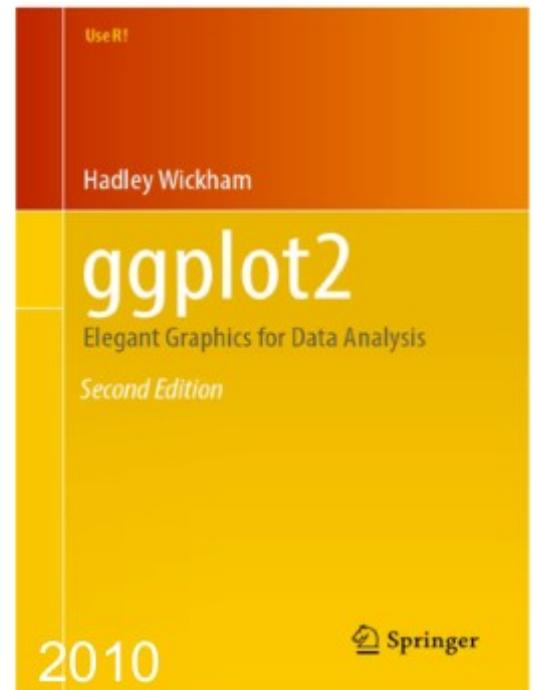


Visualization & ggplot2 Lab



Goals for the session

1. Discuss the principles of good vs bad data viz
2. Understand the grammar of graphics
4. Introduce, explain and use ggplot()
5. Discuss how to select the most appropriate plots
6. Visualization and discovery of global trends

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

base R plotting

canvas model:

a series of instructions that
sequentially fill the plotting
canvas

Great for quick data
exploration!

```
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)
```

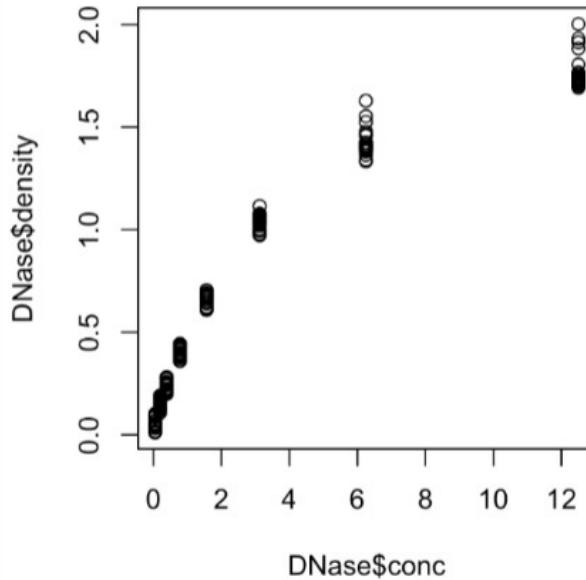


Figure 3.2: Plot of concentration vs. density
for an ELISA assay of DNase.

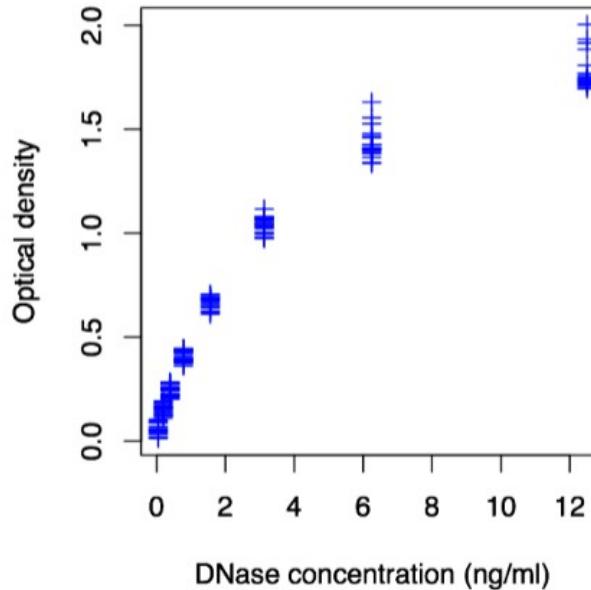
base R plotting

canvas model:

a series of instructions that
sequentially fill the plotting
canvas

Inefficient for customization
and generating complex plots.

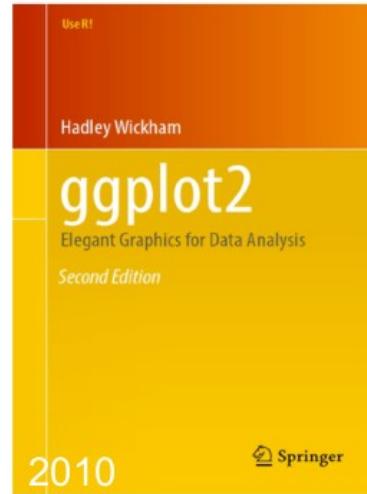
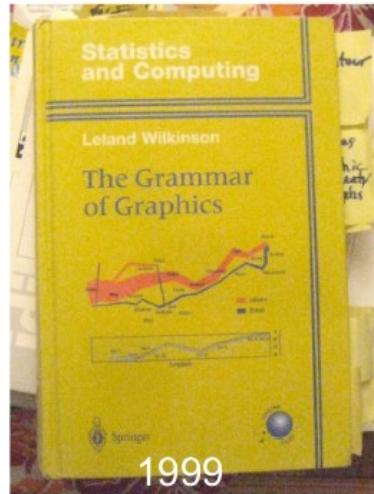
```
plot(DNase$conc, DNase$density,  
      ylab = attr(DNase, "labels")$y,  
      xlab = paste(attr(DNase, "labels")$x, attr(DNase, "units")$x),  
      pch = 3, col = "blue")
```



Goals for the session

1. Discuss the principles of good vs bad data viz
2. **Understand the grammar of graphics**
3. **Introduce, explain and use ggplot()**
4. Discuss how to select the most appropriate plots
5. Visualization and discovery of global trends

The Grammar of Graphics



Concept **coined by Leland Wilkinson in 1999**. An **abstraction** which facilitates reasoning and communicating graphics.

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.

ggplot grammar of graphics

- **datasets** (*nouns*)
- **geometric objects** (*verbs*): visual presentations of the data (points, lines, rectangles, contours..)
- **aesthetics** (*adverbs*): instructions on how to map data variables to geometric objects
- stat. transformations/summaries (line fitting, binning)
- coordinate systems and scales (linear, log, rank)
- layers: overlay
- facets: separating data into multiple subplots
- settings (text size, font, alignment, angle, positioning)

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]

[1] Cell-to-cell expression variability followed by signal reinforcement progressively segregates early mouse lineages
by Ohnishi et al., Nature Cell Biology (2014) 16(1): 27-37. doi: 10.1038/ncb2881.

ggplot() template

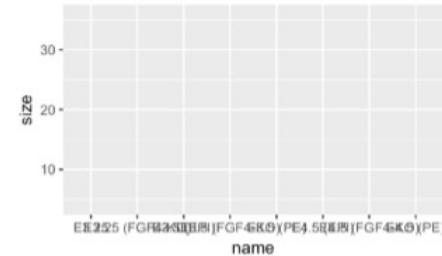
```
ggplot(data = <default data set>,
        aes(x = <default x axis variable>,
            y = <default y axis variable>,
            ... <other default aesthetic mappings>),
        ... <other plot defaults>) +
  geom_<geom type>(aes(size = <size variable for this geom>,
                        ... <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>)
```

Using the same plot, we can easily change the coordinates

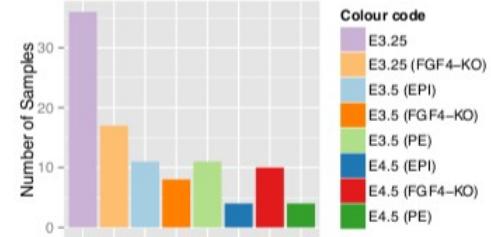
```
groupSize <- table(dftx$sampleGroup)
groupSize

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

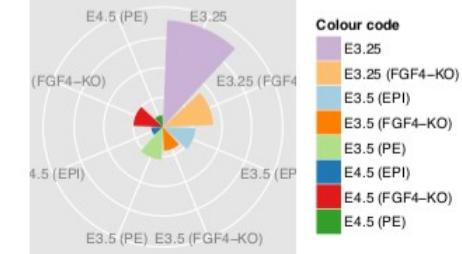
No geom defined yet!



```
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")
```

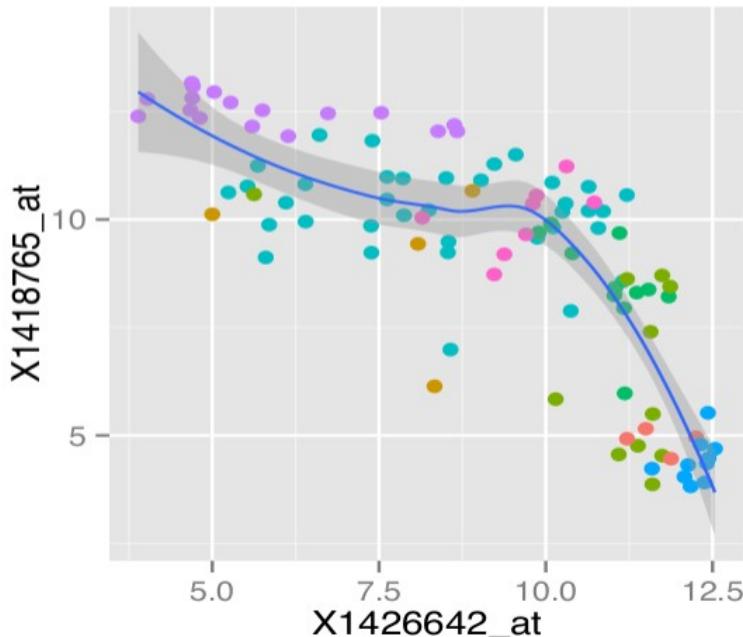


```
pb.polar <- pb + coord_polar() +
  theme(axis.text.x = element_text(angle = 0, hjust = 1),
        axis.text.y = element_blank(),
        axis.ticks = element_blank()) +
  xlab("") + ylab("")
pb.polar
```



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.

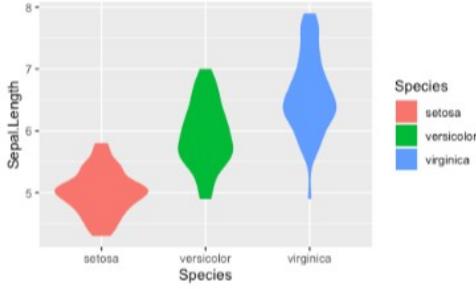
geometric objects

 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

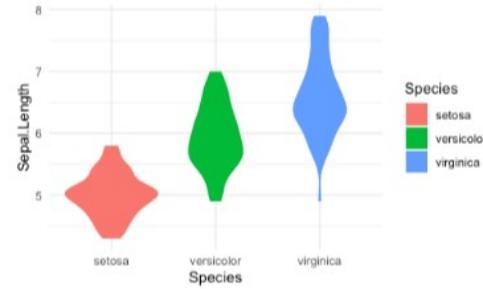
Cheat sheet: <https://www.rstudio.com/wp-content/uploads/2015/03/ggplot2-cheatsheet.pdf>

Themes can change the look

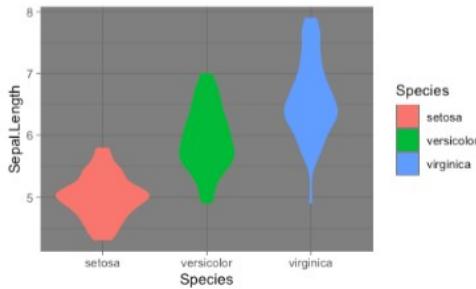
```
g = ggplot(iris,  
          aes(x = Species,  
               y = Sepal.Length,  
               fill = Species))+  
  geom_violin(col = NA)  
g
```



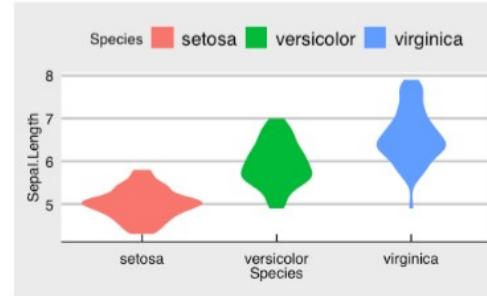
```
g + theme_minimal()
```



```
g + theme_dark()
```



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



Bar charts with error bars

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

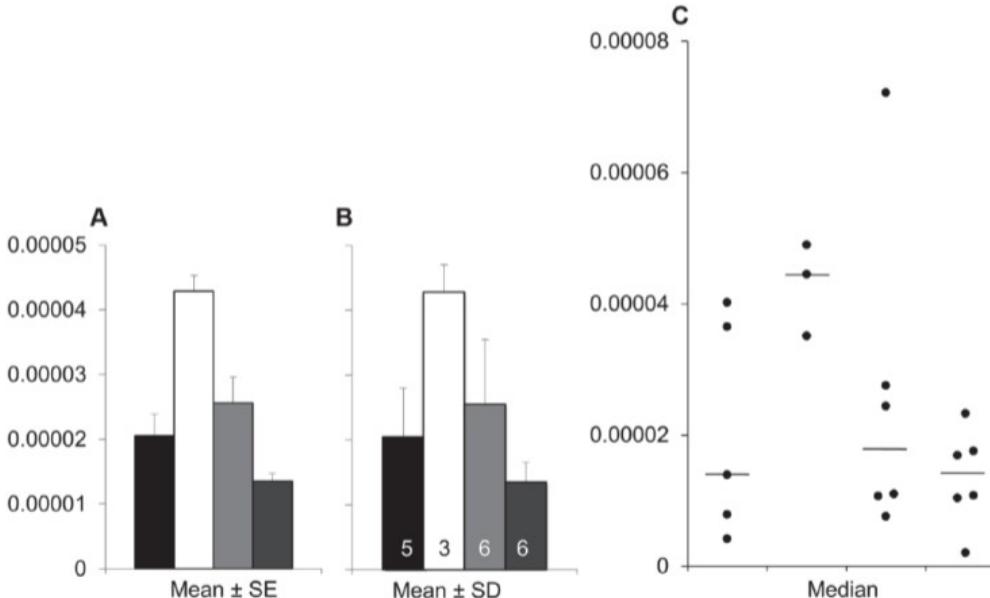


Fig 3. Bar graphs and scatterplots convey very different information. While scatterplots prompt the reader to critically evaluate the statistical tests and the authors' interpretation of the data, bar graphs discourage the reader from thinking about these issues. Placental endothelin 1 (*EDN1*) mRNA 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.

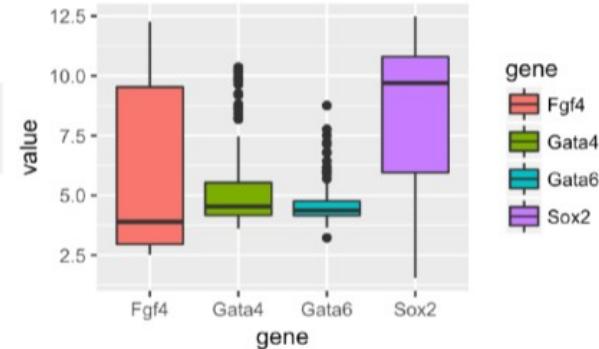
Bar charts
(with error
bars)
**not good for
showing
distributions**

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

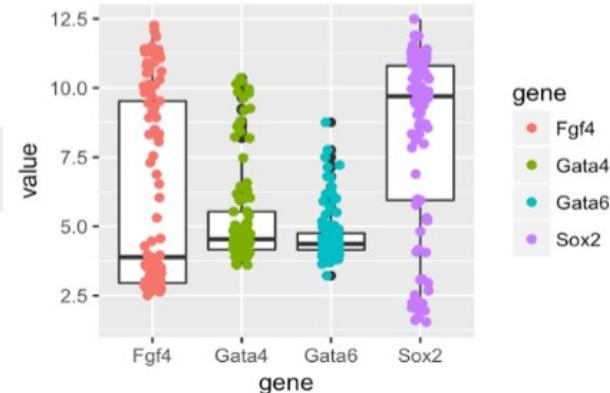
Boxplot

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))
```

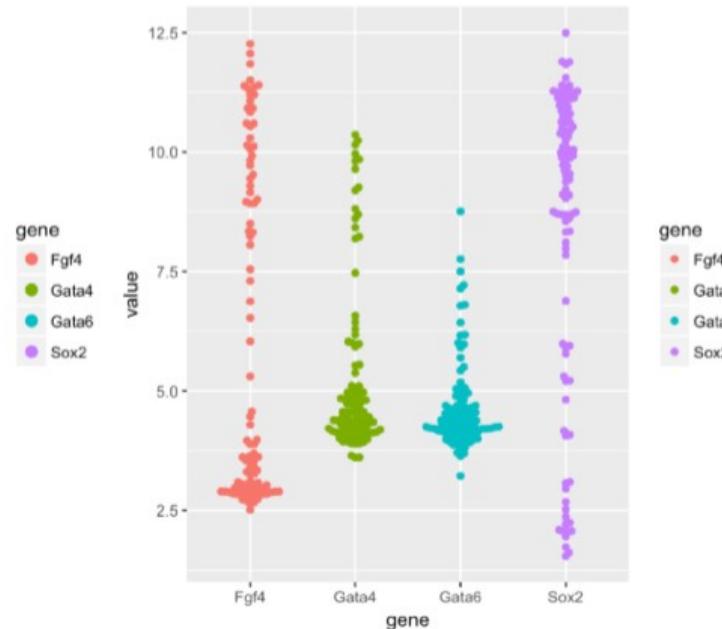
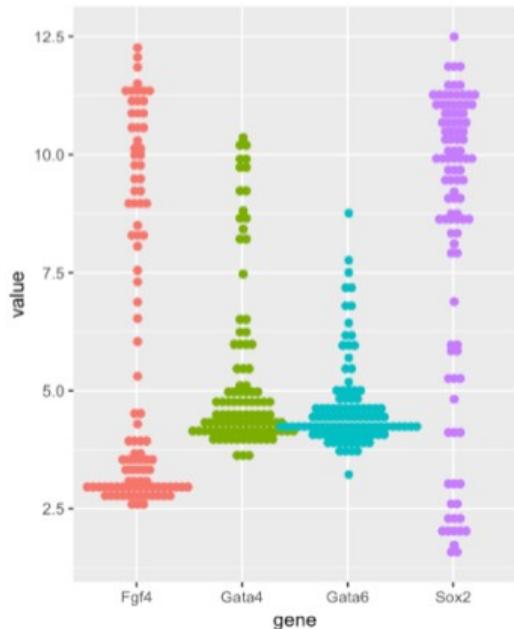


```
p + geom_boxplot() +  
  geom_jitter(aes(color = gene), width = 0.1, height = 0)
```



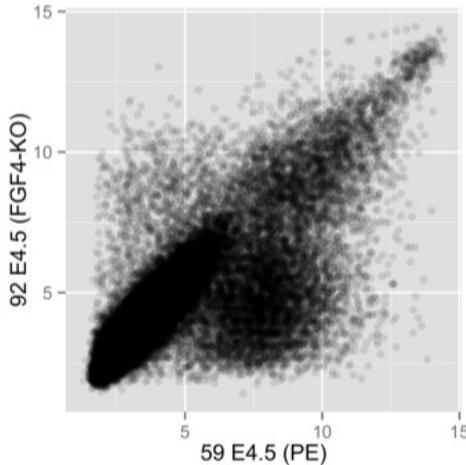
Dot & Beeswarm Plot

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

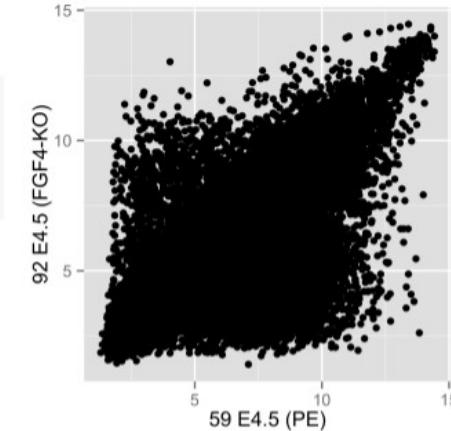


Showing distributions in 2D

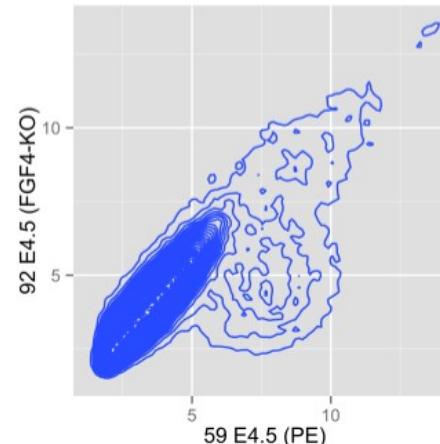
```
scp <- ggplot(dfx, aes( x = '59 E4.5 (PE)' ,  
                      y = '92 E4.5 (FGF4-KO)' ))  
scp + geom_point()
```



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



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

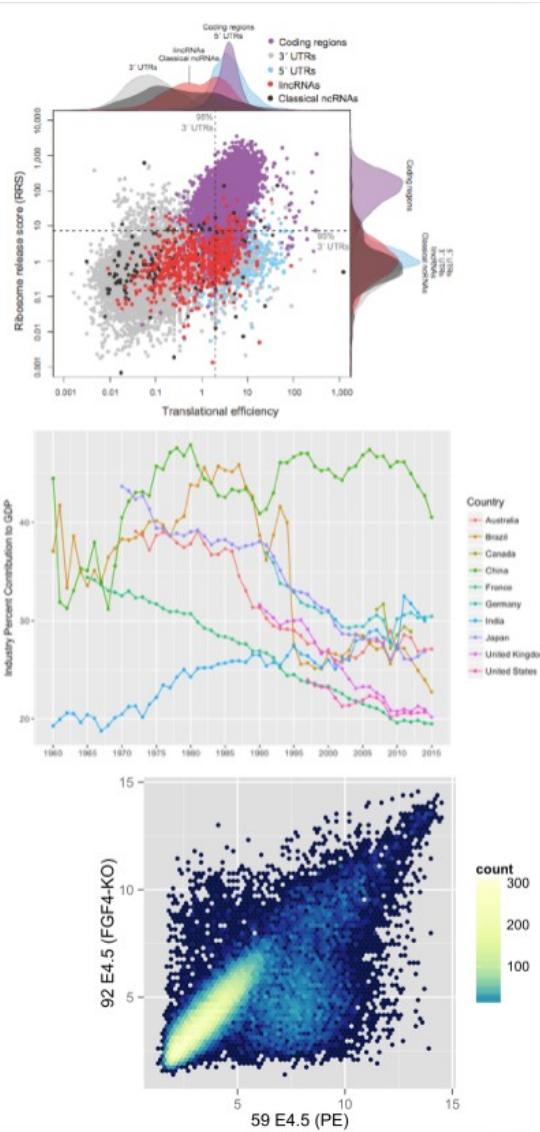


2D data plots

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)



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

geom_point's

aesthetics

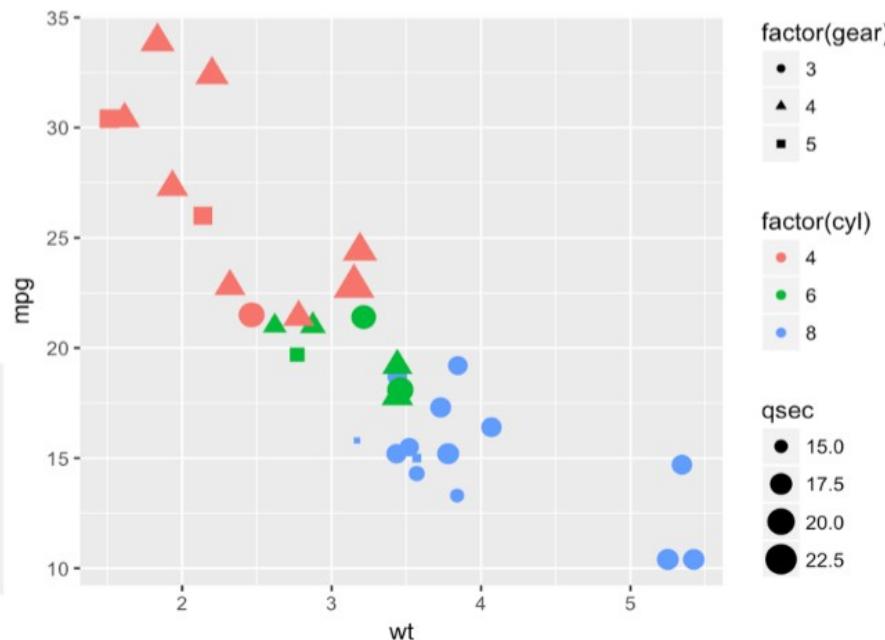
(apart from x and y):

- 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

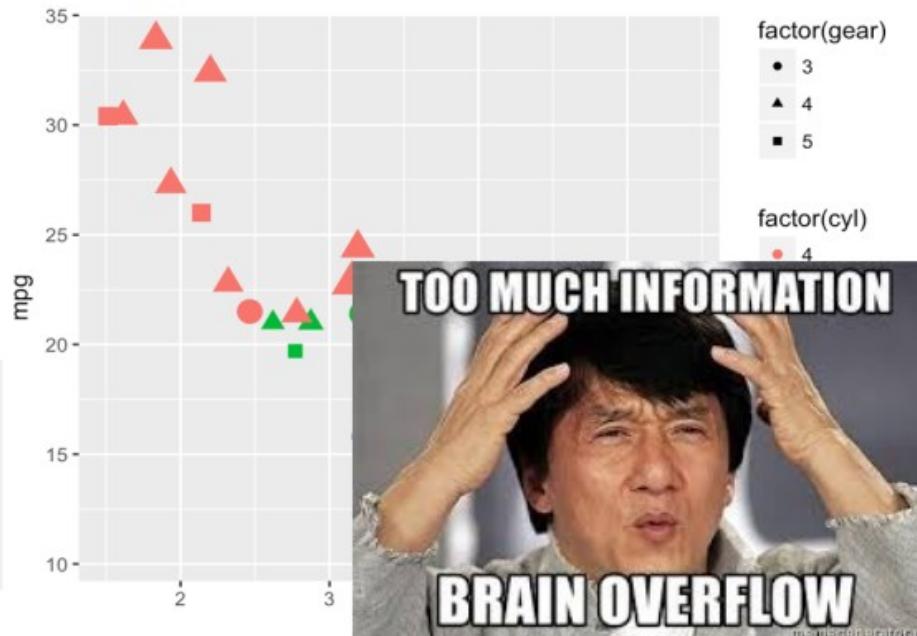
aesthetics

(apart from x and y):

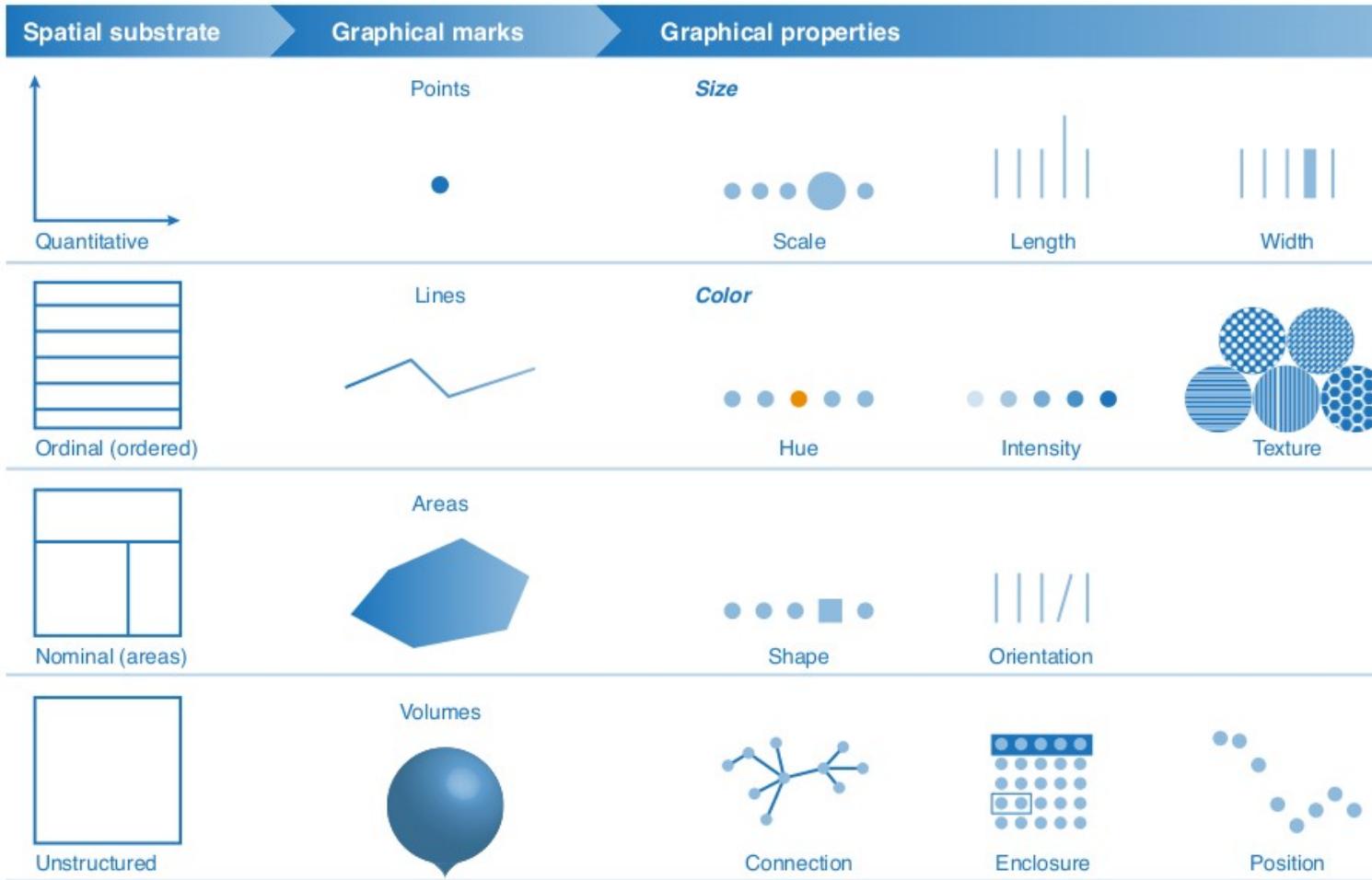
- fill / color
- shape
- size
- alpha

```
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
```



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



Faceting is useful to show more dimensions without overcrowding the graph

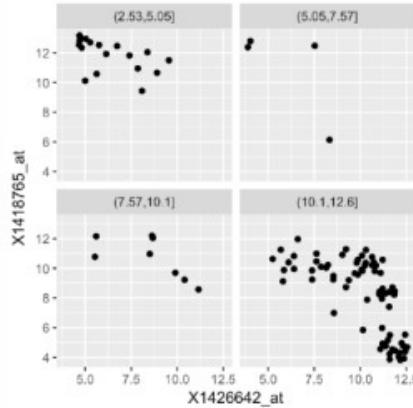


Figure 3.33: Faceting: the same data as in Figure 3.9, split by the continuous variable X1450989_at and arranged by facet_wrap.

Trellis — chart that uses multiple instances of the same chart

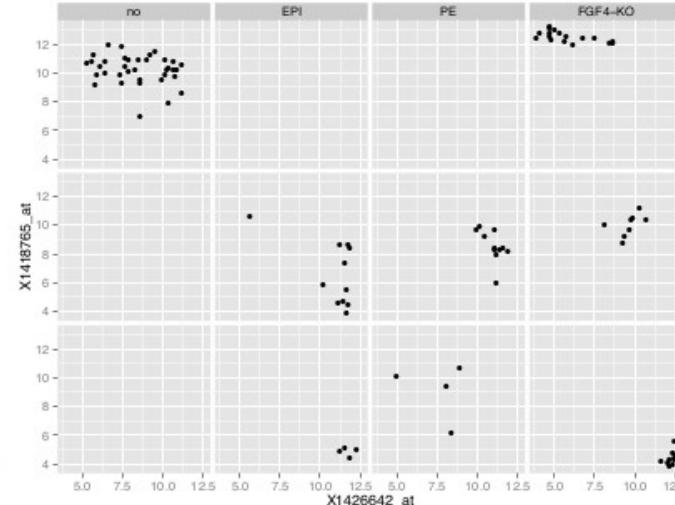
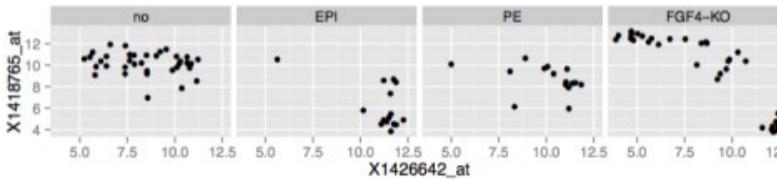
facet_wrap

```
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 )
```



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  
## 5 E3.25      8.924228    4.923580    4.629728    8.705340  
## 6 E3.25     11.325952    4.068520    4.165692    8.696228
```

e.g. a expression matrix with each raw containing a gene expression for all samples

Each **row** corresponds to a **sample** and each **column** to a **feature** (or vice versa).

long format

```
##   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  
## 4 4 E3.25 X1420085_at 9.715243  
## 5 5 E3.25 X1420085_at 8.924228  
## 6 6 E3.25 X1420085_at 11.325952
```

e.g. a collapsed expression data with each row corresponding to a gene-sample pair

Feature and **sample** information is stored separately for each measurement in data columns.

How do you switch :wide: <>> :long: ?

melt() from wide to long

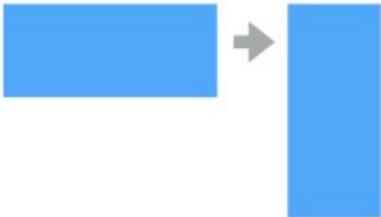
To convert between two data formats we can use functions **melt()**, and **dcast()** from package **reshape2**

```
head(genes_expression)
```

```
##          X1420085_at X1418863_at X1425463_at X1416967_at
## 1 E3.25      3.027715    4.843137    5.500618    1.731217
## 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
## 5 E3.25      8.924228    4.923580    4.629728    8.705340
## 6 E3.25     11.325952    4.068520    4.165692    8.696228
```

```
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
## 3 3 E3.25 X1420085_at 2.940142
## 4 4 E3.25 X1420085_at 9.715243
## 5 5 E3.25 X1420085_at 8.924228
## 6 6 E3.25 X1420085_at 11.325952
```



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
## 4 4 E3.25 X1420085_at 9.715243
## 5 5 E3.25 X1420085_at 8.924228
## 6 6 E3.25 X1420085_at 11.325952
```

```
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
## 2 2 E3.25    9.293016    5.530016    6.160900    9.697038
## 3 3 E3.25    2.940142    4.418059    4.584961    4.161240
## 4 4 E3.25    9.715243    5.982314    4.753439    9.540123
## 5 5 E3.25    8.924228    4.923580    4.629728    8.705340
## 6 6 E3.25   11.325952    4.068520    4.165692    8.696228
```

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

Acknowledgments

- Susan Holmes
- Wolfgang Huber
- Sudarshan Shetty
- Wisam Saleem