

# Graphics

W.Huber - Laura Symul - Susan Holmes

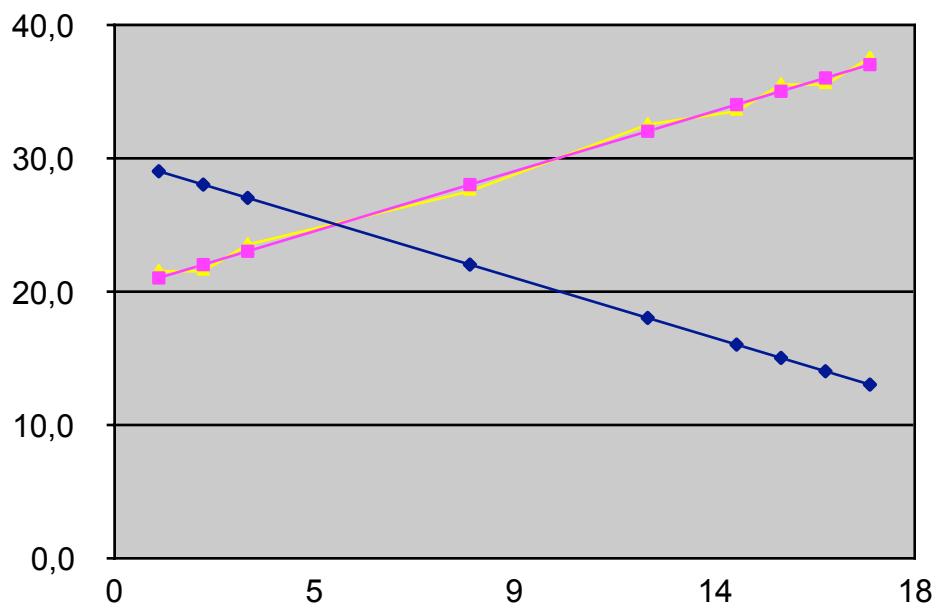
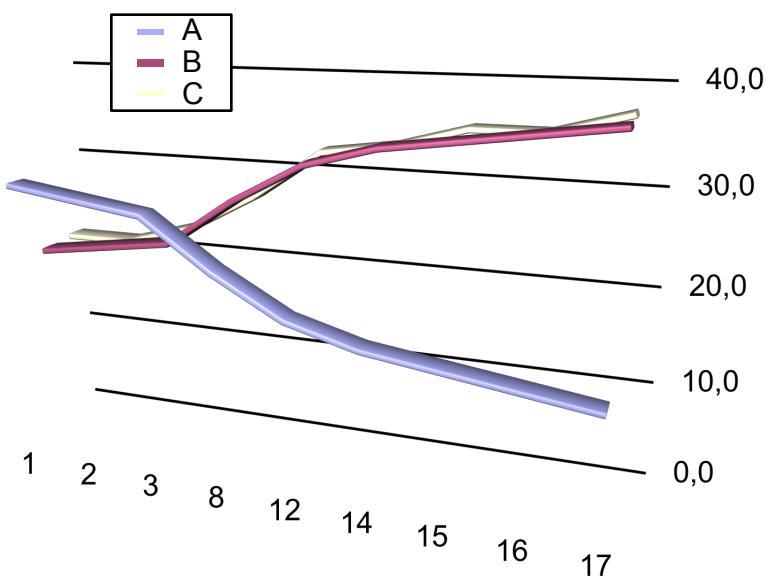
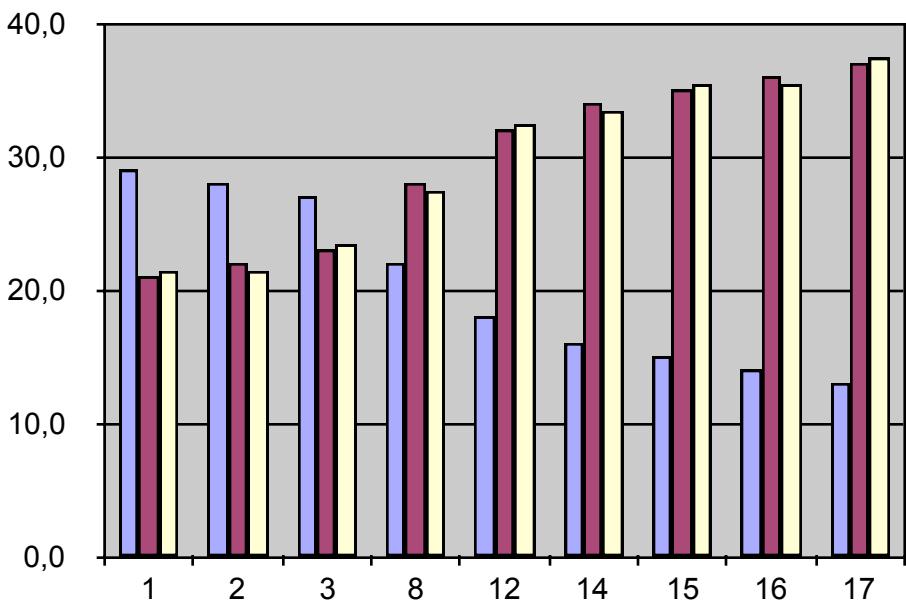
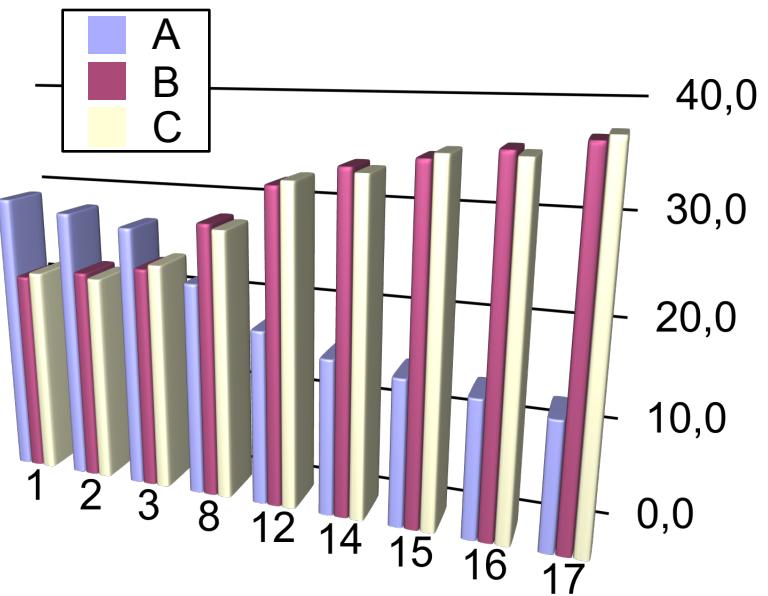
Oct 2019

# Why graphics?

- To explore data
- To communicate data patterns & preliminary insights with collaborators
- To display results and convey findings in a publication

The background of the image is a dark, teal-colored space filled with numerous tentacle-like alien creatures. These creatures have large, bulbous heads with rows of sharp, glowing green teeth. Small, red, glowing eyes are visible on the sides of their heads. The tentacles themselves are thick and dark, with some hanging down and others reaching out from behind the main cluster. The overall mood is eerie and horror-themed.

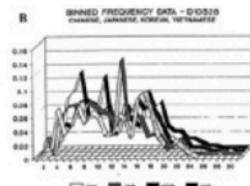
# Horror Picture Show



# The top ten worst graphs

With apologies to the authors, we provide the following list of the top ten worst graphs in the scientific literature. As these examples indicate, good scientists can make mistakes.

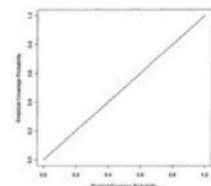
1. Roeder K (1994) DNA fingerprinting: A review of the controversy (with discussion). *Statistical Science* 9:222-278, Figure 4  
[[The article](#) | [The figure](#) | [Discussion](#)]



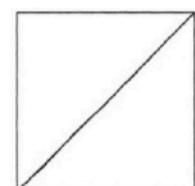
2. Wittke-Thompson JK, Pluzhnikov A, Cox NJ (2005) Rational inferences about departures from Hardy-Weinberg equilibrium. *American Journal of Human Genetics* 76:967-986, Figure 1  
[[The article](#) | [Fig 1AB](#) | [Fig 1CD](#) | [Discussion](#)]



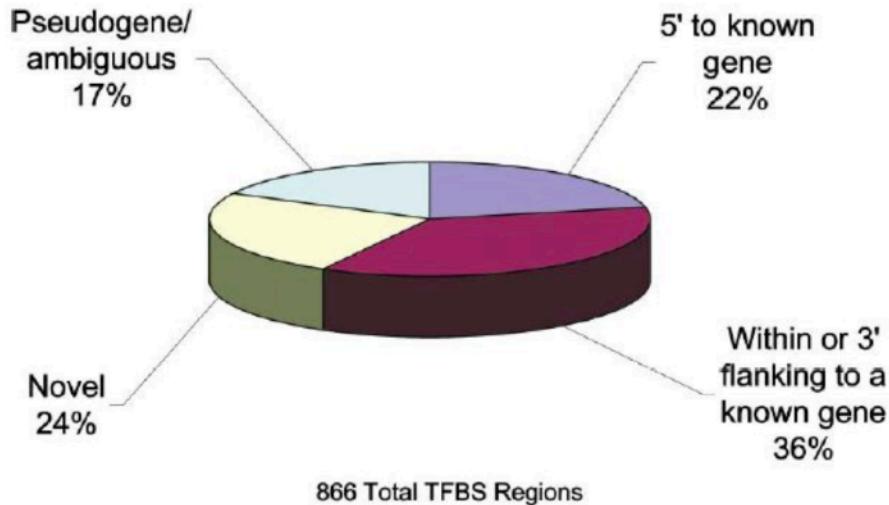
3. Epstein MP, Satten GA (2003) Inference on haplotype effects in case-control studies using unphased genotype data. *American Journal of Human Genetics* 73:1316-1329, Figure 1  
[[The article](#) | [The figure](#) | [Discussion](#)]



4. Mykland P, Tierney L, Yu B (1995) Regeneration in Markov chain samplers. *Journal of the American Statistical Association* 90:233-241, Figure 1  
[[The article](#) | [The figure](#) | [Discussion](#)]



# Distribution of All TFBS Regions



Cell

Volume 116, Issue 4, 20 February 2004, Pages 499-509

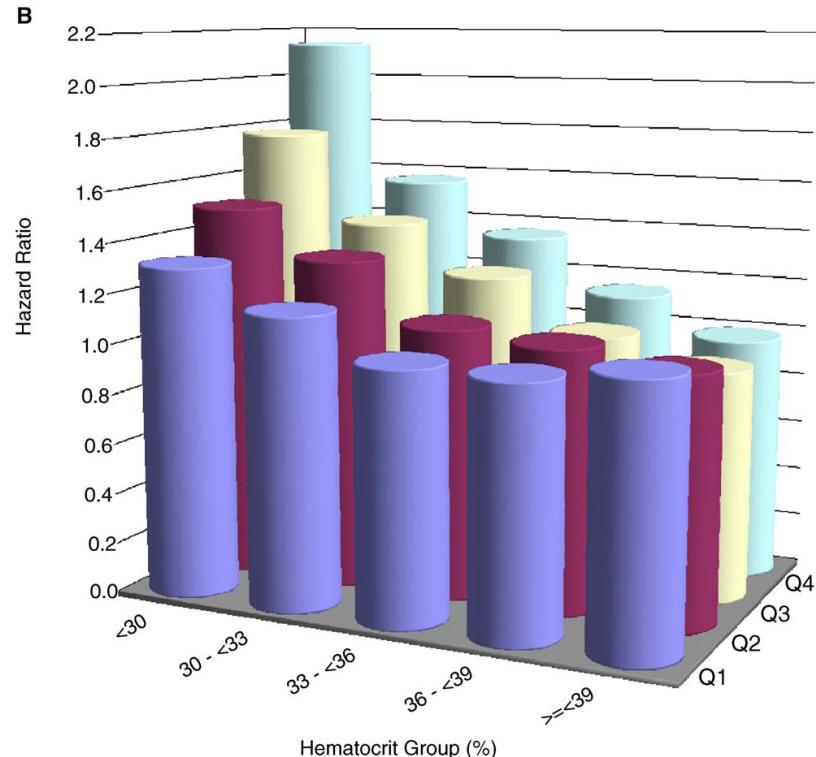


Article

## Unbiased Mapping of Transcription Factor Binding Sites along Human Chromosomes 21 and 22 Points to Widespread Regulation of Noncoding RNAs

Simon Cawley<sup>1, 5</sup>, Stefan Bekirarov<sup>1, 5</sup>, Huck H Ng<sup>2, 3, 4</sup>, Philipp Kapranov<sup>1</sup>, Edward A Sekinger<sup>2</sup>, Dione Kampa<sup>1</sup>, Antonio Piccolboni<sup>1</sup>, Victor Sementchenko<sup>1</sup>, Jill Cheng<sup>1</sup>, Alan J Williams<sup>1</sup>, Raymond Wheeler<sup>1</sup>, Brant Wong<sup>1</sup>, Jorg Drenkow<sup>1</sup>, Mark Yamanaka<sup>1</sup>, Sandeep Patel<sup>1</sup>, Shane Brubaker<sup>1</sup>, Hari Tammana<sup>1</sup>, Gregg Helt<sup>1</sup> ... Thomas R Gingeras<sup>2, 1\*</sup>

Show more



Journal of Clinical Epidemiology 57 (2004) 1086–1095

Journal of  
Clinical  
Epidemiology

Hematocrit was not validated as a surrogate end point for survival among epoetin-treated hemodialysis patients

Dennis J. Cotter<sup>a,\*</sup>, Kevin Stefanik<sup>a</sup>, Yi Zhang<sup>a</sup>, Mae Thamer<sup>a</sup>, Daniel Scharfstein<sup>b</sup>, James Kaufman<sup>c</sup>

<sup>a</sup>Medical Technology and Practice Patterns Institute, Inc., 4733 Bethesda Avenue, Suite 510, Bethesda, MD 20814

<sup>b</sup>Department of Biostatistics, Johns Hopkins Bloomberg School of Public Health, Baltimore, MD, 21205-2179

<sup>c</sup>VA Boston Healthcare System, Jamaica Plain, MA 02130

Accepted 30 April 2004

- [1] [https://doi.org/10.1016/S0092-8674\(04\)00127-8](https://doi.org/10.1016/S0092-8674(04)00127-8)
- [2] <https://doi.org/10.1016/j.jclinepi.2004.05.002>

# Goals for this lecture

1. Discuss the principles of **good vs bad** data viz
2. Review base R plotting
3. Understand the **grammar of graphics** concept
4. Introduce, explain and use the `ggplot()` function
5. Discuss how to plot 1D, 2D, 3-5D data and select the most appropriate plot type. Use facetting
6. Use visualization for the inspection of large datasets and discovery of global trends (e.g. batch effects)
7. Implement interactive (3D) visualization

# Respect **Graphical Integrity** principles

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**Representation of numbers should match the true proportions**

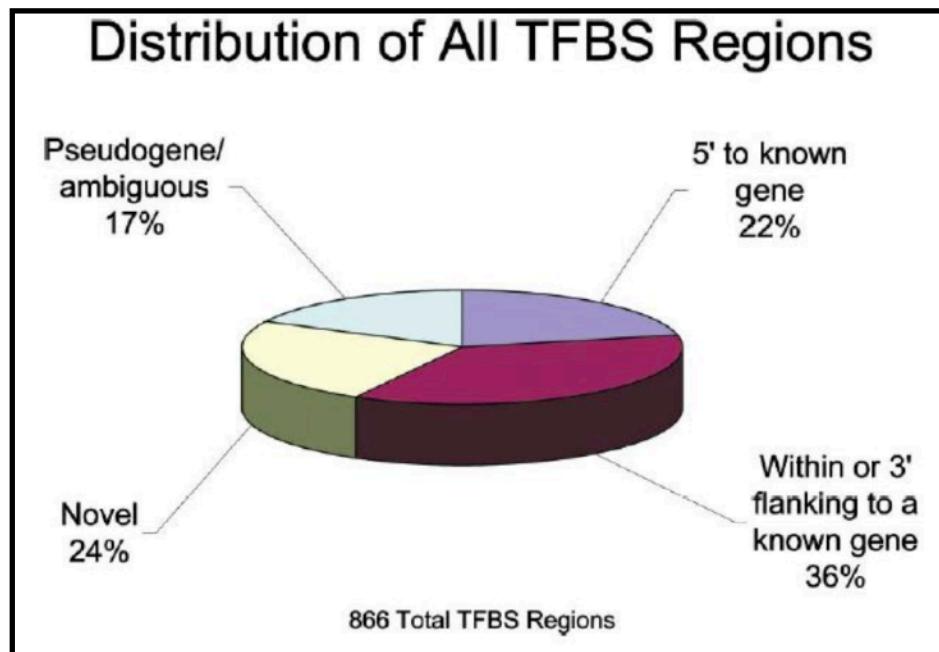
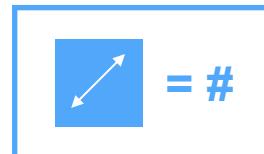
*Visual Display of Quantitative Information*  
E. Tufte



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*Visual Display of Quantitative Information*  
E. Tufte

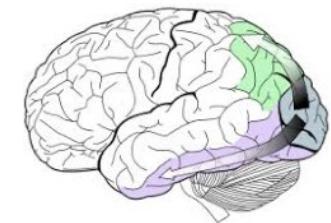


The problem with 3D

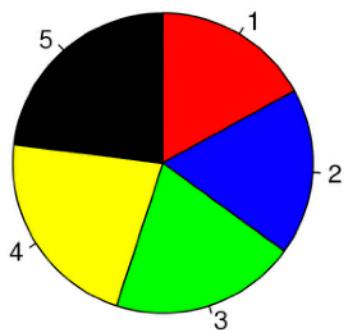
The SPACE (or even the actual angles) occupied by each category on the plot is NOT proportional to the actual numbers

This principle also applies to graphics where the origin (0) is not included.

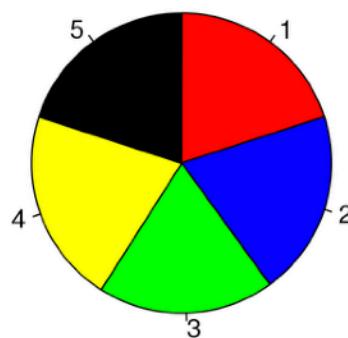
# Respect humans' visual abilities



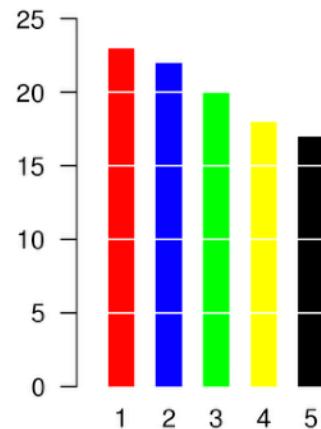
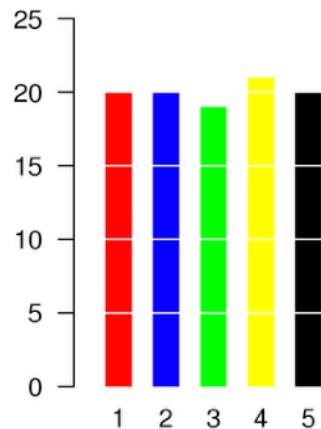
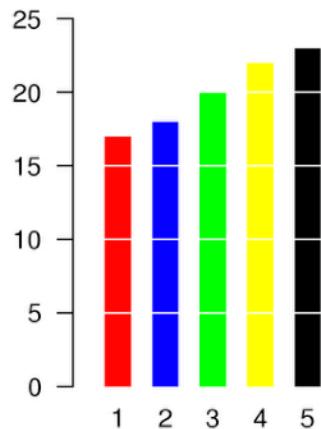
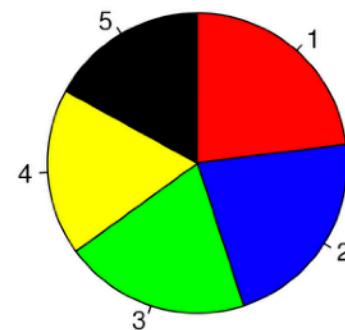
A



B

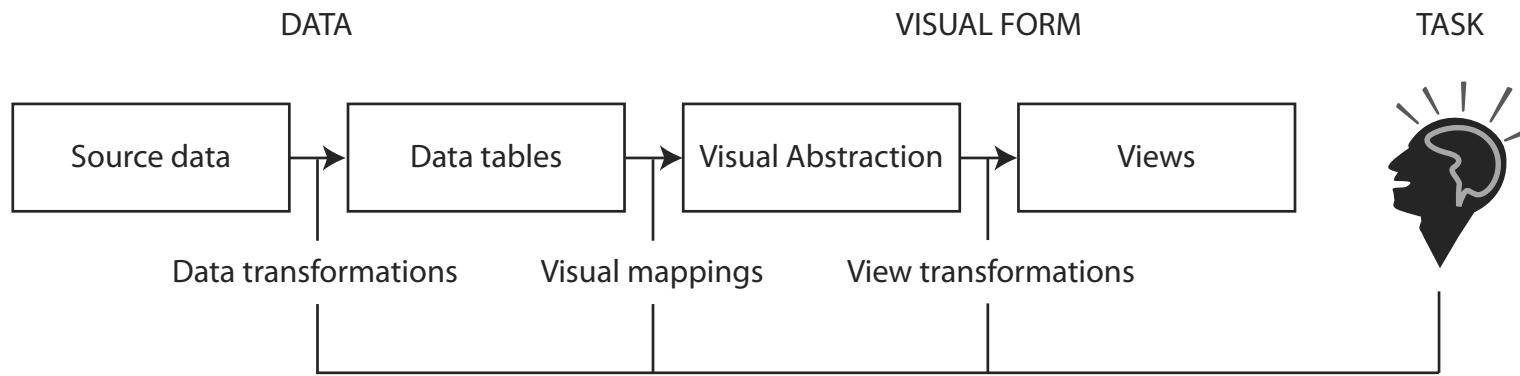


C



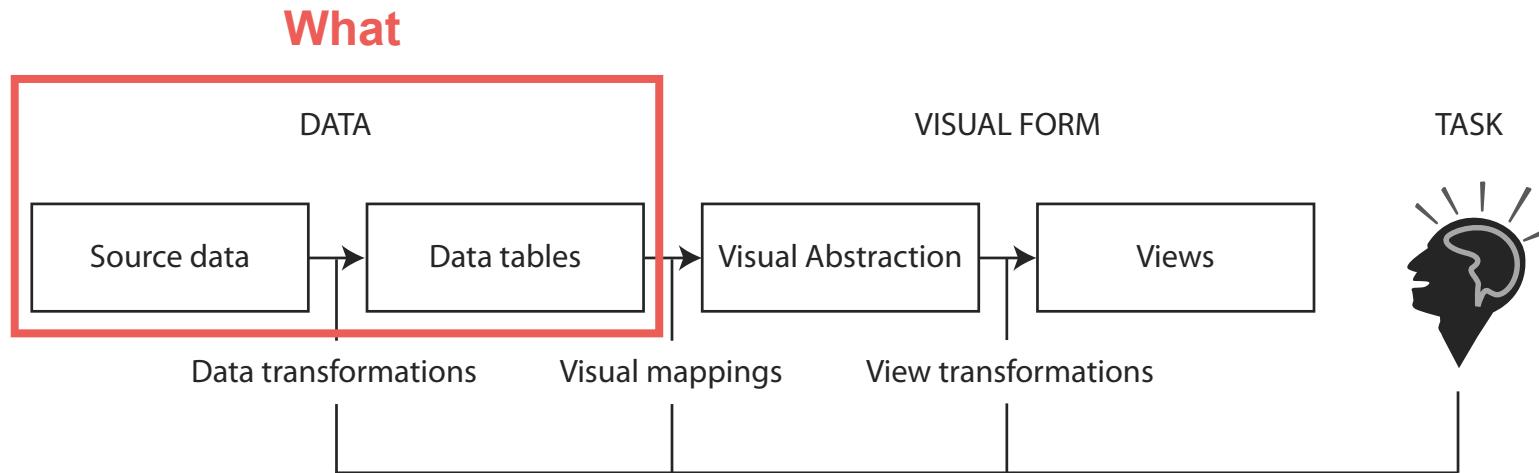
Pie charts are bad because the human brain is not good at differentiating angles. (Especially angles that do not have a horizontal or vertical edge)

# Choose a plot type that supports the task



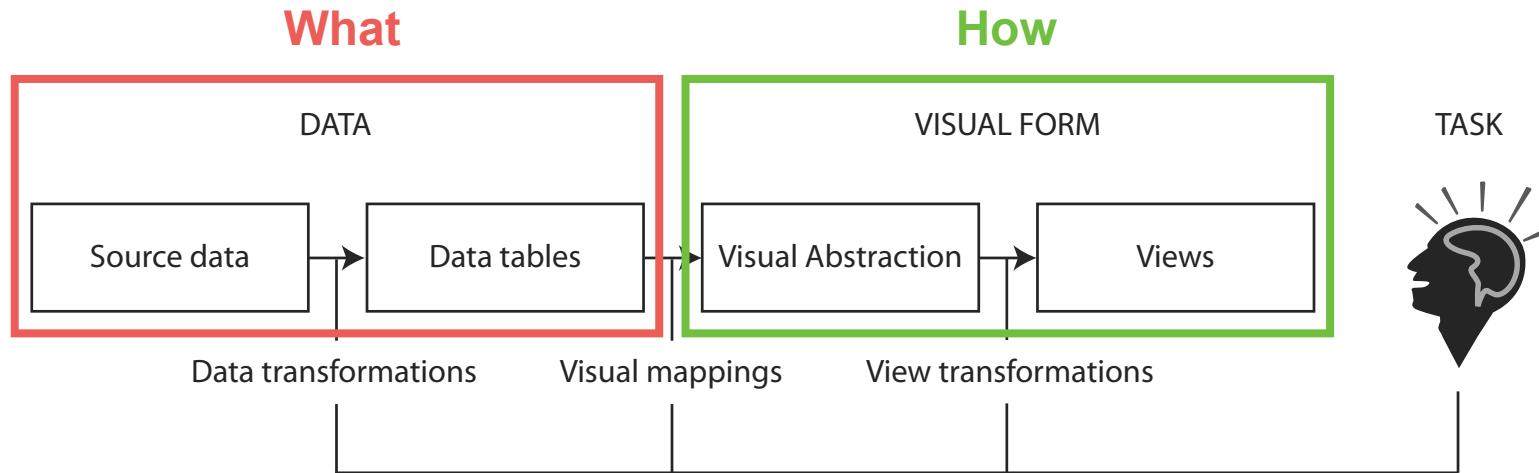
Redrawn from Card, Stuart K., Jock D. Mackinlay, and Ben Shneiderman (Editors) (1999). *Readings in Information Visualization: Using Vision to Think*. Morgan Kaufmann Publishers Inc., San Francisco, CA, USA. ISBN 1558605339.

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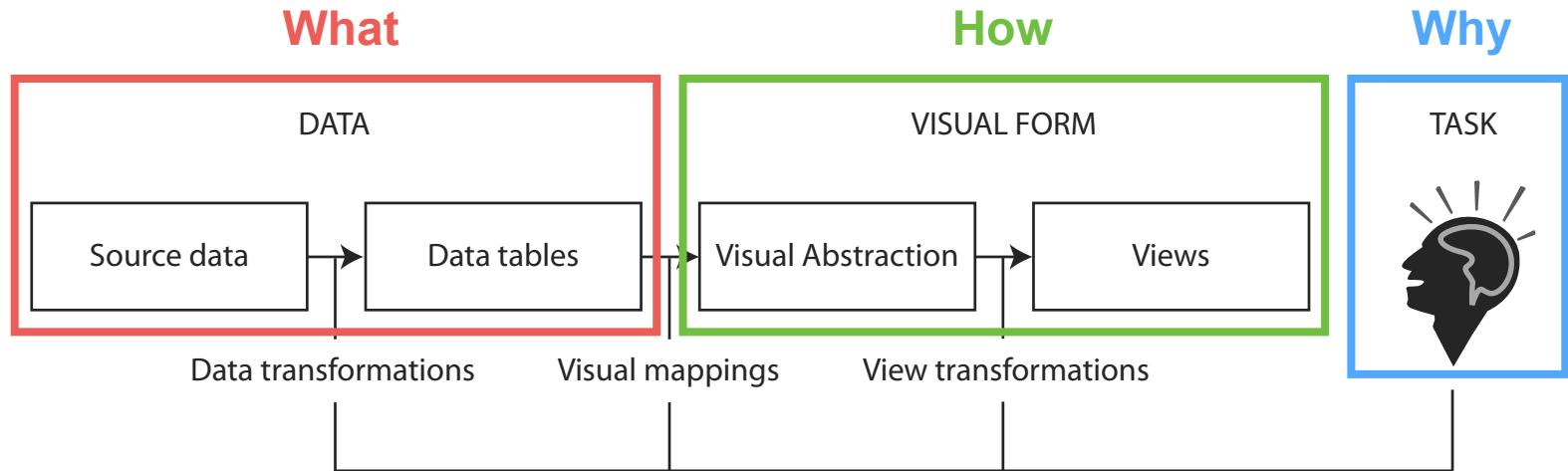
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# base R plotting

**canvas model:**

a series of instructions that  
**sequentially** fill the plotting  
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a series of instructions that  
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```
head(DNase)  
  
##   Run   conc density  
## 1  1 0.0488  0.017  
## 2  1 0.0488  0.018  
## 3  1 0.1953  0.121  
## 4  1 0.1953  0.124  
## 5  1 0.3906  0.206  
## 6  1 0.3906  0.215
```

```
plot(DNase$conc, DNase$density)
```

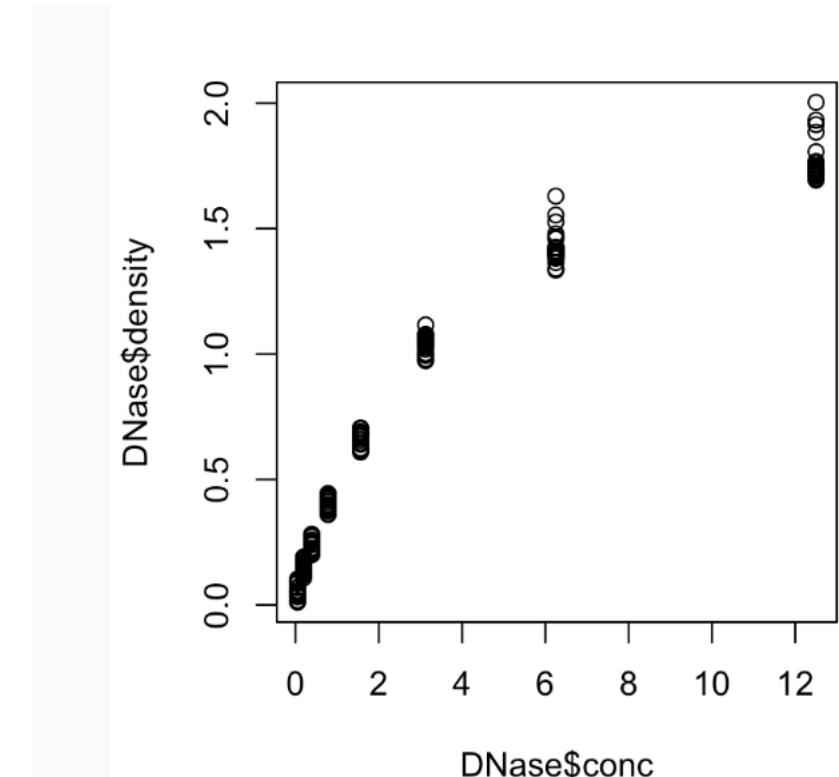


Figure 3.2: Plot of concentration vs. density for an ELISA assay of DNase.

# base R plotting

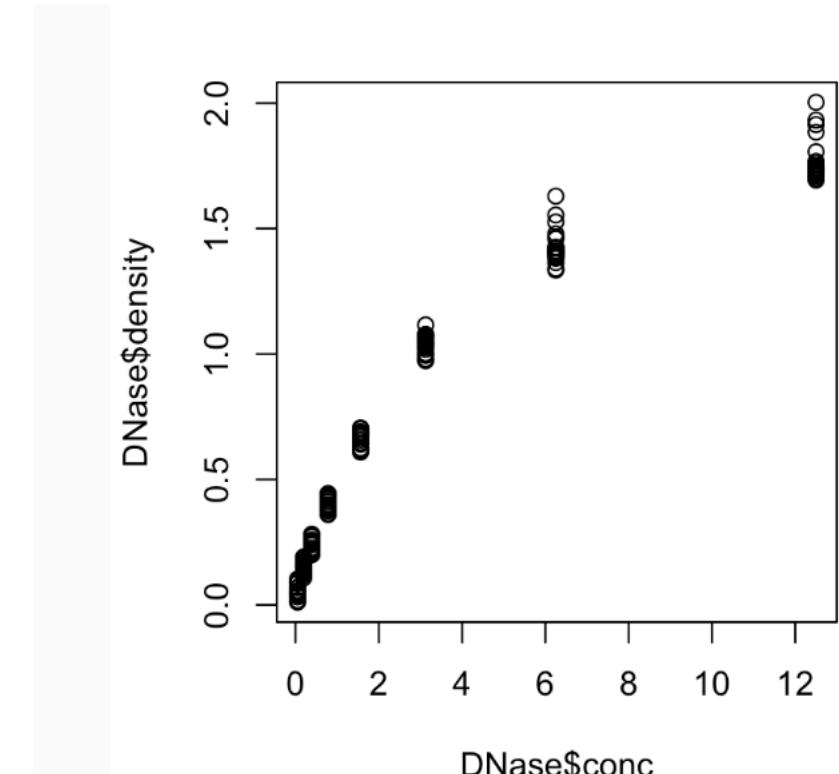
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a series of instructions that  
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**Great for quick data  
exploration!**

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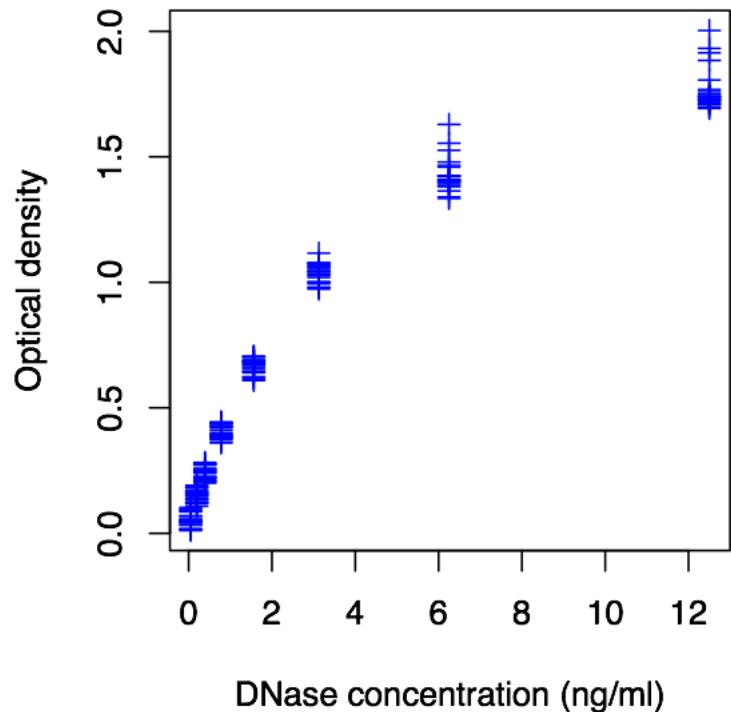
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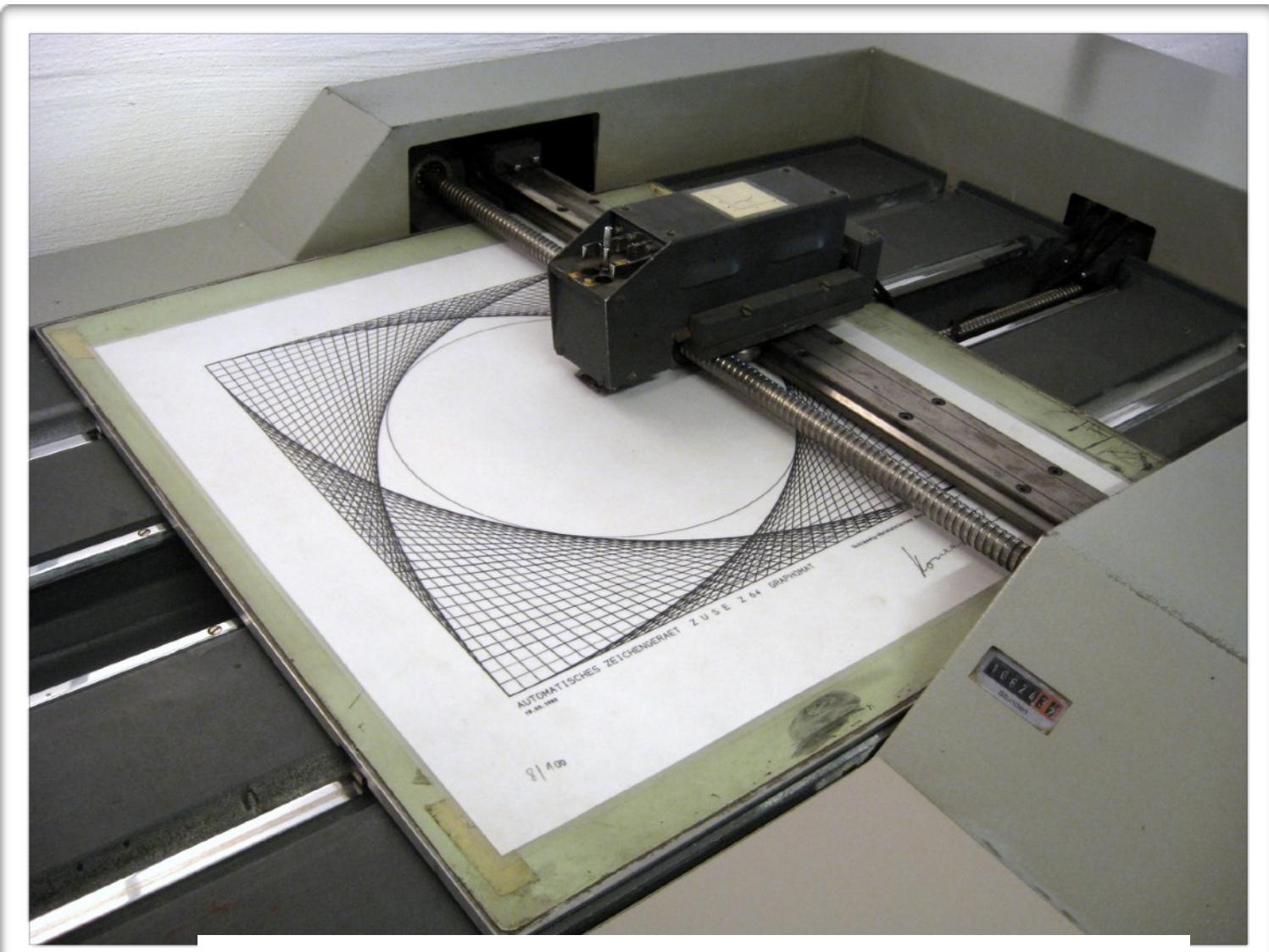
a series of instructions that  
**sequentially** fill the plotting  
canvas

**Inefficient for customization  
and generating complex plots.**

```
plot(DNase$conc, DNase$density,  
ylab = attr(DNase, "labels")$y,  
xlab = paste(attr(DNase, "labels")$x, attr(DNase, "units")$x),  
pch = 3, col = "blue")
```



# base R plotting



ZUSE Plotter Z64 (presented in 1961).

# base R plotting

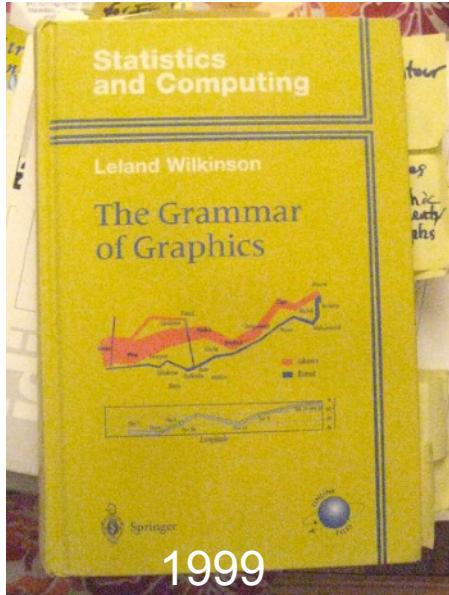
## Drawbacks:

- **Layout choices have to be made at the beginning** with no overview over what may still be coming
- **Different functions for different plot types**, with different interfaces
- Routine tasks can require lots of **boilerplate code**
- **No concept of facets / lattices**
- Only a **single global coordinate system** allowed per plot
- **Poor default colours**
- **Resizing** often leads to unsatisfactory results

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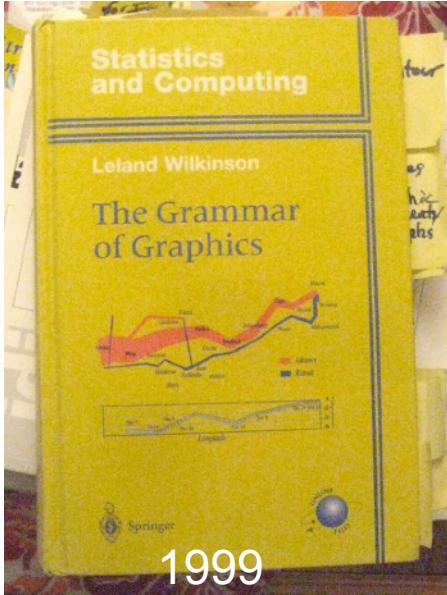
# The Grammar of Graphics



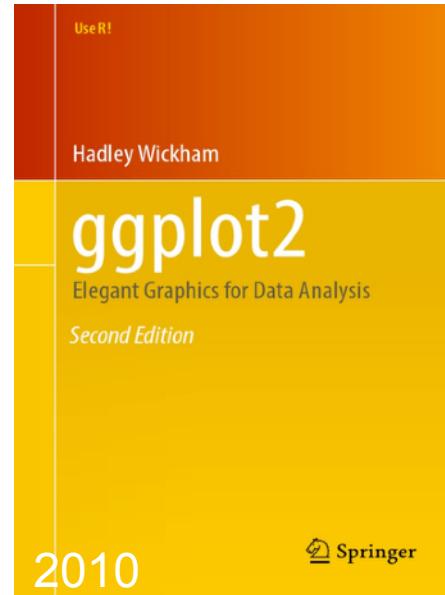
Concept **coined by**  
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An **abstraction** which  
facilitates reasoning and  
communicating graphics.

# The Grammar of Graphics



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ggplot2 is an implementation of a **layered grammar of graphics** that enables users to independently specify the building blocks of a plot and combine them to create just about any kind of graphical display.

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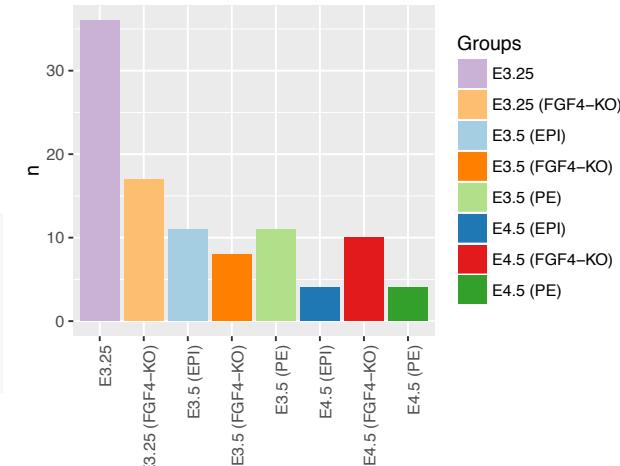
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```
ggplot(groups, aes(x = sampleGroup, y = n, fill = sampleGroup)) +  
  geom_bar(stat = "identity") +  
  scale_fill_manual(values = groupColour, name = "Groups") +  
  theme(axis.text.x = element_text(angle = 90, hjust = 1))
```



# geometric objects

 geom_boxplot() stat_boxplot()	A box and whiskers plot (in the style of Tukey)
 geom_violin() stat_ydensity()	Violin plot
 geom_path() geom_line() geom_step()	Connect observations
 geom_point()	Points
 geom_smooth() stat_smooth()	Smoothed conditional means
 geom_raster() geom_rect() geom_tile()	Rectangles
 geom_density() stat_density()	Smoothed density estimates
geom_density_2d() stat_density_2d()	Contours of a 2d density estimate

# ggplot( ) template

```
ggplot(data = <default data set>,
        aes(x = <default x axis variable>,
            y = <default y axis variable>,
            ... <other default aesthetic mappings>),
        ... <other plot defaults>) +
  geom_<geom type>(aes(size = <size variable for this geom>,
                        ... <other aesthetic mappings>),
                     data = <data for this point geom>,
                     stat = <statistic string or function>,
                     position = <position string or function>,
                     color = <"fixed color specification">,
                     ... <other arguments, possibly passed to the _stat_ function>) +
  scale_<aesthetic>_<type>(name = <"scale label">,
                            breaks = <where to put tick marks>,
                            labels = <labels for tick marks>,
                            ... <other options for the scale>) +
  theme(plot.background = element_rect(fill = "gray"),
        ... <other theme elements>)
```

# Data must be in *dataframe* format

```
library(Hiragi2013)
data(x)
expression <- Biobase::exprs(x)
dftx <- data.frame(pData(x), t(expression))
head(pData(x))
```

```
##           File.name Embryonic.day Total.number.of.cells lineage genotype
## 1 E3.25    1_C32_IN      E3.25                  32       WT
## 2 E3.25    2_C32_IN      E3.25                  32       WT
## 3 E3.25    3_C32_IN      E3.25                  32       WT
## 4 E3.25    4_C32_IN      E3.25                  32       WT
## 5 E3.25    5_C32_IN      E3.25                  32       WT
## 6 E3.25    6_C32_IN      E3.25                  32       WT
```

```
##           ScanDate sampleGroup sampleColour
## 1 E3.25 2011-03-16      E3.25      #CAB2D6
## 2 E3.25 2011-03-16      E3.25      #CAB2D6
## 3 E3.25 2011-03-16      E3.25      #CAB2D6
## 4 E3.25 2011-03-16      E3.25      #CAB2D6
## 5 E3.25 2011-03-16      E3.25      #CAB2D6
## 6 E3.25 2011-03-16      E3.25      #CAB2D6
```

```
dim(expression)
```

```
## [1] 45101 101
```

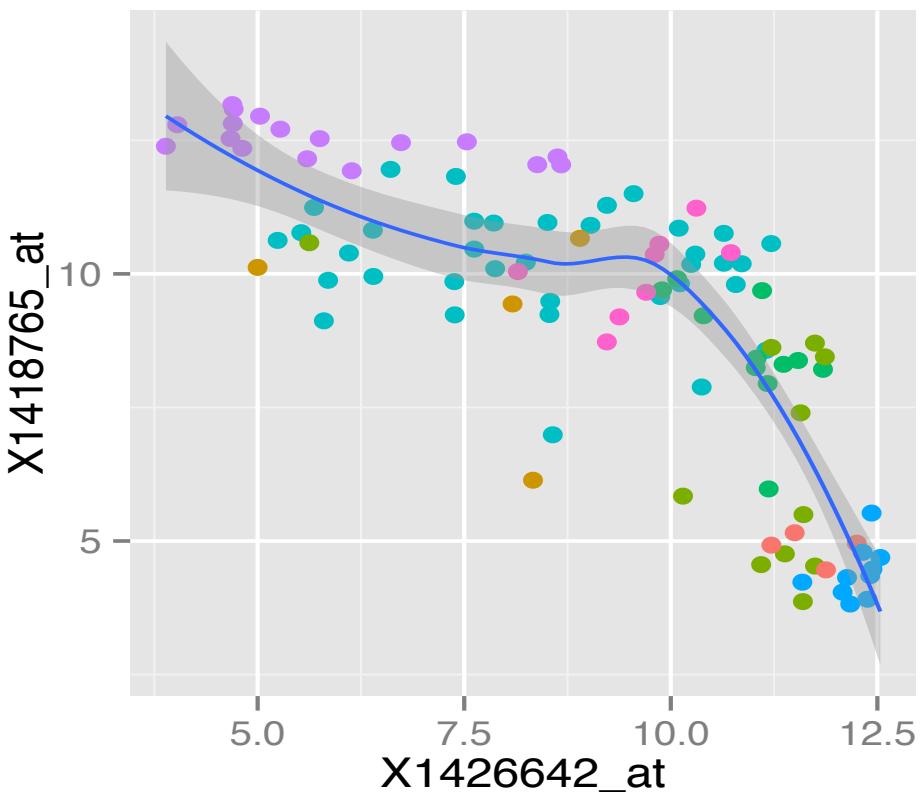
ggplot()  
requires input  
data in form of a  
dataframe

Gene expression  
**microarray**  
**dataset on early**  
**development of**  
**mouse embryos**

transcriptomes of  
~100 individual  
cells at different  
time points in. [1]

# Multiple layers can be superposed

```
ggplot( dftx, aes( x = X1426642_at, y = X1418765_at ) ) +  
  geom_point( aes( colour = sampleColour), shape = 19 ) +  
  geom_smooth( method = "loess" ) +  
  scale_colour_discrete( guide = FALSE )
```



Here, the first layer holds the points, the second holds the smoothed average.

# Using the same plot, we can easily change the coordinates

```
groupSize <- table(dftx$sampleGroup)  
groupSize
```

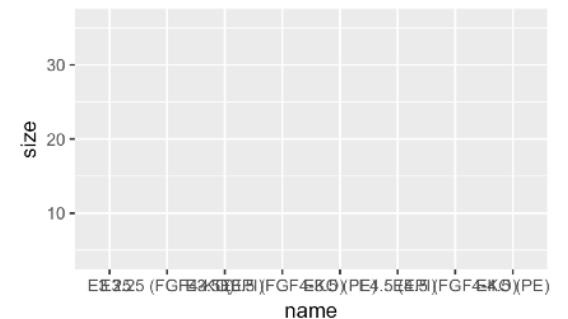
```
pb <- ggplot(data.frame(  
    name = names(groupSize),  
    size = as.vector(groupSize)),  
    aes(x = name, y = size))
```

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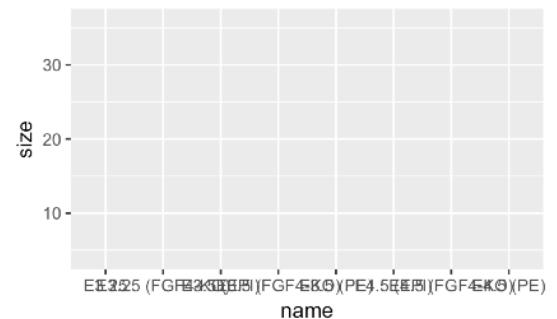
No geom defined yet!



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No geom defined yet!



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    aes(x = name, y = size))
```

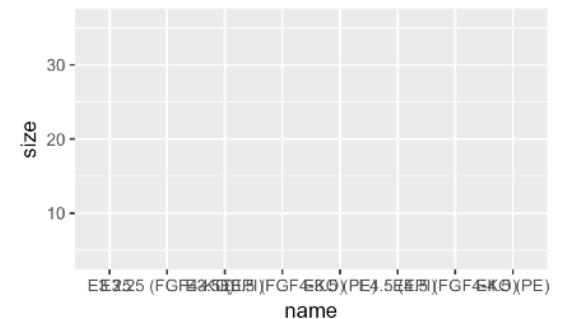
```
pb <- pb + geom_bar(stat = "identity") +  
  aes(fill = name) +  
  scale_fill_manual(values = groupColour, name = "Colour code") +  
  theme(axis.text.x = element_text(angle = 90, hjust = 1)) +  
  xlab("Groups") + ylab("Number of Samples")
```

# Using the same plot, we can easily change the coordinates

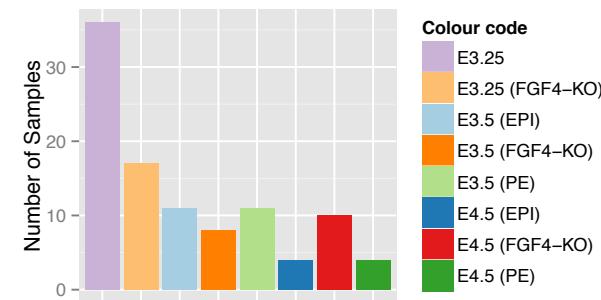
```
groupSize <- table(dftx$sampleGroup)  
groupSize
```

```
pb <- ggplot(data.frame(  
    name = names(groupSize),  
    size = as.vector(groupSize)),  
    aes(x = name, y = size))
```

No geom defined yet!



```
pb <- pb + geom_bar(stat = "identity") +  
  aes(fill = name) +  
  scale_fill_manual(values = groupColour, name = "Colour code") +  
  theme(axis.text.x = element_text(angle = 90, hjust = 1)) +  
  xlab("Groups") + ylab("Number of Samples")
```

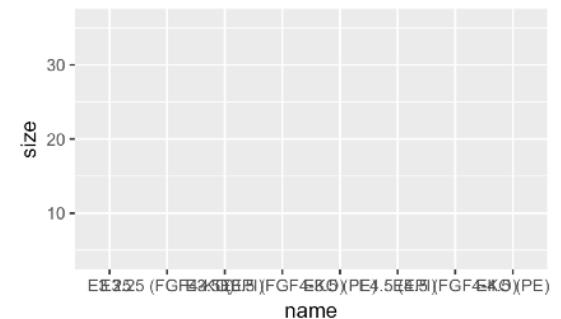


# Using the same plot, we can easily change the coordinates

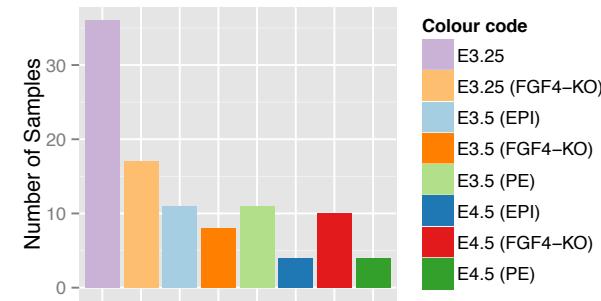
```
groupSize <- table(dftx$sampleGroup)  
groupSize
```

```
pb <- ggplot(data.frame(  
    name = names(groupSize),  
    size = as.vector(groupSize)),  
    aes(x = name, y = size))
```

No geom defined yet!



```
pb <- pb + geom_bar(stat = "identity") +  
  aes(fill = name) +  
  scale_fill_manual(values = groupColour, name = "Colour code") +  
  theme(axis.text.x = element_text(angle = 90, hjust = 1)) +  
  xlab("Groups") + ylab("Number of Samples")
```



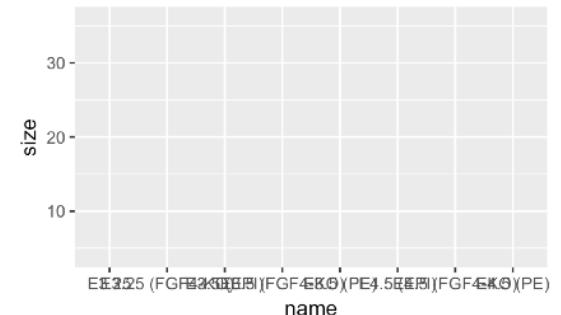
```
pb.polar <- pb + coord_polar() +  
  theme(axis.text.x = element_text(angle = 0, hjust = 1),  
        axis.text.y = element_blank(),  
        axis.ticks = element_blank()) +  
  xlab("") + ylab("")  
pb.polar
```

# Using the same plot, we can easily change the coordinates

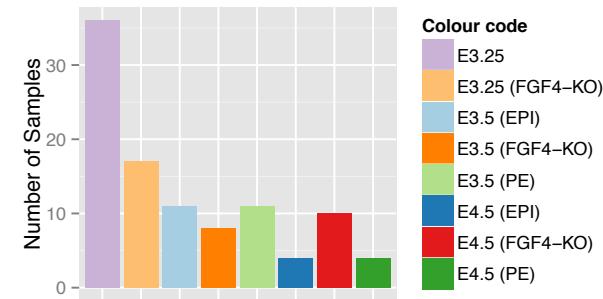
```
groupSize <- table(dftx$sampleGroup)  
groupSize
```

```
pb <- ggplot(data.frame(  
    name = names(groupSize),  
    size = as.vector(groupSize)),  
    aes(x = name, y = size))
```

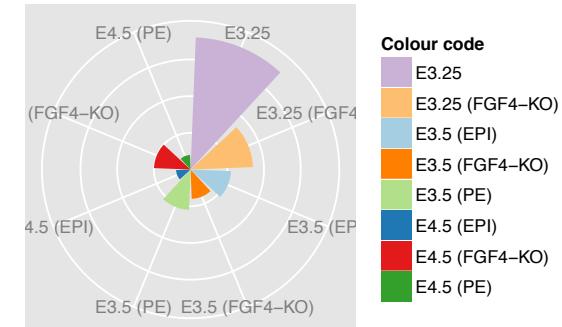
No geom defined yet!



```
pb <- pb + geom_bar(stat = "identity") +  
  aes(fill = name) +  
  scale_fill_manual(values = groupColour, name = "Colour code") +  
  theme(axis.text.x = element_text(angle = 90, hjust = 1)) +  
  xlab("Groups") + ylab("Number of Samples")
```



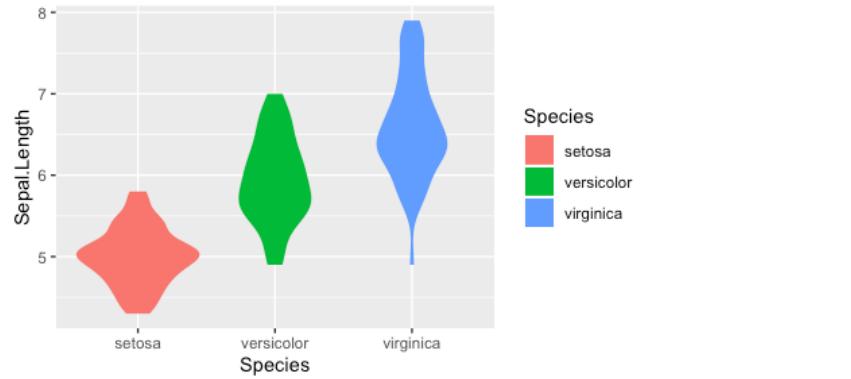
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pb.polar <- pb + coord_polar() +  
  theme(axis.text.x = element_text(angle = 0, hjust = 1),  
        axis.text.y = element_blank(),  
        axis.ticks = element_blank()) +  
  xlab("") + ylab("")  
pb.polar
```



# Themes can change the look

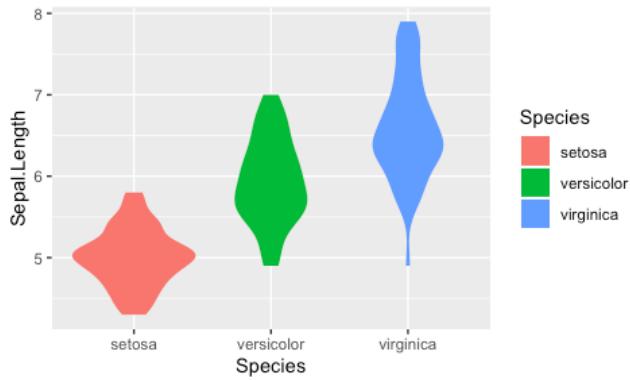
# Themes can change the look

```
g = ggplot(iris,  
           aes(x = Species,  
                 y = Sepal.Length,  
                 fill = Species))+  
  geom_violin(col = NA)  
g
```

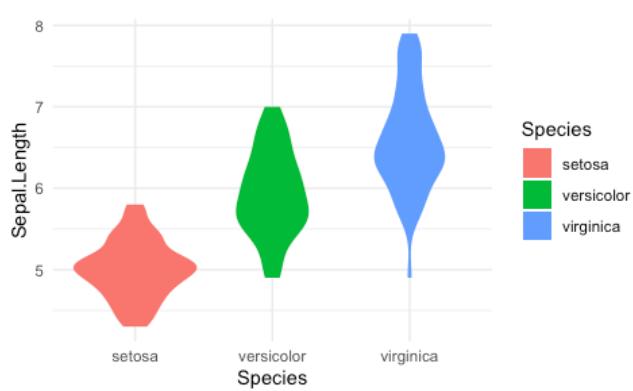


# Themes can change the look

```
g = ggplot(iris,  
           aes(x = Species,  
                 y = Sepal.Length,  
                 fill = Species))+  
  geom_violin(col = NA)  
g
```

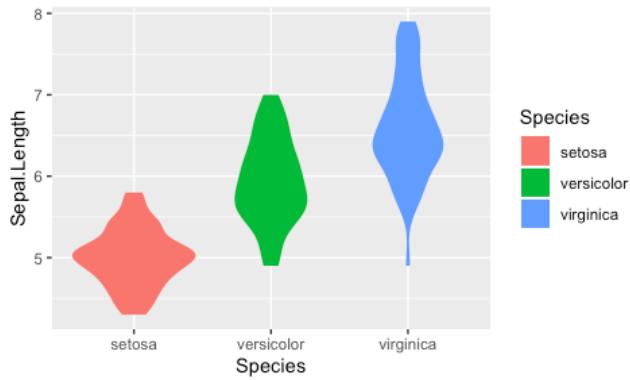


```
g + theme_minimal()
```

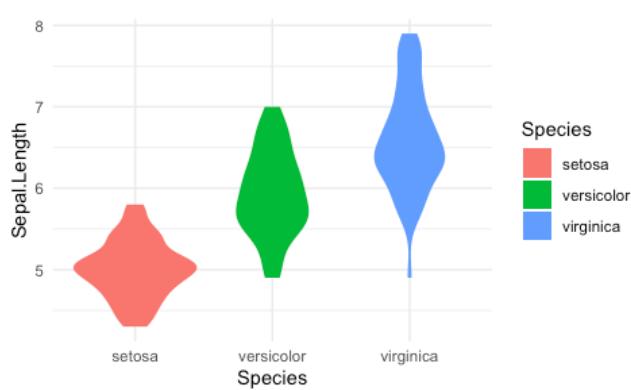


# Themes can change the look

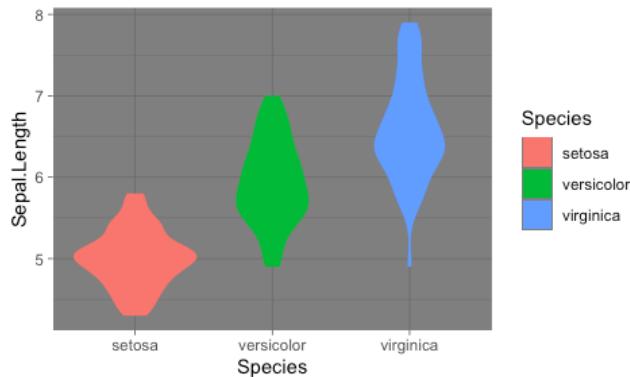
```
g = ggplot(iris,  
           aes(x = Species,  
                 y = Sepal.Length,  
                 fill = Species))+  
  geom_violin(col = NA)  
g
```



```
g + theme_minimal()
```

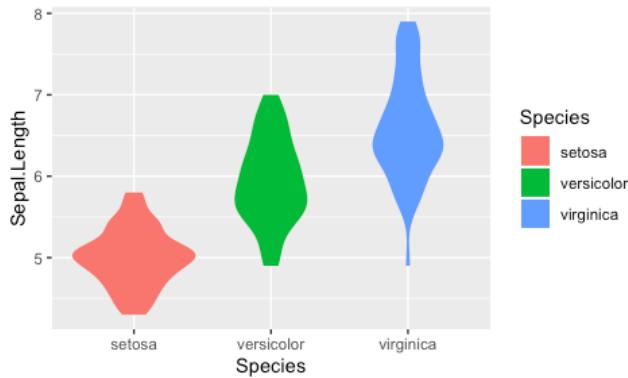


```
g + theme_dark()
```

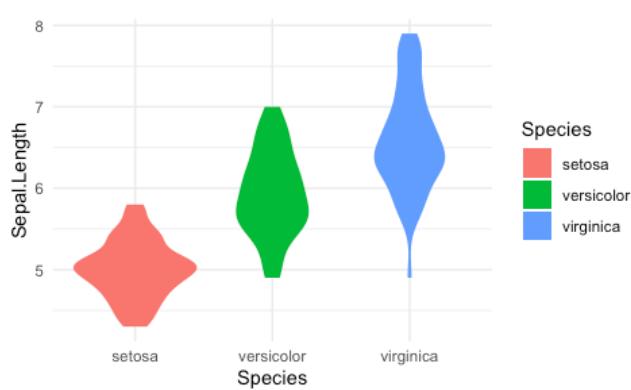


# Themes can change the look

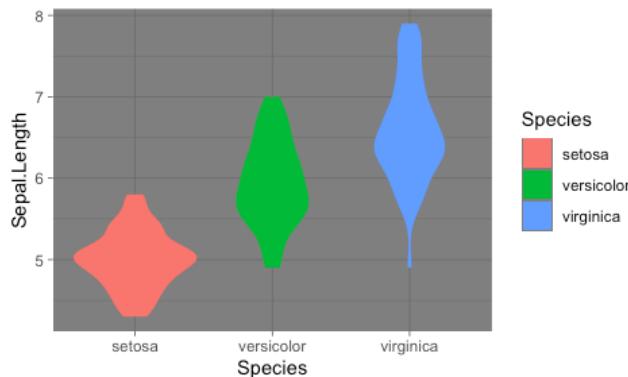
```
g = ggplot(iris,  
           aes(x = Species,  
                 y = Sepal.Length,  
                 fill = Species))+  
  geom_violin(col = NA)  
g
```



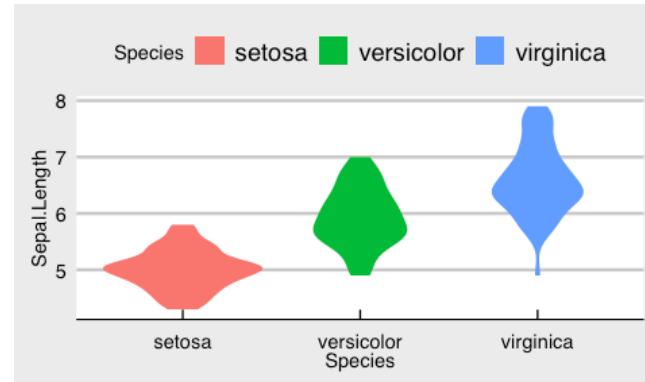
```
g + theme_minimal()
```



```
g + theme_dark()
```



```
library(ggthemes)  
g + theme_economist_white()
```



# Goals for this lecture

1. Discuss the principles of **good vs bad** data viz
2. Review base R plotting
3. Understand the **grammar of graphics** concept
4. Introduce, explain and use the `ggplot()` function
5. Discuss how to plot 1D, 2D, 3-5D data and select the most appropriate plot type. Use facetting
6. Use visualization for the inspection of large datasets and discovery of global trends (e.g. batch effects)
7. Implement interactive (3D) visualization

# 1D plot types

# 1D plot types

What do you use to show or compare 1D distributions?

# 1D plot types

What do you use to show or compare 1D distributions?

[Boxplot](#) makes sense for **unimodal** distributions

[Histogram](#) requires definition of bins/binwidths/break positions. It can create visual artifacts esp. if the number of data points is not large

[Density](#) requires setting of **bandwidth parameter**; obscures the sample size (i.e. the uncertainty of the estimate)

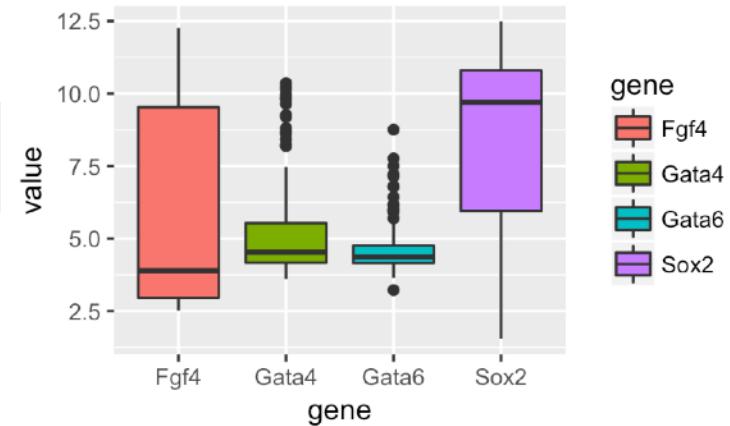
[ECDF](#) (Empirical Cumulative Density Function) does not have these problems, but is more abstract and its interpretation requires more training.

If you have only up to a **few dozens of points** just **show the raw data!** (e.g. with [beeswarm](#))

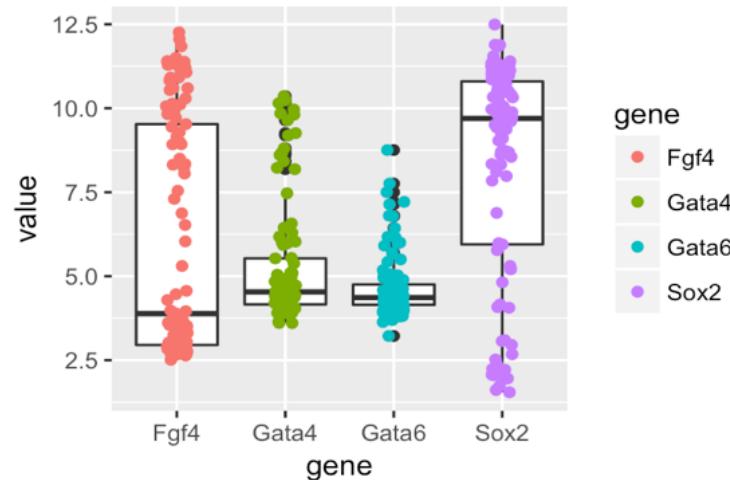
# Boxplot

Boxplots are good for plotting summary of 1D continuous data; they allow you to **compare quantiles of data distributions**.

```
p = ggplot(genes, aes(x = gene, y = value))  
p + geom_boxplot(aes(fill = gene))
```



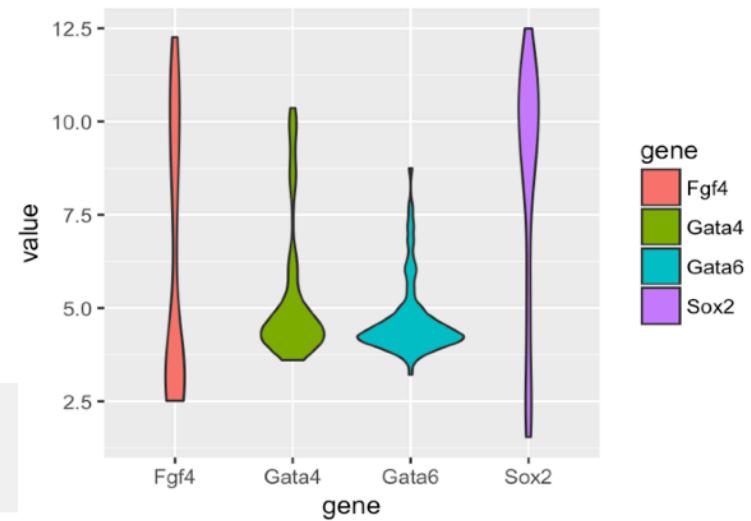
```
p + geom_boxplot() +  
  geom_jitter(aes(color = gene), width = 0.1, height = 0)
```



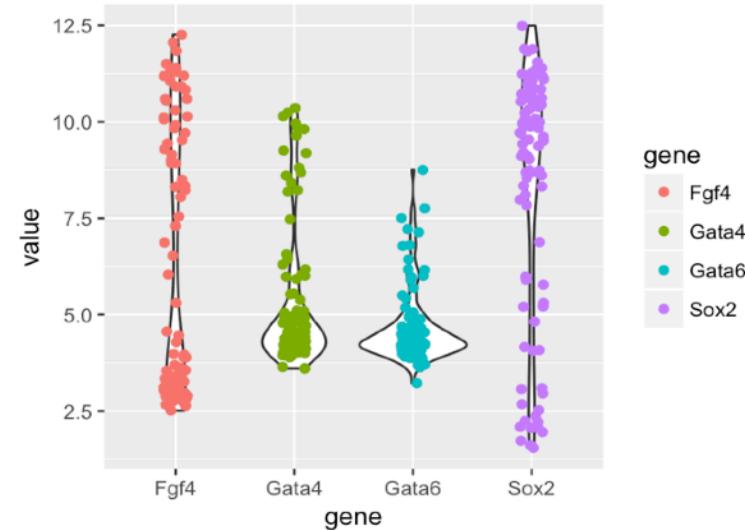
# Violin Plot

If there are many observations in the dataset, we can **show the estimated distribution with violin plots.**

```
p = ggplot(genes, aes( x = gene, y = value))  
p + geom_violin(aes(fill = gene))
```

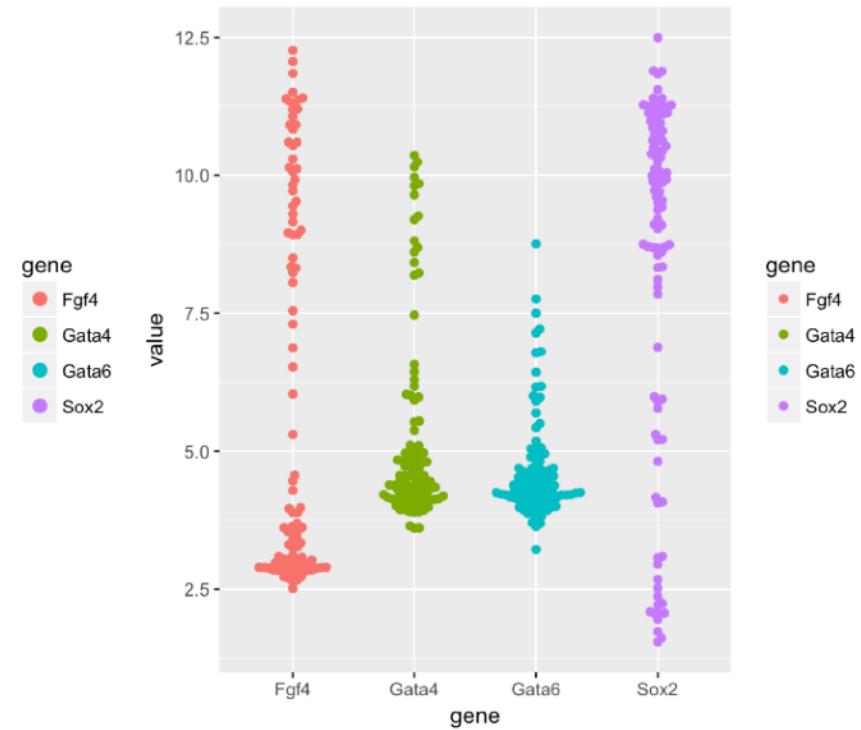
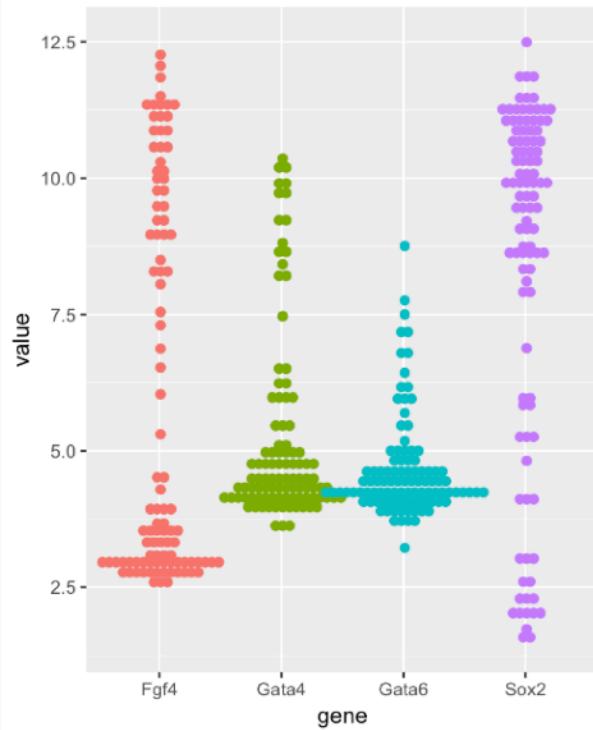


```
p + geom_boxplot() +  
  geom_jitter(aes(color = gene), width = 0.1, height = 0)
```



# Dot & Beeswarm Plot

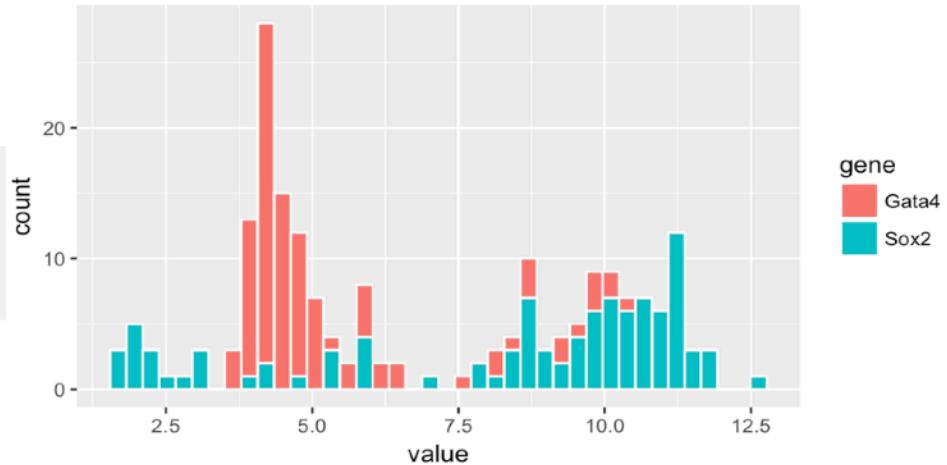
```
p + geom_dotplot(binaxis = "y", binwidth = 1/6,  
                  stackdir = "center", stackratio = 0.75,  
                  aes(color = gene))  
  
library("ggbeeswarm")  
p + geom_beeswarm(aes(color = gene))
```



# Histograms

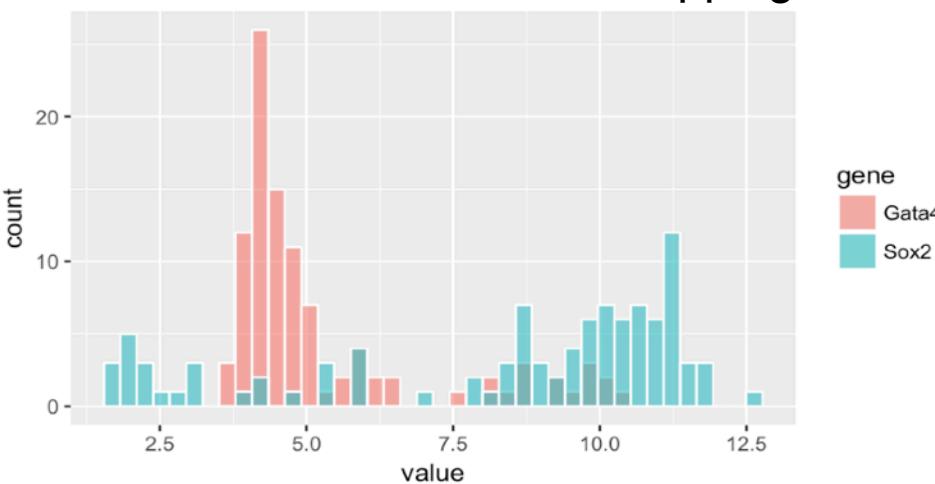
Stacked

```
p = ggplot(genes %>% filter(gene %in% c("Gata4", "Sox2")),
            aes(x = value))
p + geom_histogram(aes(fill = gene),
                   color = "white", bins = 40)
```



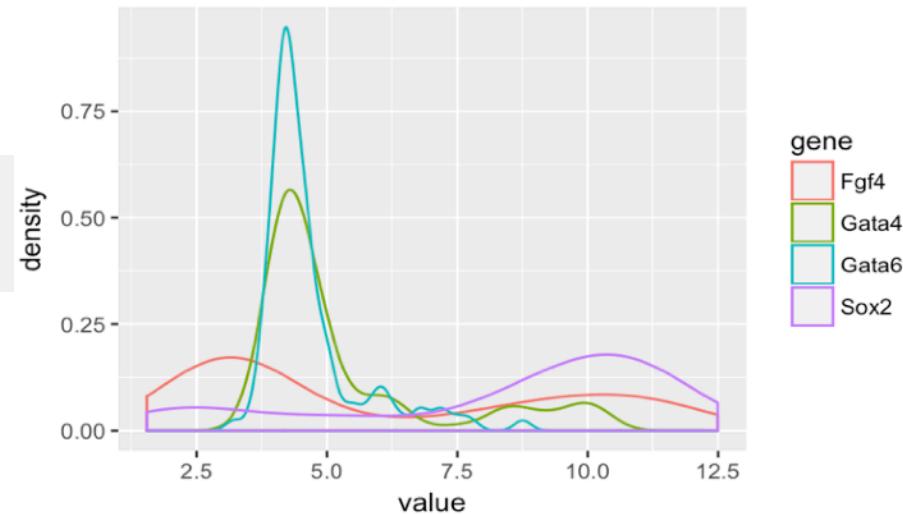
Overlapping

```
p + geom_histogram(
  aes(fill = gene), color="white", alpha=0.6,
  bins = 40, position = "identity")
```

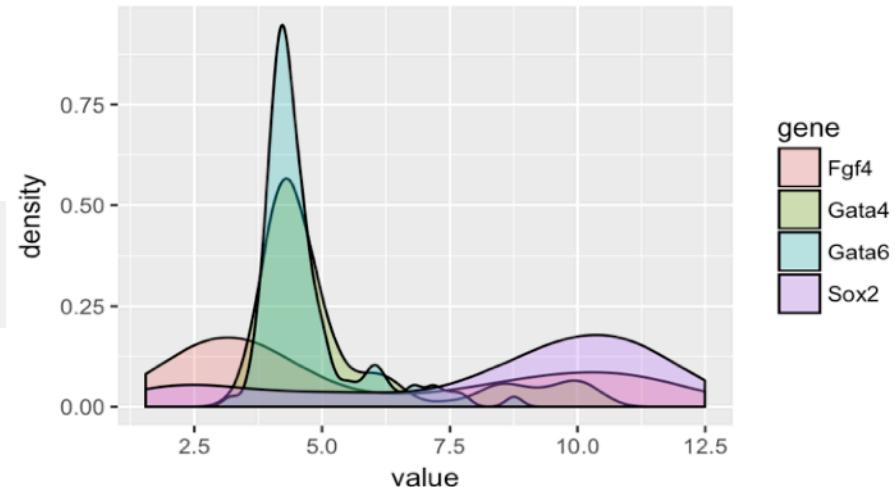


# Density plots

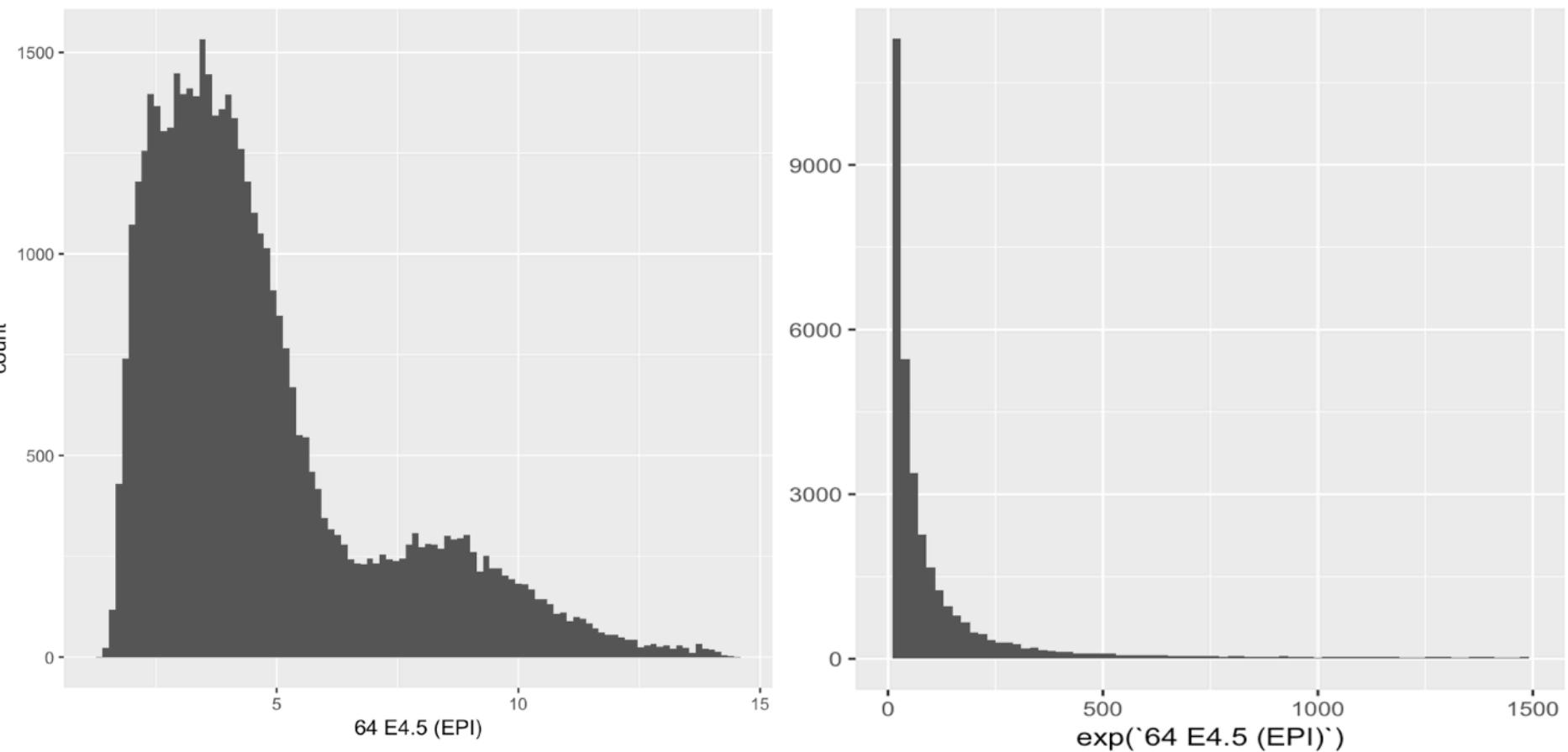
```
p = ggplot(genes, aes( x = value, color = gene))  
p + geom_density()
```



```
p = ggplot(genes, aes( x = value, fill = gene))  
p + geom_density(alpha = 0.3)
```



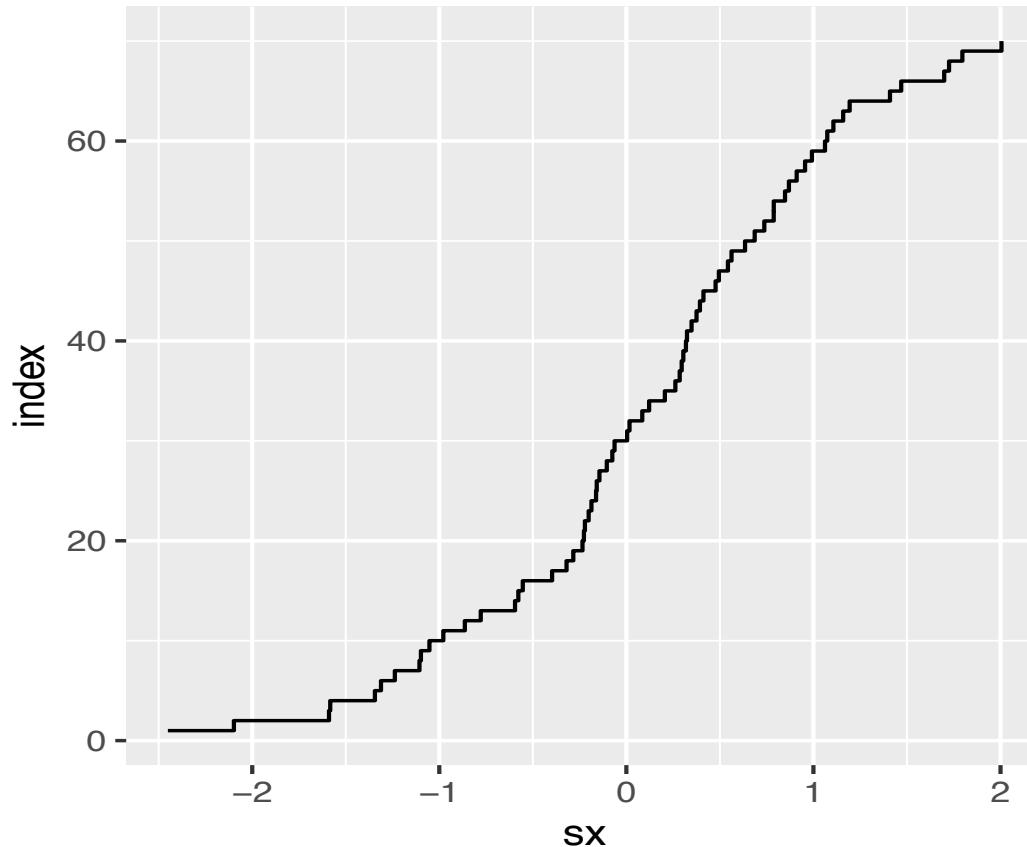
# Non-linear transformations change the shape of a density



- The **mode** of a distribution is an **infinitesimal concept**.
- Need either an infinite amount of data or choose smoothing / binning bandwidth
- **Number of modes (let alone their positions) can change under non-linear data transformations**

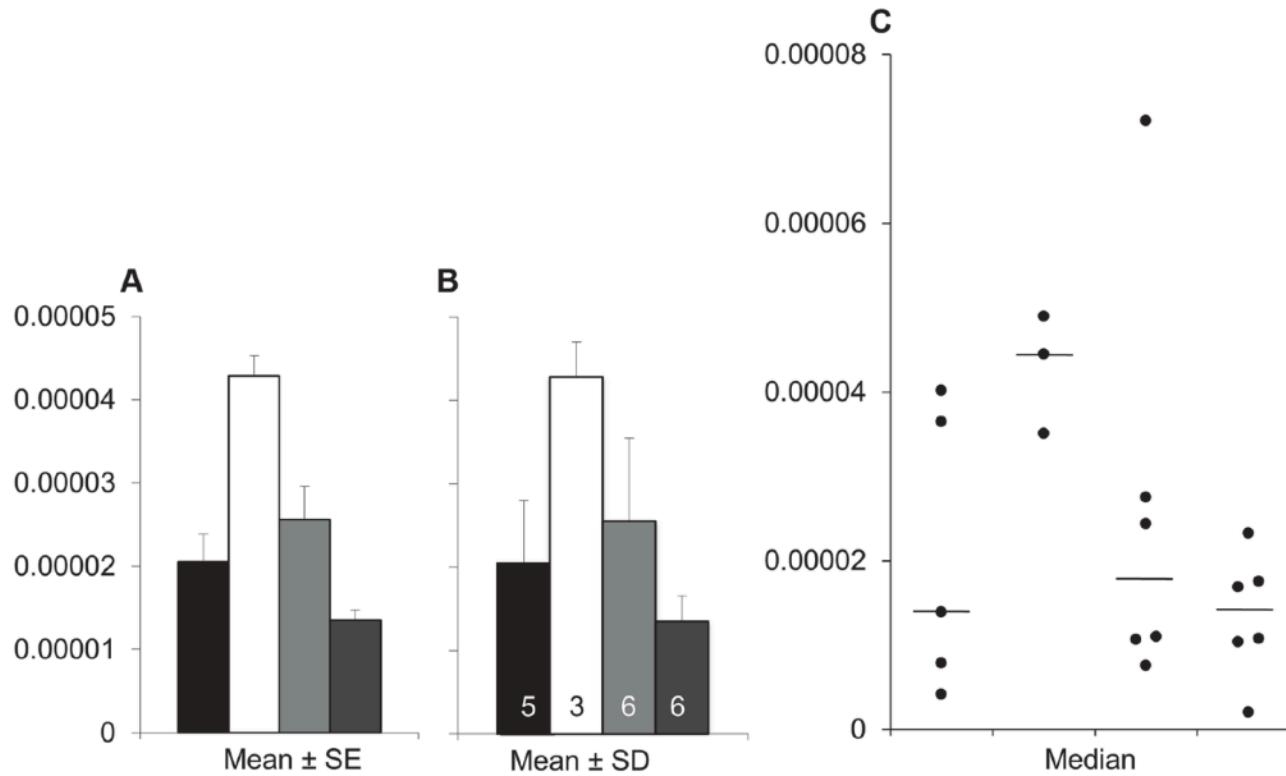
# The empirical cumulative distribution

$$F_n(x) = \frac{\text{number of } i \text{ for which } x_i \leq x}{n} = \frac{1}{n} \sum_{i=1}^n \mathbb{1}(x \leq x_i)$$



```
simdata = rnorm(70)
simdf <- data.frame(index = seq(along = simdata), sx = sort(simdata))
ggplot(simdf, aes(x = sx, y = index)) + geom_step()
```

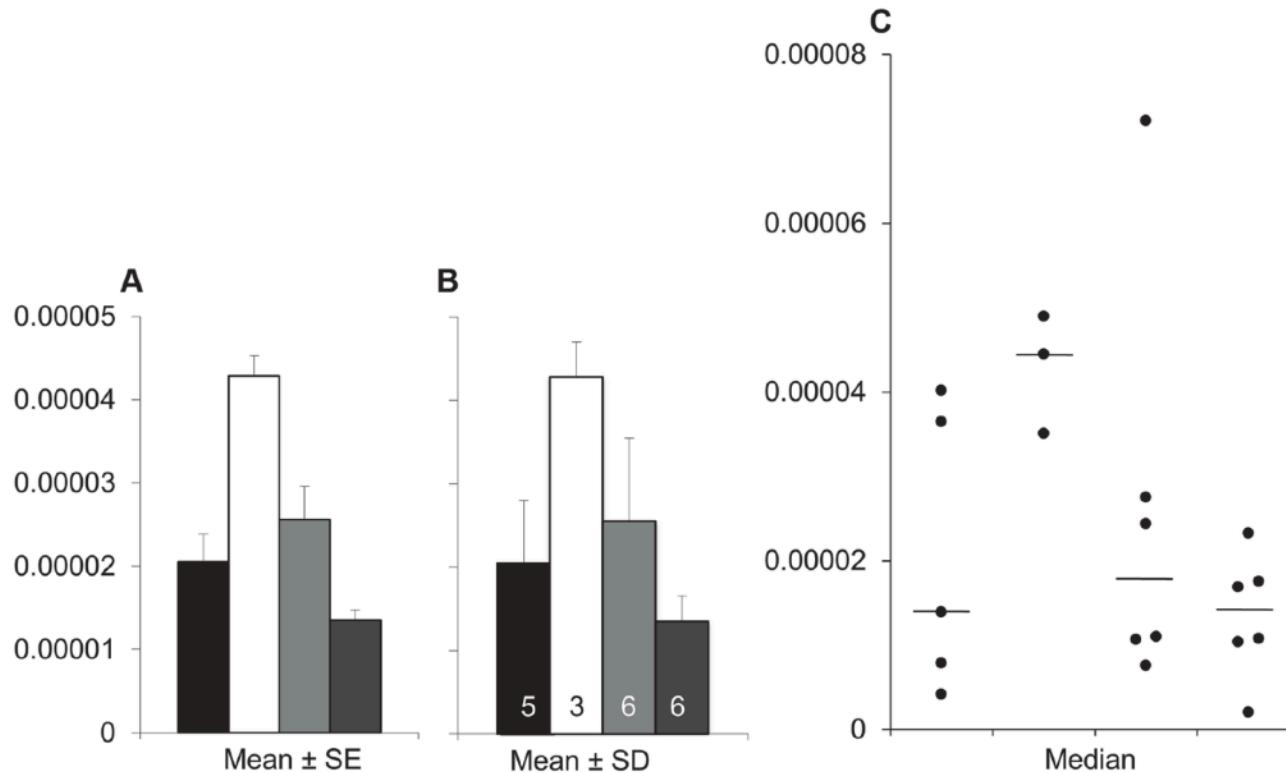
# Bar charts with error bars



**Fig 3. Bar graphs and scatterplots convey very different information.** While scatterplots prompt the reader to critically evaluate the statistical tests and the authors' interpretation of the data, bar graphs discourage the reader from thinking about these issues. Placental endothelin 1 (*EDN1*) mRNA data for four different groups of participants is presented in bar graphs showing mean  $\pm$  SE (Panel A), or mean  $\pm$  SD (Panel B), and in a univariate scatterplot (Panel C). Panel A (mean  $\pm$  SE) suggests that the second group has higher values than the remaining groups; however, Panel B (mean  $\pm$  SD) reveals that there is considerable overlap between groups. Showing SE rather than SD magnifies the apparent visual differences between groups, and this is exacerbated by the fact that SE obscures any effect of unequal sample size. The scatterplot (Panel C) clearly shows that the sample sizes are small, group one has a much larger variance than the other groups, and there is an outlier in group three. These problems are not apparent in the bar graphs shown in Panels A and B.

# Bar charts with error bars

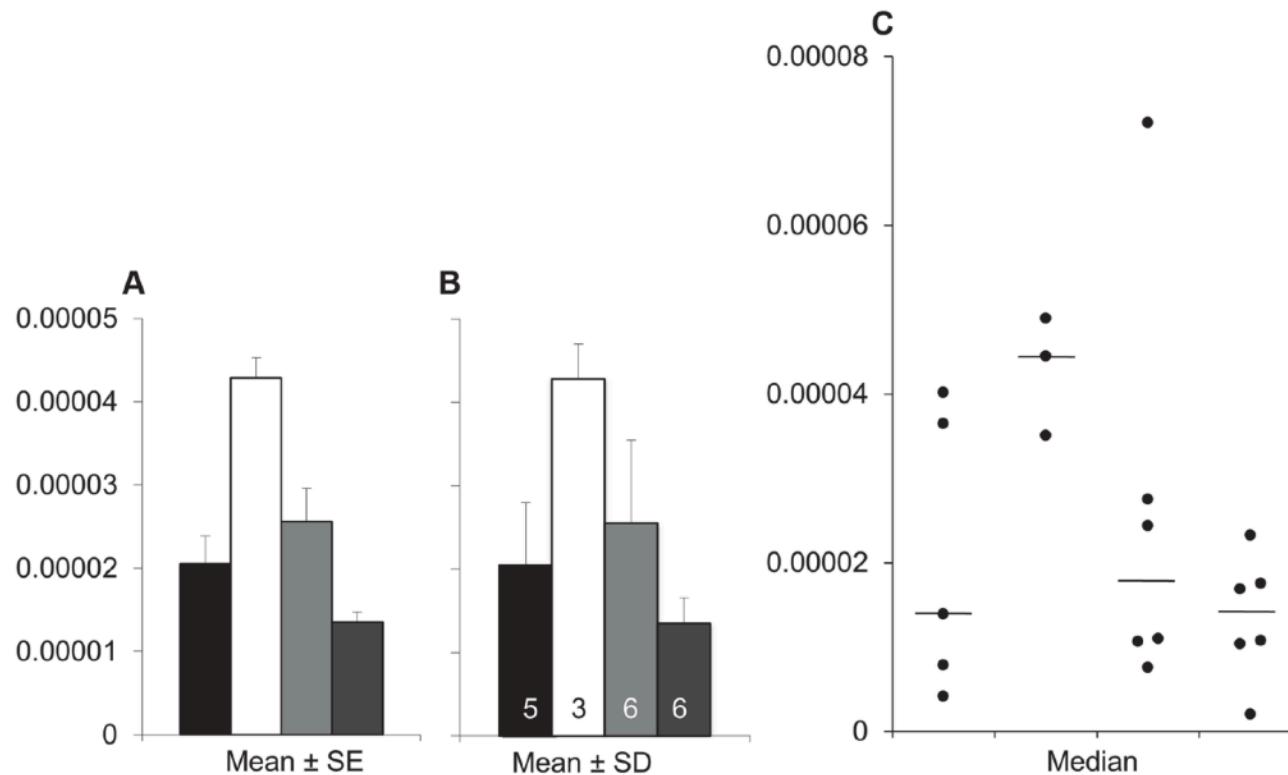
What is wrong with {bar charts + error bars} ?



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# Bar charts with error bars

## What is wrong with {bar charts + error bars} ?



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doi:10.1371/journal.pbio.1002128.g003

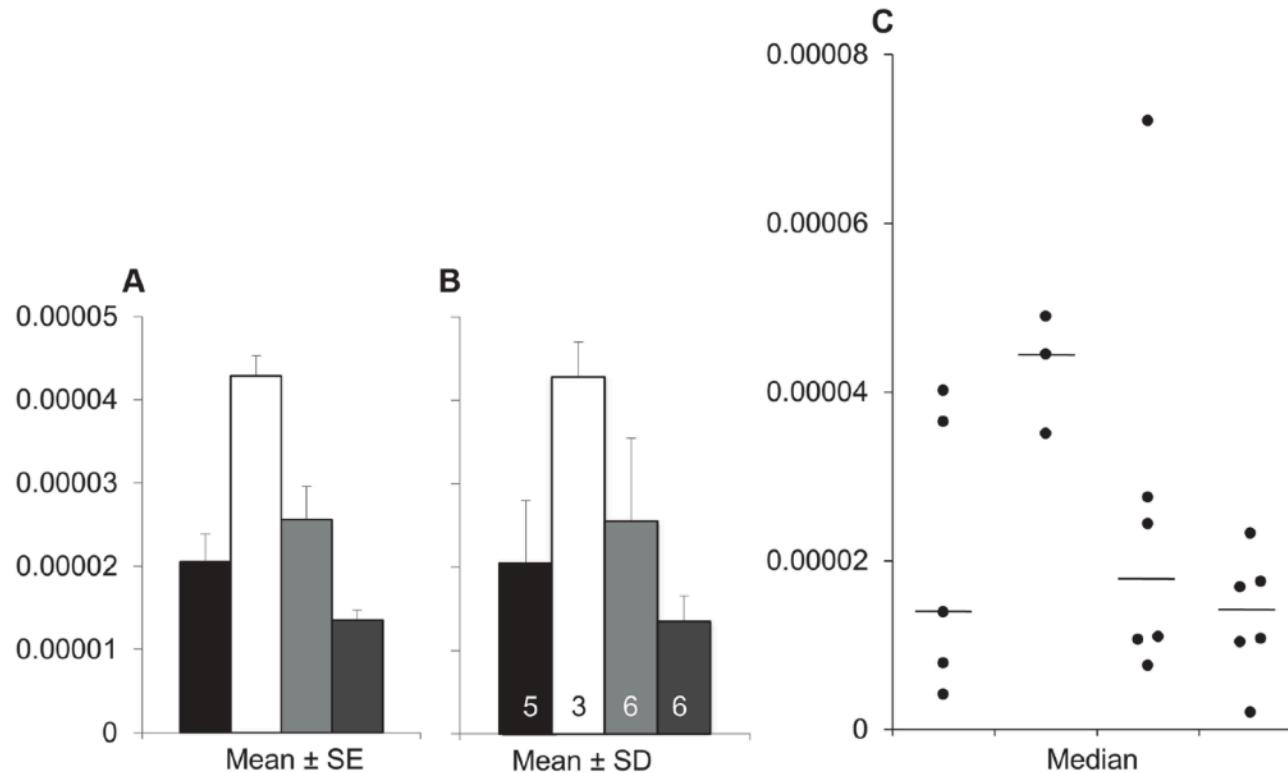
Weissgerber TL, et al. (2015) Beyond Bar and Line Graphs: Time for a New Data Presentation Paradigm. PLOS Biology 13(4): e1002128.

Bar charts  
(with error  
bars)  
**not good for  
showing  
distributions**

Use bar charts  
**only to show  
class counts.**

# Bar charts with error bars

What is wrong with {bar charts + error bars} ?



**Fig 3. Bar graphs and scatterplots convey very different information.** While scatterplots prompt the reader to critically evaluate the statistical tests and the authors' interpretation of the data, bar graphs discourage the reader from thinking about these issues. Placental endothelin 1 (*EDN1*) mRNA data for four different groups of participants is presented in bar graphs showing mean  $\pm$  SE (Panel A), or mean  $\pm$  SD (Panel B), and in a univariate scatterplot (Panel C). Panel A (mean  $\pm$  SE) suggests that the second group has higher values than the remaining groups; however, Panel B (mean  $\pm$  SD) reveals that there is considerable overlap between groups. Showing SE rather than SD magnifies the apparent visual differences between groups, and this is exacerbated by the fact that SE obscures any effect of unequal sample size. The scatterplot (Panel C) clearly shows that the sample sizes are small, group one has a much larger variance than the other groups, and there is an outlier in group three. These problems are not apparent in the bar graphs shown in Panels A and B.

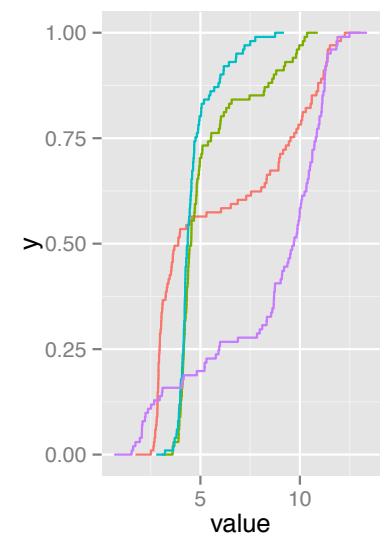
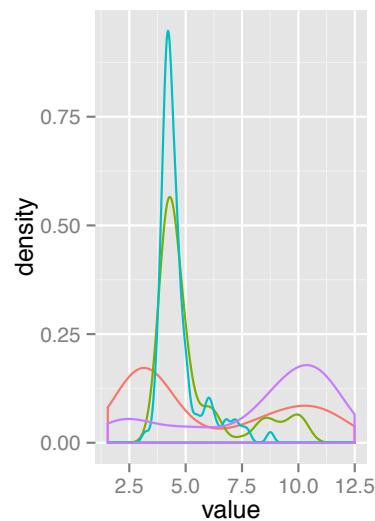
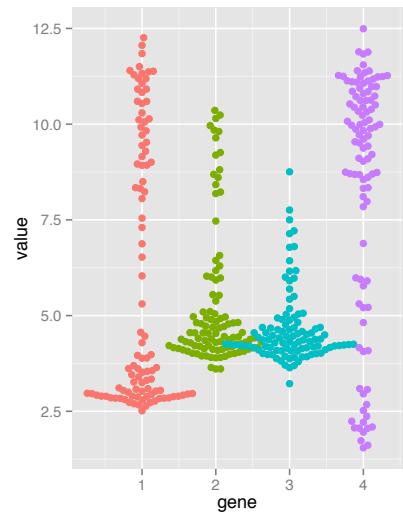
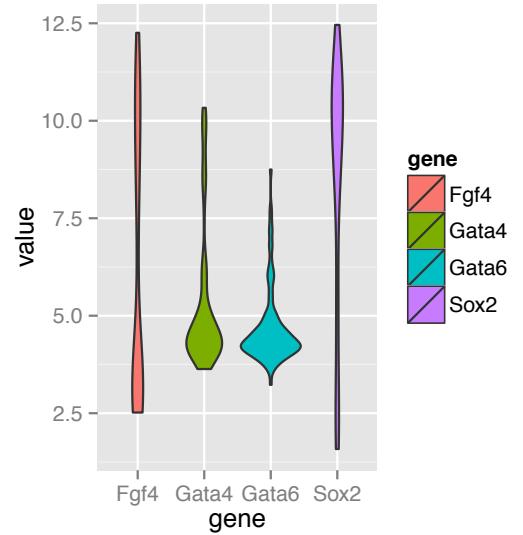
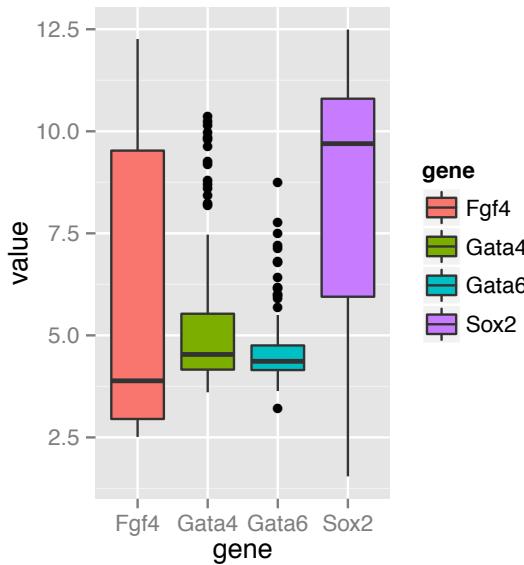
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(with error  
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class counts.**

# Summary: Visualizing distributions in 1D



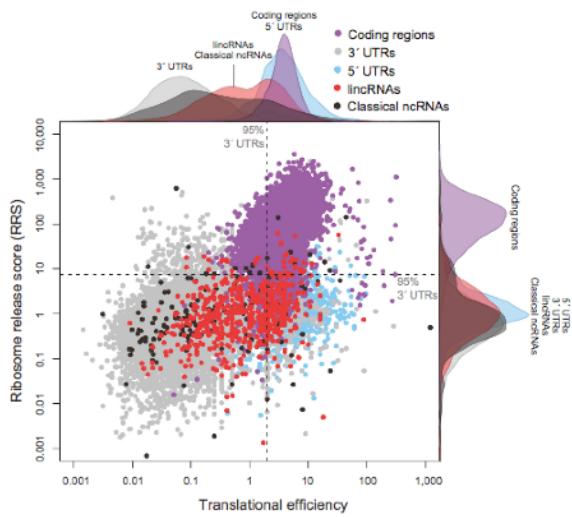
# 2D data plots

# 2D data plots

Scatterplots (x,y)-point plots

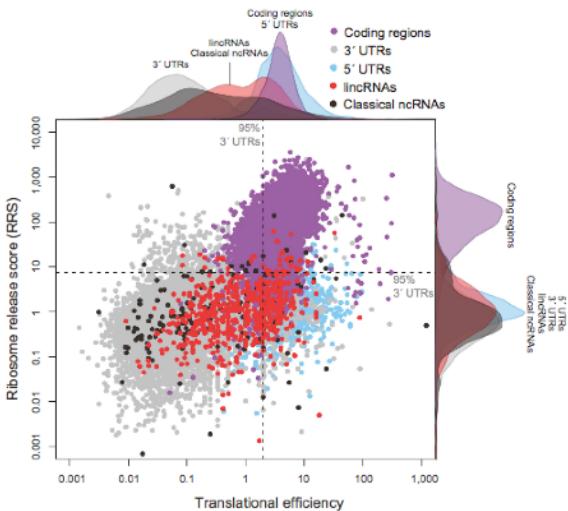
# 2D data plots

## Scatterplots (x,y)-point plots

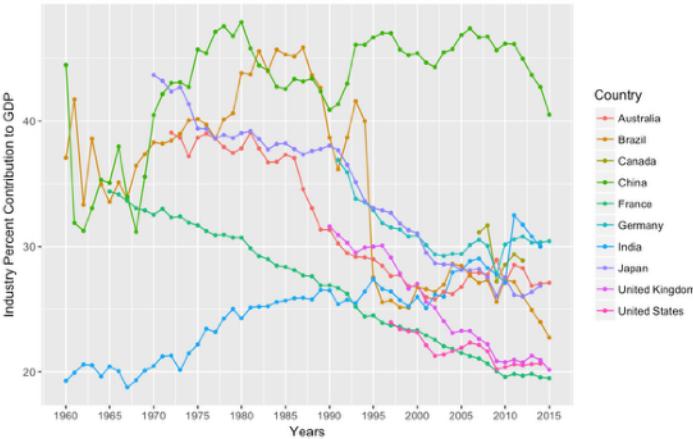


# 2D data plots

## Scatterplots (x,y)-point plots

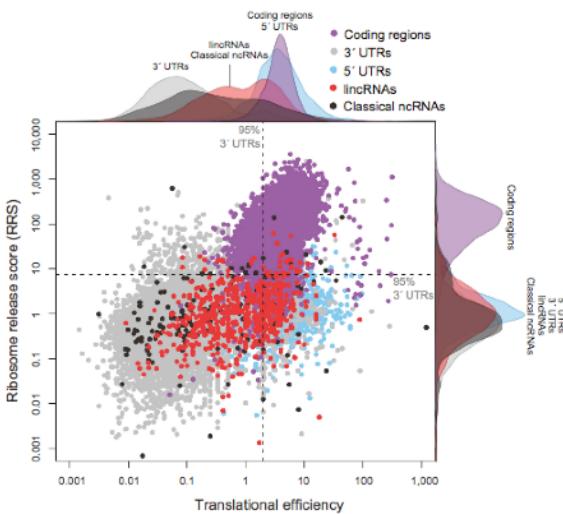


## Line plots (x,y)-line plots

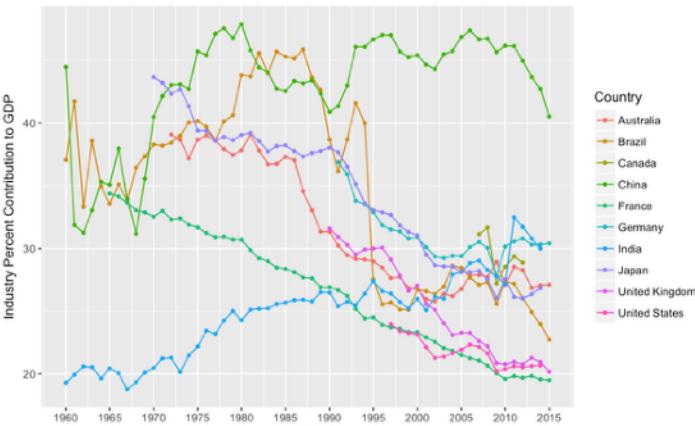


# 2D data plots

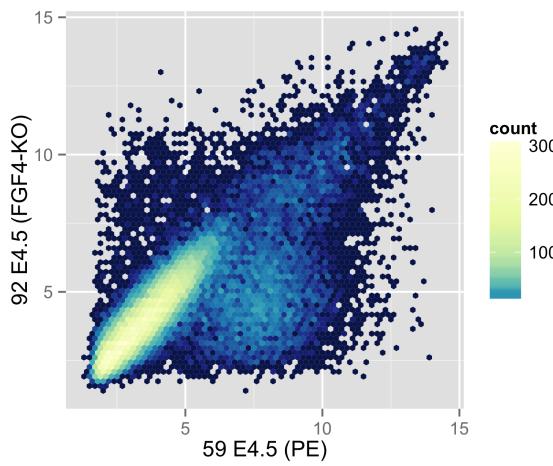
## Scatterplots (x,y)-point plots



## Line plots (x,y)-line plots

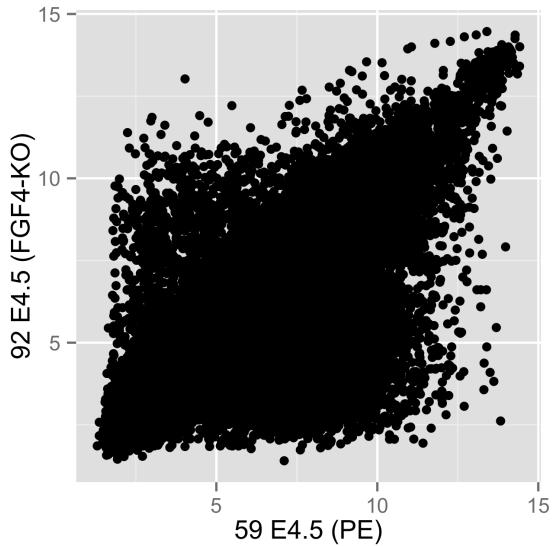


2D density requires the choice of bandwidth; obscures the sample size (i.e. the uncertainty of the estimate)



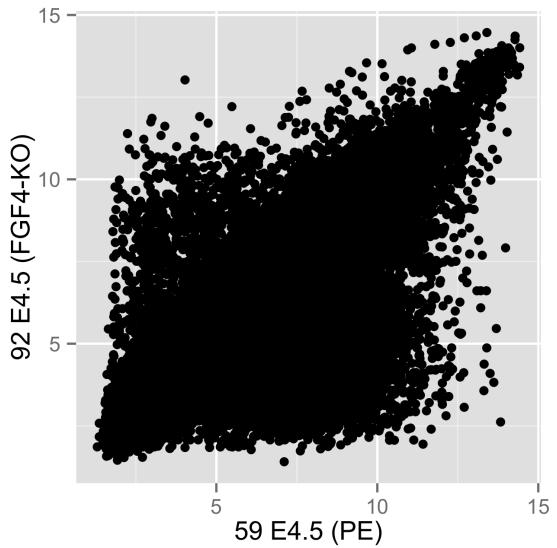
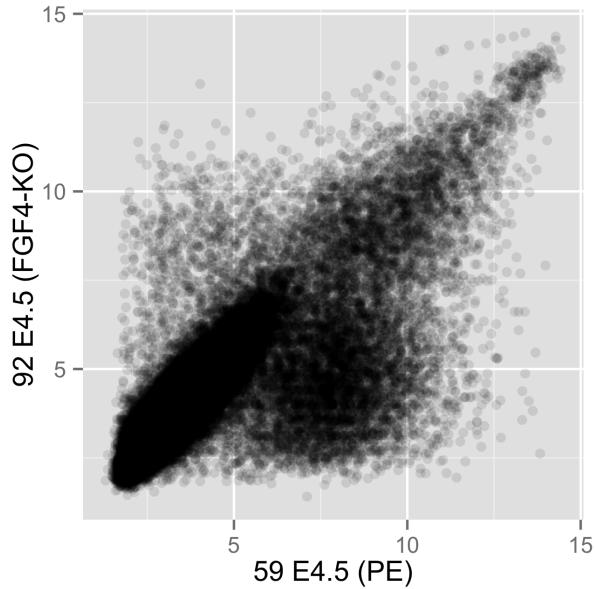
# Showing distributions in 2D

```
scp <- ggplot(dfx, aes( x = '59 E4.5 (PE)' ,  
                      y = '92 E4.5 (FGF4-KO)' ))  
scp + geom_point()
```



# Showing distributions in 2D

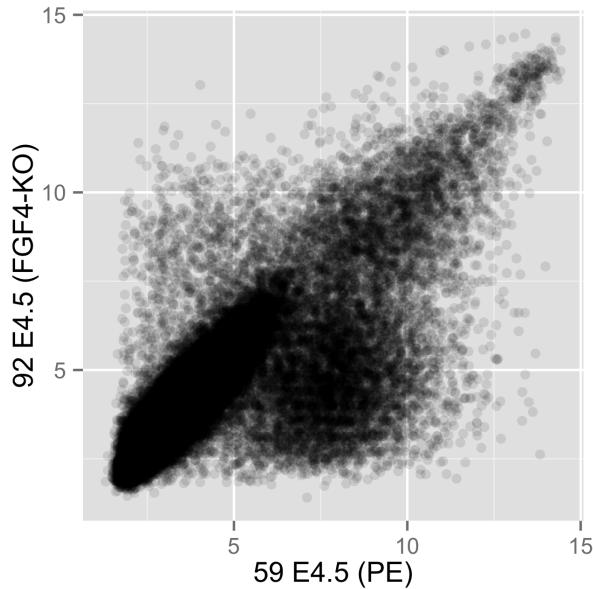
```
scp <- ggplot(dfx, aes( x = '59 E4.5 (PE)' ,  
y = '92 E4.5 (FGF4-KO)' ))  
scp + geom_point()
```



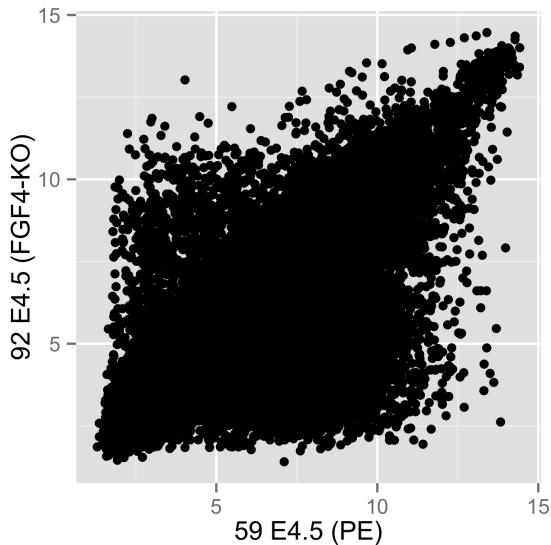
```
scp + geom_point(alpha = 0.1)
```

# Showing distributions in 2D

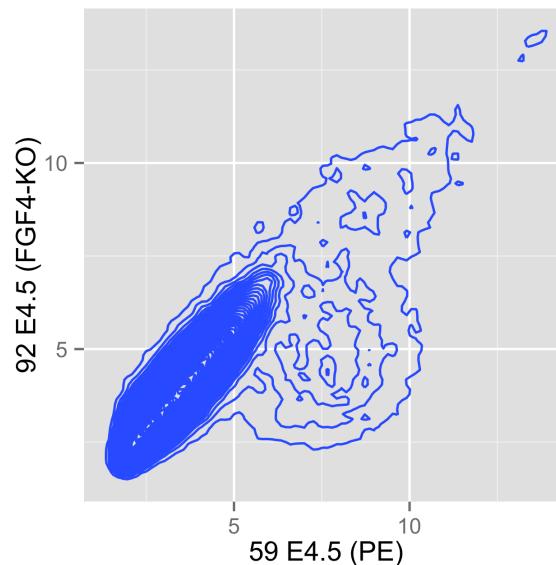
```
scp <- ggplot(dfx, aes( x = '59 E4.5 (PE)' ,  
y = '92 E4.5 (FGF4-KO)' ))  
scp + geom_point()
```



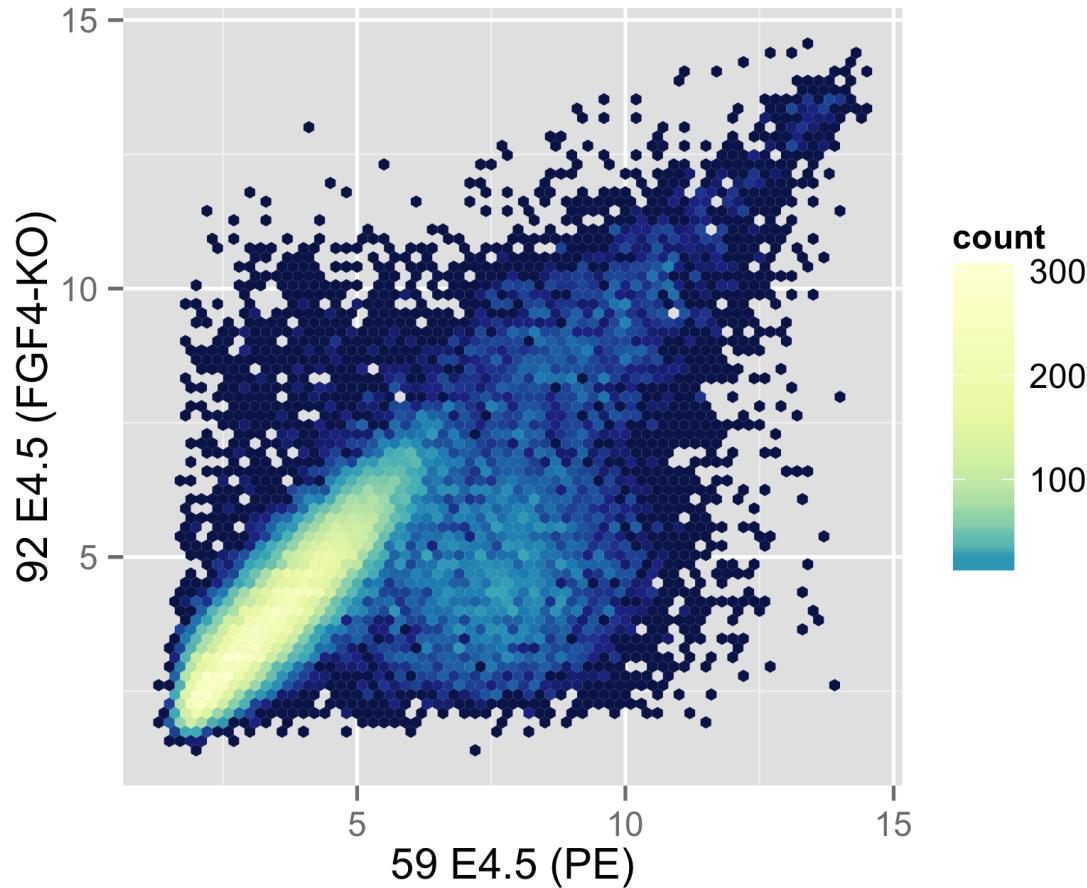
```
scp + geom_point(alpha = 0.1)
```



```
scp + geom_density2d(h = 0.5, bins = 60)
```



**binhex** is a good, easy to read, option to show 2D density



```
scp + stat_binhex(binwidth = c(0.2, 0.2)) + colourscale +  
coord_fixed()
```

# How to show more than 2D?

## How to show more than 2D?

What tricks do you use for >2D?

# 3-5D: aesthetics allow to show more than 2D

## geom\_point's

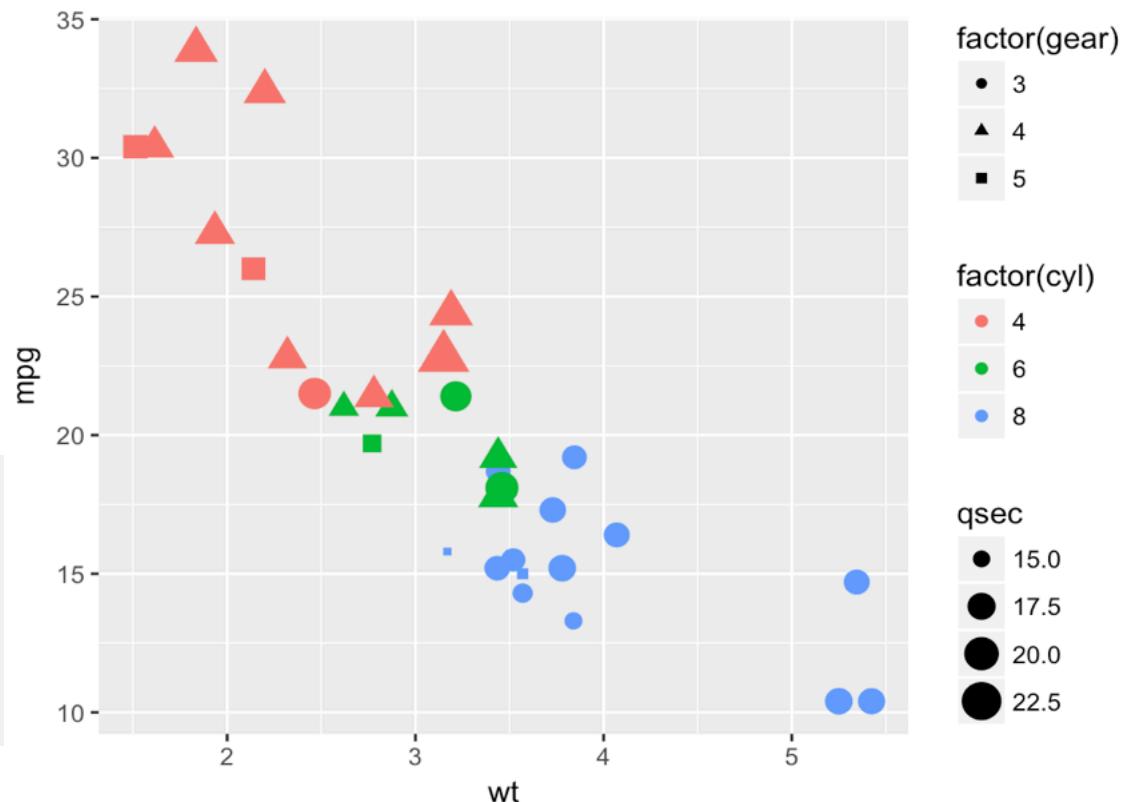
### aesthetics

(apart from x and y):

- fill / color
- shape
- size
- alpha

```
ggplot(data = mtcars) +  
  geom_point(  
    aes(x = wt, y = mpg,  
        shape = factor(gear),  
        color = factor(cyl),  
        size = qsec))
```

```
head(mtcars)  
##          mpg cyl disp  hp drat    wt  qsec vs am gear carb  
## Mazda RX4   21.0   6 160 110 3.90 2.620 16.46  0  1    4    4  
## Mazda RX4 Wag 21.0   6 160 110 3.90 2.875 17.02  0  1    4    4  
## Datsun 710  22.8   4 108  93 3.85 2.320 18.61  1  1    4    1  
## Hornet 4 Drive 21.4   6 258 110 3.08 3.215 19.44  1  0    3    1  
## Hornet Sportabout 18.7   8 360 175 3.15 3.440 17.02  0  0    3    2  
## Valiant   18.1   6 225 105 2.76 3.460 20.22  1  0    3    1
```



# 3-5D: aesthetics allow to show more than 2D

## geom\_point's

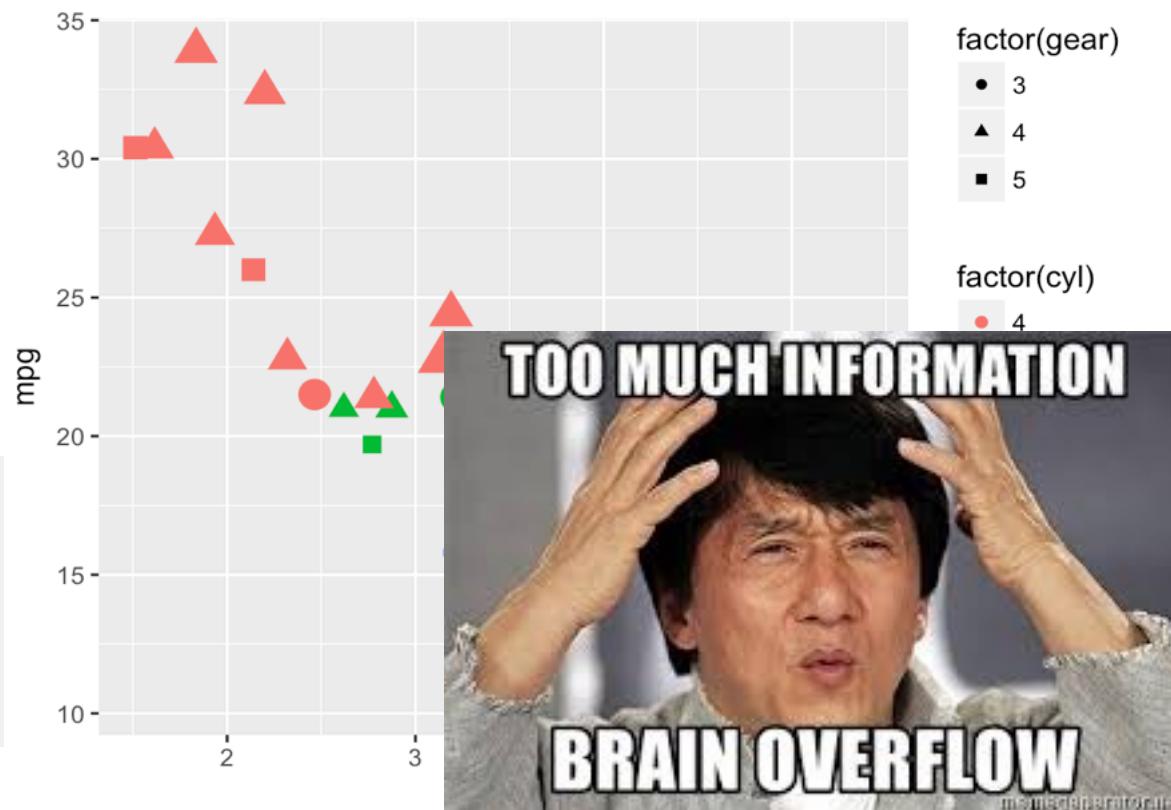
### aesthetics

(apart from x and y):

- fill / color
- shape
- size
- alpha

```
ggplot(data = mtcars) +  
  geom_point(  
    aes(x = wt, y = mpg,  
        shape = factor(gear),  
        color = factor(cyl),  
        size = qsec))
```

```
head(mtcars)  
##          mpg cyl disp  hp drat    wt  qsec vs am gear carb  
## Mazda RX4   21.0   6 160 110 3.90 2.620 16.46  0  1    4    4  
## Mazda RX4 Wag 21.0   6 160 110 3.90 2.875 17.02  0  1    4    4  
## Datsun 710   22.8   4 108  93 3.85 2.320 18.61  1  1    4    1  
## Hornet 4 Drive 21.4   6 258 110 3.08 3.215 19.44  1  0    3    1  
## Hornet Sportabout 18.7   8 360 175 3.15 3.440 17.02  0  0    3    2  
## Valiant     18.1   6 225 105 2.76 3.460 20.22  1  0    3    1
```



# 3-5D: aesthetics allow to show more than 2D

## geom\_point's

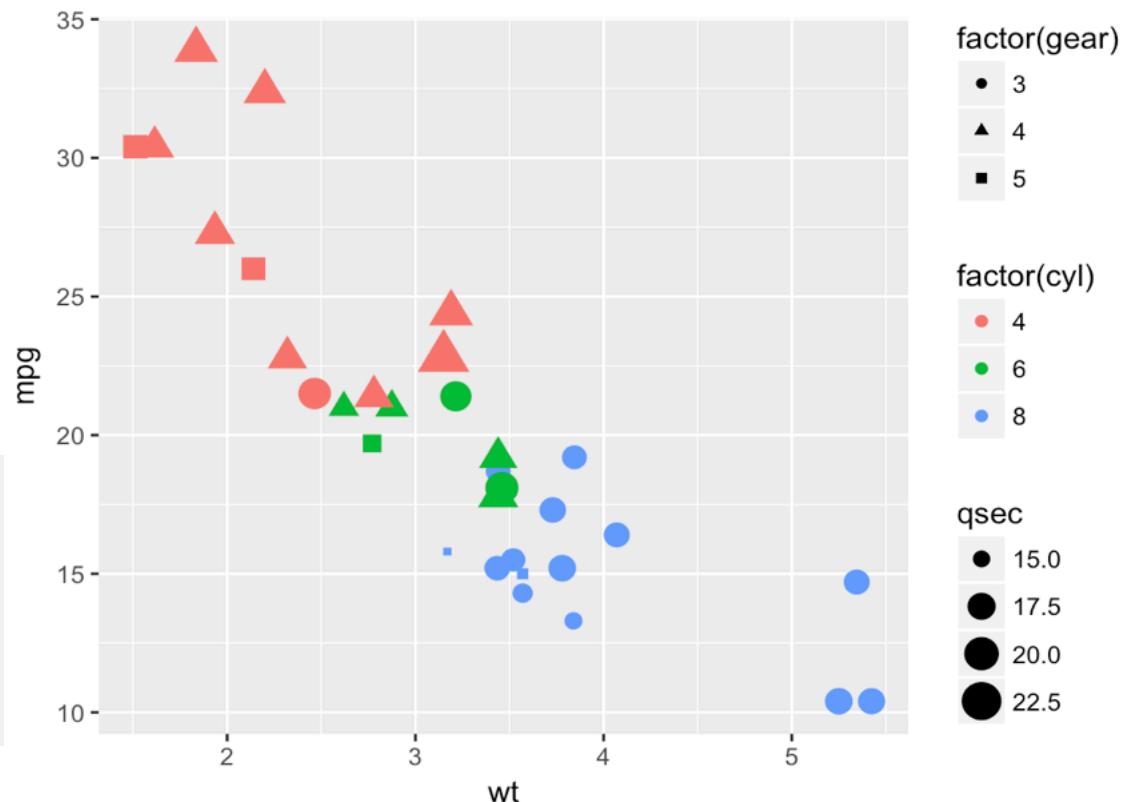
### aesthetics

(apart from x and y):

- fill / color
- shape
- size
- alpha

```
ggplot(data = mtcars) +  
  geom_point(  
    aes(x = wt, y = mpg,  
        shape = factor(gear),  
        color = factor(cyl),  
        size = qsec))
```

```
head(mtcars)  
##          mpg cyl disp  hp drat    wt  qsec vs am gear carb  
## Mazda RX4   21.0   6 160 110 3.90 2.620 16.46  0  1    4    4  
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## Datsun 710  22.8   4 108  93 3.85 2.320 18.61  1  1    4    1  
## Hornet 4 Drive 21.4   6 258 110 3.08 3.215 19.44  1  0    3    1  
## Hornet Sportabout 18.7   8 360 175 3.15 3.440 17.02  0  0    3    2  
## Valiant   18.1   6 225 105 2.76 3.460 20.22  1  0    3    1
```



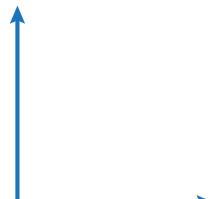
A diversity of **graphical properties (aesthetics)** are available to show dimensions

# A diversity of graphical properties (aesthetics) are available to show dimensions

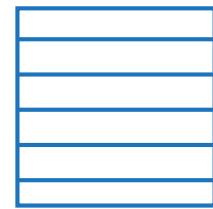
Spatial substrate

Graphical marks

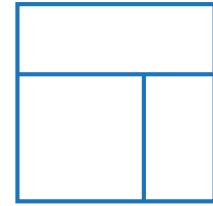
Graphical properties



Quantitative



Ordinal (ordered)



Nominal (areas)



Unstructured

Points



Size



Scale



Length



Width

Lines



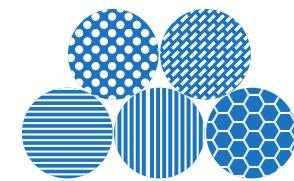
Color



Hue

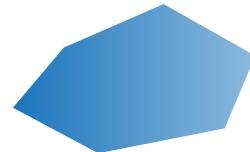


Intensity



Texture

Areas



Shape

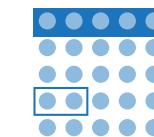


Orientation

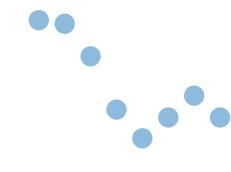
Volumes



Connection



Enclosure



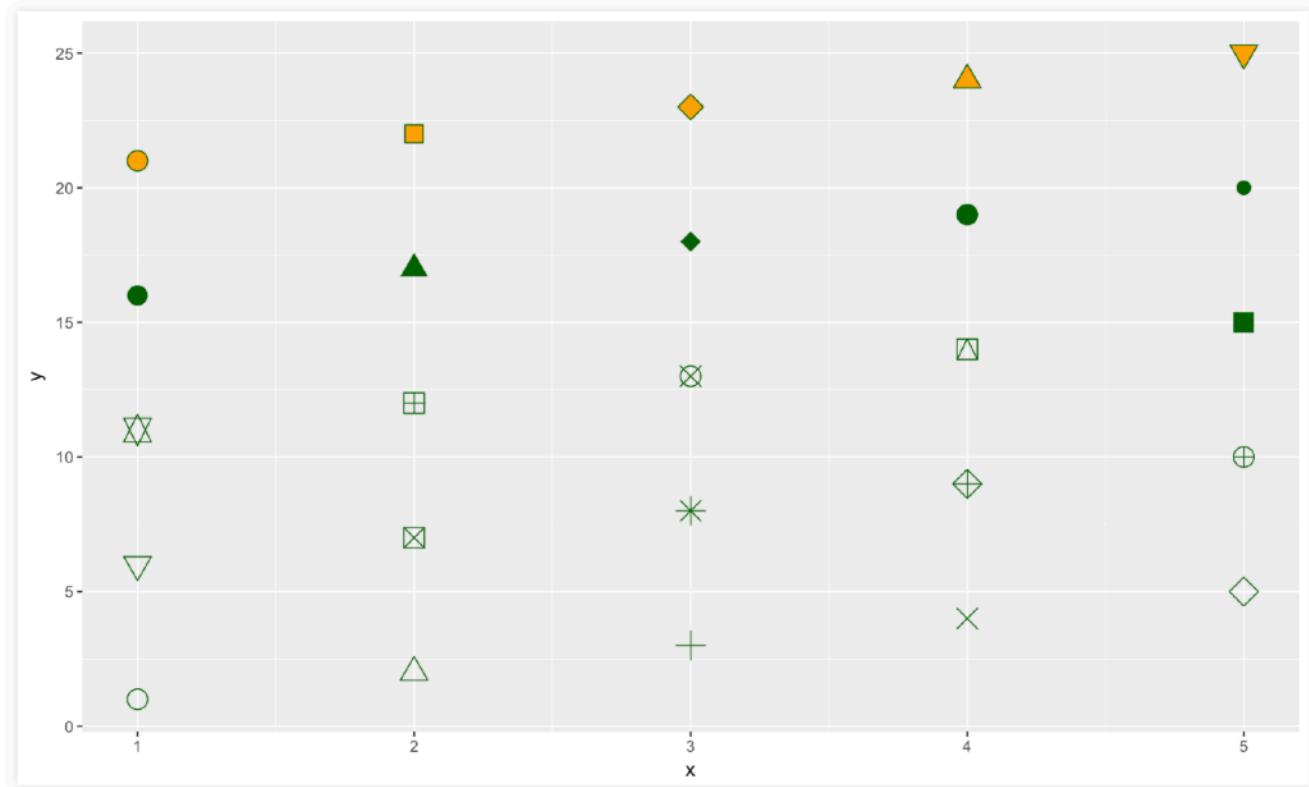
Position

# Marker shapes and colors in R

## **geom\_point's**

aesthetics  
(beyond x and y):

- **fill / color**
- **shape**
- size
- alpha

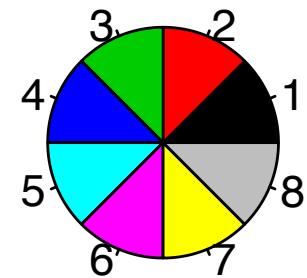


```
ggplot(data.frame(x = 1:5, y = 1:25, z = 1:25), aes(x = x, y = y)) +  
  geom_point(aes(shape = z), size = 5, colour = "darkgreen", fill = "orange") +  
  scale_shape_identity()
```

# Color Usage

Default color scheme in base R plot:

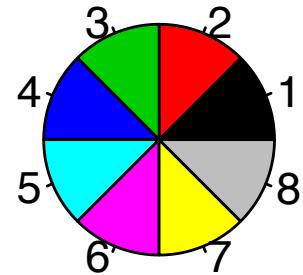
```
pie(rep(1, 8), col=1:8)
```



# Color Usage

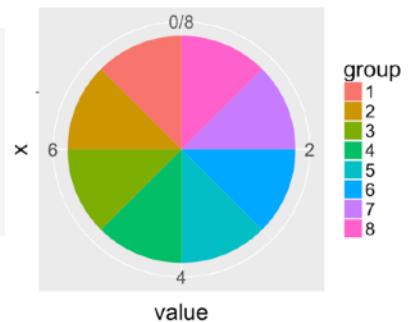
Default color scheme in base R plot:

```
pie(rep(1, 8), col=1:8)
```



Default color scheme in ggplot:

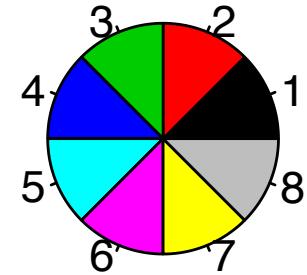
```
ggplot(data.frame(group = factor(seq_len(8)), value = rep(1, 8)),
       aes(x="", y=value, fill=group)) +
  geom_bar(width = 1, stat = "identity") +
  coord_polar("y", start=0) +
  theme(text = element_text(size = 20))
```



# Color Usage

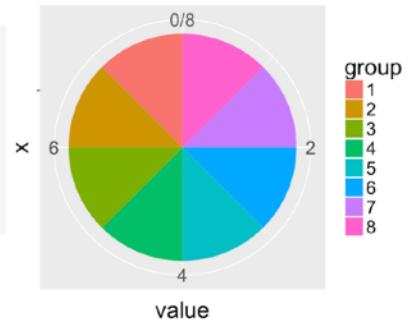
Default color scheme in base R plot:

```
pie(rep(1, 8), col=1:8)
```



Default color scheme in ggplot:

```
ggplot(data.frame(group = factor(seq_len(8)), value = rep(1, 8)),
       aes(x="", y=value, fill=group)) +
  geom_bar(width = 1, stat = "identity") +
  coord_polar("y", start=0) +
  theme(text = element_text(size = 20))
```



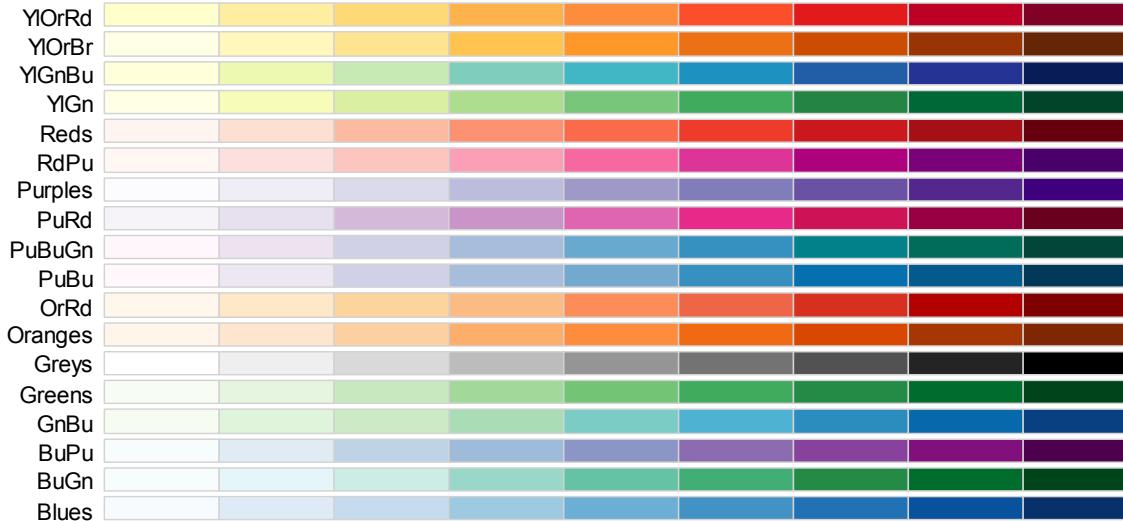
When choosing a coloring scheme, consider these:

- Different requirements for line & area colors
- Many people are **red-green color-blind**
- Lighter colors tend to make areas look larger than darker colors  
→ **use colors of equal luminance for filled areas.**

# RColorBrewer

```
display.brewer.all()
```

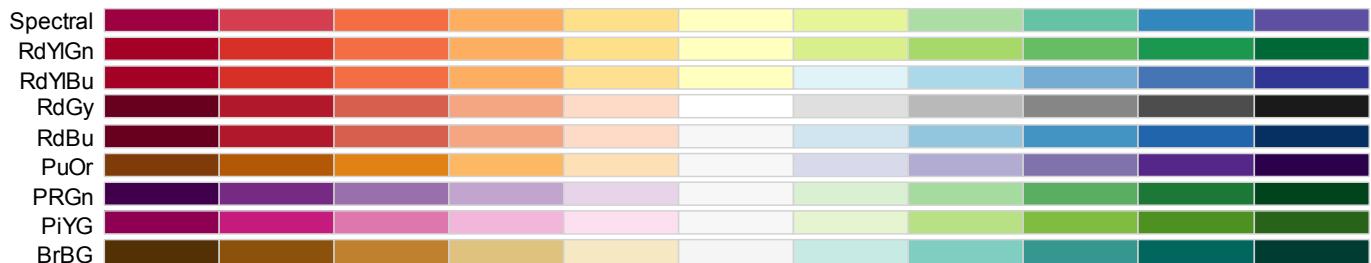
**sequential**



**qualitative**



**diverging**



# Viridis Palettes

```
install.packages("viridis")
library(viridis)
```

Simply add: `scale_color_viridis()`  
`scale_fill_viridis()`.

to your plot



# Viridis Palettes

Color scales are designed to be:

- **Colorful and Pretty**, spanning as wide a palette as possible so as to make differences easy to see,
- **Perceptually uniform**, the perceived difference between two colors is proportional to the Euclidian distance within the color space
- **Robust to colorblindness**, looks good in grey scale and to people with common forms of colorblindness

You can hear more about the science behind creating these color scales, on Walt and Smith's [talk at SciPy 2015](#).

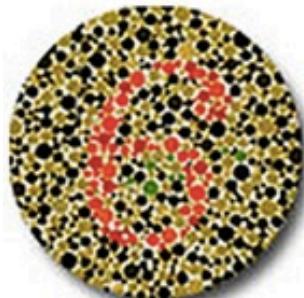


not perceptually uniform

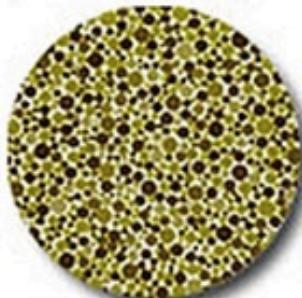


perceptually uniform

# Be kind to colorblind people



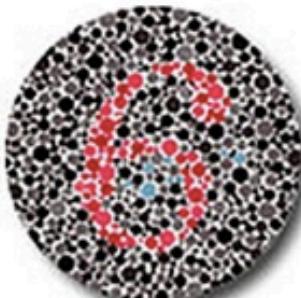
Normal  
Vision



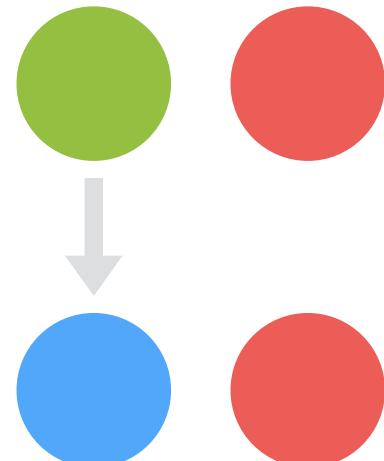
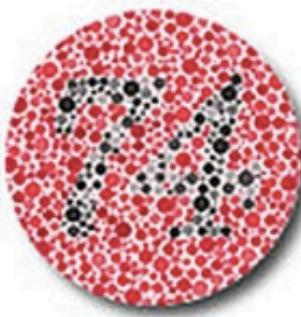
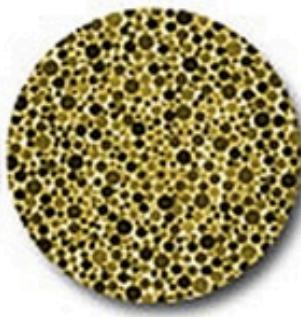
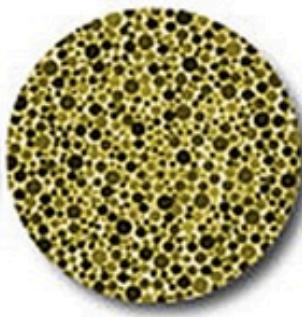
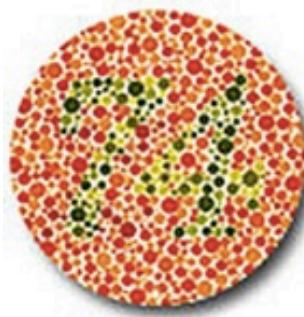
Protanope  
Vision



Deuteranope  
Vision



Tritanope  
Vision



Simple solution: replace greens by blues.

Blues also display better on most monitors than greens.

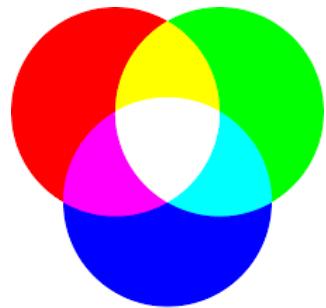
# Color models

# Color models

How are colors defined?

# Color models

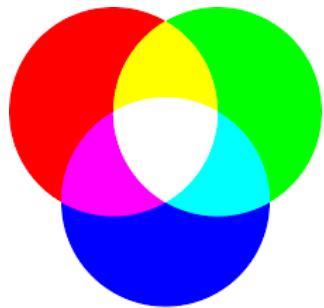
How are colors defined?



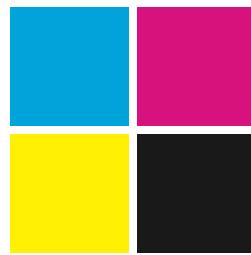
**RGB**

# Color models

How are colors defined?



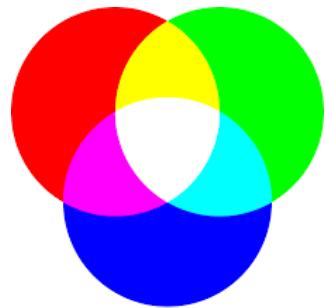
**RGB**



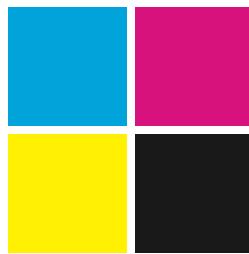
**CMYK**

# Color models

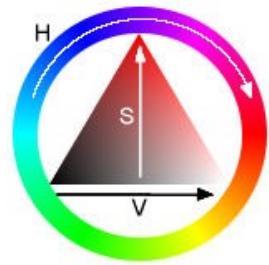
How are colors defined?



**RGB**



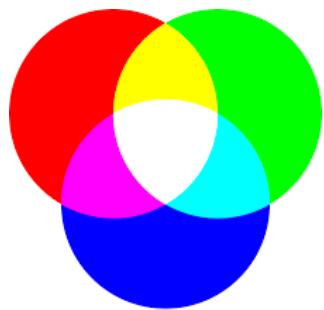
**CMYK**



**HSV**  
**HSB**

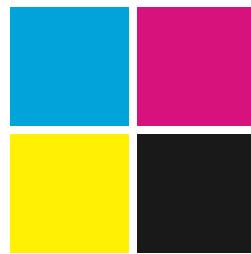
# Color models

How are colors defined?



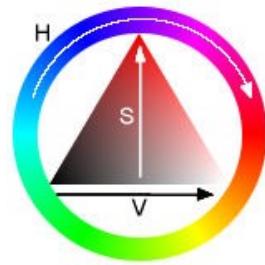
**RGB**

light



**CMYK**

ink



**HSV**  
**HSB**

human perception

**Faceting** is useful to show more dimensions without overcrowding the graph

# Faceting is useful to show more dimensions without overcrowding the graph

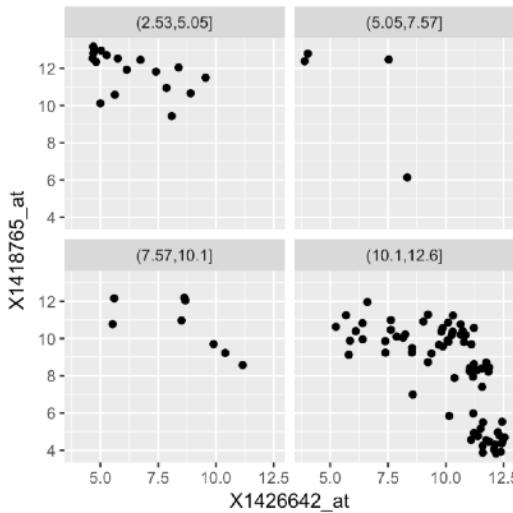


Figure 3.33: Faceting: the same data as in Figure 3.9, split by the continuous variable X1450989\_at and arranged by facet\_wrap.

**Trellis** — chart that uses multiple instances of the same chart

facet\_wrap

```
ggplot(mutate(dftx, Tdgf1 = cut(X1450989_at, breaks = 4)),  
       aes( x = X1426642_at, y = X1418765_at)) + geom_point() +  
       facet_wrap( ~ Tdgf1, ncol = 2 )
```

# Faceting is useful to show more dimensions without overcrowding the graph

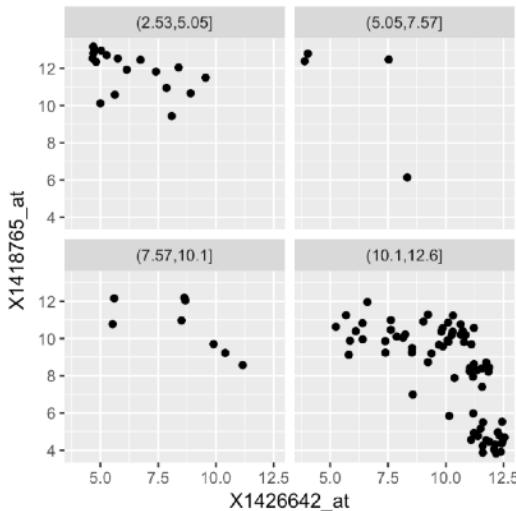


Figure 3.33: Faceting: the same data as in Figure 3.9, split by the continuous variable X1450989\_at and arranged by facet\_wrap.

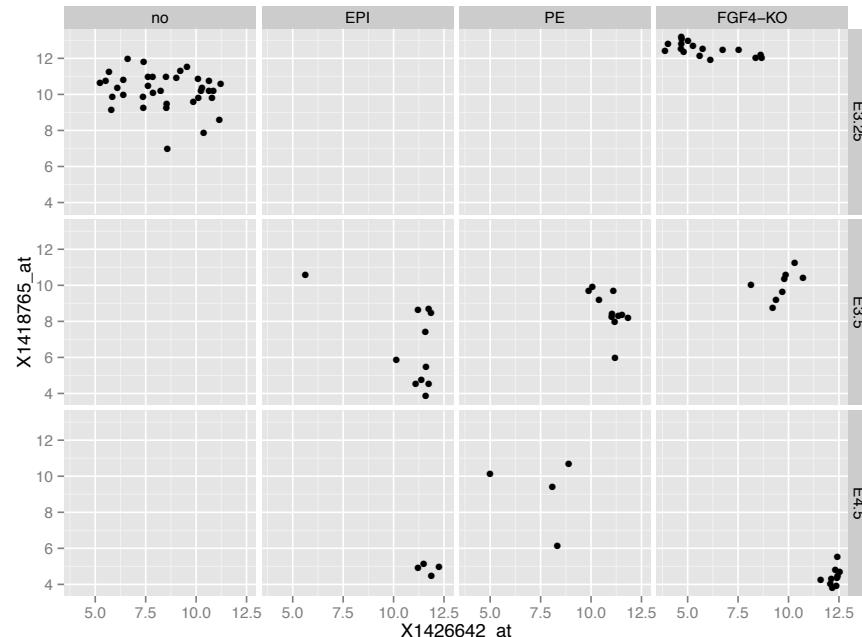
**Trellis** — chart that uses multiple instances of the same chart

facet\_wrap

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ggplot(mutate(dftx, Tdgf1 = cut(X1450989_at, breaks = 4)),  
       aes( x = X1426642_at, y = X1418765_at)) + geom_point() +  
       facet_wrap( ~ Tdgf1, ncol = 2 )
```

facet\_grid

```
ggplot( dftx,  
       aes( x = X1426642_at, y = X1418765_at)) + geom_point() +  
       facet_grid( Embryonic.day ~ lineage )
```



# Faceting is useful to show more dimensions without overcrowding the graph

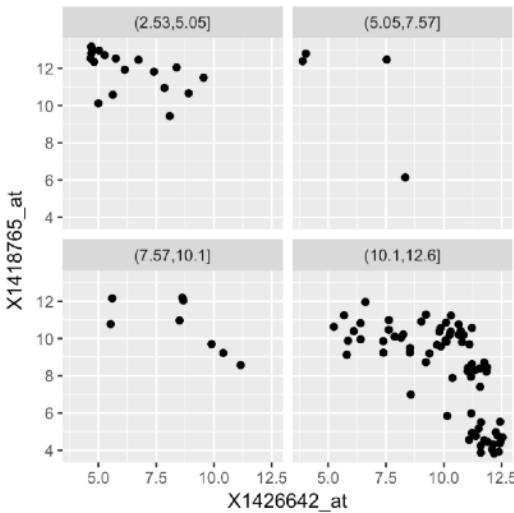


Figure 3.33: Faceting: the same data as in Figure 3.9, split by the continuous variable X1450989\_at and arranged by facet\_wrap.

**Trellis** — chart that uses multiple instances of the same chart

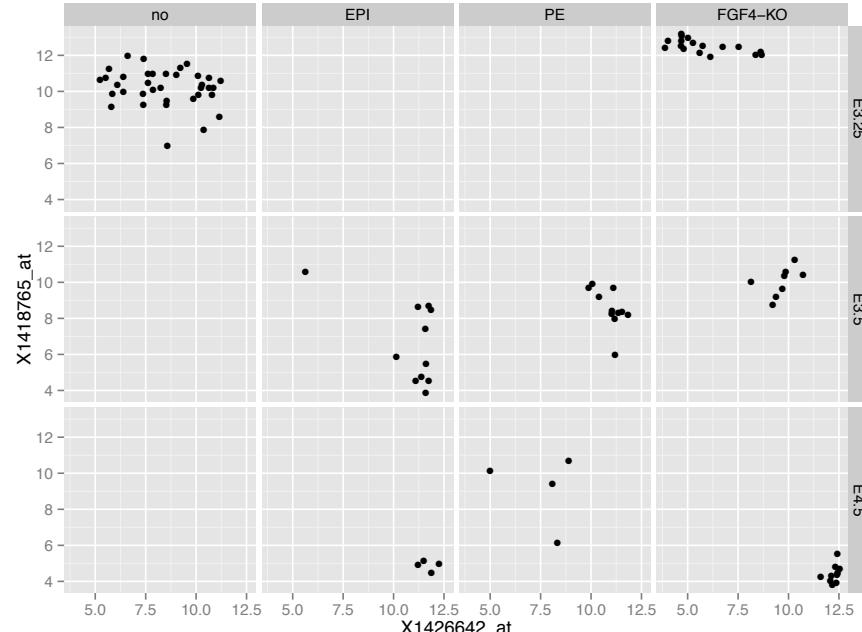
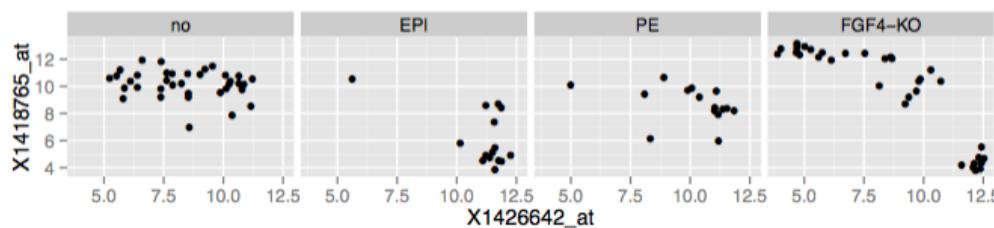
facet\_wrap

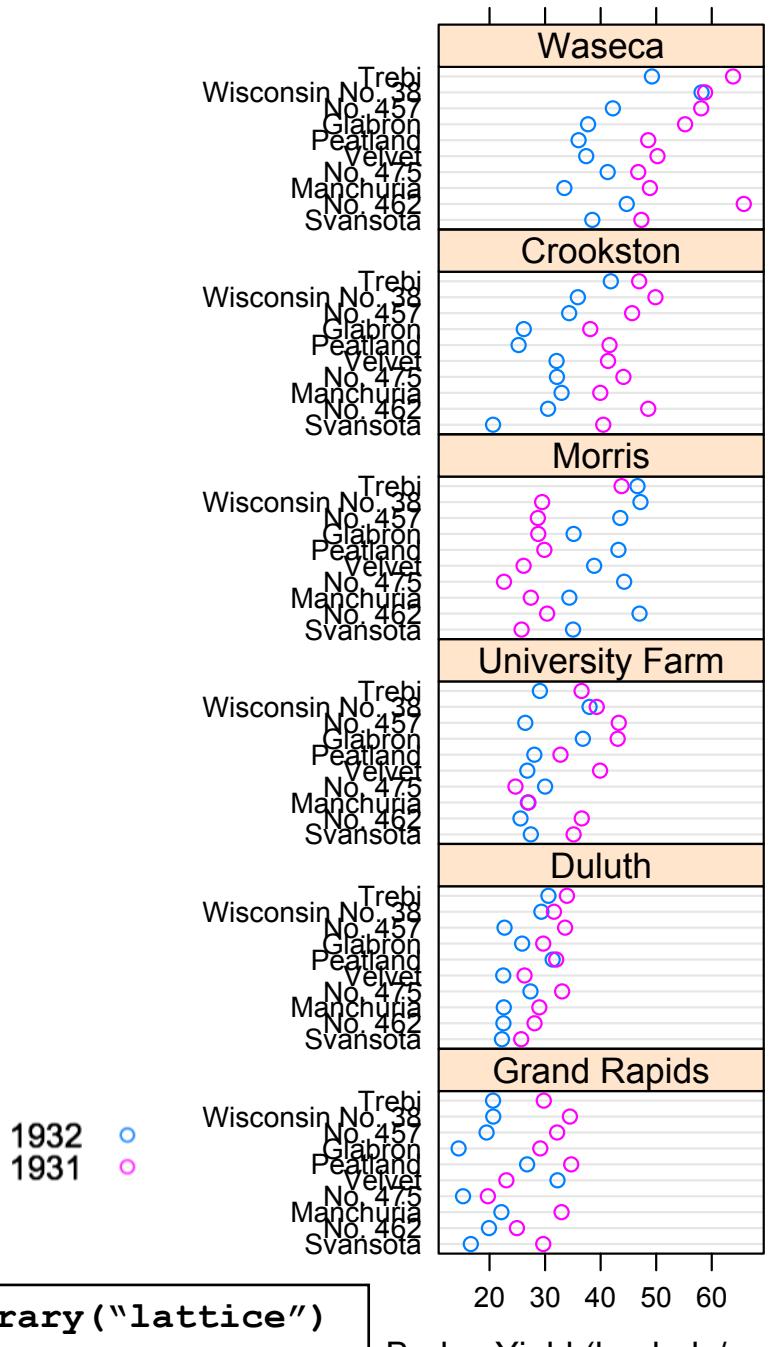
```
ggplot(mutate(dftx, Tdgf1 = cut(X1450989_at, breaks = 4)),  
       aes( x = X1426642_at, y = X1418765_at)) + geom_point() +  
       facet_wrap( ~ Tdgf1, ncol = 2 )
```

facet\_grid

```
ggplot( dftx,  
       aes( x = X1426642_at, y = X1418765_at)) + geom_point() +  
       facet_grid( Embryonic.day ~ lineage )
```

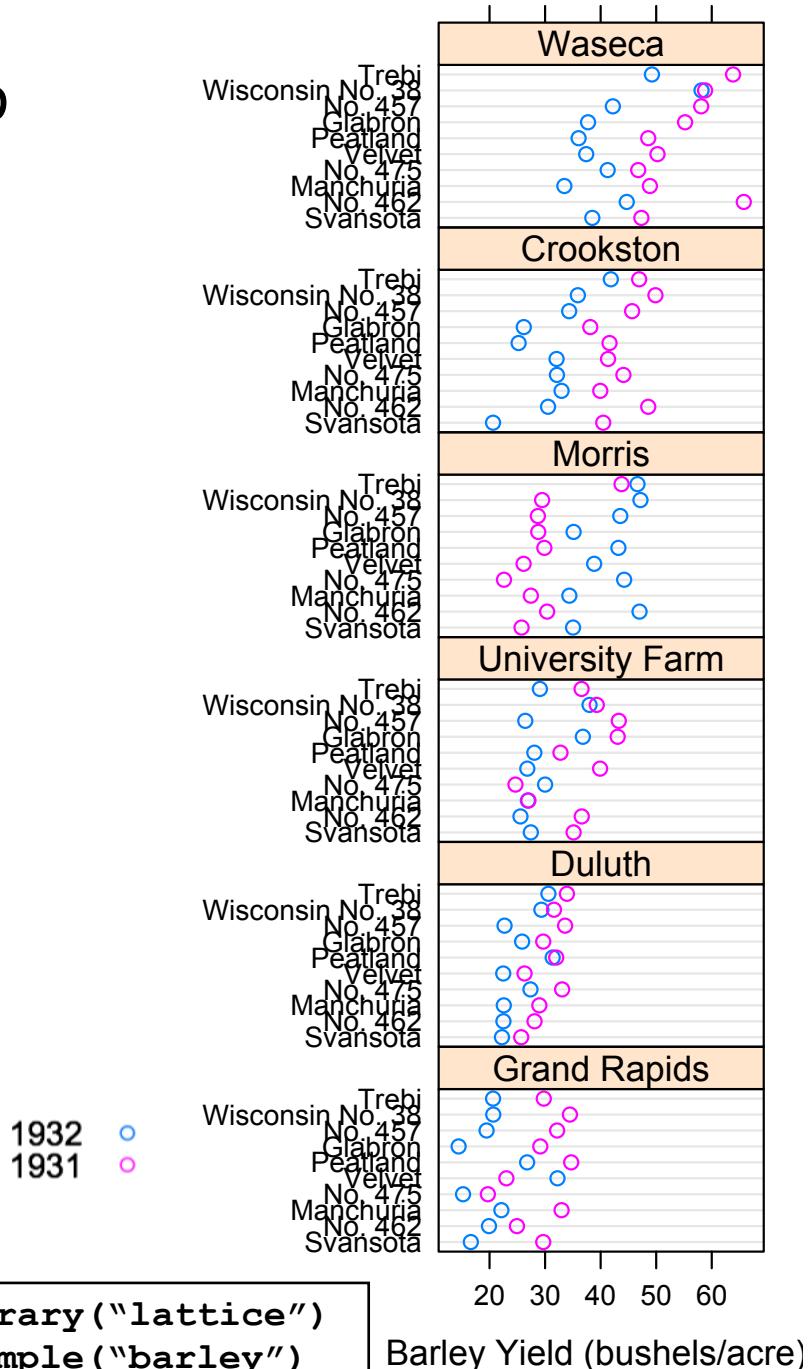
```
ggplot(dftx, aes( x = X1426642_at, y = X1418765_at)) +  
       geom_point() + facet_grid( . ~ lineage )
```





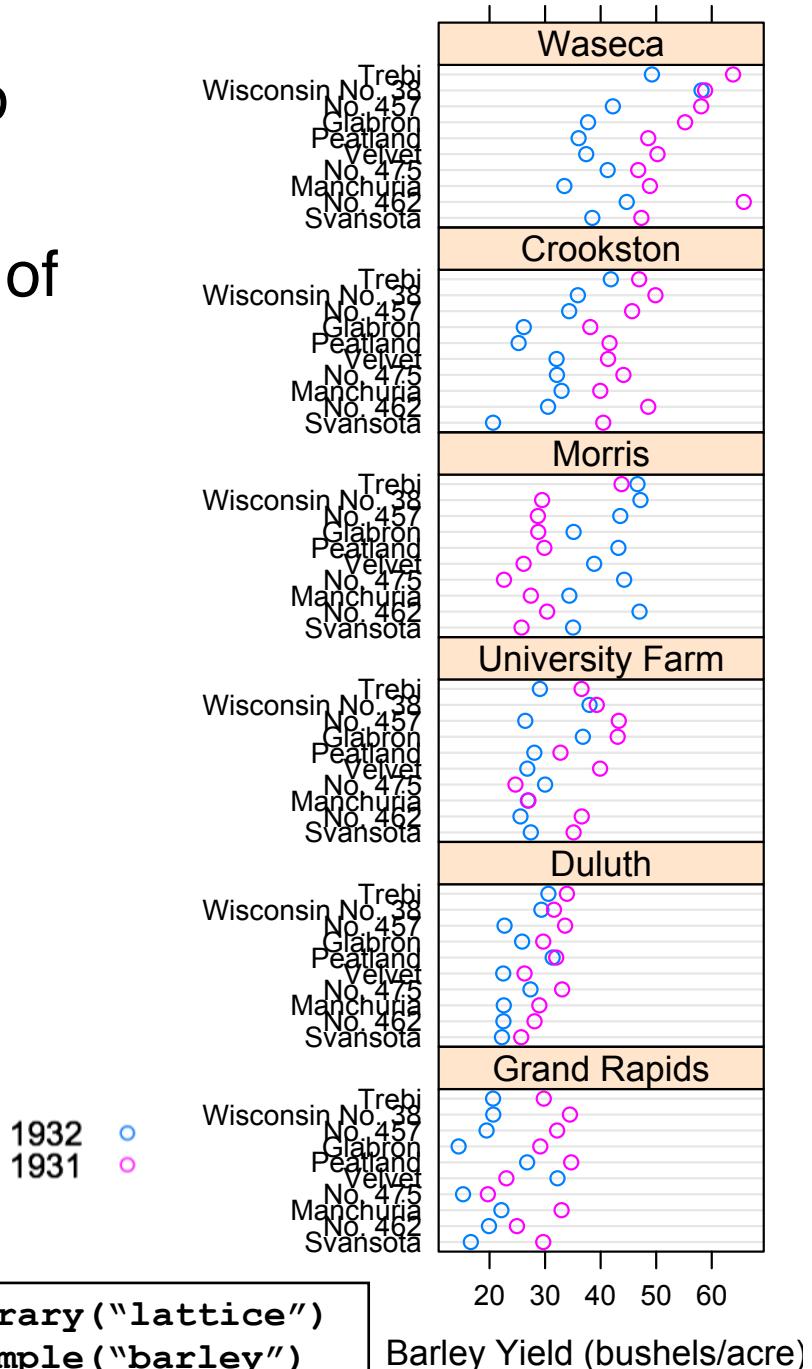
```
library("lattice")
example("barley")
```

# Data from an agricultural field trial to study the crop barley.



# Data from an agricultural field trial to study the crop barley.

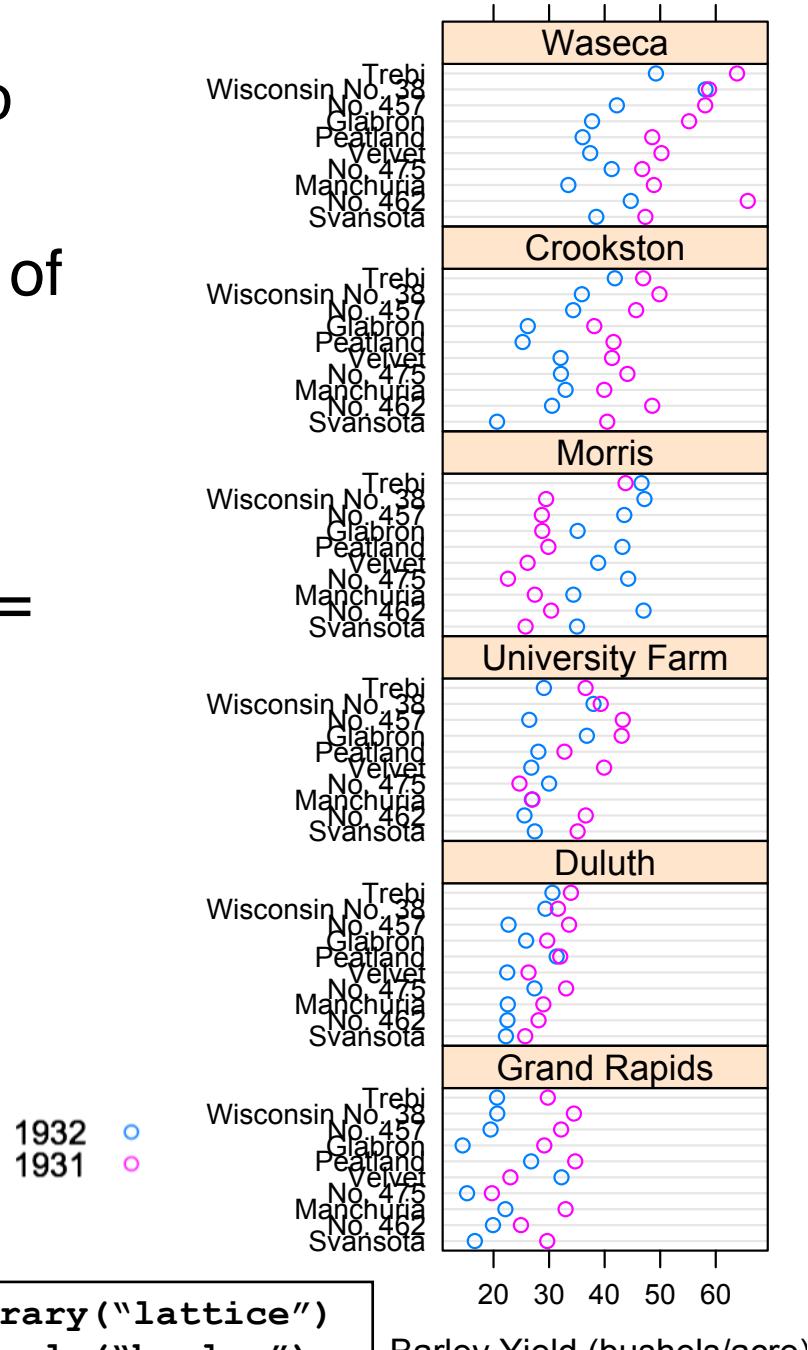
At 6 sites in Minnesota, 10 varieties of barley were grown in each of two years.



Data from an agricultural field trial to study the crop barley.

At 6 sites in Minnesota, 10 varieties of barley were grown in each of two years.

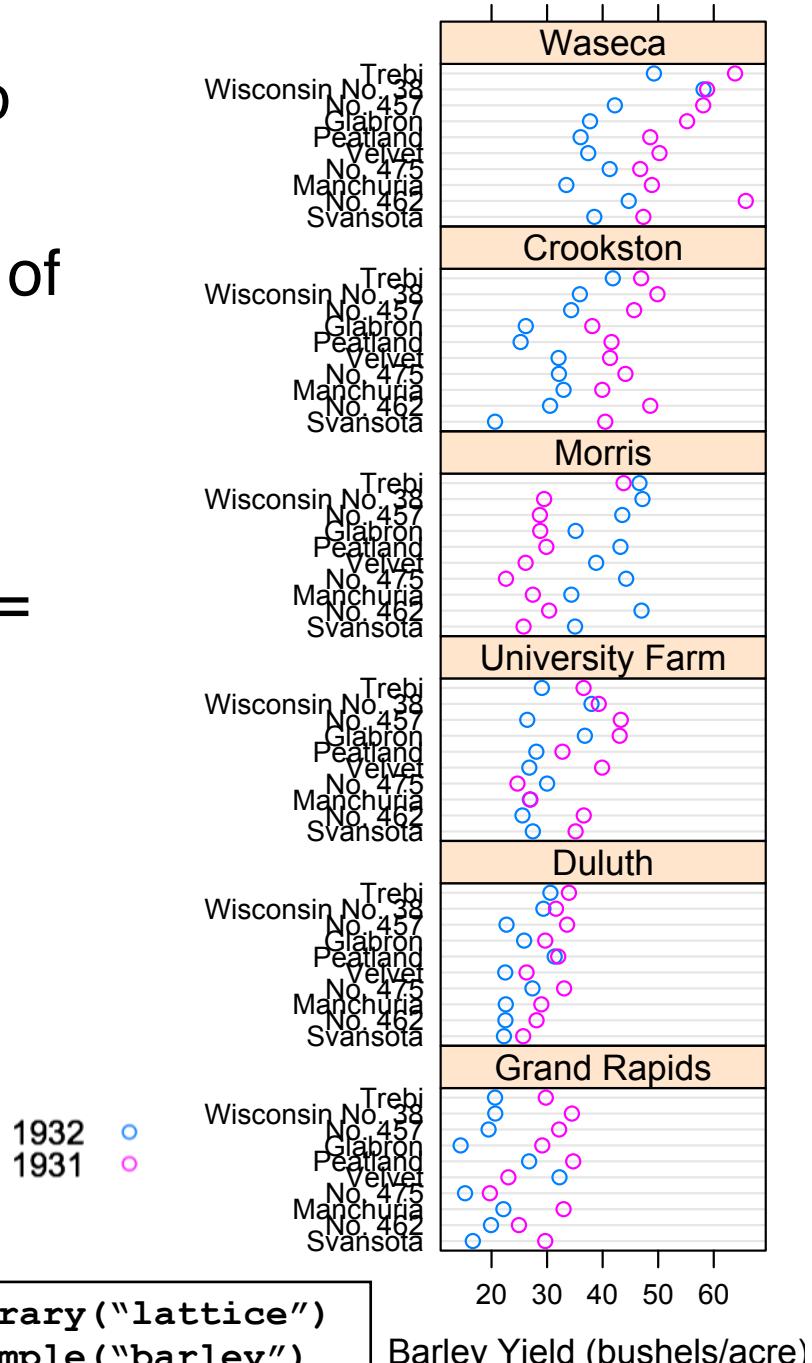
Data: yield, for all combinations of site, variety, and year ( $6 \times 10 \times 2 = 120$  observations)



Data from an agricultural field trial to study the crop barley.

At 6 sites in Minnesota, 10 varieties of barley were grown in each of two years.

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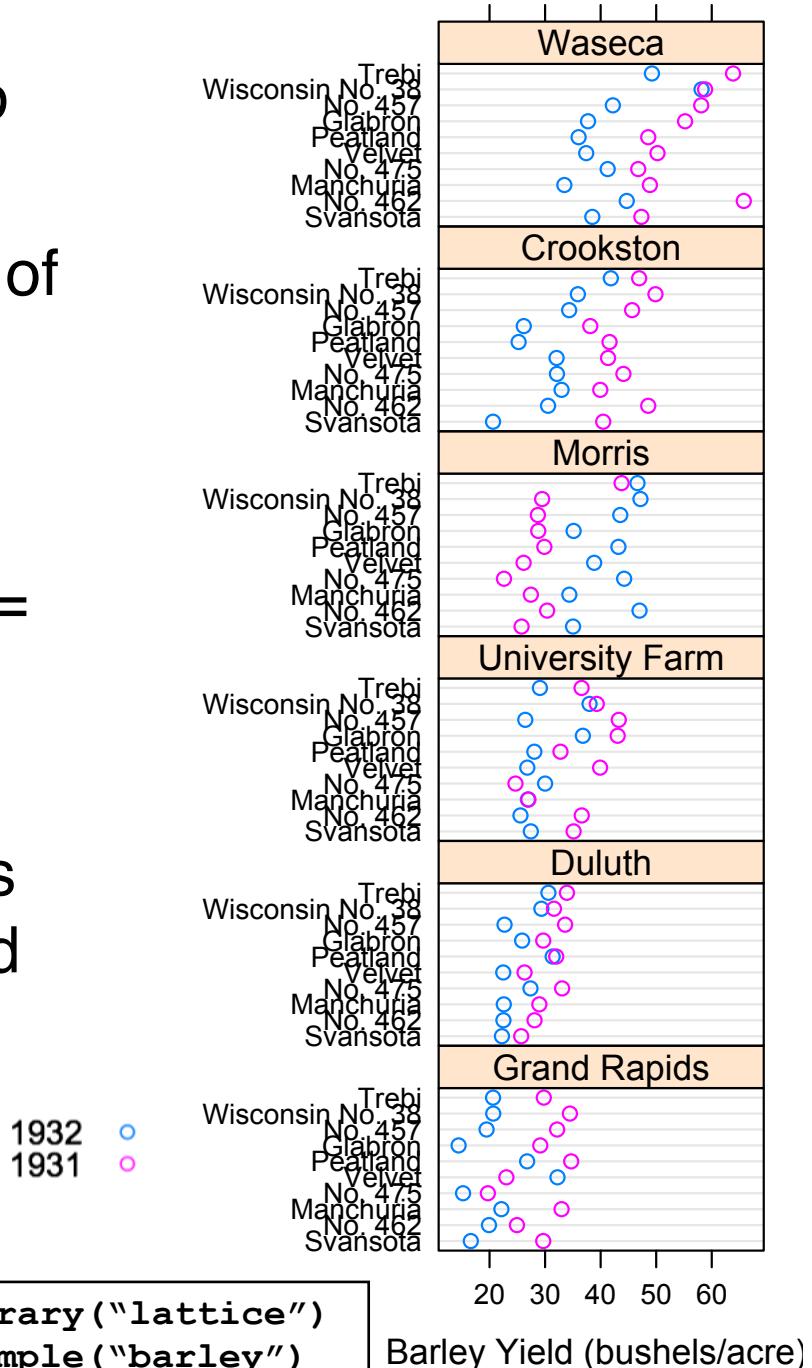


Data from an agricultural field trial to study the crop barley.

At 6 sites in Minnesota, 10 varieties of barley were grown in each of two years.

Data: yield, for all combinations of site, variety, and year ( $6 \times 10 \times 2 = 120$  observations)

Note the data for **Morris** - reanalysis in the 1990s using Trellis revealed that the years had been flipped!



Data from an agricultural field trial to study the crop barley.

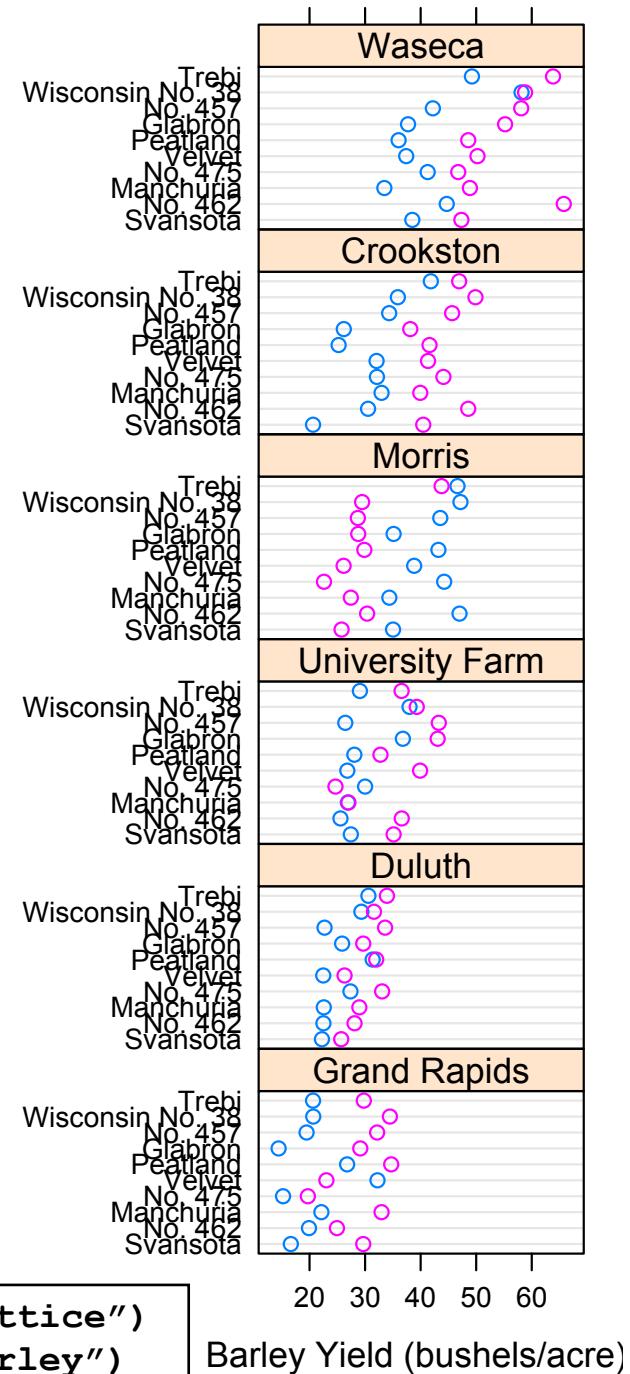
At 6 sites in Minnesota, 10 varieties of barley were grown in each of two years.

Data: yield, for all combinations of site, variety, and year ( $6 \times 10 \times 2 = 120$  observations)

Note the data for **Morris** - reanalysis in the 1990s using Trellis revealed that the years had been flipped!

1932      ○  
1931      ●

```
library("lattice")
example("barley")
```



How could you quickly check for potential batch effects?

# Tidying data to use columns as aesthetics

```
ggplot( dftx,  
  aes( x = X1426642_at, y = X1418765_at)) + geom_point() +  
  facet_grid( Embryonic.day ~ lineage )
```

# Tidying data to use columns as aesthetics

```
ggplot( dftx,  
  aes( x = X1426642_at, y = X1418765_at)) + geom_point() +  
  facet_grid( Embryonic.day ~ lineage )
```

Data.frame in R can be in:

# Tidying data to use columns as aesthetics

```
ggplot( dftx,  
        aes( x = X1426642_at, y = X1418765_at)) + geom_point() +  
        facet_grid( Embryonic.day ~ lineage )
```

Data.frame in R can be in:

## wide format

```
##          X1420085_at X1418863_at X1425463_at X1416967_at  
## 1 E3.25      3.027715    4.843137    5.500618    1.731217  
## 2 E3.25      9.293016    5.530016    6.160900    9.697038  
## 3 E3.25      2.940142    4.418059    4.584961    4.161240  
## 4 E3.25      9.715243    5.982314    4.753439    9.540123  
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e.g. a expression matrix with each raw containing  
a gene expression for all samples

# Tidying data to use columns as aesthetics

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ggplot( dftx,  
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Data.frame in R can be in:

## wide format

```
##           X1420085_at X1418863_at X1425463_at X1416967_at  
## 1 E3.25      3.027715    4.843137    5.500618    1.731217  
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## long format

```
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## 3 3 E3.25 X1420085_at 2.940142  
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```
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How do you switch :wide: <> :long: ?

# melt() from wide to long

To convert between two data formats we can use functions **melt()**, and **dcast()** from package **reshape2**

```
head(genes_expression)
```

```
##           X1420085_at X1418863_at X1425463_at X1416967_at
## 1 E3.25      3.027715    4.843137    5.500618    1.731217
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```

```
library("reshape2")
genes = melt(genes_expression, varnames = c("sample", "probe"))
head(genes)
```

```
##   sample     probe   value
## 1 1 E3.25 X1420085_at 3.027715
## 2 2 E3.25 X1420085_at 9.293016
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```

# dcast( ) from long to wide

To convert between two data formats we can use functions **melt()**, and **dcast()** from package **reshape2**

```
head(genes)
```

```
##      sample      probe      value
## 1 1 E3.25 X1420085_at 3.027715
## 2 2 E3.25 X1420085_at 9.293016
## 3 3 E3.25 X1420085_at 2.940142
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## 5 5 E3.25 X1420085_at 8.924228
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```

```
wide <- dcast(genes, formula = sample ~ probe, value.var = "value")
head(wide)
```

```
##      sample X1420085_at X1418863_at X1425463_at X1416967_at
## 1 1 E3.25    3.027715    4.843137    5.500618    1.731217
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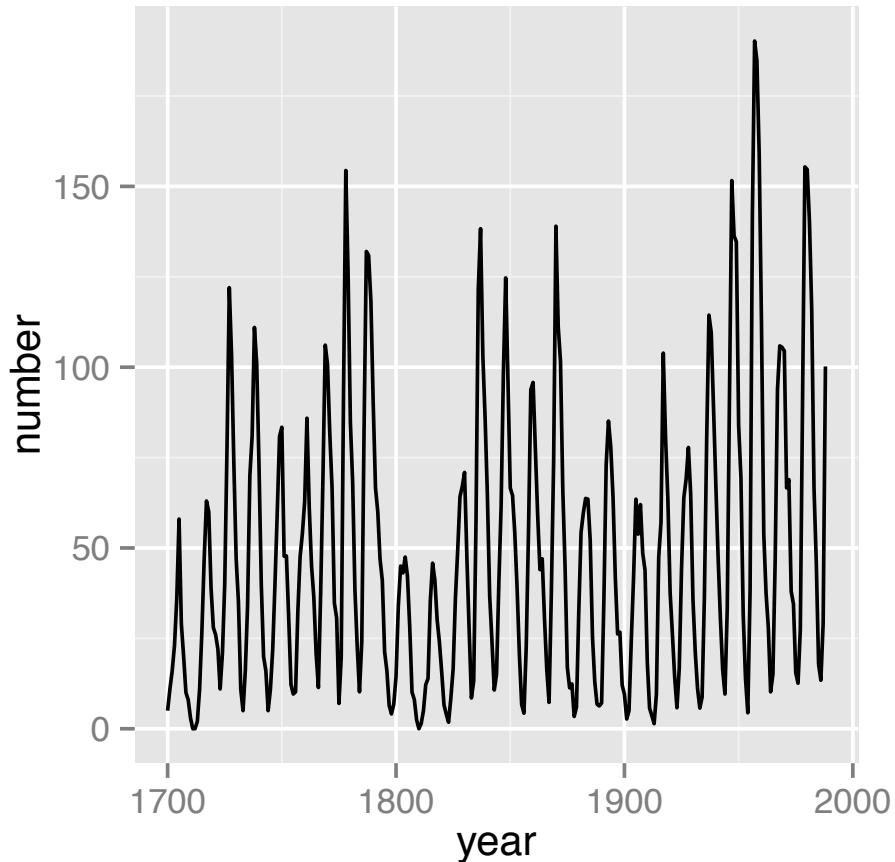
# Choose aspect ratio so that banking = 45%

Yearly sunspot numbers 1849-1924 - changes in amplitude

## Banking to 45 degrees:

Choose aspect ratio so that the median absolute slope is 1, i.e. at 45 degrees angle.

**Sawtooth:** Sunspot cycles typically rise more rapidly than they fall — steep rise and slow decline.



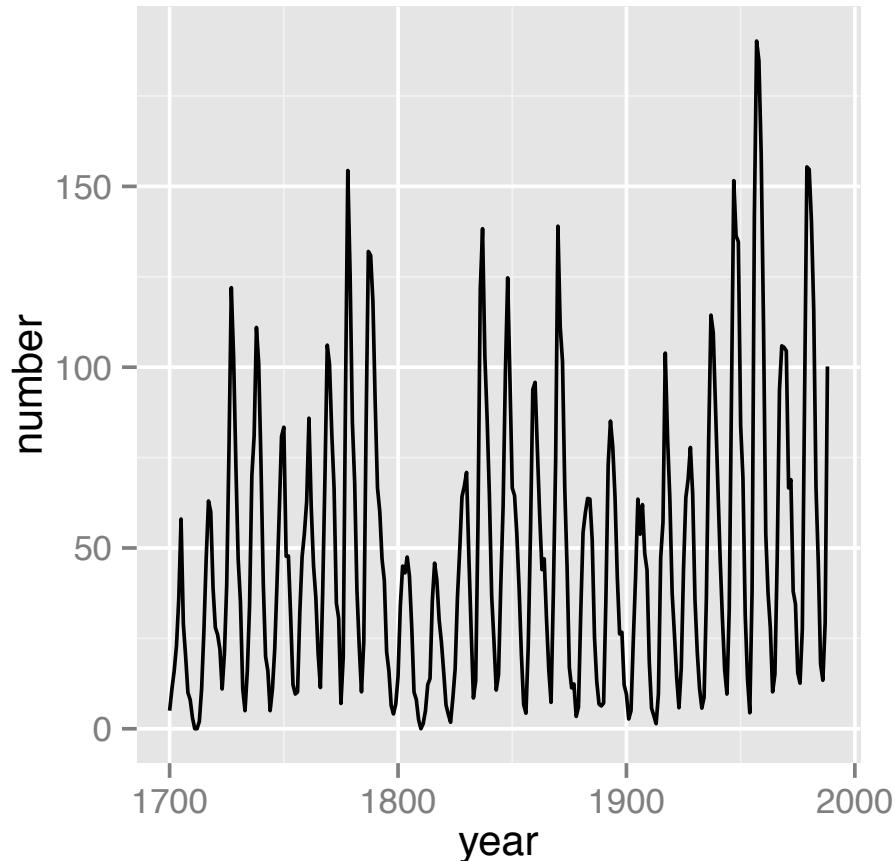
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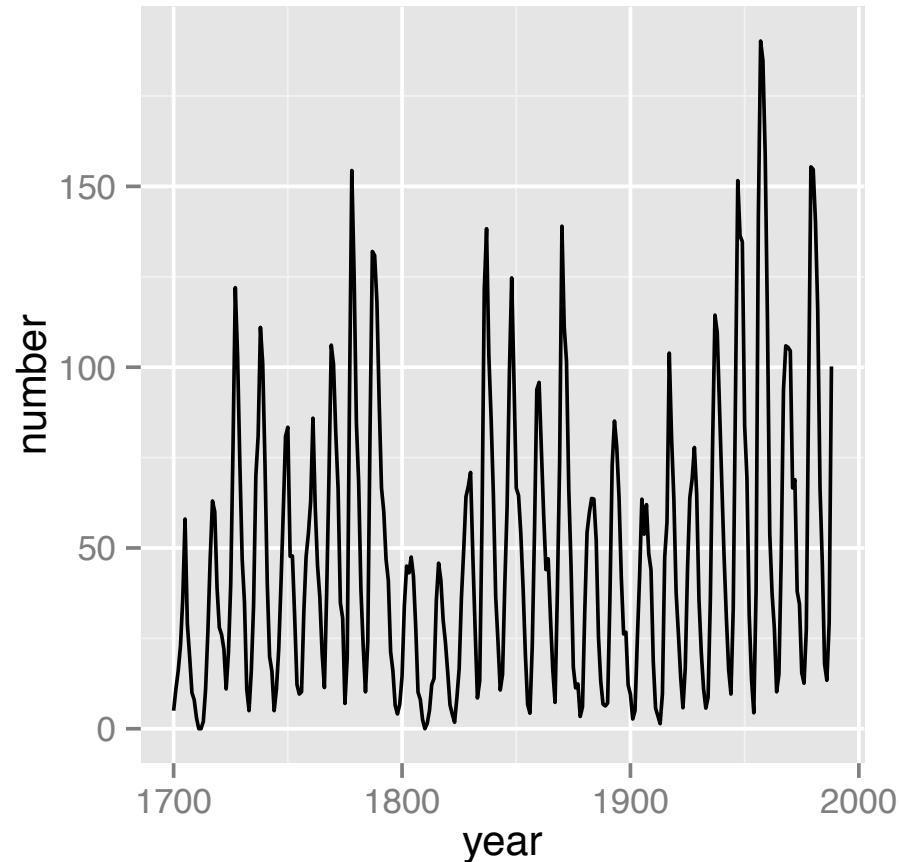
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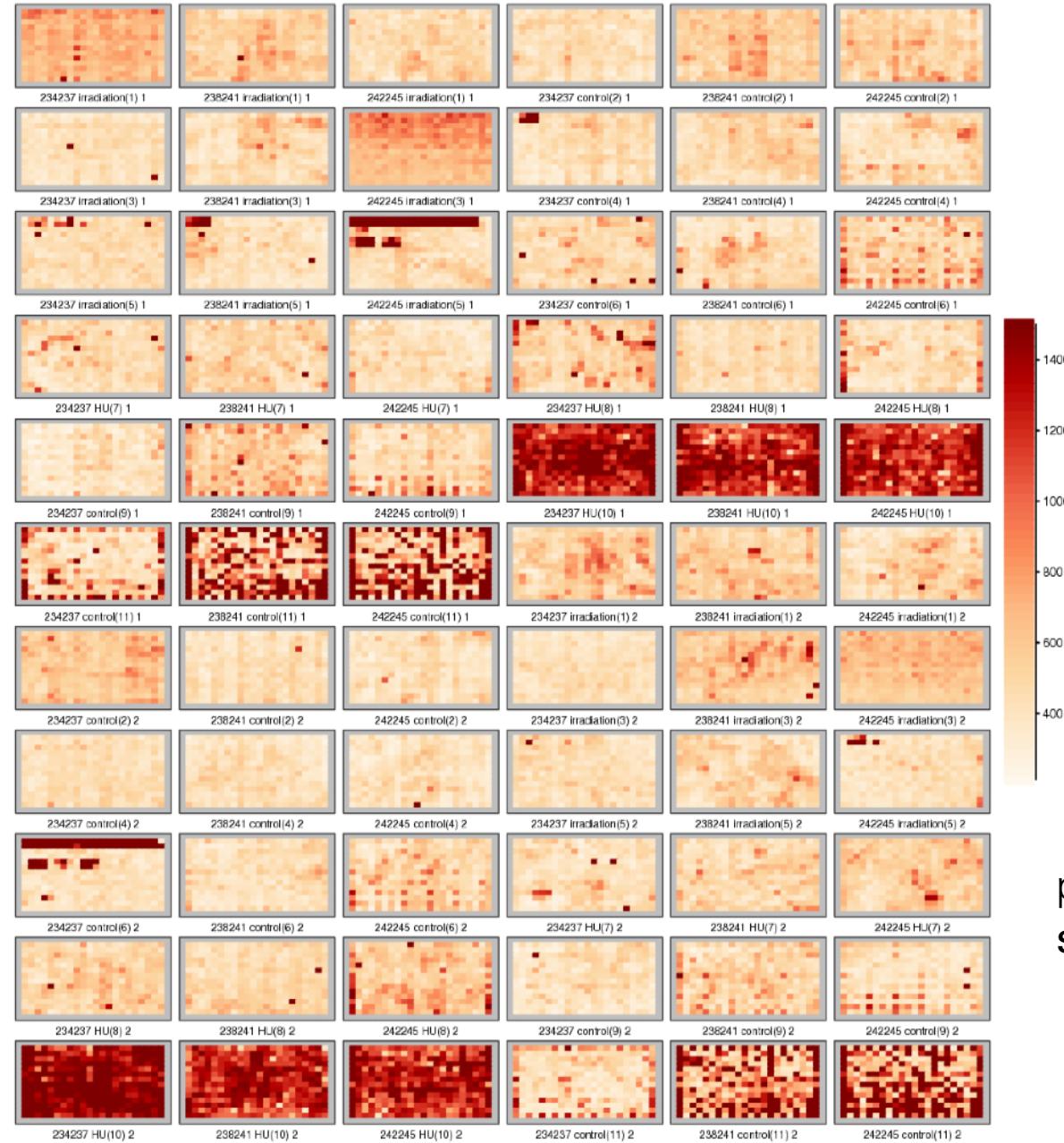
**Sawtooth:** Sunspot cycles typically rise more rapidly than they fall — steep rise and slow decline.



For plots where x- and y-axis have same units:  
use 1:1 aspect ratio

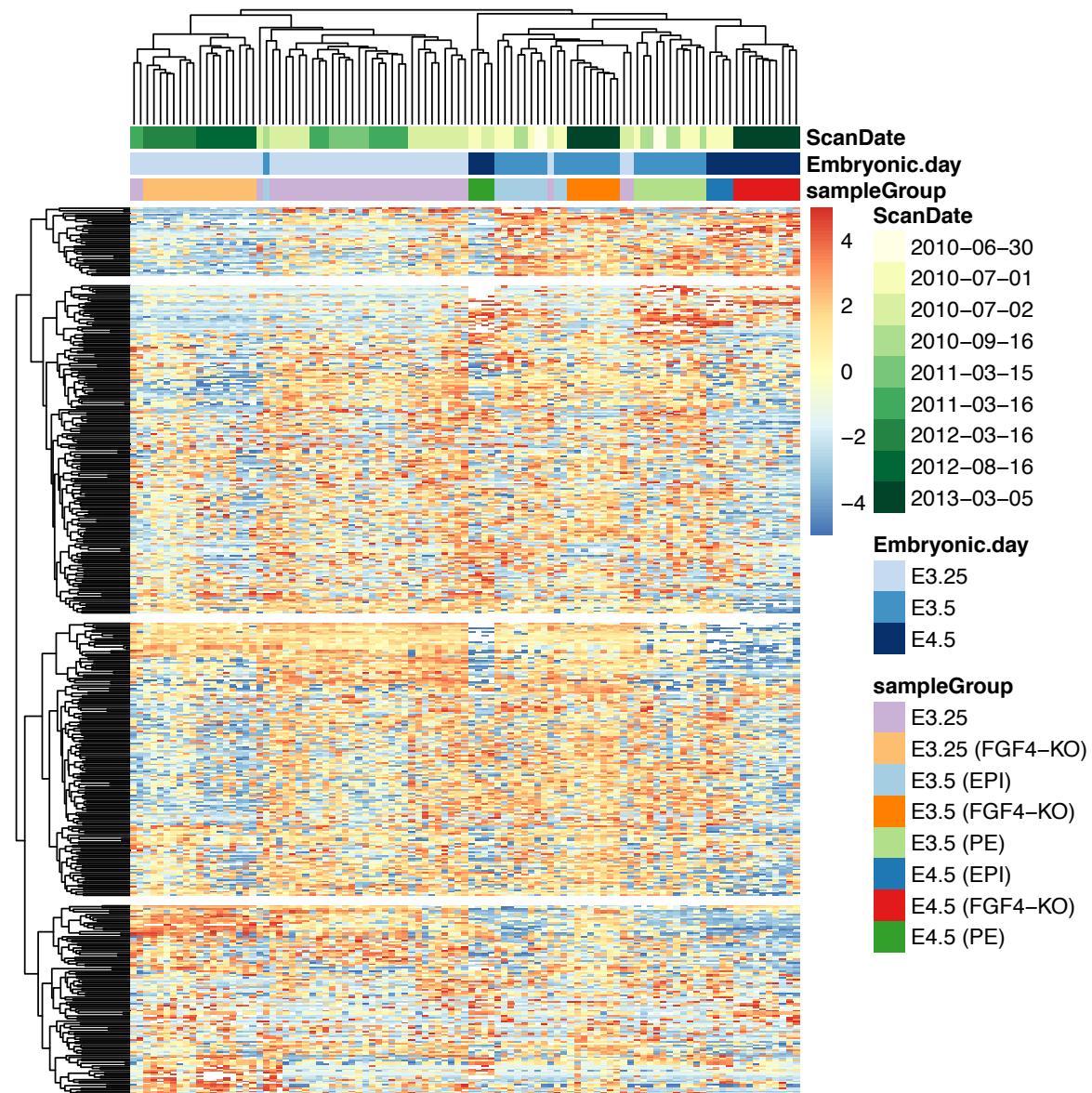


# EDA for finding batch effects

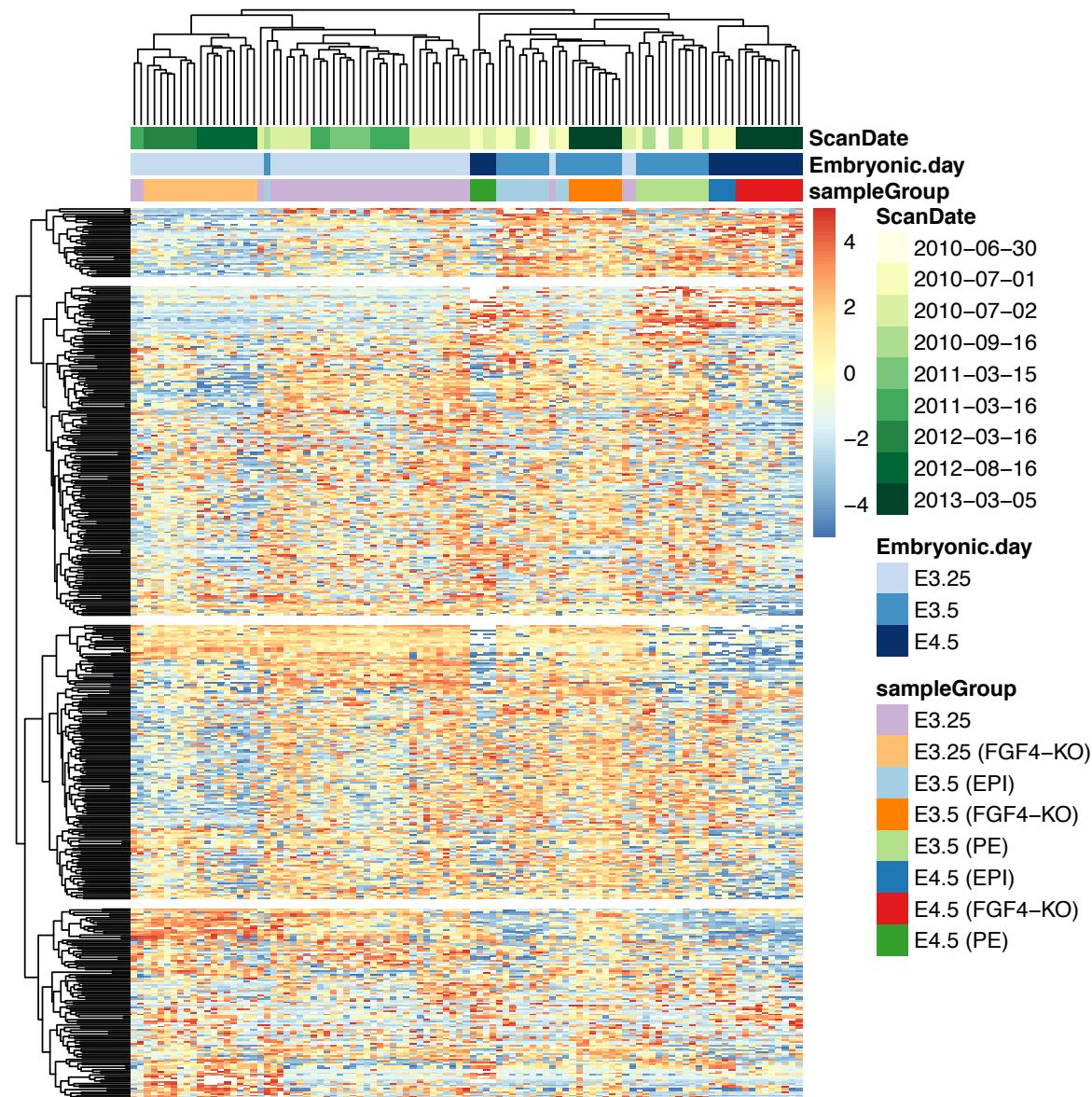


# Heatmaps for visualizing large matrices

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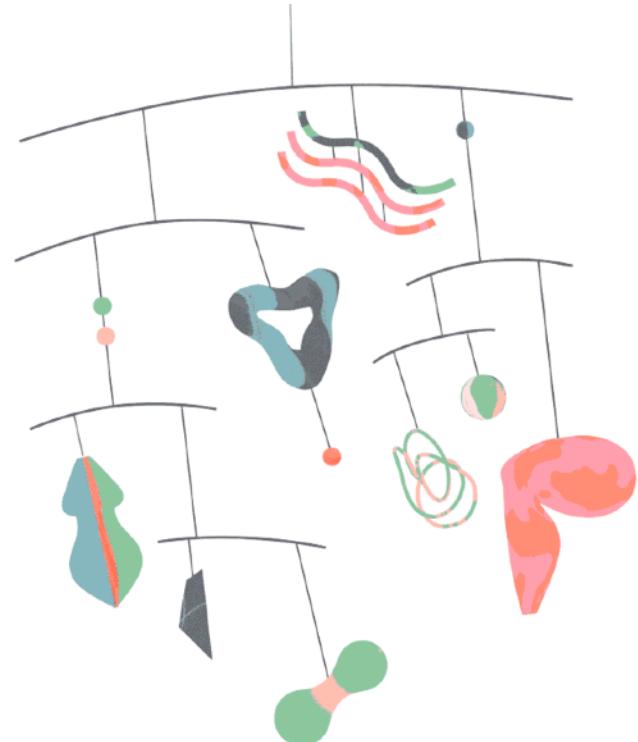
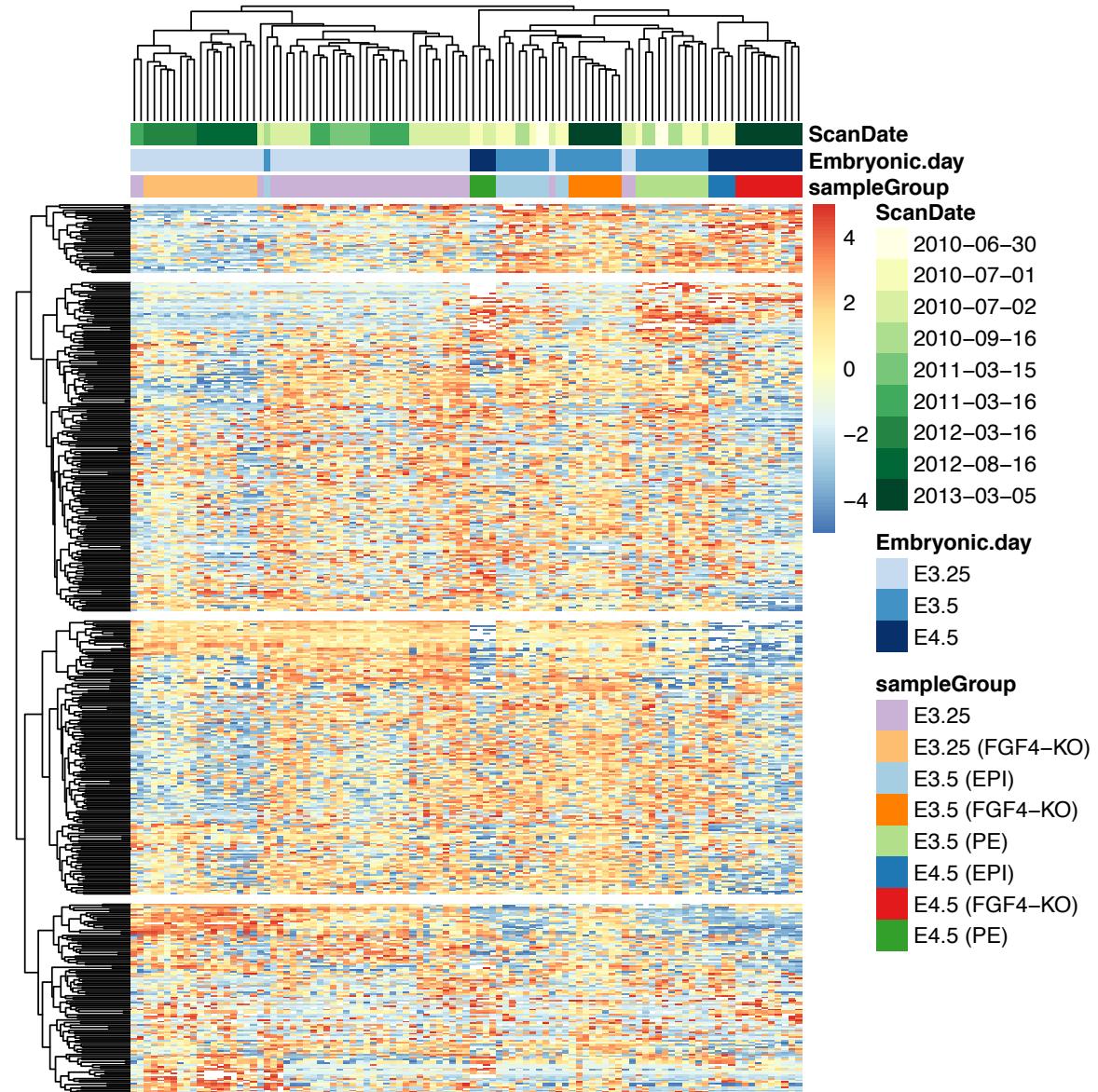
## pheatmap

- many “reasonable” defaults
- easy to add column and row ‘metadata’ at the sides

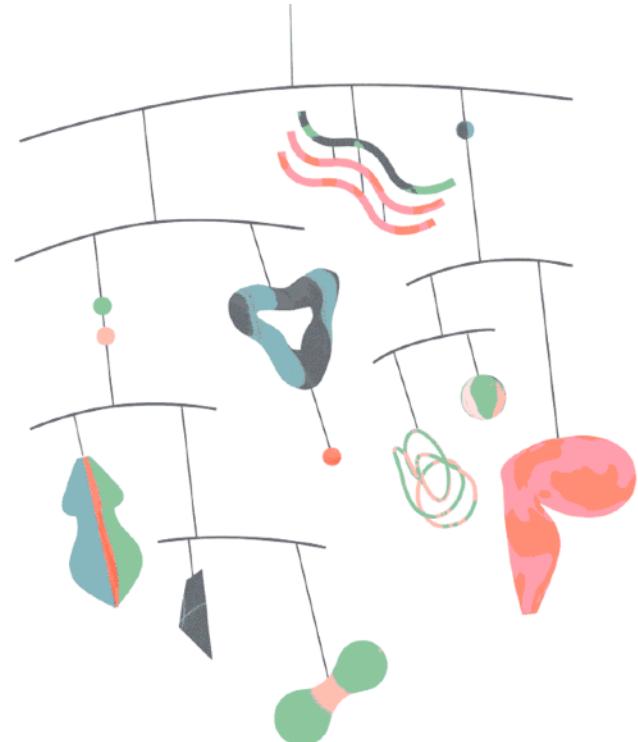
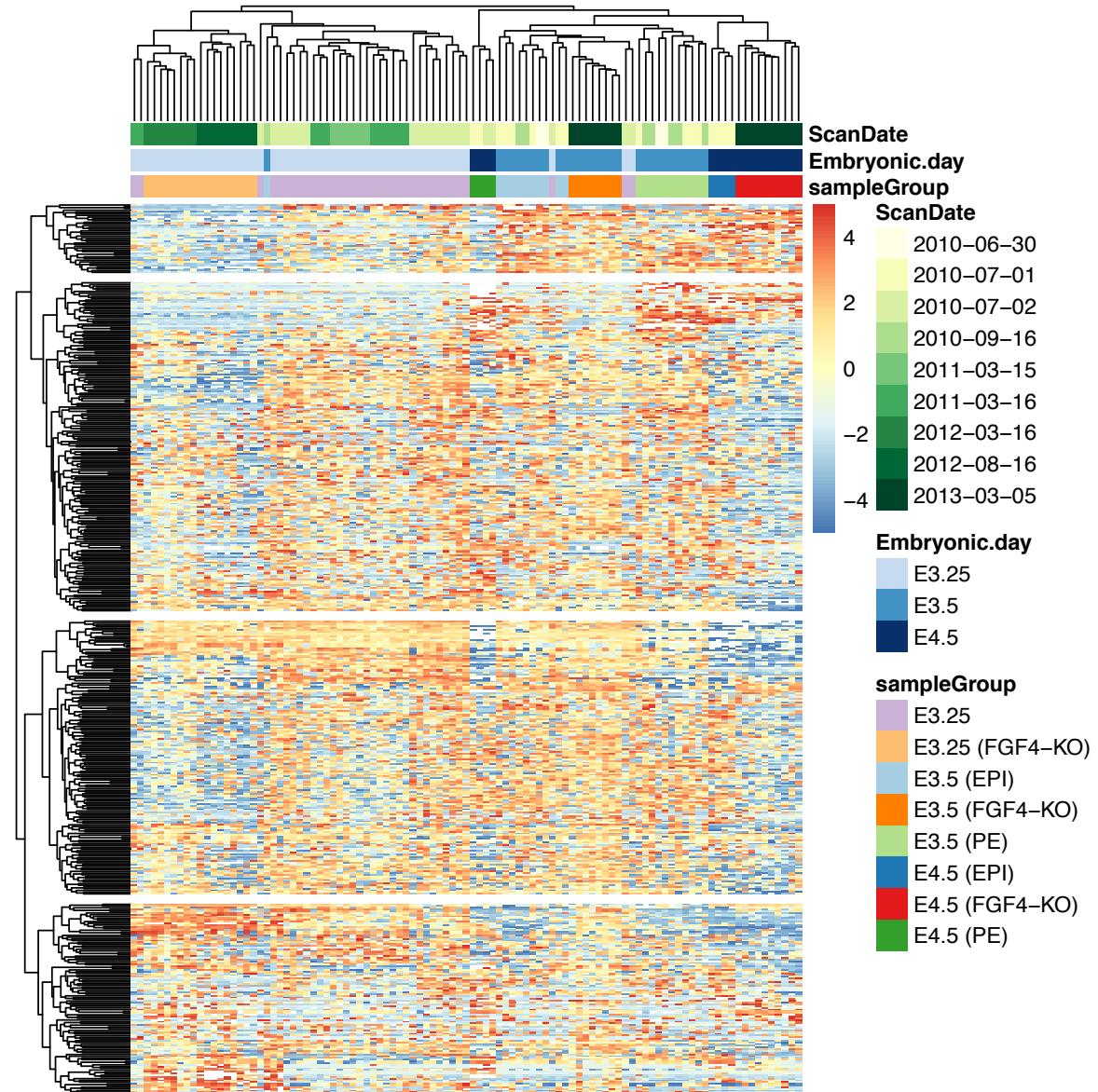
See also

*ComplexHeatmap*  
package

# The order of dendrogram branches is not unique



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# Goals for this lecture

1. Discuss the principles of **good vs bad** data viz
2. Review base R plotting
3. Understand the **grammar of graphics** concept
4. Introduce, explain and use the `ggplot()` function
5. Discuss how to plot 1D, 2D, 3-5D data and select the most appropriate plot type. Use facetting
6. Use visualization for the inspection of large datasets and discovery of global trends (e.g. batch effects)
7. Implement interactive (3D) visualization

# Interactivity

Use shiny or plotly

<https://shiny.rstudio.com/gallery/genome-browser.html>

Animations (time-dependent plots):

<https://gganimate.com>

Linked Charts

<https://anders-biostat.github.io/linked-charts/>

NB: ggvis is senescent

# plotly interactive graphics

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More on plotly can be found at <https://plotly-book.cpsievert.me/>

# plotly interactive graphics demo

see 2019\_Lec3\_graphics\_plots.html

# Acknowledgements

Susan Holmes

Laura Marie J Symul

Hadley Wickham

Lan Huong Nguyen

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What is your main take-away from each section?

# Questions

