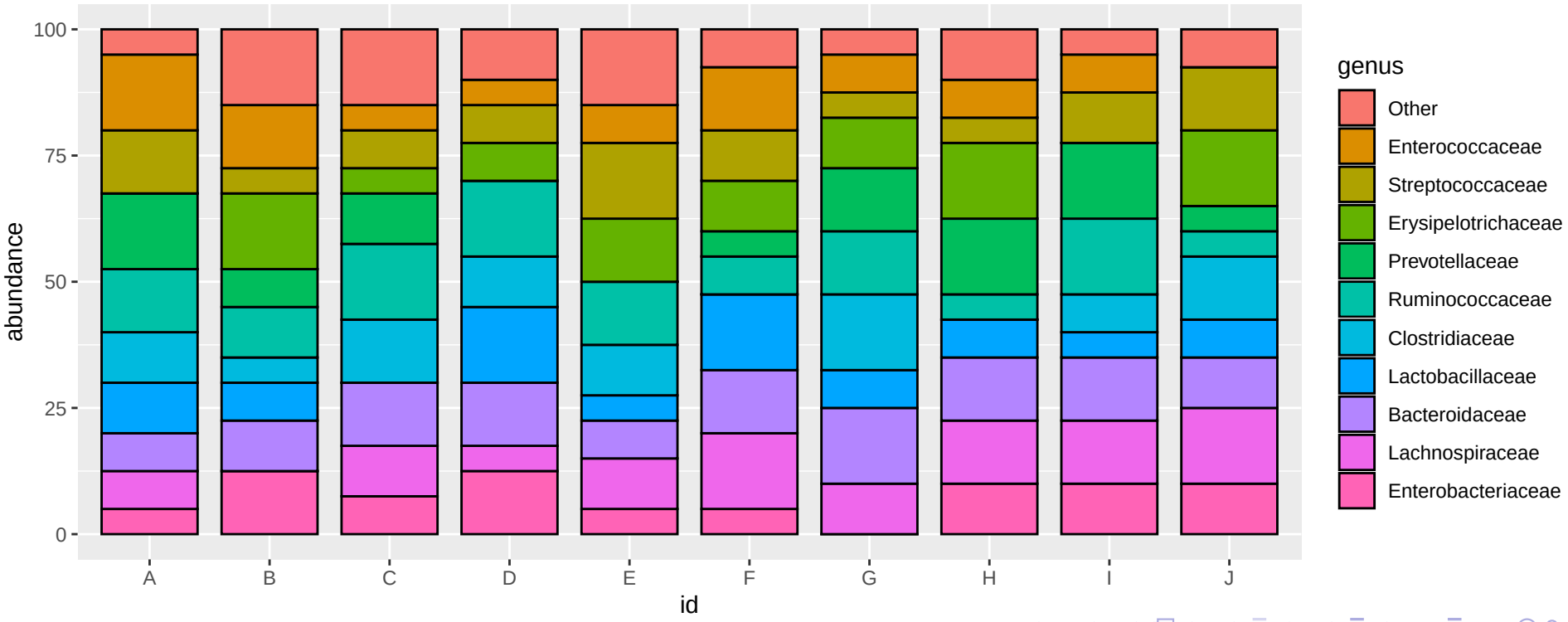
```
ggplot( speabu, aes( x = id, y = abundance, fill = genus ) ) +
  geom_bar( stat = "identity", position = "stack", color = "black", width = 0.8 );
```



指定 Genus 展示顺序

factor 的操纵详见第 4 章。

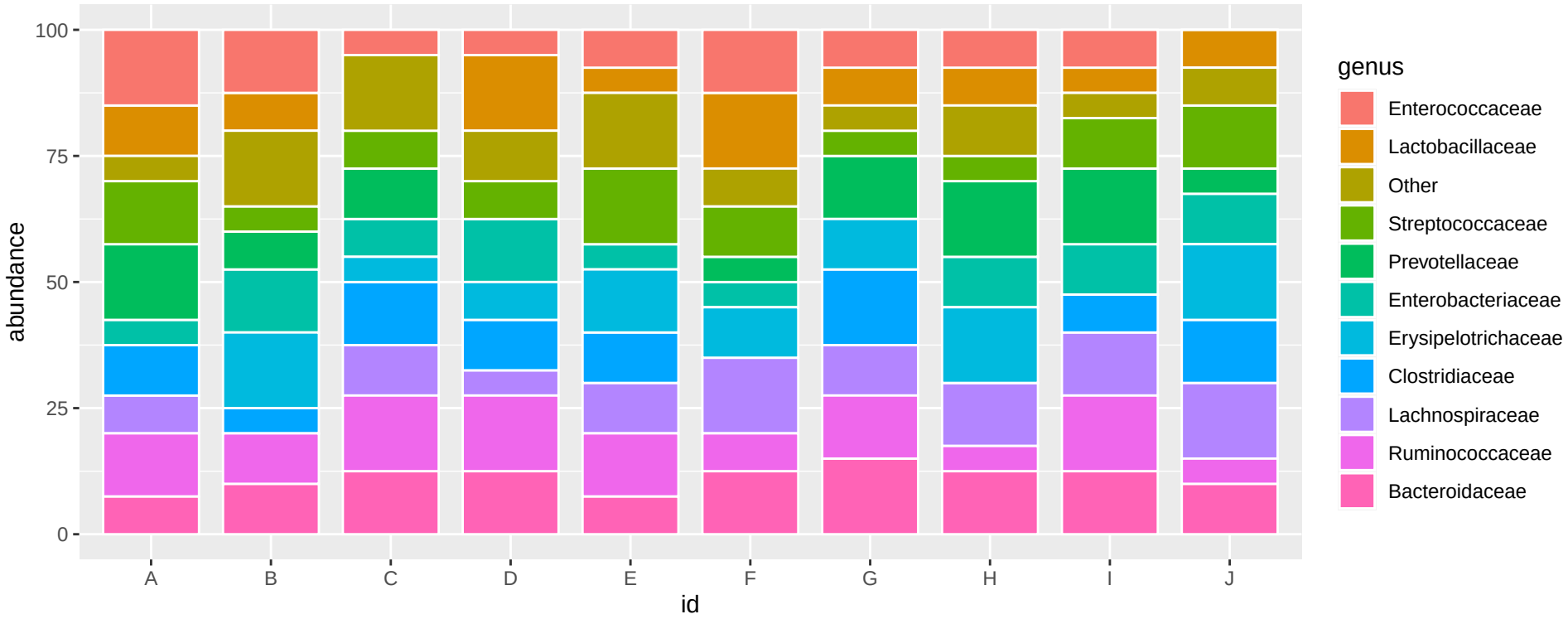
```
speabu$genus <- factor( speabu$genus, levels = rev( c( "Enterobacteriaceae", "Lachnospiraceae",
       "Clostridiaceae", "Ruminococcaceae", "Prevotellaceae", "Erysipelotrichaceae", "Streptoco
ggplot( speabu, aes( x = id, y = abundance, fill = genus ) ) +
  geom_bar( stat = "identity", position = "stack", color = "black", width = 0.8 );
```



按丰度排序

按丰度中值大小排序

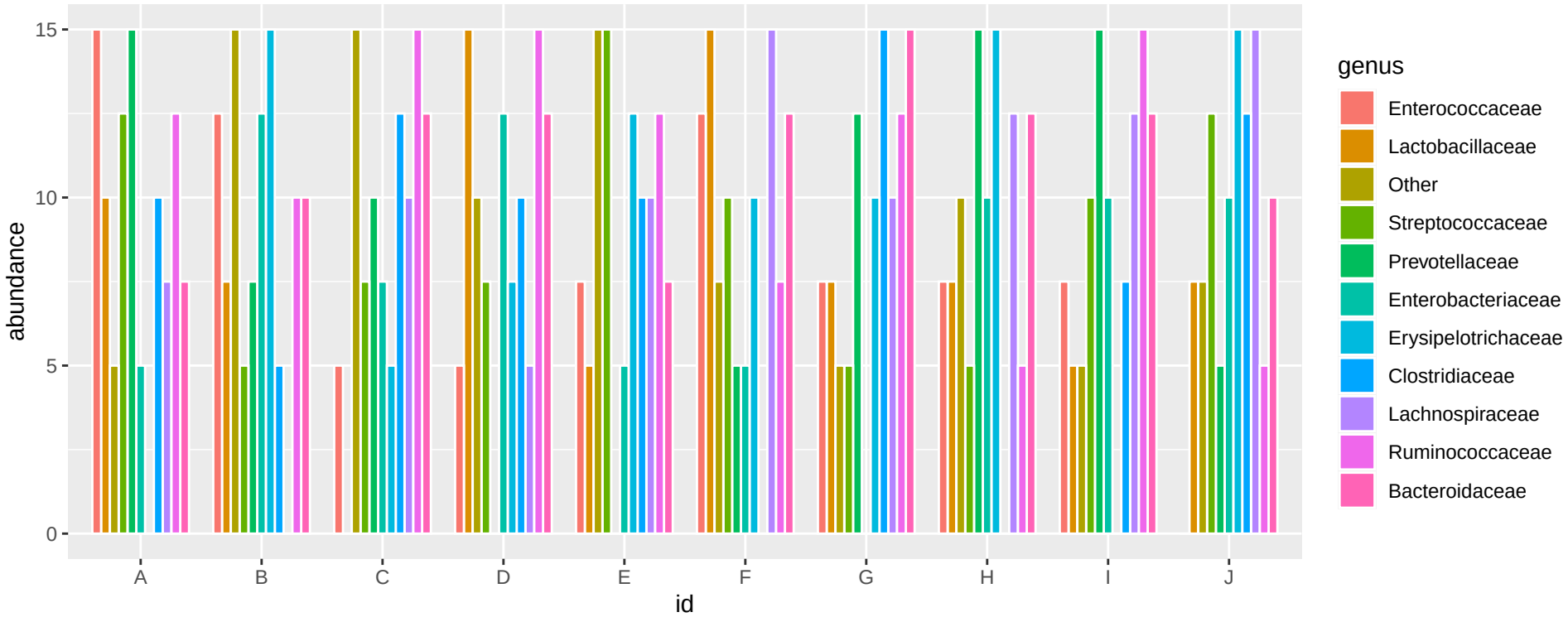
```
speabu$genus <- reorder( speabu$genus, speabu$abundance, median );
ggplot( speabu, aes( x = id, y = abundance, fill = genus ) ) +
  geom_bar( stat = "identity", position = "stack", color = "white", width = 0.8 );
```



position = "stack" 又是什么 ??

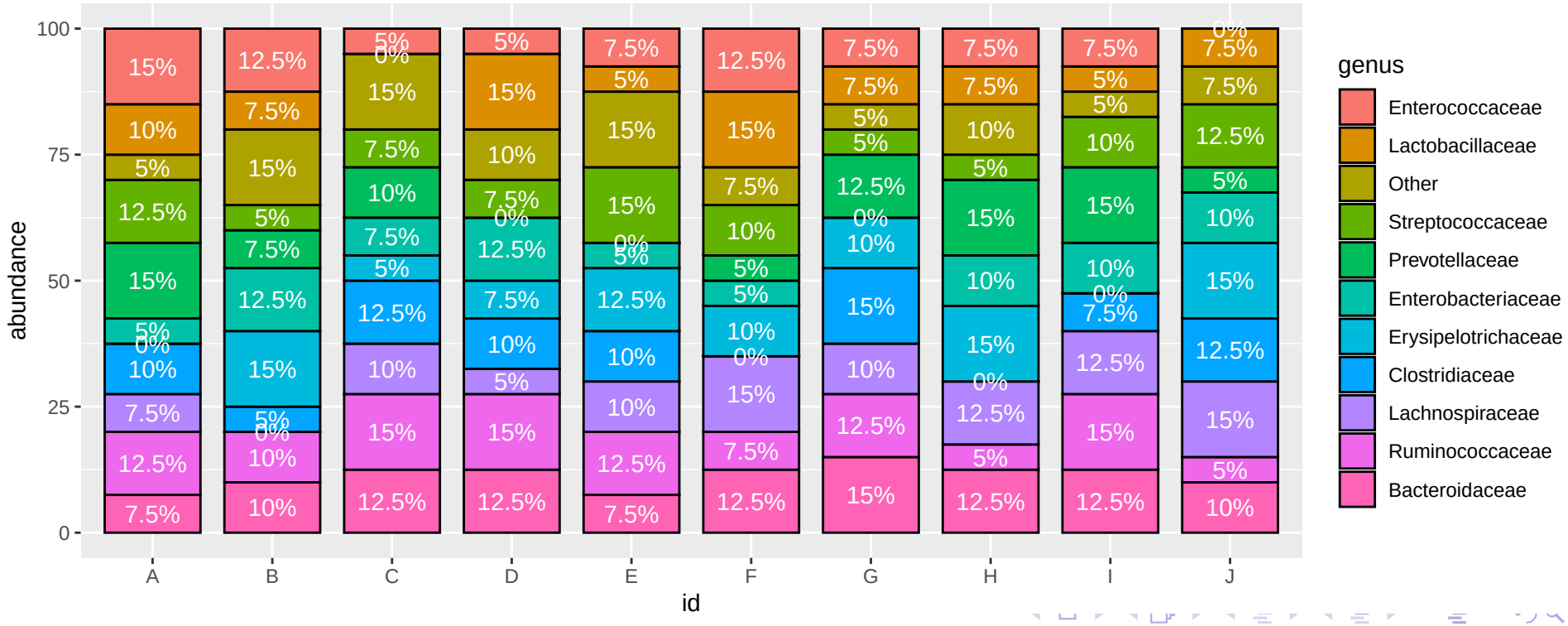
position = "dodge" : plot bars next to each other ...

```
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( ypos = 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" );
```



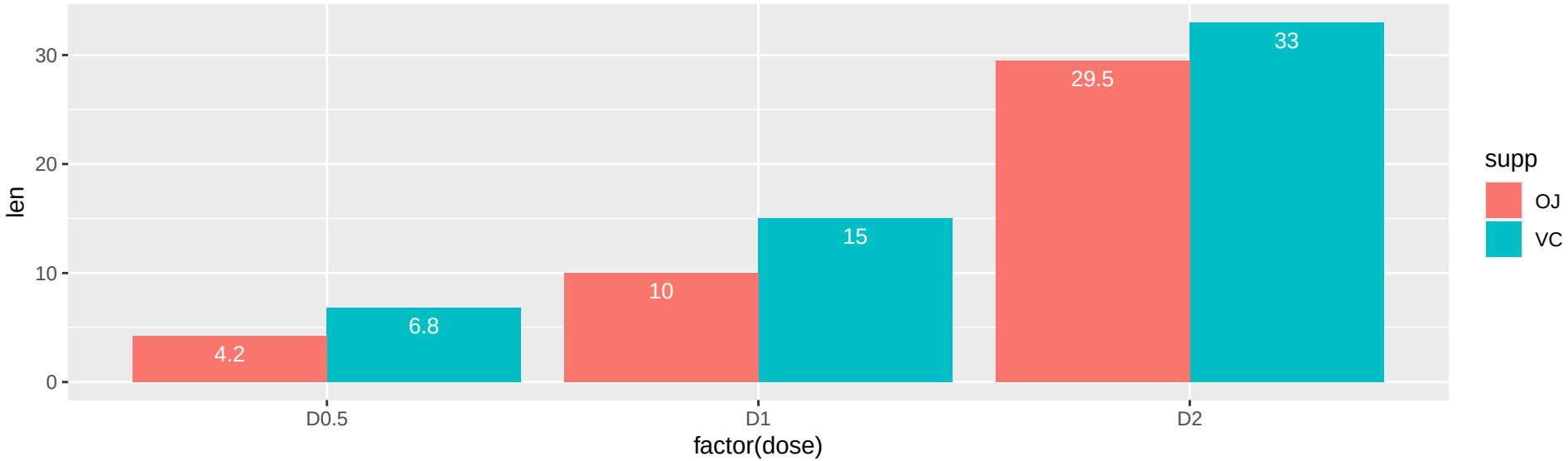
显示数值 ... ，cont.

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

```
df2 <- data.frame(supp=rep(c("VC", "OJ"), each=3),
                  dose=rep(c("D0.5", "D1", "D2"),2),
                 len=c(6.8, 15, 33, 4.2, 10, 29.5))
ggplot( df2, aes(x=factor(dose), y=len, fill=supp)) +
  geom_bar(stat="identity", position=position_dodge())+
  geom_text(aes(label=len), vjust=1.6, color="white",
            position = position_dodge(0.9), size=3.5)
```



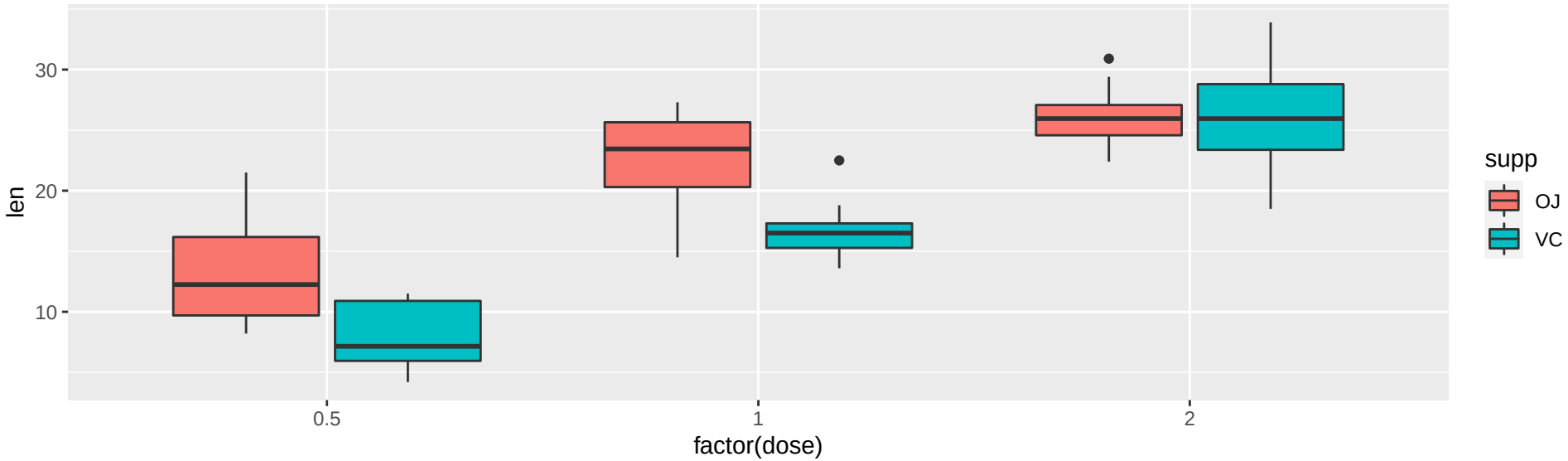
position 的其它取值

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

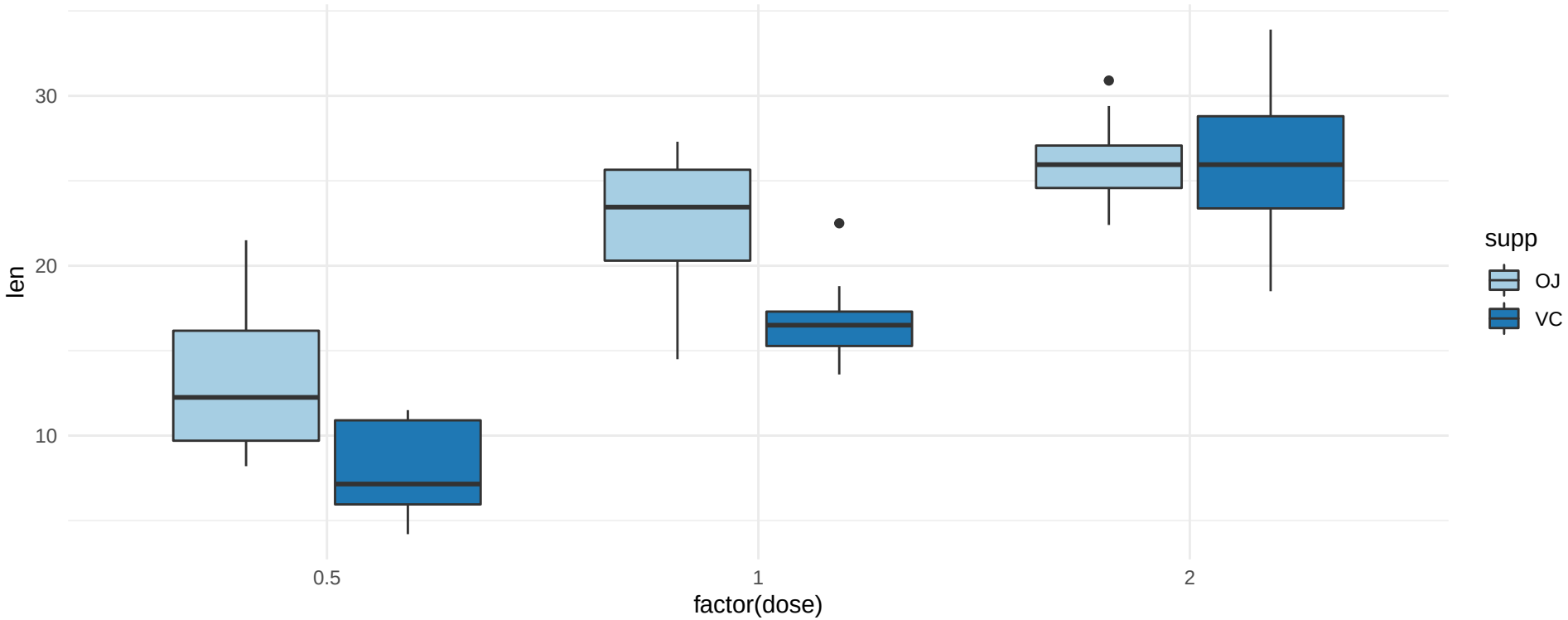
```
ggplot(ToothGrowth, aes(x=factor( dose ), y=len, fill=supp)) +
  geom_boxplot()
```



geom_boxplot()：默认为 dodge

change color palette

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



要点

1. 颜色 palette 的用法
2. theme 系统

theme in ggplot2

- `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。

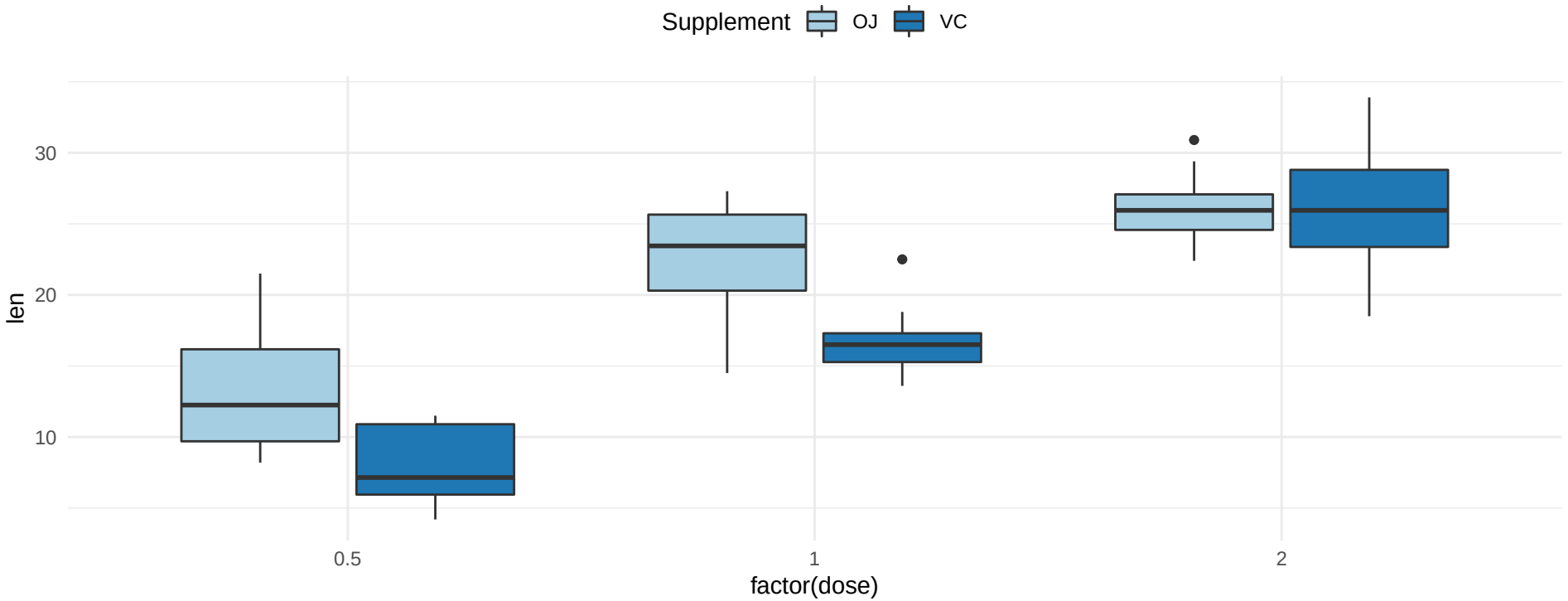
- line, rect, text, title：整体框架
- axis.<compoment>：调整坐标轴
- legend.<parameter>：调整图例
- plot.<>：控制 title, subtitle 等细节
- panel.<...>：调整 facet 情况下的 panel （facet 下面会介绍）
- strip.<...>：调整 facet 的标题细节 ...

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" ) + theme_minimal() +
  labs( fill = "Supplement" ) + theme( legend.position = "top" );
```



ggsci: palette for scientific journals!!!

```
# Install ggsci from CRAN:
install.packages("ggsci");

# Or try the development version on GitHub:
# install.packages("devtools")
devtools::install_github("nanxstats/ggsci")
```

提供了一系列

scale_color_<journal> 和 scale_fill_<journal> 函数

详见：https://cran.r-project.org/web/packages/ggsci/vignettes/ggsci.html

ggsci 举例

```
library("ggsci")
library("ggplot2")
library("gridExtra")
data("diamonds")
p1 <- ggplot(
  subset(diamonds, carat >= 2.2),
  aes(x = table, y = price, colour = cut)
) +
  geom_point(alpha = 0.7) +
  geom_smooth(method = "loess", alpha = 0.05, size = 1, span = 1) +
  theme_bw()

p2 <- ggplot(
  subset(diamonds, carat > 2.2 & depth > 55 & depth < 70),
  aes(x = depth, fill = cut)
) +
  geom_histogram(colour = "black", binwidth = 1, position = "dodge") +
  theme_bw()
```

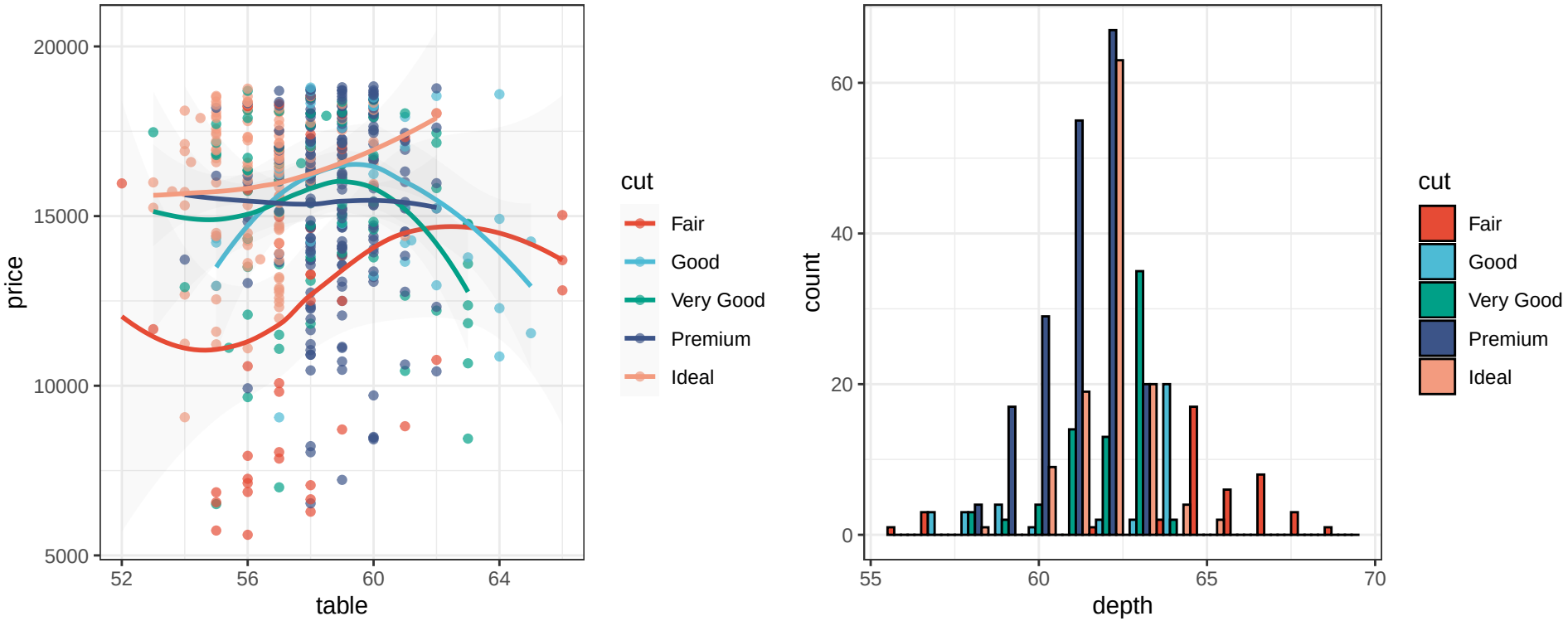
要点

- library(gridExtra)

ggsci 结果, Nature Style !!

```
p1_npg <- p1 + scale_color_npg()
p2_npg <- p2 + scale_fill_npg()
grid.arrange(p1_npg, p2_npg, ncol = 2)
```

```
## `geom_smooth()` using formula 'y ~ x'
```

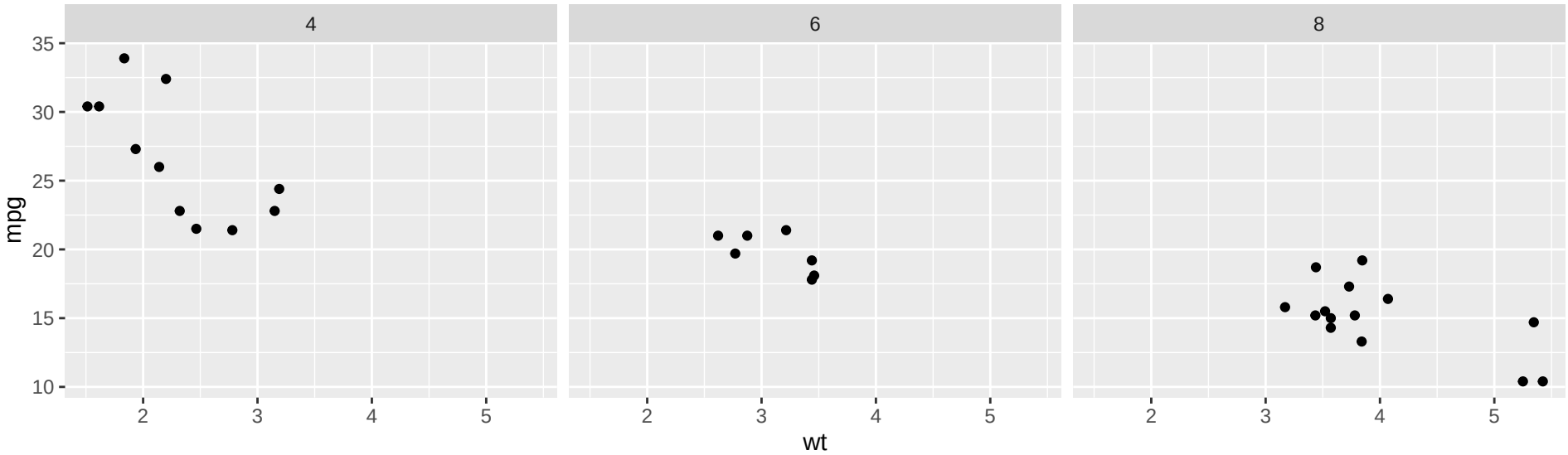


faceting ...

Faceting generates small multiples each showing a different subset of the data.

`facet_grid( <by_row> ~ <by_col> )` 汽缸、车重与燃油效率间的关系

```
ggplot( mtcars, aes( x = wt, y = mpg ) ) +
  geom_point() +
  facet_grid( . ~ cyl );
```



faceting , cont.

by col: 请自行尝试 ~

```
ggplot( mtcars, aes( x = wt, y = mpg ) ) +
  geom_point() +
  facet_grid( cyl ~ . );
```

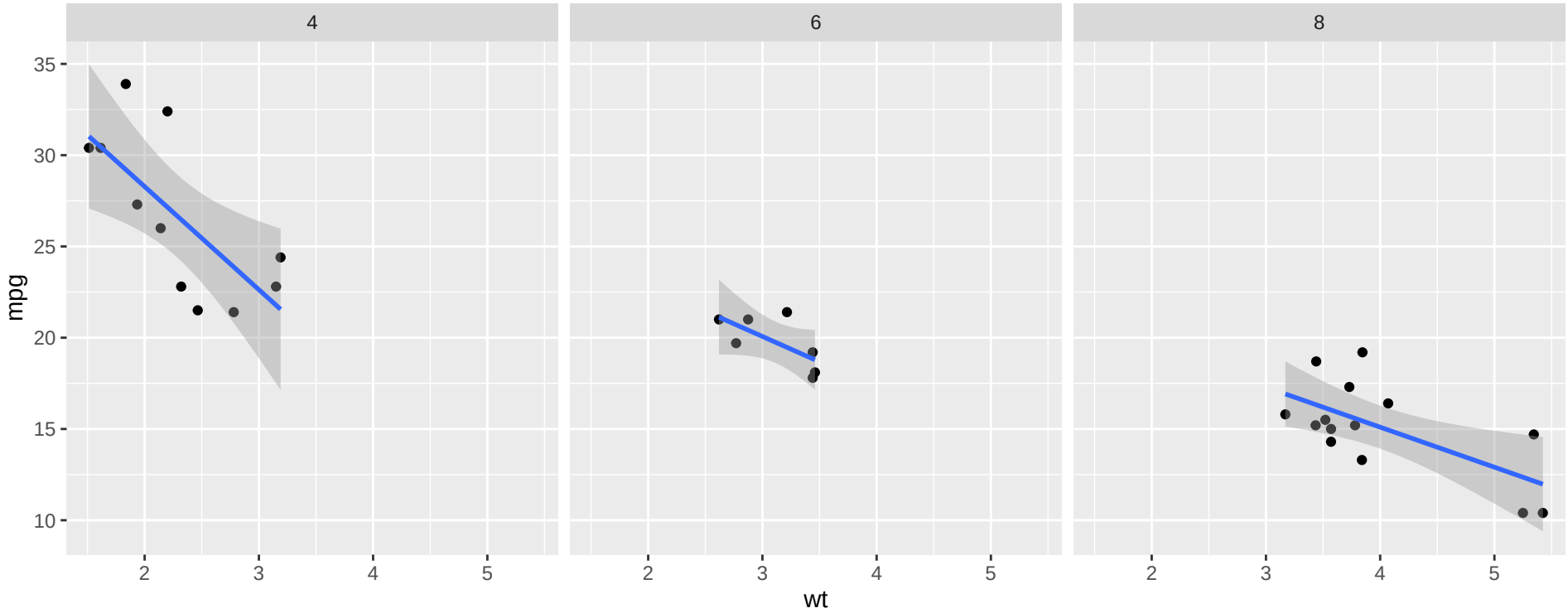
** 注意 **

作图相关概念：panel, strip, axis, tick, tick label, axis label

facet_grid 的适用范围是全局

```
ggplot( mtcars, aes( x = wt, y = mpg ) ) +
  geom_point() + geom_smooth( method = "lm" ) +
  facet_grid( . ~ cyl );
```

```
## `geom_smooth()` using formula 'y ~ x'
```

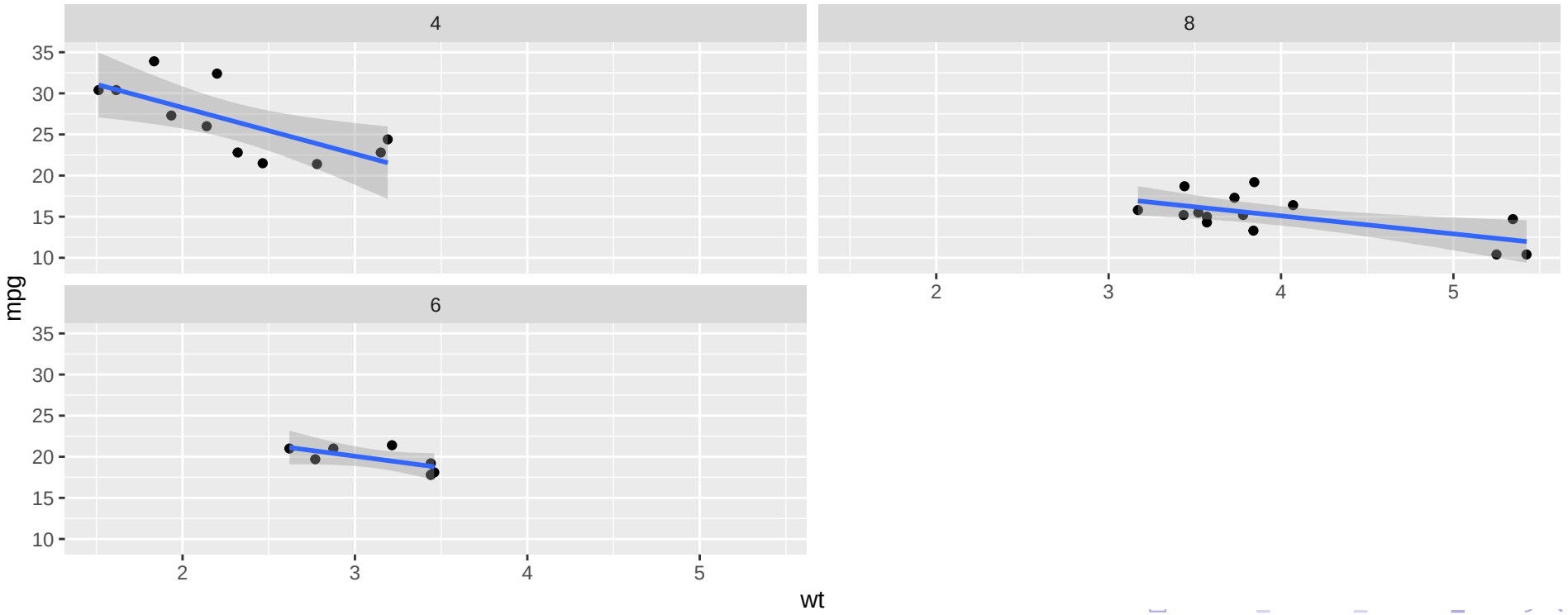


facet_wrap

指定行、列数和方向

```
ggplot( mtcars, aes( x = wt, y = mpg ) ) +
  geom_point() + geom_smooth( method = "lm" ) +
  facet_wrap( . ~ cyl , ncol = 2, dir = "v" );
```

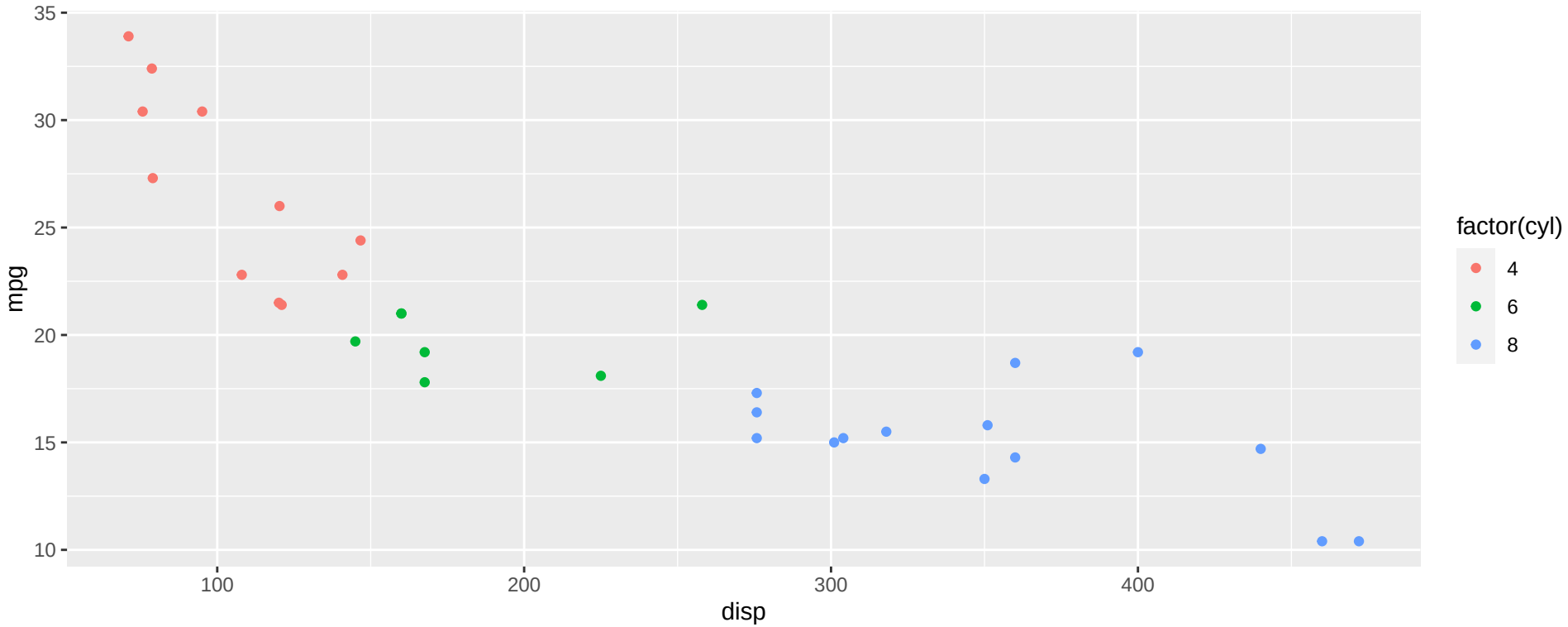
```
## `geom_smooth()` using formula 'y ~ x'
```



重点讲述：ggplot2 的颜色系统

非连续颜色

```
mtcars %>% ggplot( aes(disp, mpg) ) + geom_point( aes( color = factor(cyl) ) )
```



默认使用 scale_colour_hue() 颜色；

scale_colour_hue()

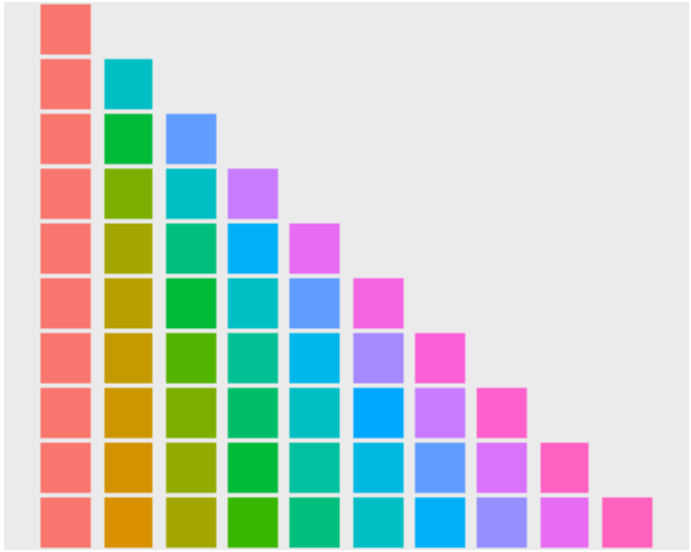


Figure 8: default discrete colour palette

```
scale_colour_hue(
  ...,
  h = c(0, 360) + 15,
  c = 100,
  l = 65,
  h.start = 0,
  direction = 1,
  na.value = "grey50",
  aesthetics = "colour"
)
```

scale_colour_brewer() 更易用

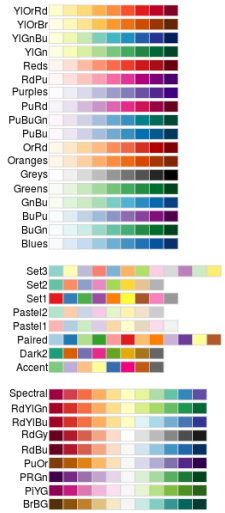
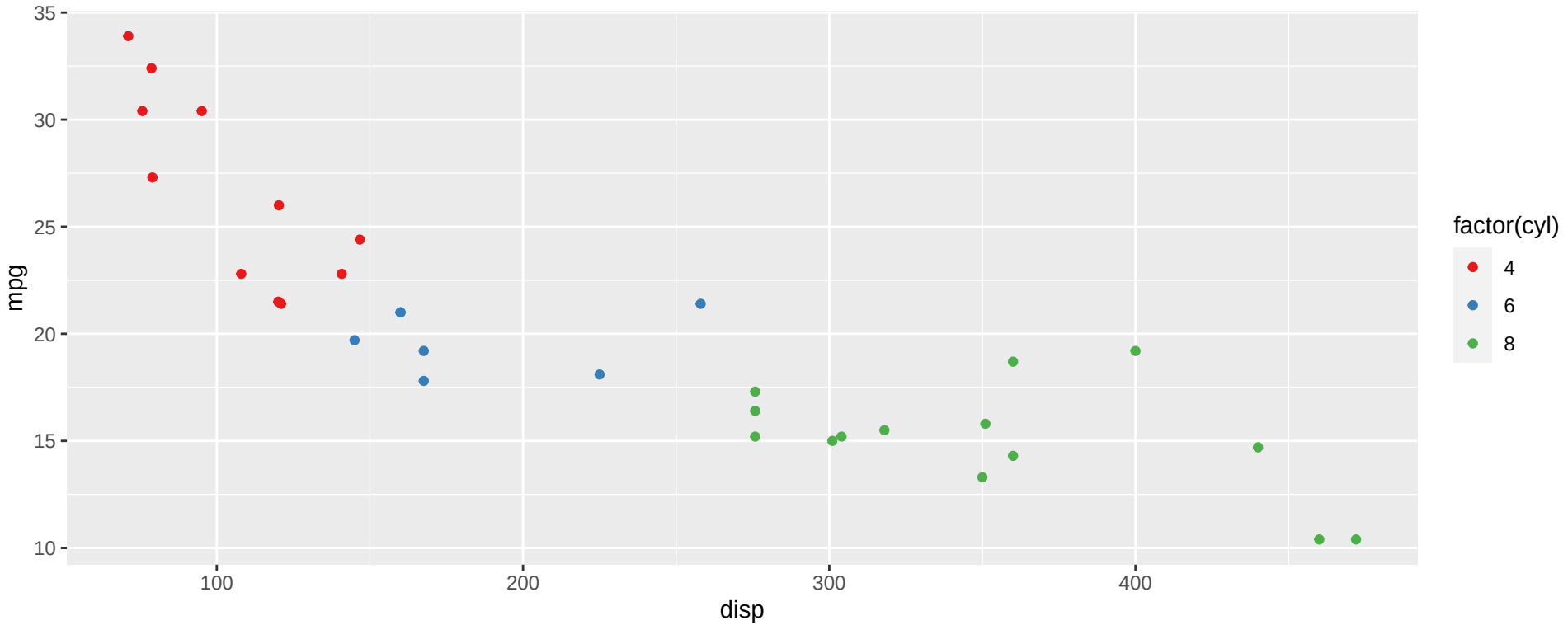


Figure 9: default discrete colour palette

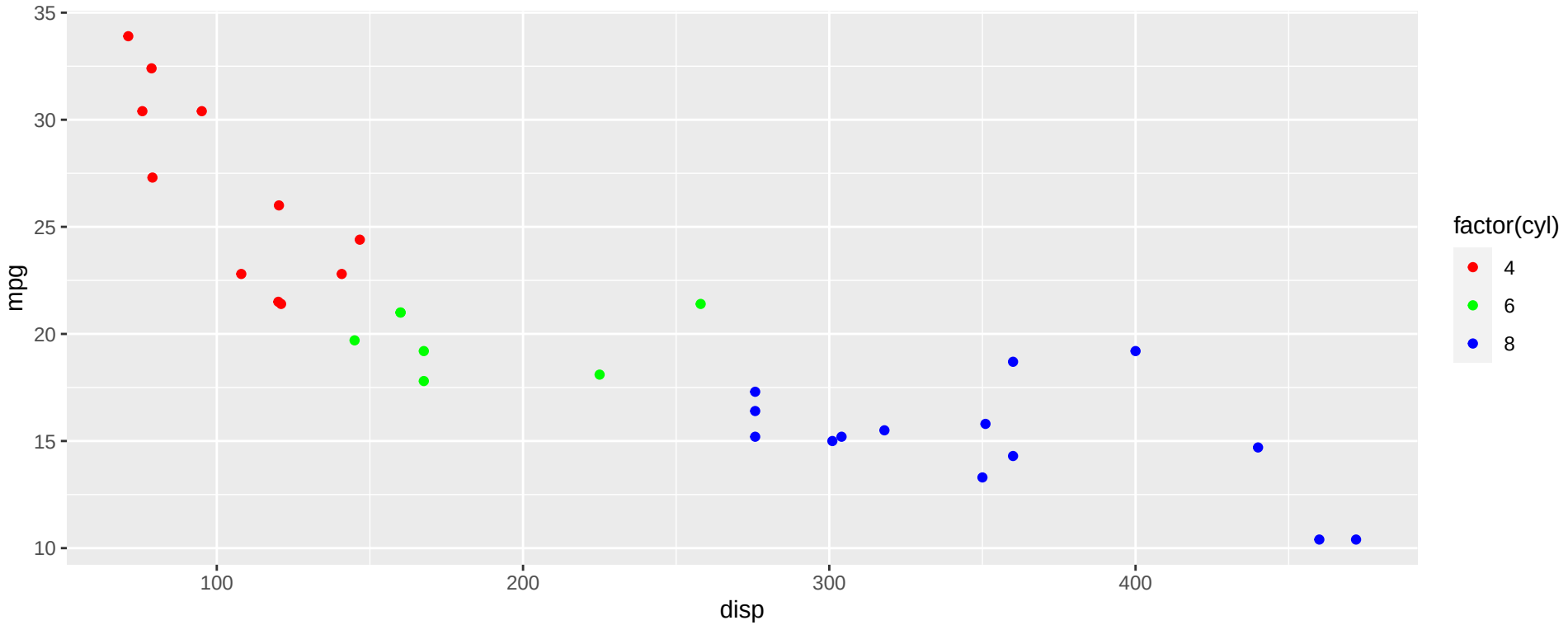
scale_colour_brewer(), cont.

```
mtcars %>% ggplot( aes(disp, mpg) ) + geom_point( aes( color = factor(cyl) ) ) +
  scale_color_brewer( palette = "Set1" );
```



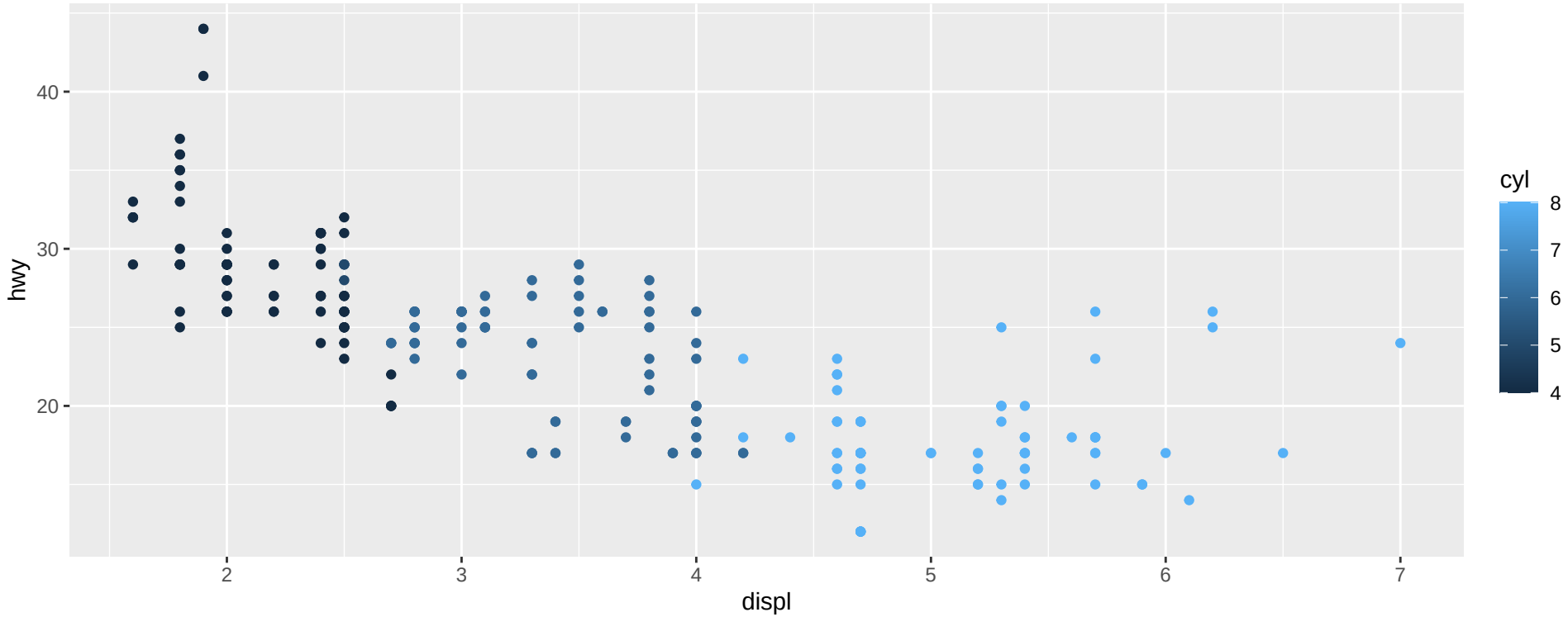
scale_colour_manual()

```
mtcars %>% ggplot( aes(disp, mpg) ) + geom_point( aes( color = factor(cyl) ) ) +
  scale_color_manual( breaks = c("4","6","8"), values = c("red","green","blue") );
```



连续颜色

```
mpg %>% ggplot( aes(displ, hwy) ) + geom_point( aes( color = cyl ) );
```



默认为：scale_color_gradient()

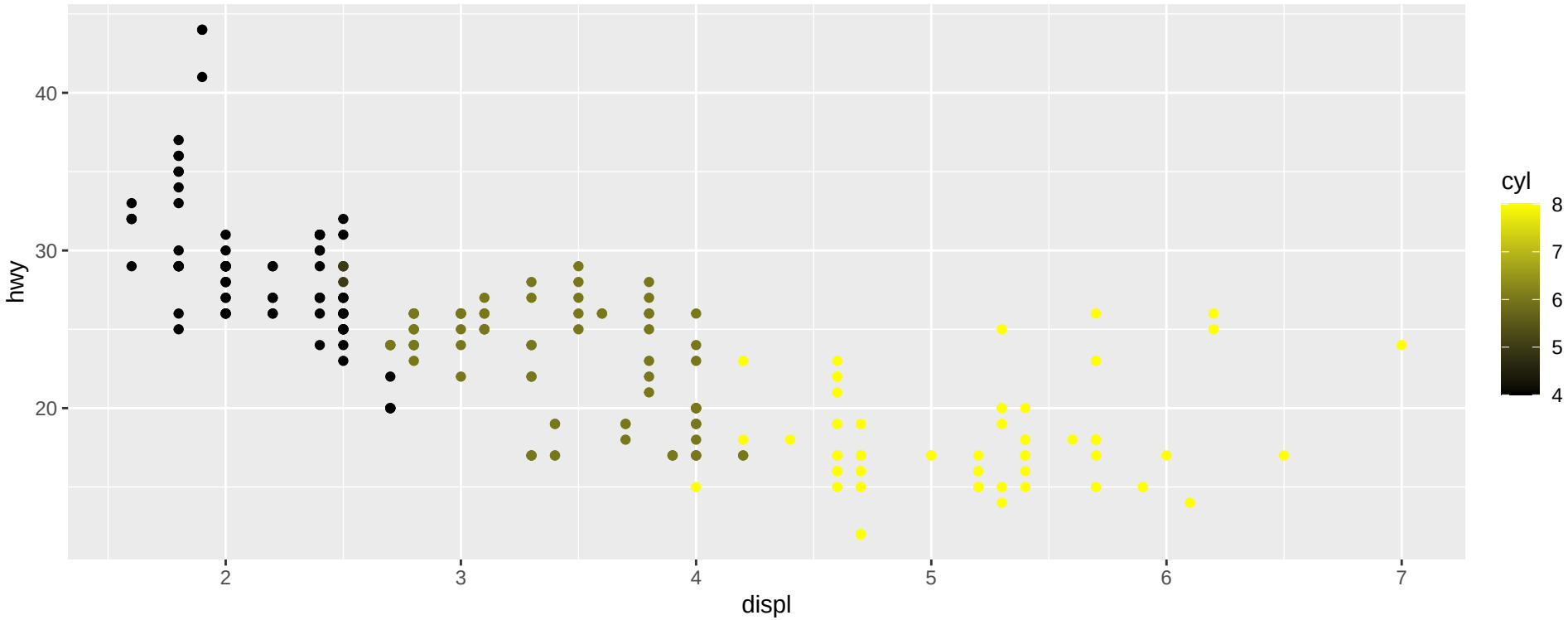
scale_color_gradient() 改变颜色更容易一些

```
scale_colour_gradient(
  ...,
  low = "#132B43",
  high = "#56B1F7",
  space = "Lab",
  na.value = "grey50",
  guide = "colourbar",
  aesthetics = "colour"
)
```

改变 low 和 high 的值即可；

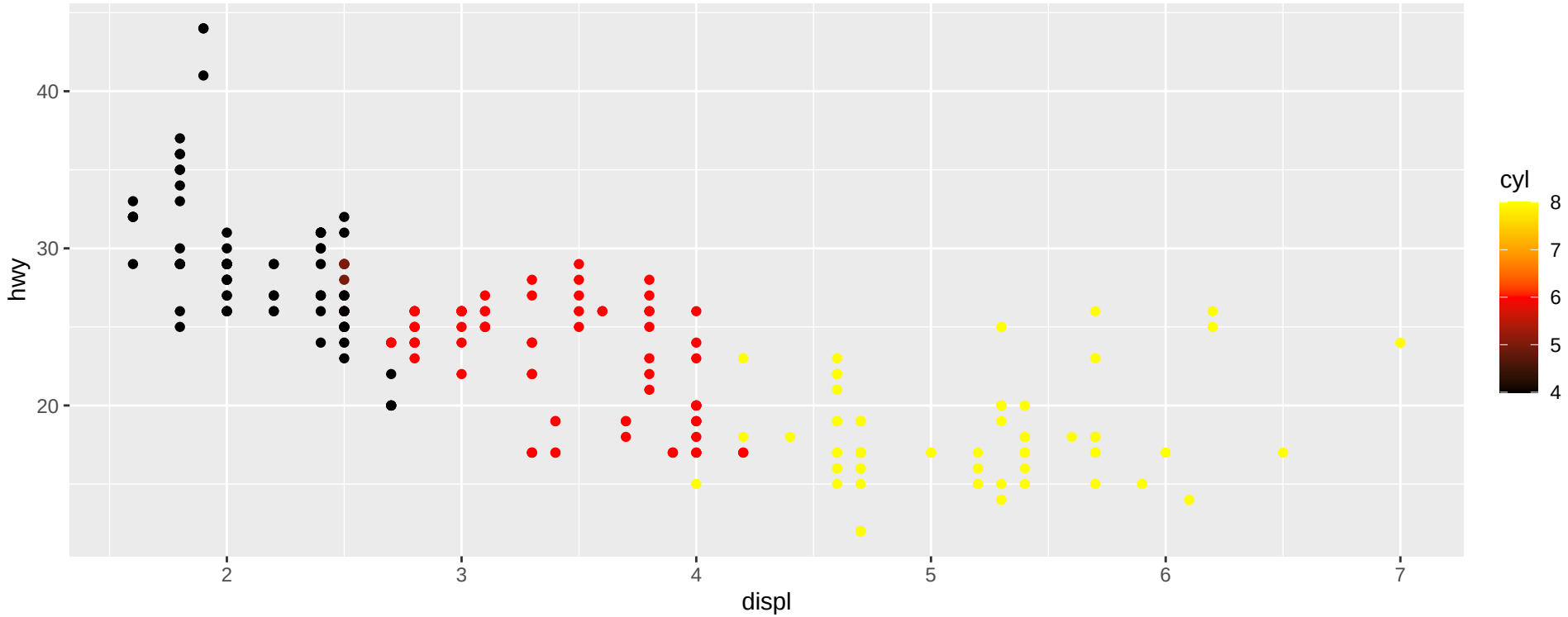
scale_color_gradient() 举例

```
mpg %>% ggplot( aes(displ, hwy) ) + geom_point( aes( color = cyl ) ) +
  scale_color_gradient( low = "black", high = "yellow" );
```



scale_color_gradient2() 3 个颜色

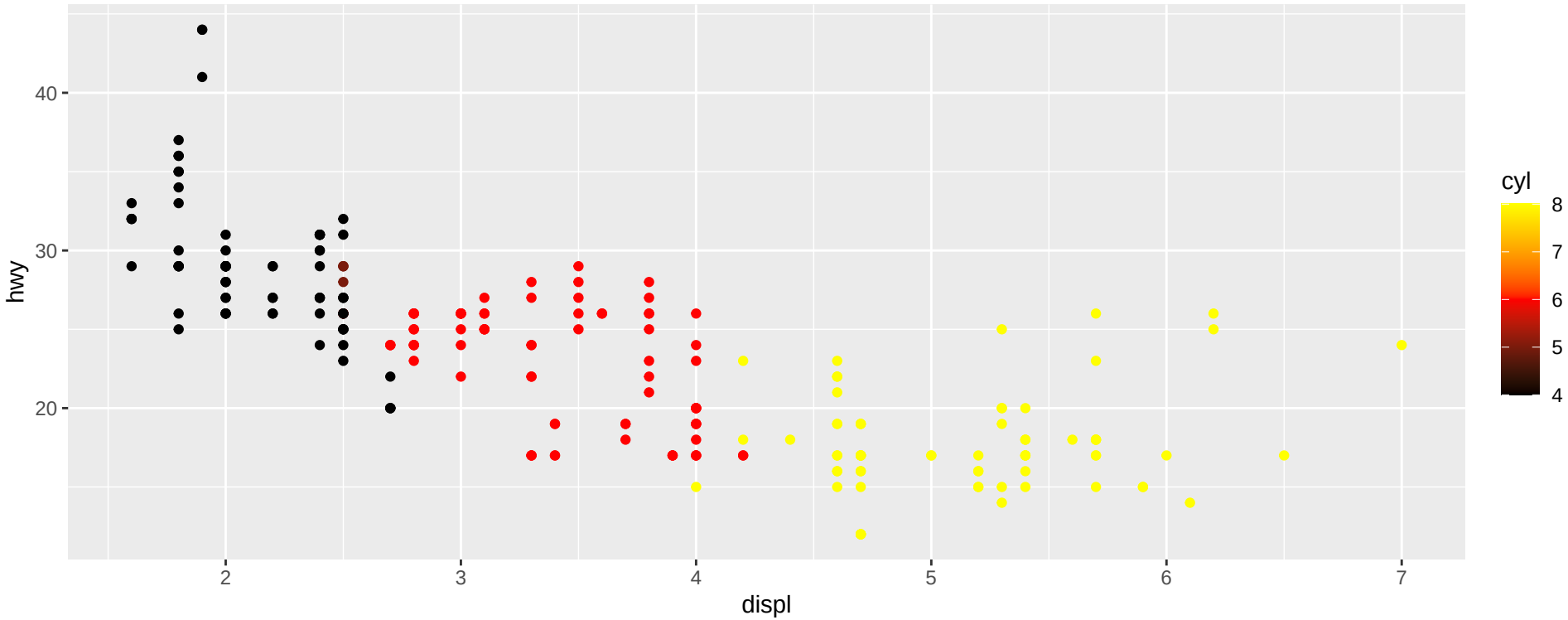
```
mpg %>% ggplot( aes(displ, hwy) ) + geom_point( aes( color = cyl ) ) +
  scale_colour_gradient2( low = "black", mid = "red", high = "yellow", midpoint = 6 );
```



注意 midpoint 参数

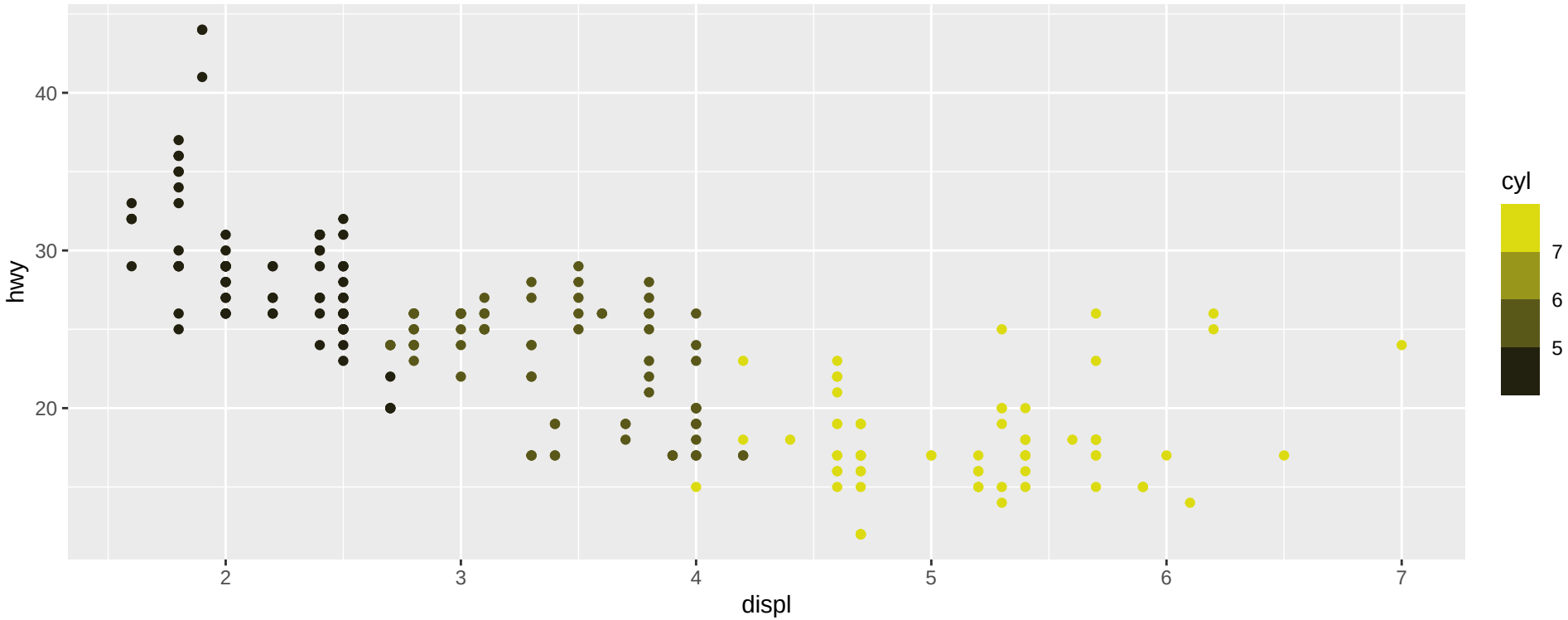
scale_colour_gradientn 多个颜色

```
mpg %>% ggplot( aes(displ, hwy) ) + geom_point( aes( color = cyl ) ) +
  scale_colour_gradientn( colors = c("black","red", "yellow") );
```



scale_colour_binned gradient 颜色的另一种方式

```
mpg %>% ggplot( aes(displ, hwy) ) + geom_point( aes( color = cyl ) ) +
  scale_color_binned( low = "black", high = "yellow" );
```



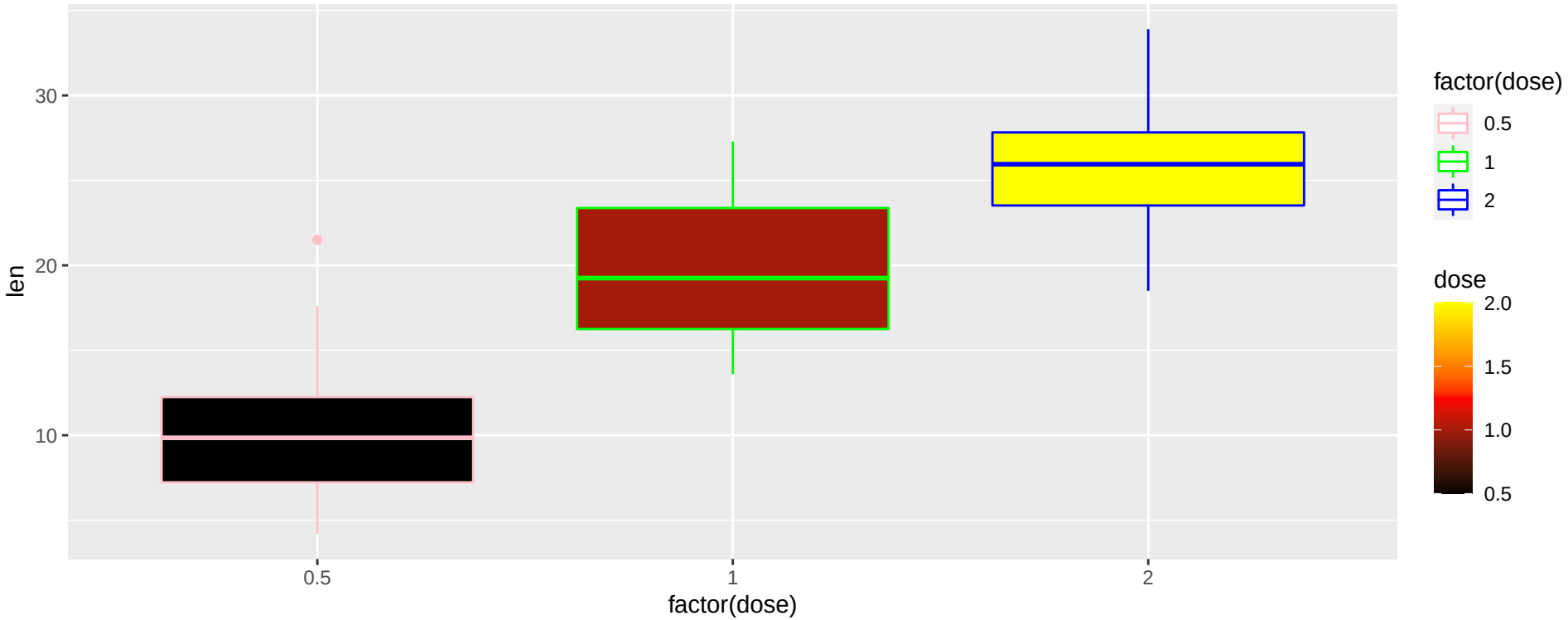
scale_fill_XX

- 颜色的使用与 aes 是配套的：

```
## color --> scale_colour_xxx
mpg %>% ggplot( aes(displ, hwy) ) + geom_point( aes( color = cyl ) ) +
  scale_colour_gradientn( colors = c("black","red", "yellow") );
```

更多举例

```
ggplot(ToothGrowth, aes(x=factor(dose), y=len, fill=dose, color = factor(dose))) +
  geom_boxplot() + scale_fill_gradientn( colors = c("black","red", "yellow") ) +
  scale_colour_manual( values = c("pink", "green", "blue") )
```



查看 RColorBrewer palette

```
library(RColorBrewer);
## 画图
display.brewer.pal(n = 8, name = 'Dark2')
```

Dark2 (qualitative)

```
## 查看颜色的值
brewer.pal(n = 8, name = "Dark2")
```

```
## [1] "#1B9E77" "#D95F02" "#7570B3" "#E7298A" "#66A61E" "#E6AB02" "#A6761D"
## [8] "#666666"
```

ggplot2 小结

layered grammer（图层语法）的成分

- 图层（ geom_xxx ）
- scale（ scale_xxx ）
- faceting（ facet_xxx ）
- 坐标系统

图象类型

- 点图
- bars
- boxplots

其它重要内容（部分需要自学）

- colours
- theme
- 其它图像类型
- 图例（legends）和坐标轴
- 图形注释和其它定制

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
3. 太多记忆点
4. 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。

请见 “ggplot2 : elegant graphics for data analysis” 一书!!

section 7: Exercise and home work

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