

Graphics

Wolfgang Huber

Horror Picture Show

40.0

30.0

20.0

10.0

0.0



1

2

3

8

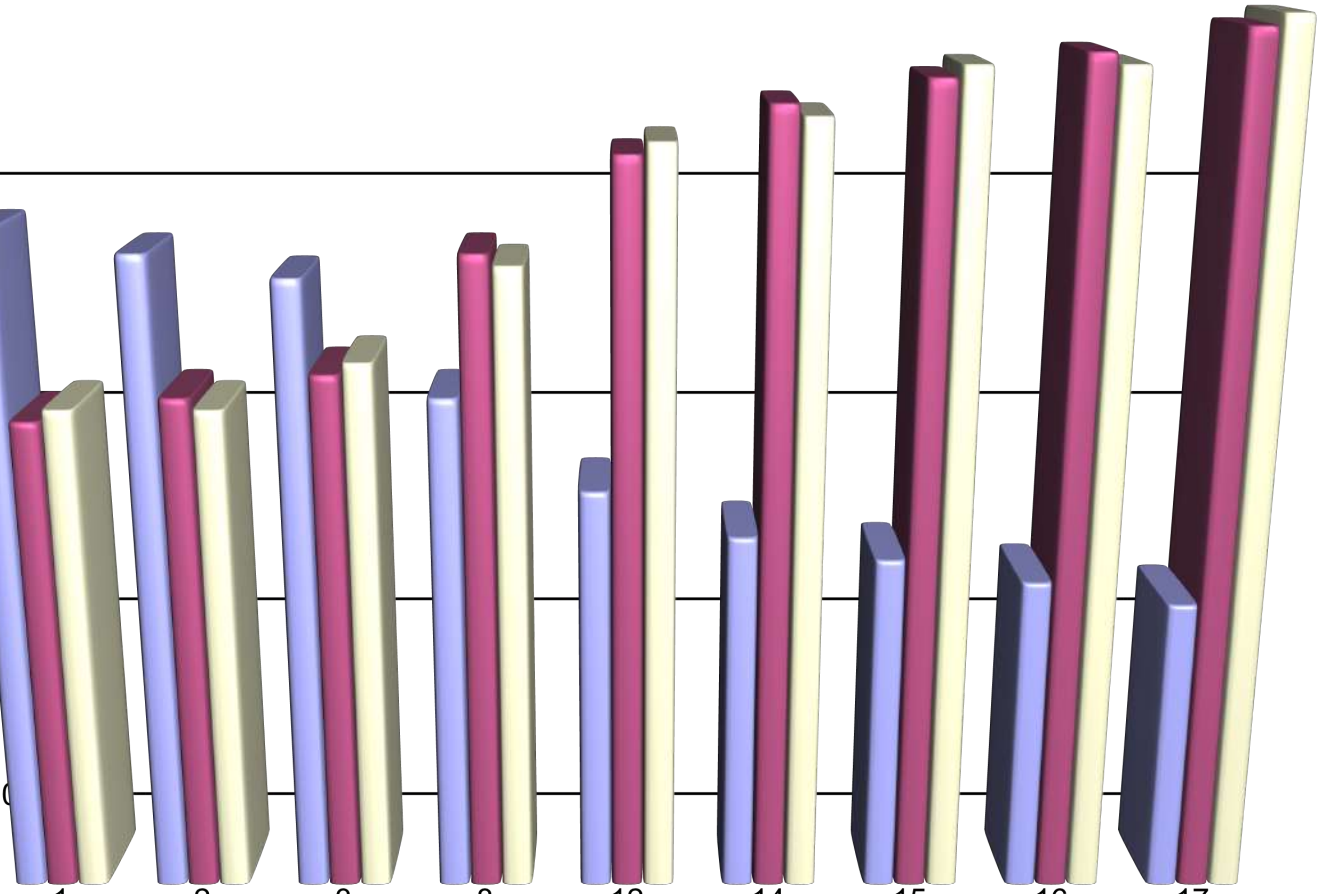
12

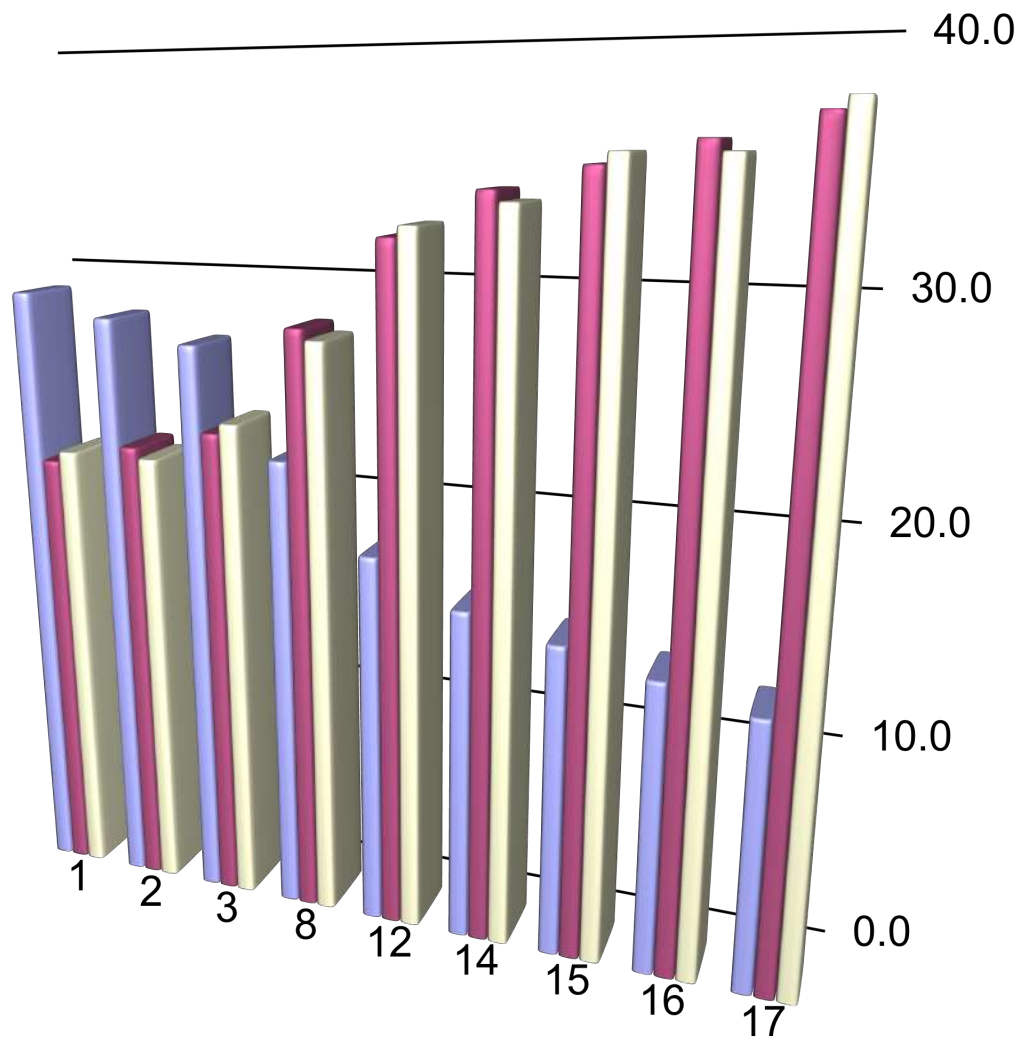
14

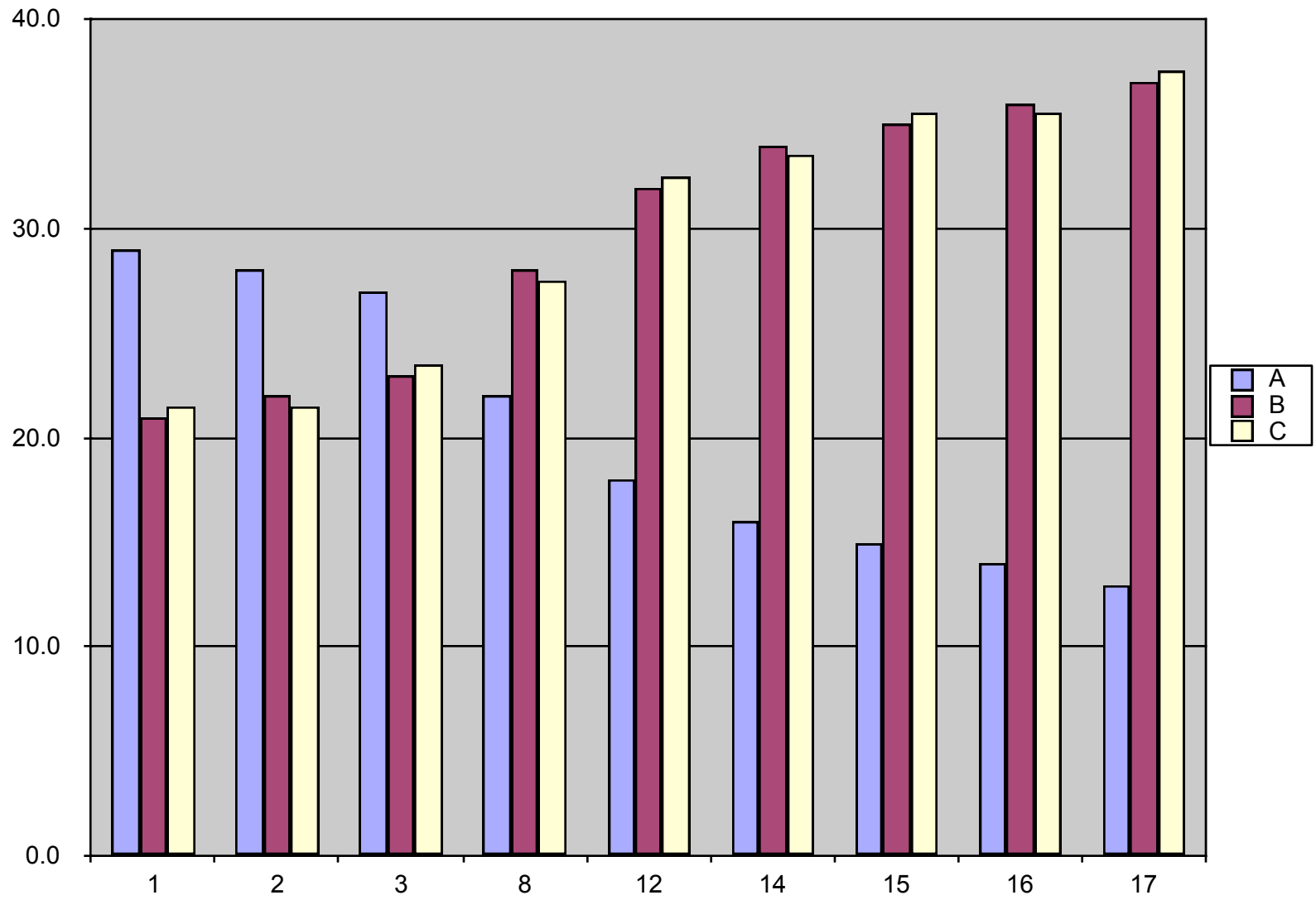
15

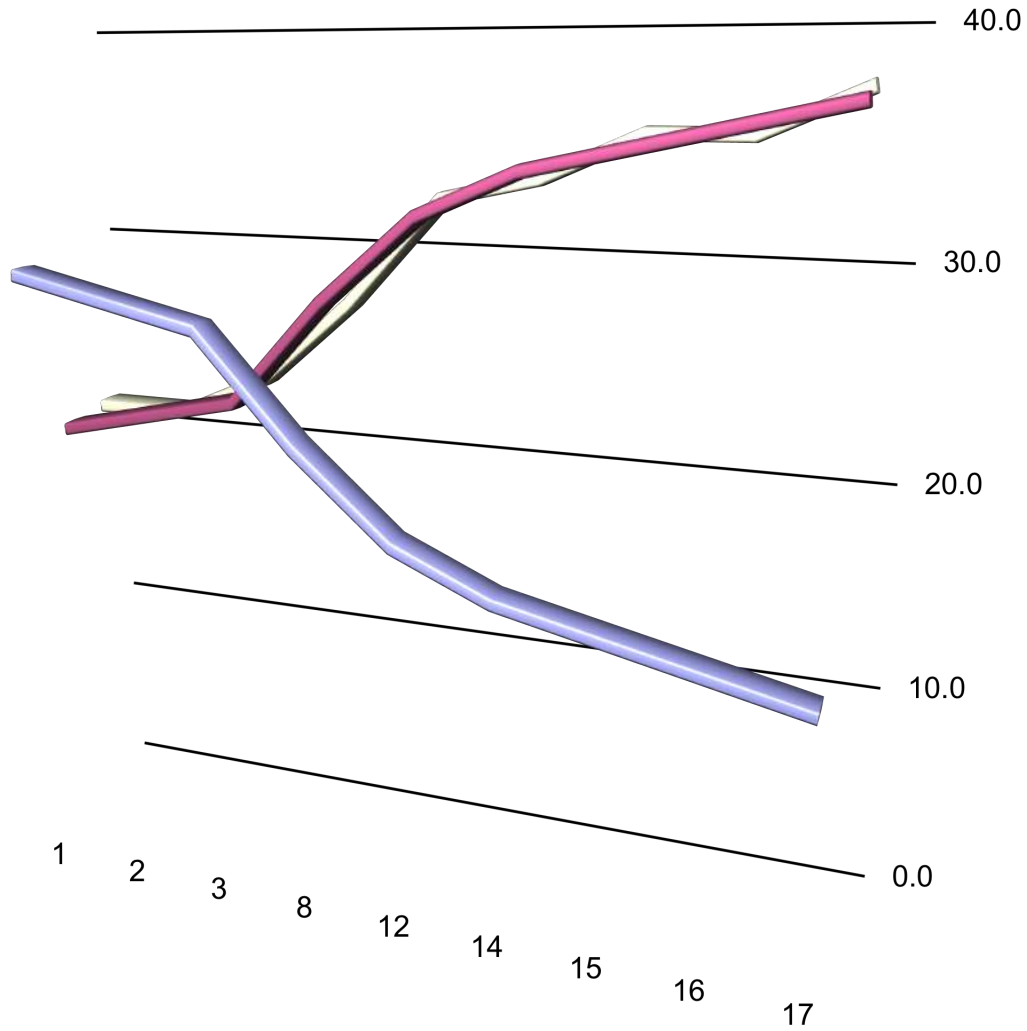
16

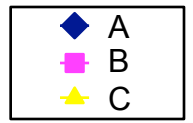
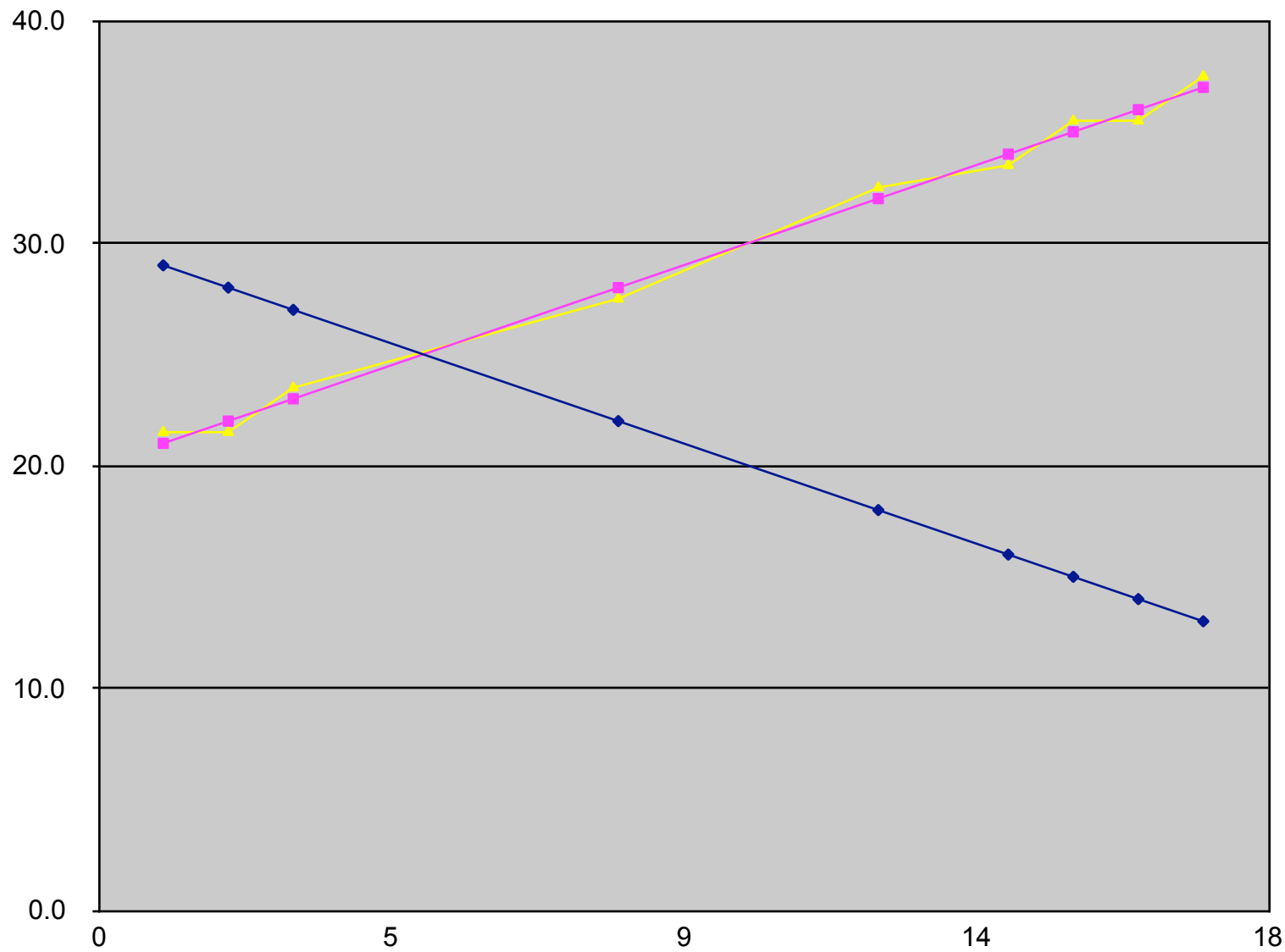
17











Why graphics?

1. To explore data (interactively)
2. To communicate data & preliminary insights with collaborators
3. To publish results

Goals for this lecture

- Review base R plotting
- Understand the **grammar of graphics** concept
- Introduce ggplot2's ggplot function
- See how to plot 1D, 2D, 3-5D data and understand faceting
- Visualisation for quickling viewing large datasets and discover large-scale trends (e.g. batch effects)
- Use colours like a pro

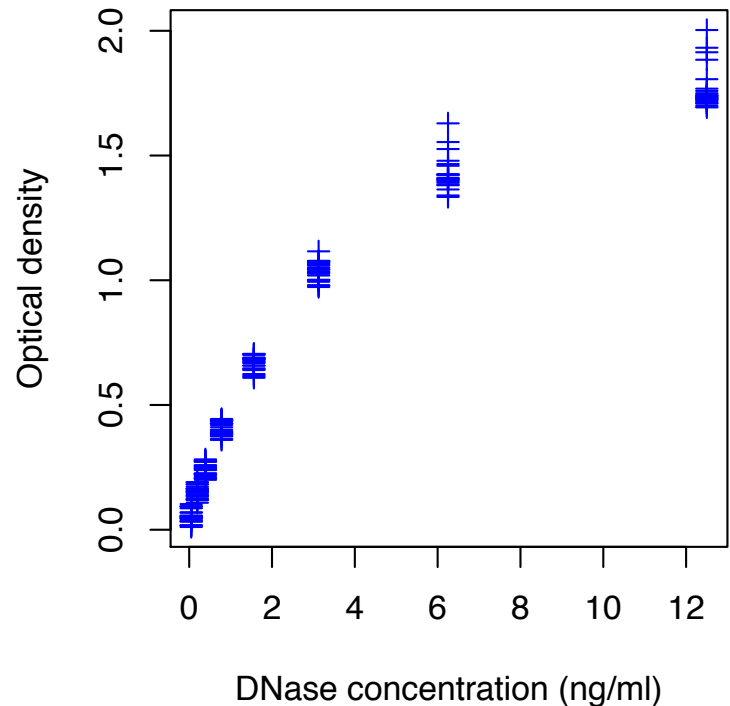
base R plotting

Canvas model: a series of instructions that sequentially fill the plotting canvas

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



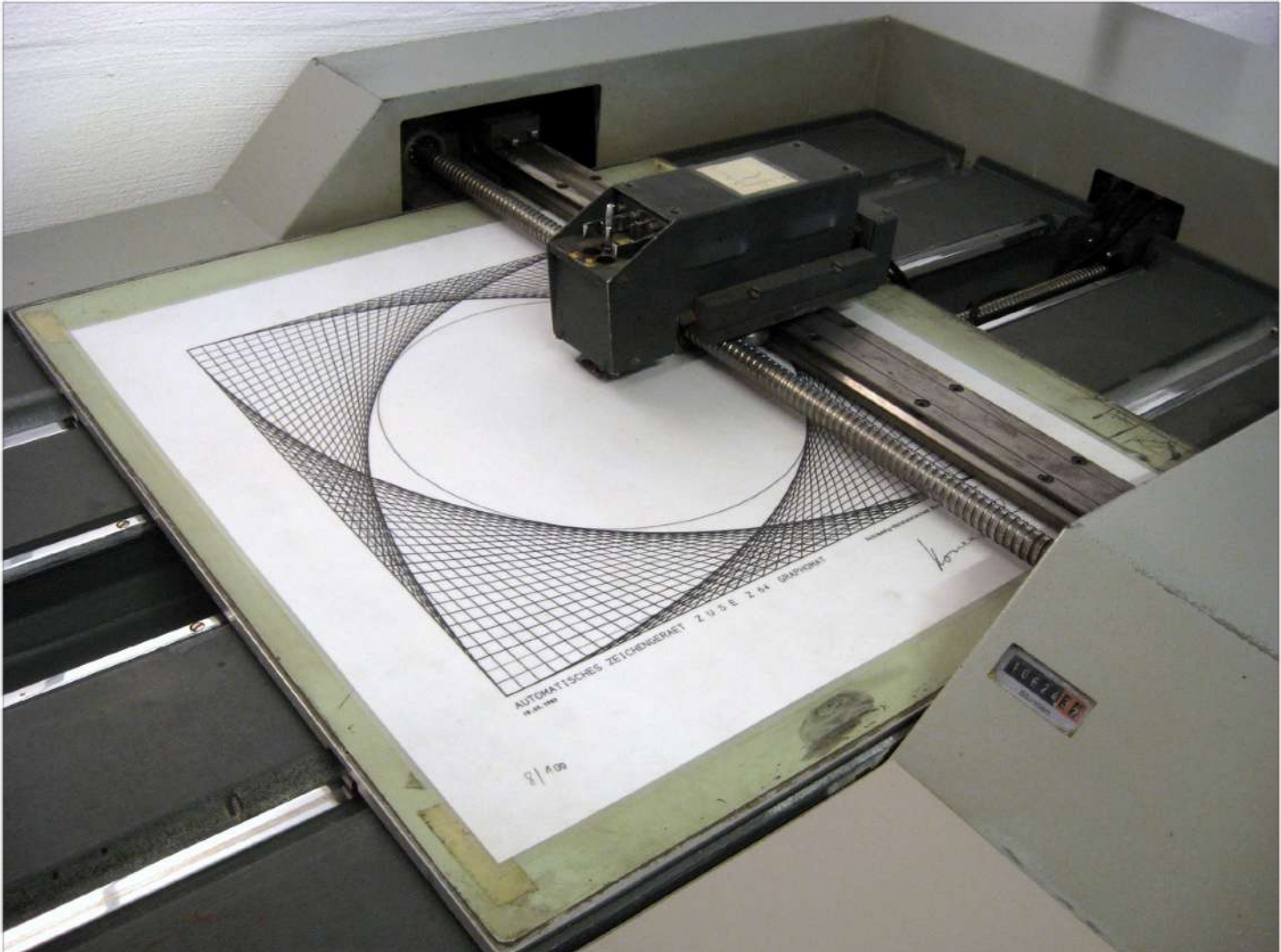
base R plotting

Canvas
of i
sec
plo

```
head(DNase)
```

```
## Run c
## 1 1 0.0
## 2 1 0.0
## 3 1 0.1
## 4 1 0.1
## 5 1 0.3
## 6 1 0.3
```

```
plot(DNase$c
ylab = attr(
xlab = paste
pch = 3, col
```



ZUSE Plotter Z64 (presented in 1961).

12
l)

base R plotting

Canvas
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Drawbacks:

- Layout choices have to be made with no 'global' overview over what may still be coming
- Resizing often leads to unsatisfactory results
- Different functions for different plot types with different interfaces
- Many routine tasks require a lot of 'boilerplate' code
- No concept of facets / lattices / viewports
- Default colours are poor

```
head(DNase
## Run
## 1 1 G
## 2 1 G
## 3 1 G
## 4 1 G
## 5 1 G
## 6 1 G

plot(DNase
ylab = att
xlab = paste
pch = 3, col
```

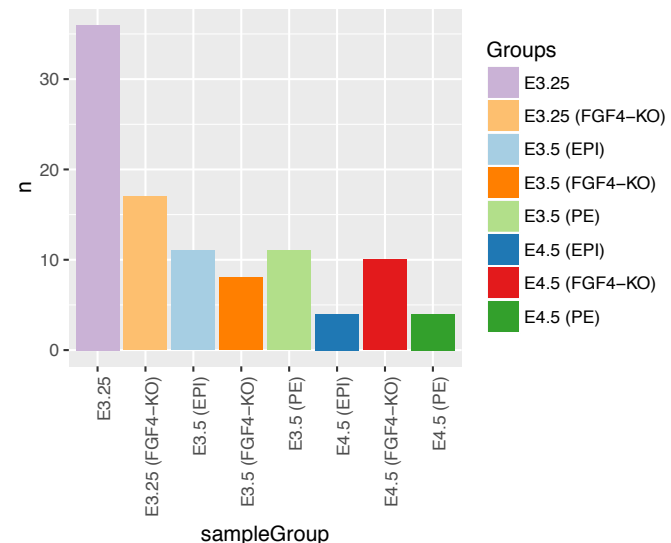
ZUSE Plotter Z64 (presented in 1961).

The grammar of graphics

The components of *ggplot2*'s grammar of graphics are

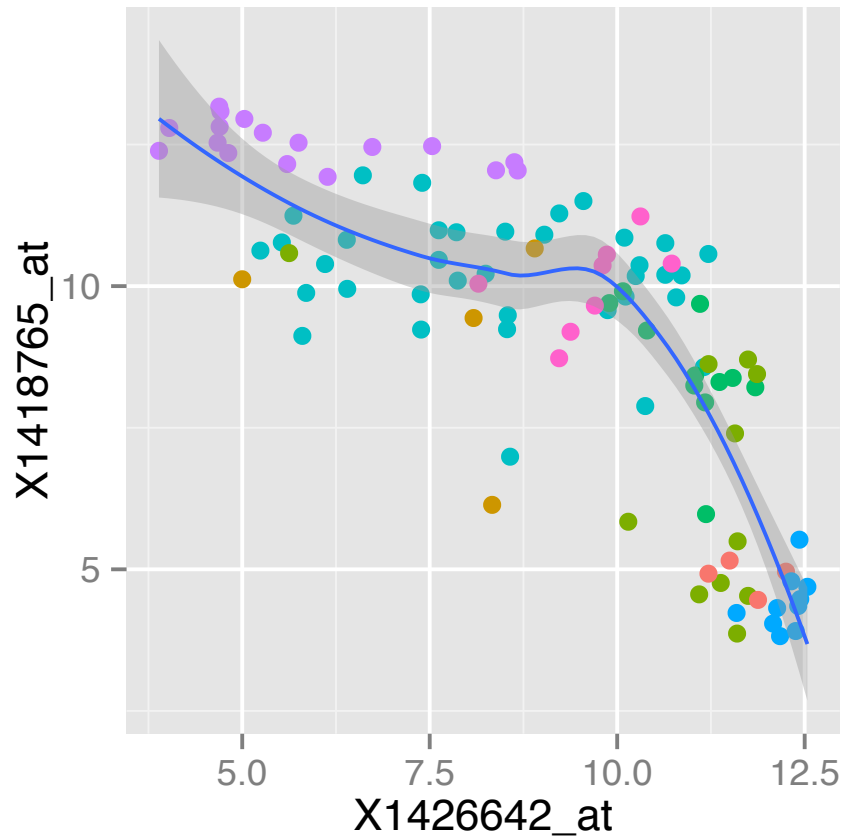
1. a dataset
2. a choice of geometric object that serves as the visual representations of the data – for instance, points, lines, rectangles, contours
3. a description of how the variables in the data are mapped to visual properties (aesthetics) of the geometric objects, and an associated scale, (e. g., linear, logarithmic, rank)
4. a statistical summarisation rule
5. a coordinate system
6. a facet specification, i. e. the use of several plots to look at the same data

```
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))
```



Layers

```
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 )
```

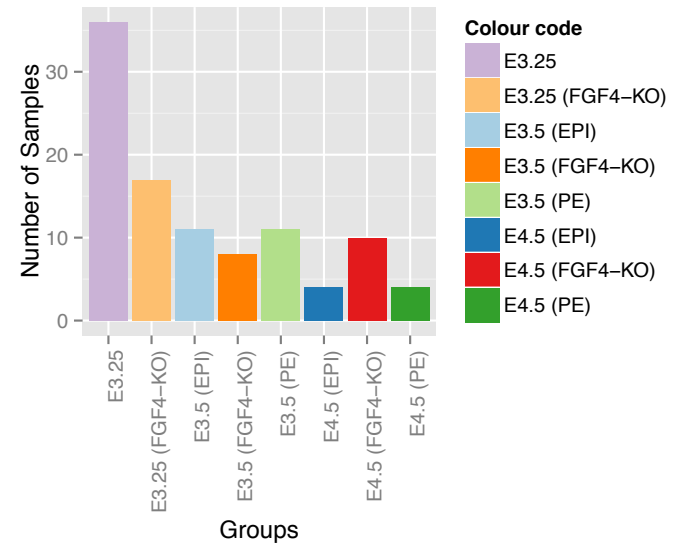


A more complex example: themes

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

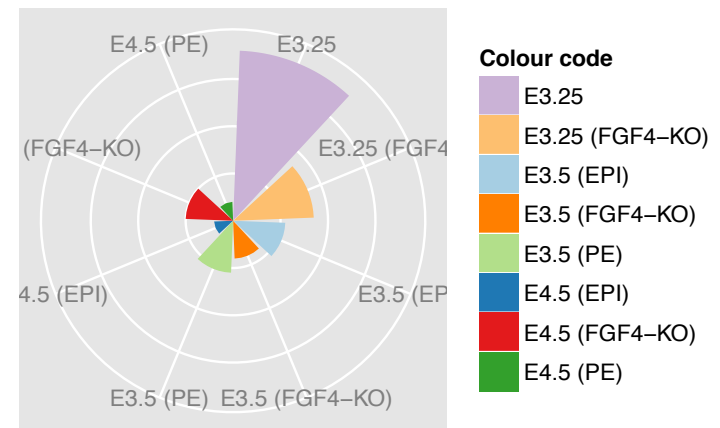
No geom defined yet!

```
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")
```

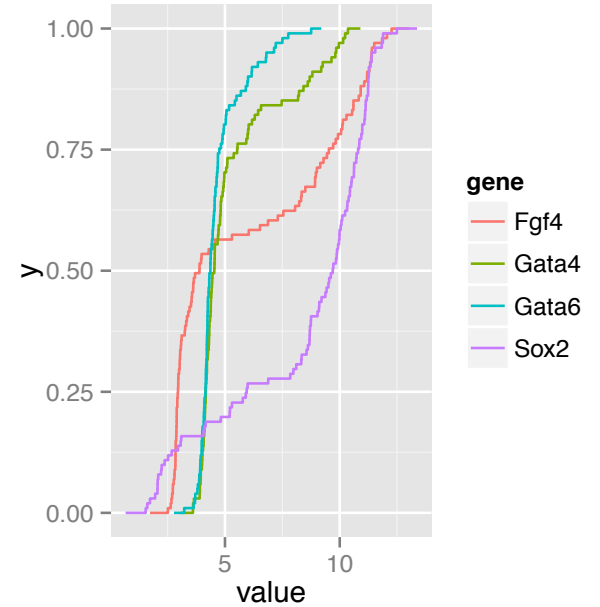
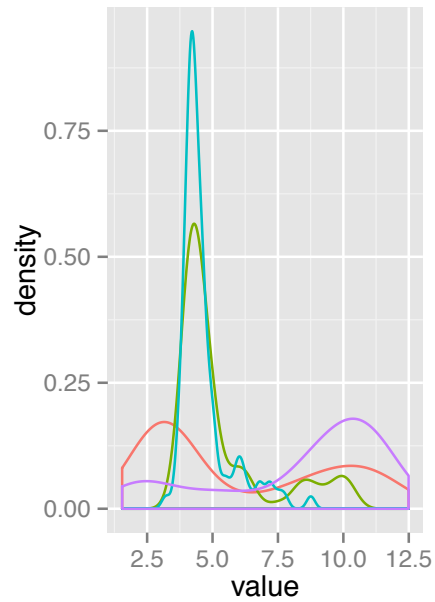
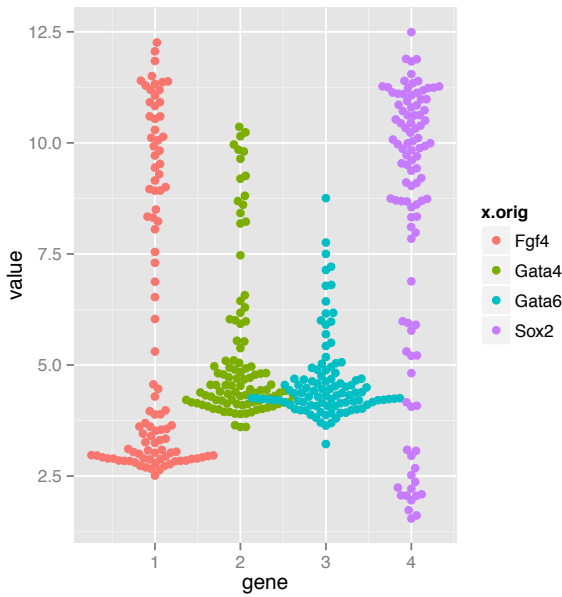
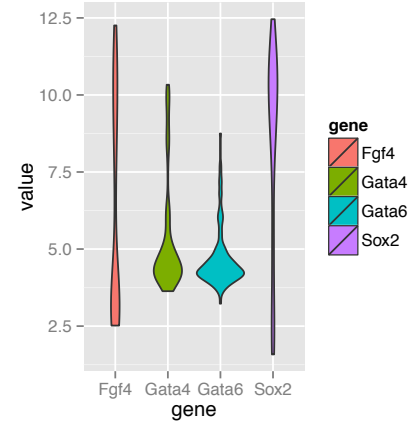
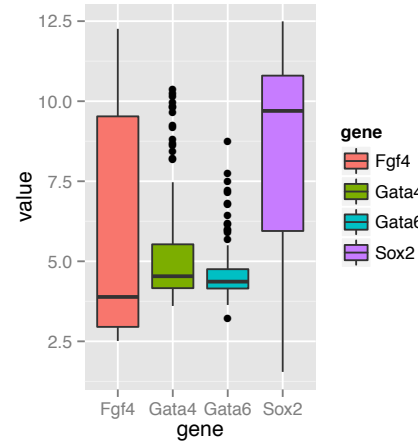
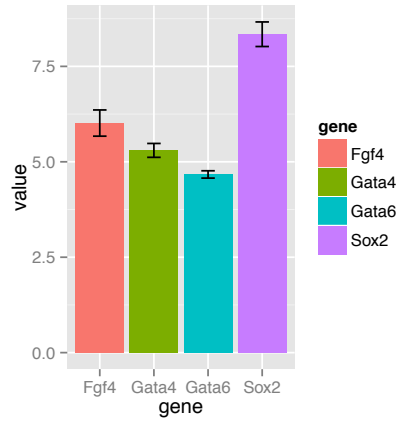
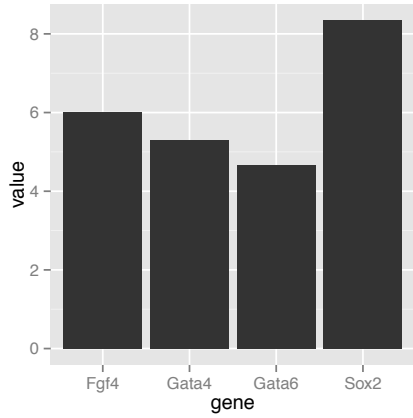


```
pb.polar <- pb + coord_polar() +  
  theme(axis.text.x = element_text(angle = 0, hjust = 1),  
        axis.text.y = element_blank(),  
        axis.ticks = element_blank()) +  
  xlab("") + ylab("")
```

pb.polar



Showing 1D data



Discussion of 1D plot types

Boxplot makes sense for unimodal distributions

Histogram requires definition of bins (width, positions) and can create visual artifacts esp. if the number of data points is not large

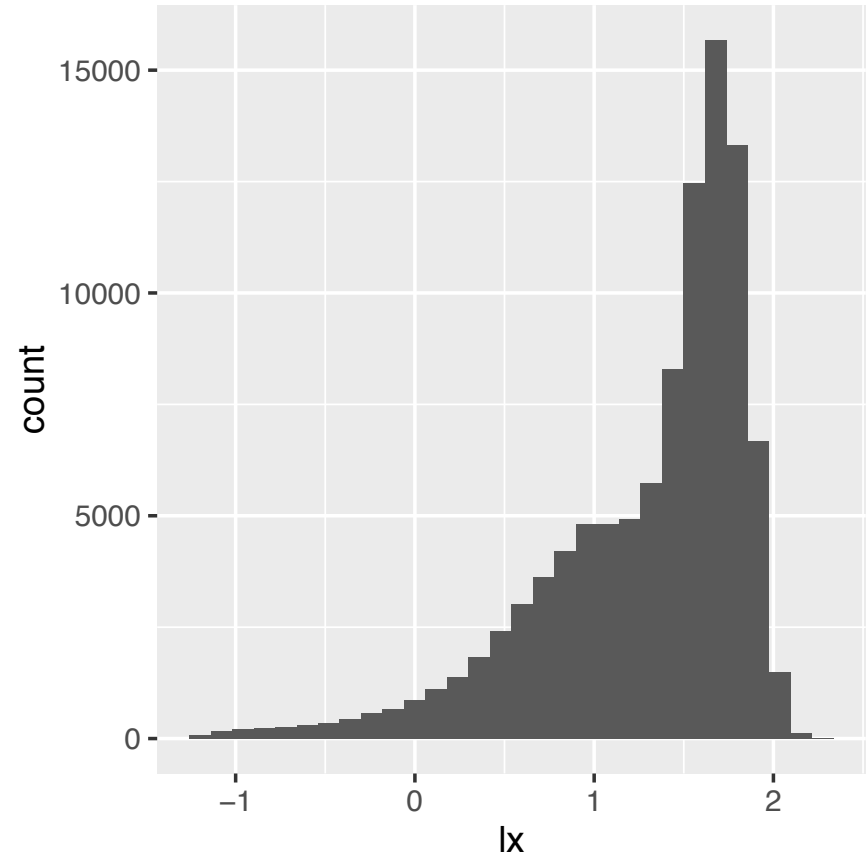
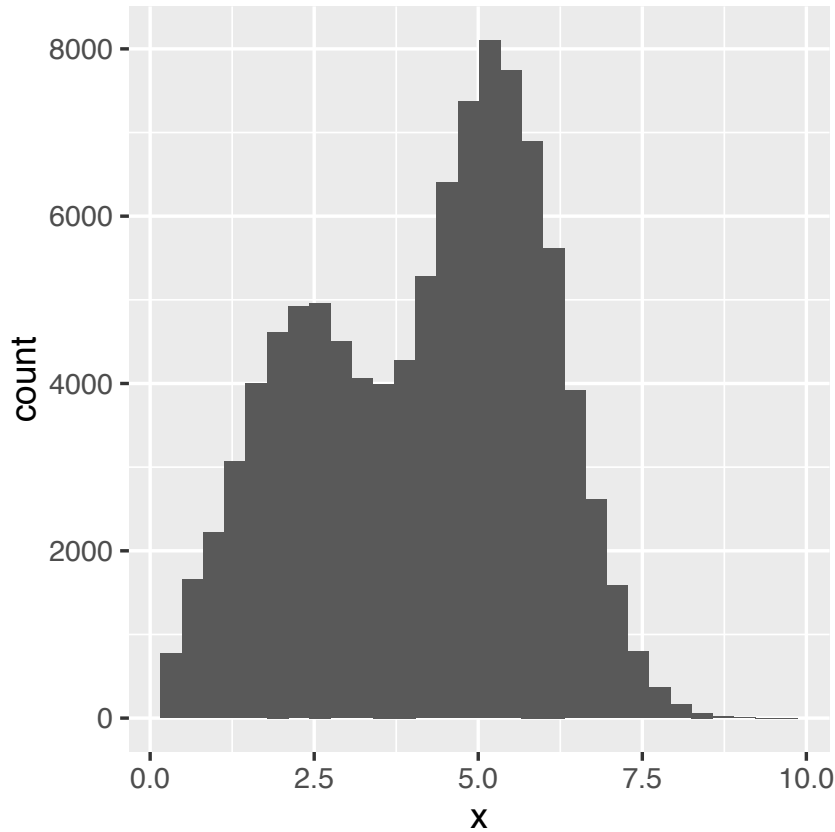
Density requires the choice of bandwidth; obscures the sample size (i.e. the uncertainty of the estimate)

ecdf does not have these problems; but is more abstract and interpretation requires more training. Good for reading off quantiles and shifts in location in comparative plots; OK for detecting differences in scale; less good for detecting multimodality.

Up to a few dozens of points - just show the data! (**beeswarm**)

Impact of non-linear transformation on the shape of a density

mixture of two normal distributions

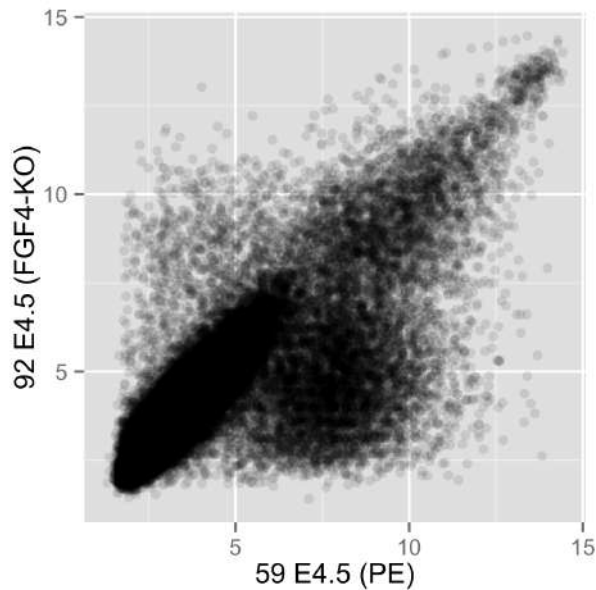
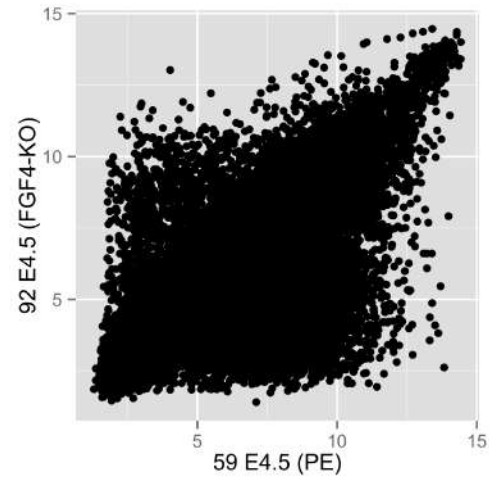


[Code example](#)

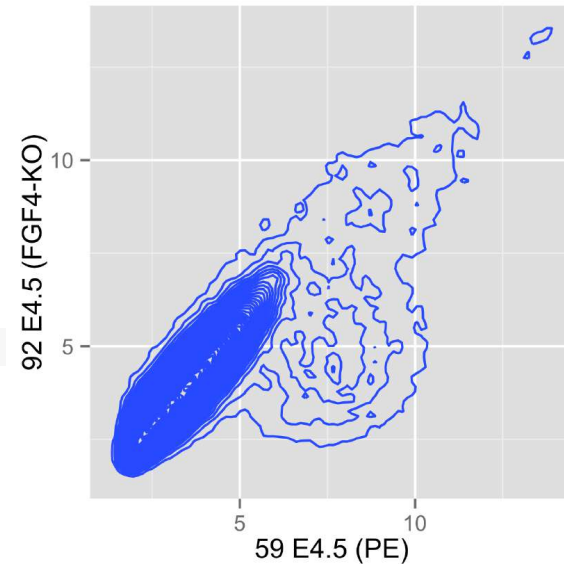
Figure 3.22: Histograms of the same data, with and without logarithmic transformation. The number of modes is different.

Showing 2D data

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

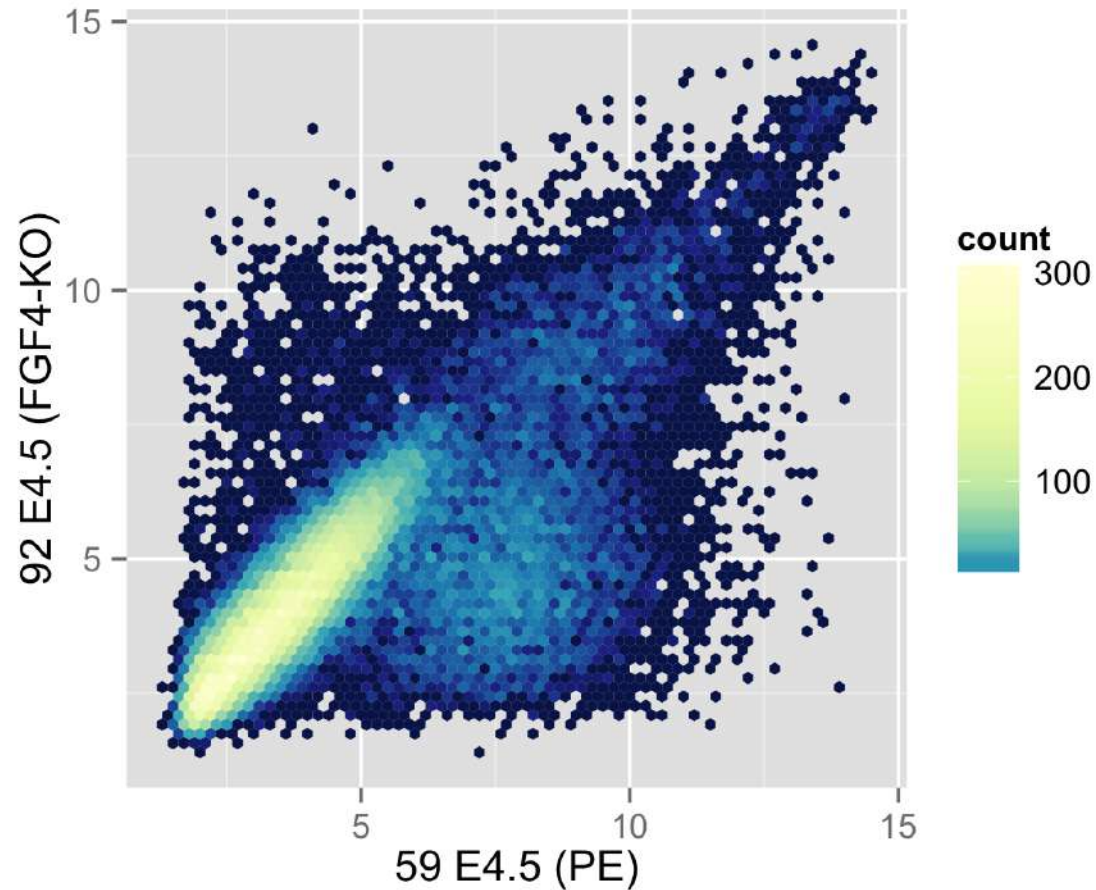


```
scp + geom_point(alpha = 0.1)
```



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

Showing 2D data



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

Plot shape, banking

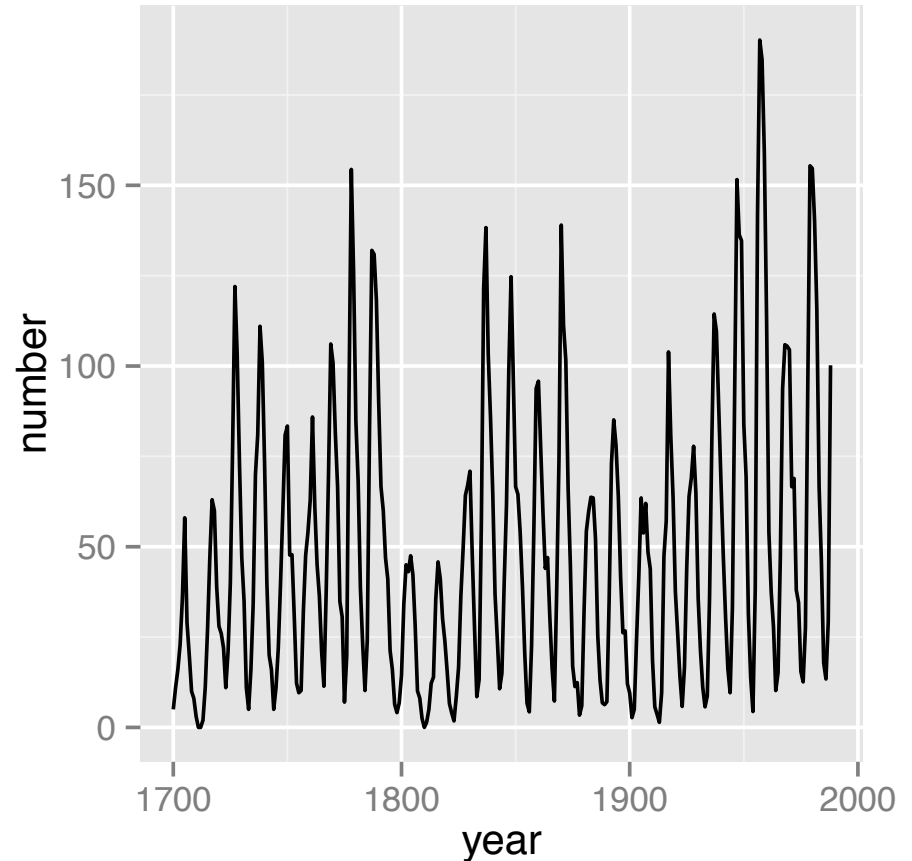
Yearly sunspot numbers
1849-1924

Changes in amplitude

Banking to 45 degrees:

Choose aspect ratio so that
center of absolute values of
slopes is 45 degrees

Sawtooth: Sunspot cycles
typically rise more rapidly than
they fall (pronounced for high
peaks, less for medium and
not for lowest)



Plot shape, banking

Yearly sunspot numbers
1849-1924

Changes in amplitude

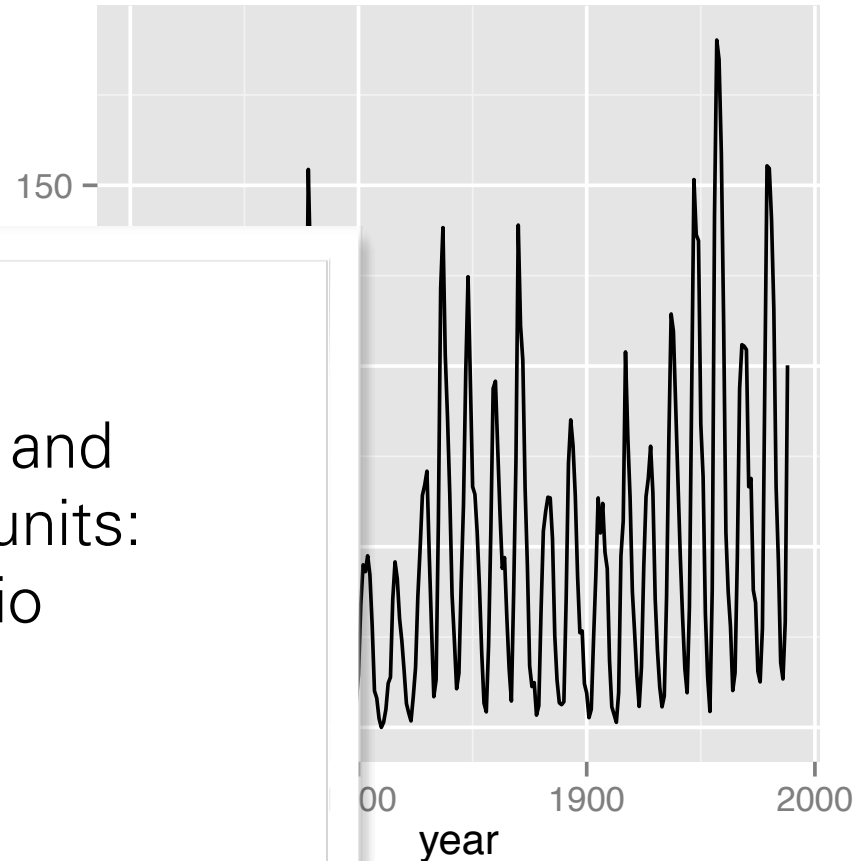
Banking

Choose
center of
slopes is

Sawtooth
typically

they fall (pronounced for high
peaks, less for medium and
not for lowest)

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

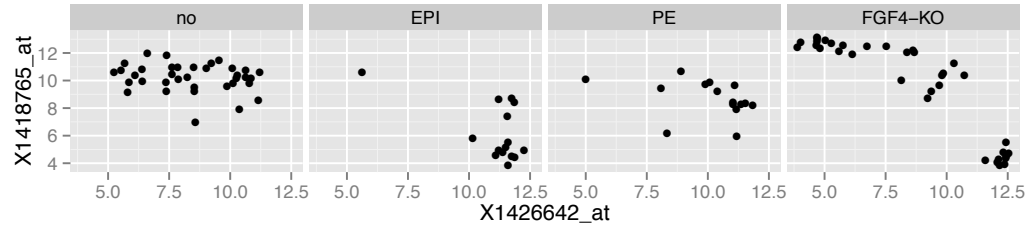


3-5 D and faceting

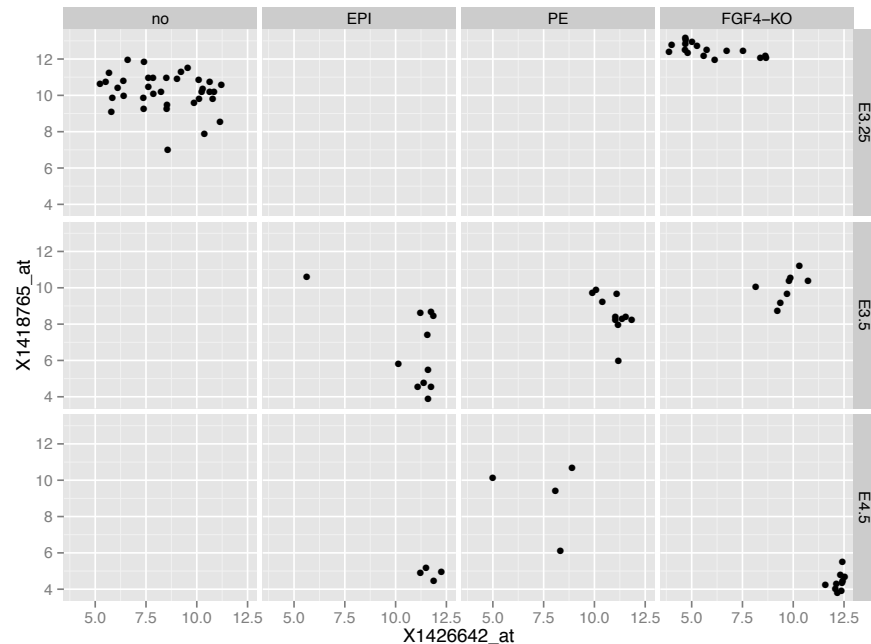
```
ggplot(dftx, aes( x = X1426642_at, y = X1418765_at)) +  
  geom_point() + facet_grid( . ~ lineage )
```

geom_point
offers these
aesthetics
(beyond x and y):

- fill
- colour
- shape
- size
- alpha



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

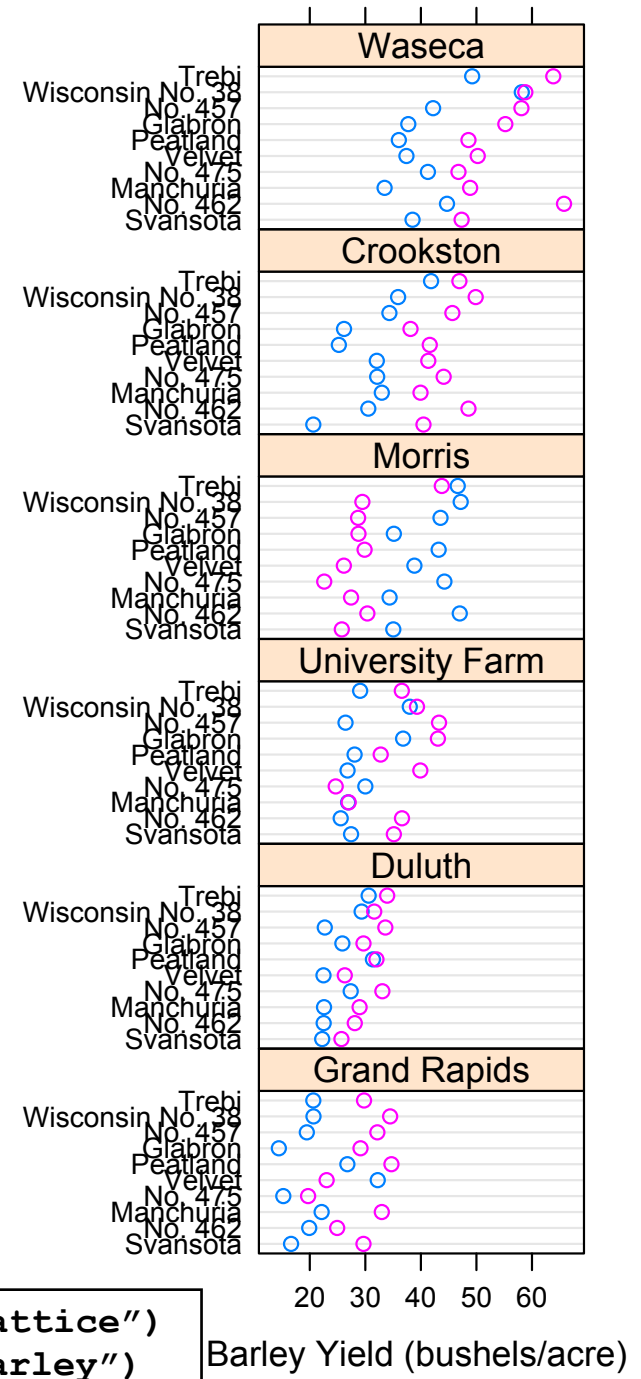


Data from an agricultural field trial to study the crop barley.

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 x 10 x 2 = 120 observations)

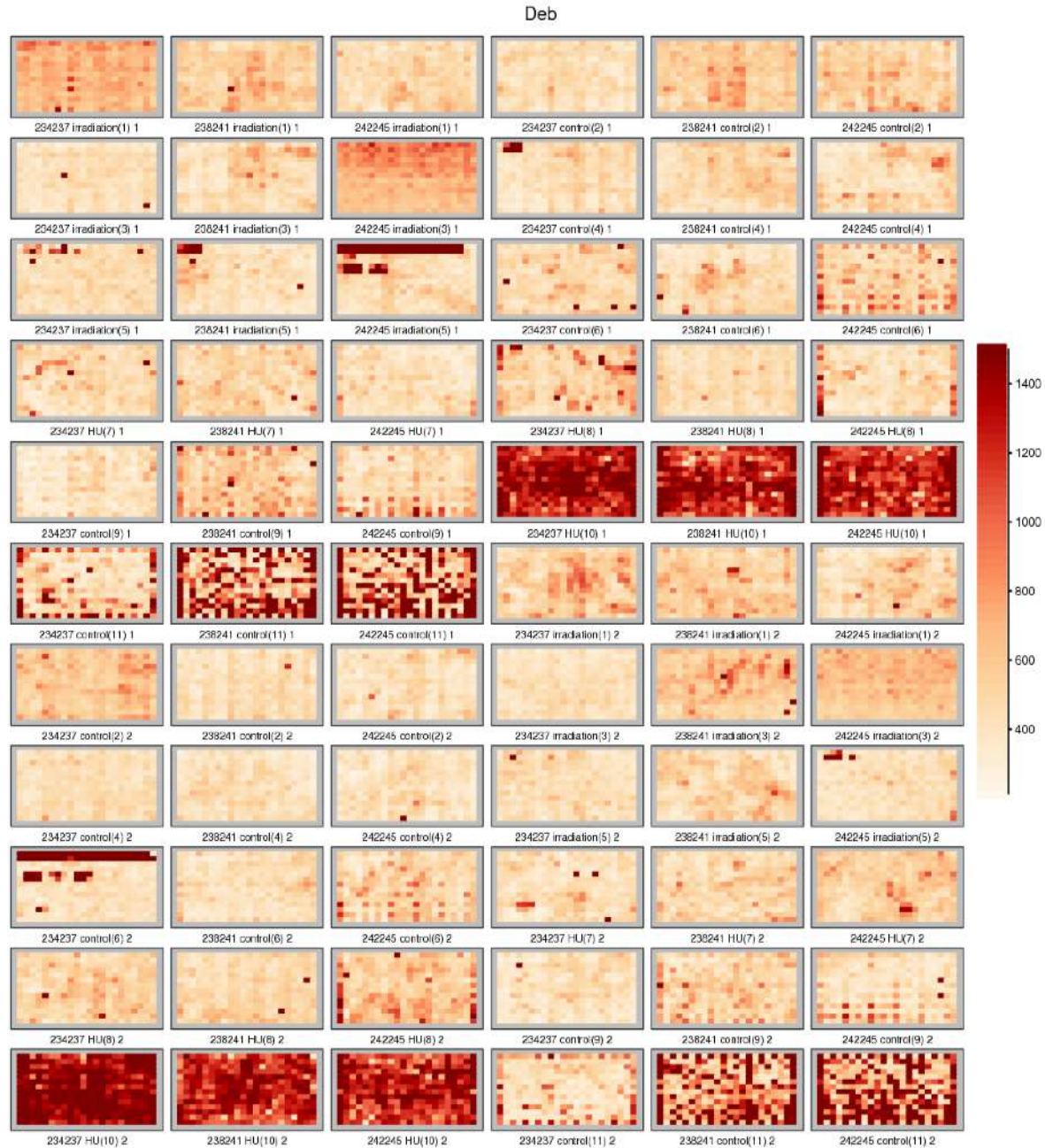
Note the data for Morris - reanalysis in the 1990s using Trellis revealed that the years had been flipped!



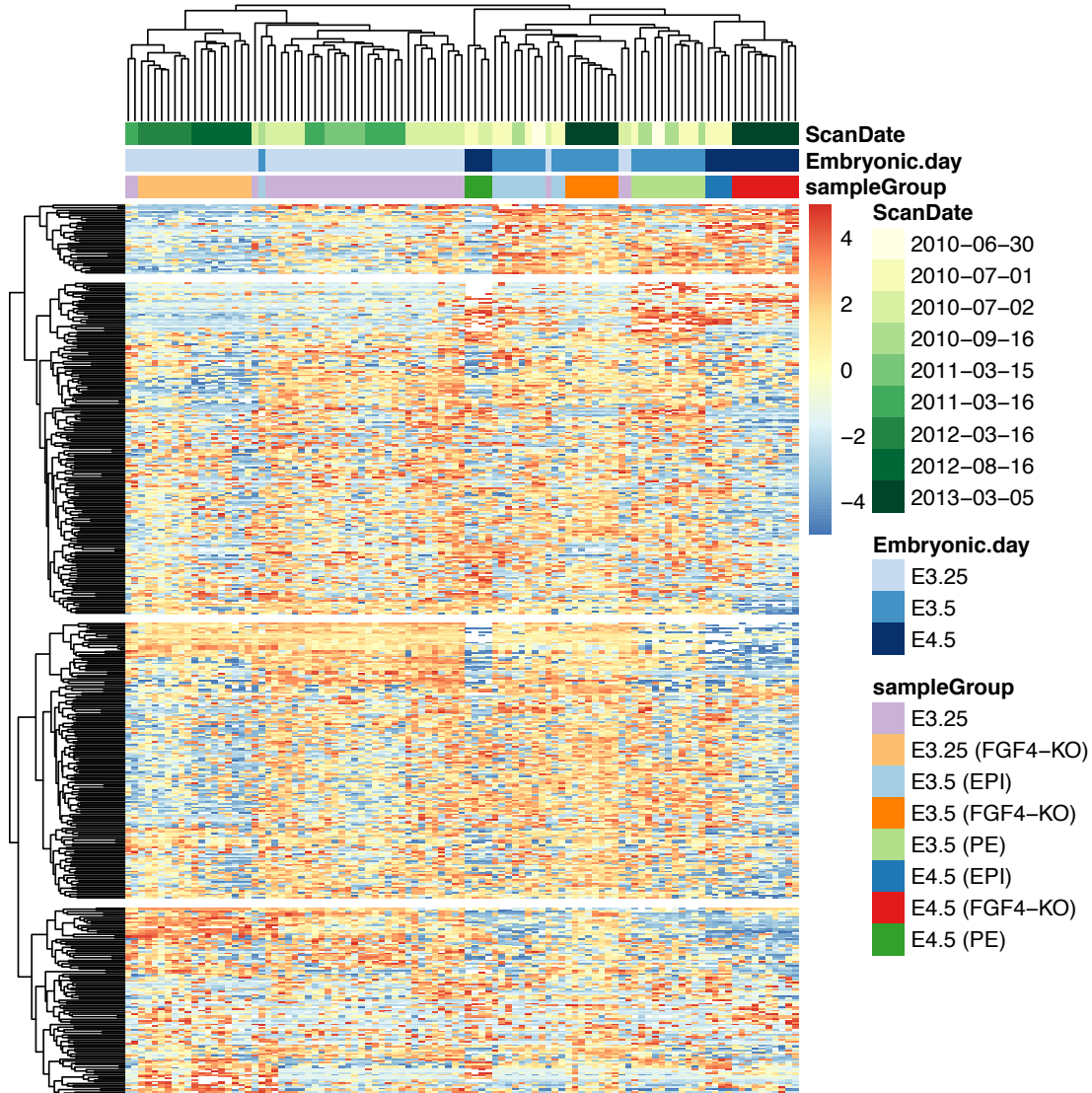
Demo ggvis

1. in R-Studio
2. <http://ggvis.rstudio.com/interactivity.html>

EDA for finding batch effects



pheatmap

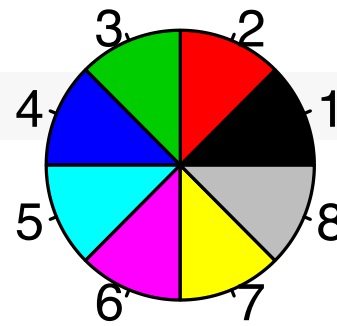


Many reasonable defaults

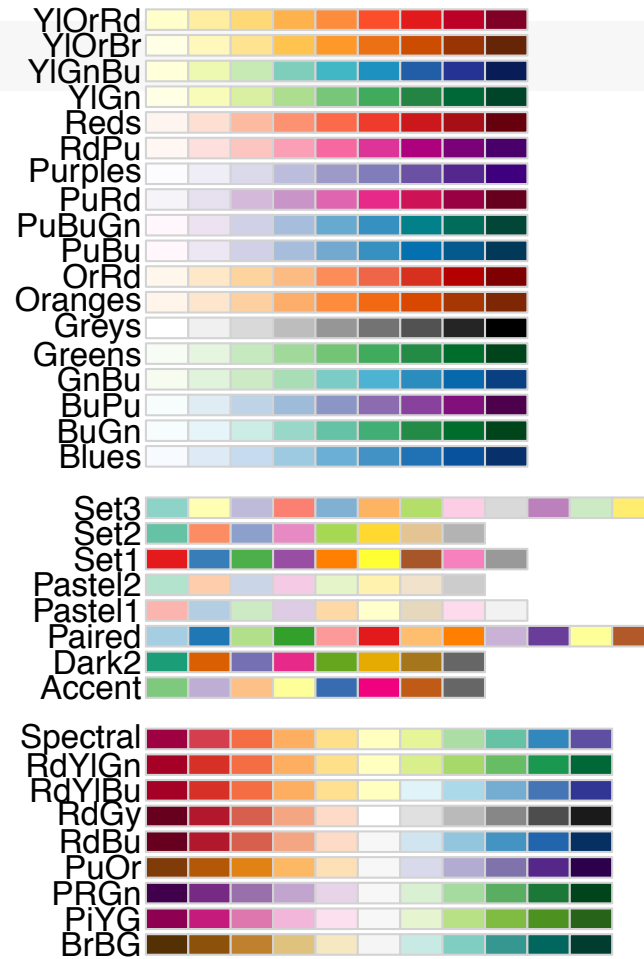
Easy to add column and row 'metadata' at the sides

See also [ComplexHeatmaps](#) package

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



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



```
pie(rep(1, 8), c
```

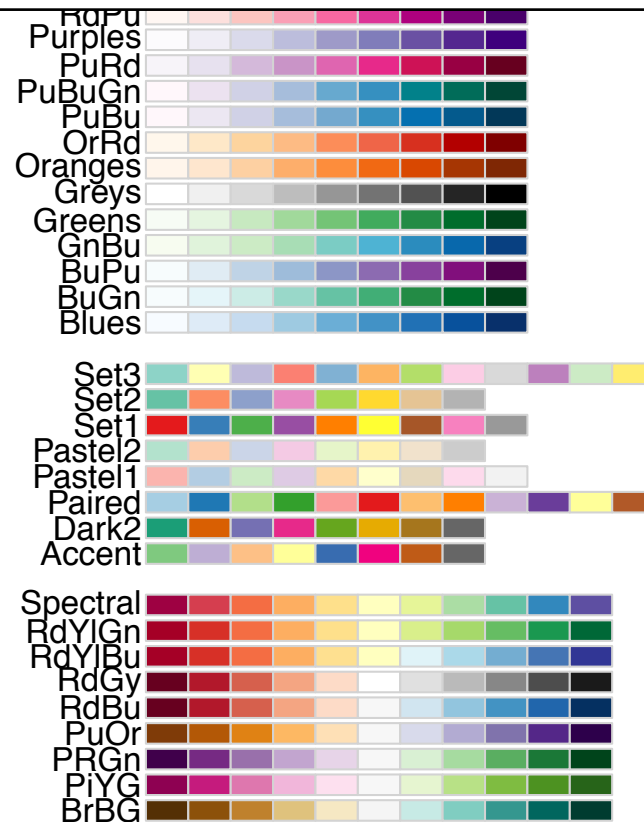
Consider these:

Different requirements for line & area colours

Many people are red-green colour blind

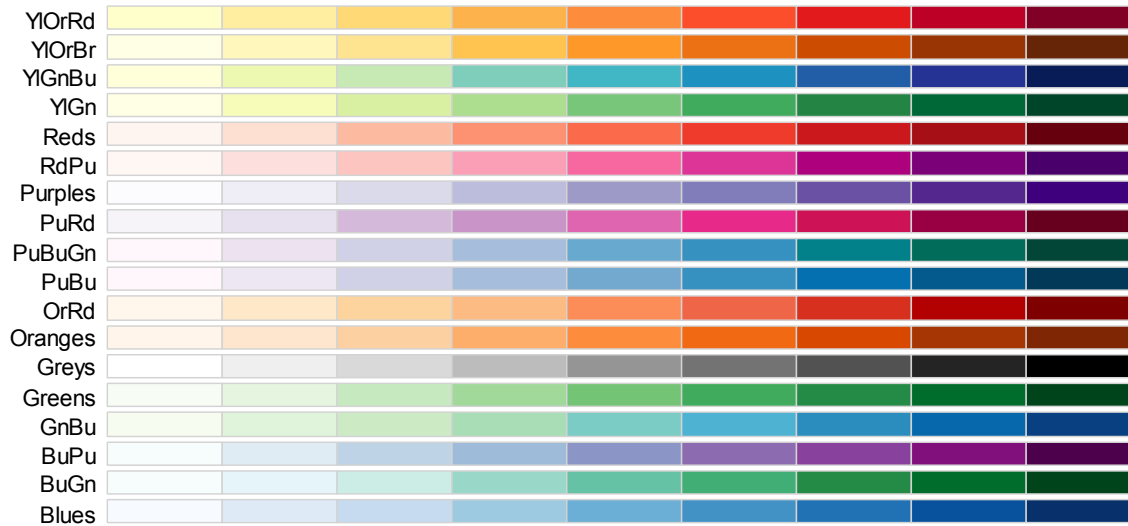
Lighter colours tend to make areas look larger than darker colours → use colors of equal luminance for filled areas.

```
display.brewer.
```

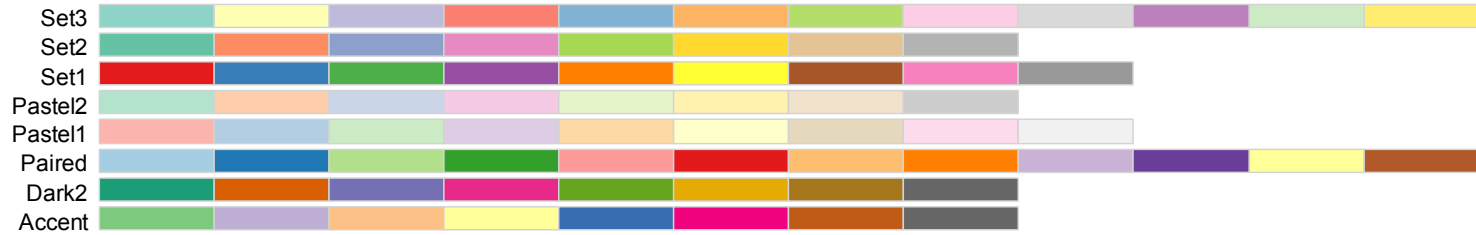


RColorBrewer

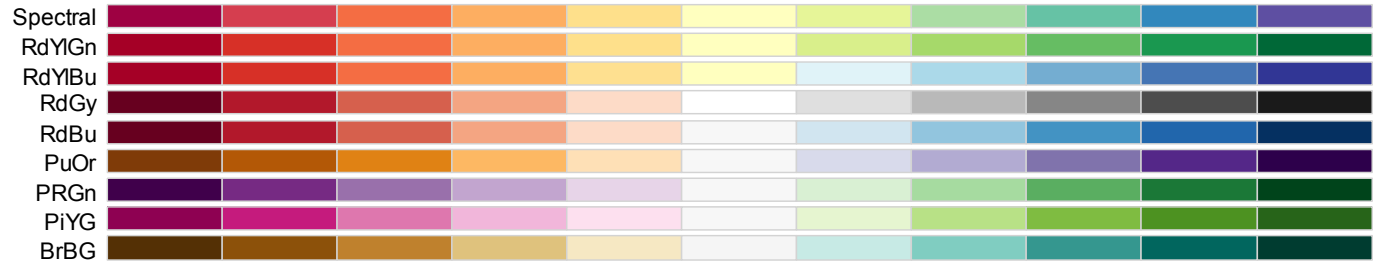
sequential



qualitative

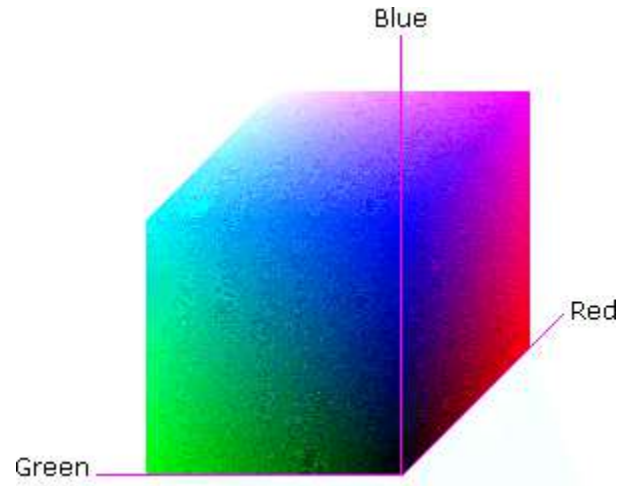
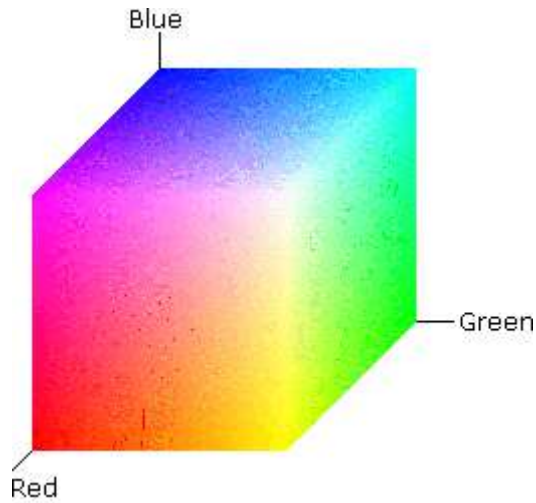


diverging



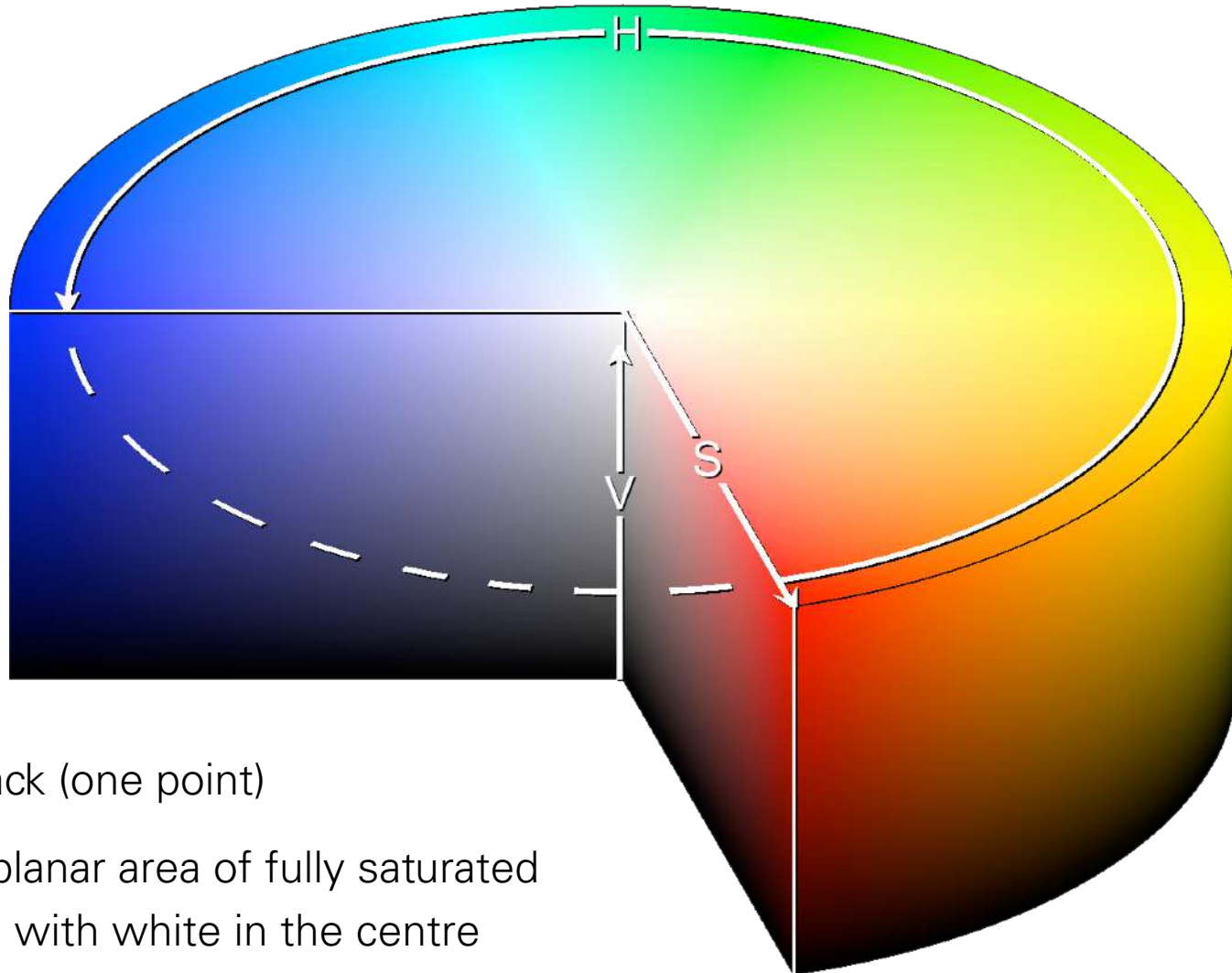
RGB color space

Motivated by computer screen hardware



HSV color space

Hue-Saturation-Value (Smith 1978)



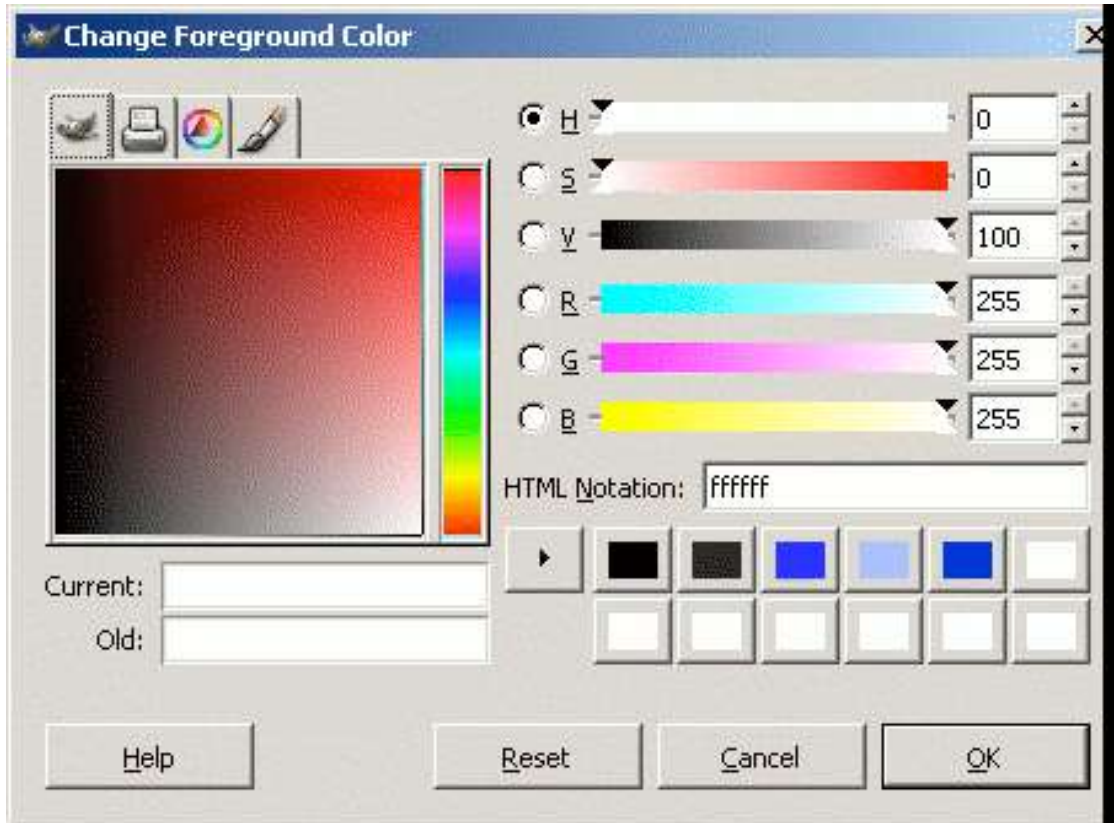
V_{\min} : black (one point)

V_{\max} : a planar area of fully saturated colours, with white in the centre

wikipedia

HSV color space

GIMP colour selector



linear or circular hue
chooser

and

a two-dimensional
area (usually a square
or a triangle) to choose
saturation and value/
lightness for the
selected hue

(almost) 1:1 mapping between RGB and HSV space

Conversion from RGB to HSL or HSV

Let $r, g, b \in [0, 1]$ be the red, green, and blue coordinates, respectively, of a color in RGB space.

Let \max be the greatest of $r, g,$ and $b,$ and \min the least.

To find the hue angle $h \in [0, 360]$ for either HSL or HSV space, compute:

$$h = \begin{cases} 0 & \text{if } \max = \min \\ (60^\circ \times \frac{g-b}{\max-\min} + 0^\circ) \bmod 360^\circ, & \text{if } \max = r \\ 60^\circ \times \frac{b-r}{\max-\min} + 120^\circ, & \text{if } \max = g \\ 60^\circ \times \frac{r-g}{\max-\min} + 240^\circ, & \text{if } \max = b \end{cases}$$

To find saturation and lightness $s, l \in [0, 1]$ for HSL space, compute:

$$s = \begin{cases} 0 & \text{if } \max = \min \\ \frac{\max - \min}{\max + \min} = \frac{\max - \min}{2l}, & \text{if } l \leq \frac{1}{2} \\ \frac{\max - \min}{2 - (\max + \min)} = \frac{\max - \min}{2 - 2l}, & \text{if } l > \frac{1}{2} \end{cases}$$
$$l = \frac{1}{2}(\max + \min)$$

wikipedia

The value of h is generally normalized to lie between 0 and 360° , and $h = 0$ is used when $\max = \min$ (that is, for grays) though the hue has no geometric meaning there, where the saturation s is zero. Similarly, the choice of 0 as the value for s when l is equal to 0 or 1 is arbitrary.

HSL and HSV have the same definition of [hue](#), but the other components differ. The values for s and v of an HSV color are defined as follows:

$$s = \begin{cases} 0, & \text{if } \max = 0 \\ \frac{\max - \min}{\max} = 1 - \frac{\min}{\max}, & \text{otherwise} \end{cases}$$

$$v = \max$$

The range of HSV and HSL vectors is a cube in the [cartesian coordinate system](#); but since hue is really a cyclic property, with a cut at red, visualizations of these spaces invariably involve hue circles;^[4] [cylindrical](#) and conical (bi-conical for HSL) depictions are most popular; [Spherical](#) depictions are also possible.

Perceptual colour spaces

Human perception of colour corresponds neither to RGB nor HSV coordinates, and neither to the physiological axes light-dark, yellow-blue, red-green

Rather to polar coordinates in the colour plane (yellow/blue vs. green/red) plus a third light/dark axis. Perceptually-based colour spaces try to capture these perceptual axes:

1. hue (dominant wavelength)
2. chroma (colourfulness, intensity of color as compared to grey)
3. luminance (brightness, amount of grey)

CIELUV and HCL

Commission Internationale de l'Éclairage (CIE) in 1931, on the basis of extensive colour matching experiments with people, defined a “standard observer” who represents a typical human colour response (response of the three light cones + their processing in the brain) to a triplet (x,y,z) of primary light sources (in principle, this could be monochromatic R, G, B; but CIE choose something a bit more subtle)

1976: CIELUV and CIELAB are perceptually based coordinates of colour space.

CIELUV (L, u, v) -coordinates is preferred by those who work with emissive colour technologies (such as computer displays) and CIELAB by those working with dyes and pigments (such as in the printing and textile industries)

HCL colours

$$(u,v) = \text{chroma} * (\cos h, \sin h)$$

L the same as in CIELUV, (C, H) are simply polar coordinates for (u,v)

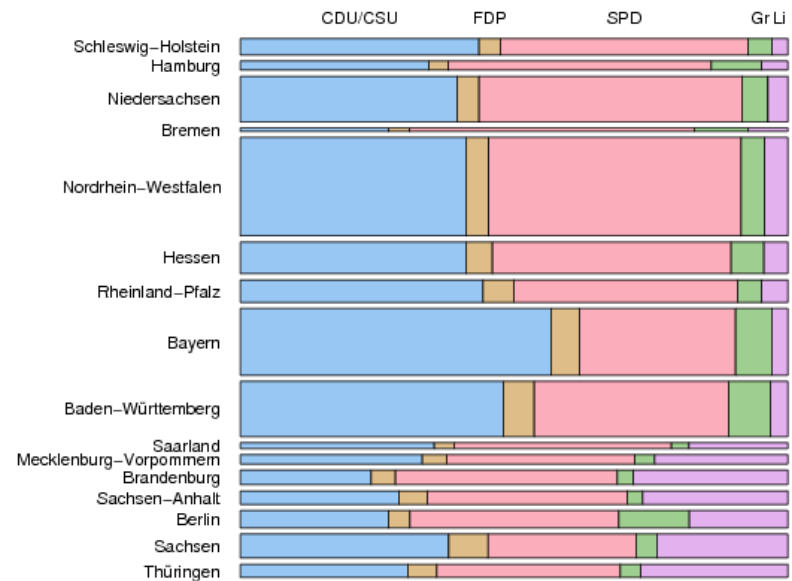
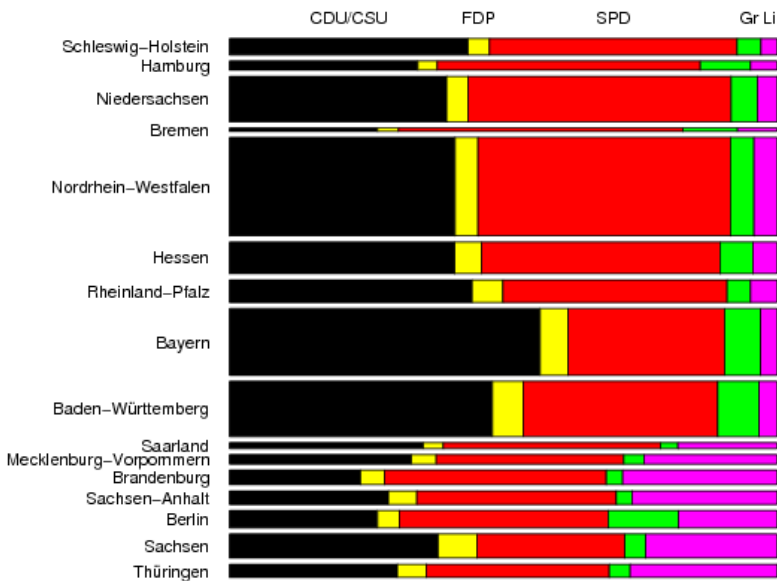
1. hue (dominant wavelength)
2. chroma (colorfulness, intensity of color as compared to gray)
3. luminance (brightness, amount of gray)



a**b**

Figure 2: Circles in HCL colorspace. *a*: circles in HCL space at constant $L = 75$, with the angular coordinate H varying from 0 to 360 and the radial coordinate $C = 0, 10, \dots, 60$. *b*: constant $C = 50$, and $L = 10, 20, \dots, 90$.

Pick your favourite

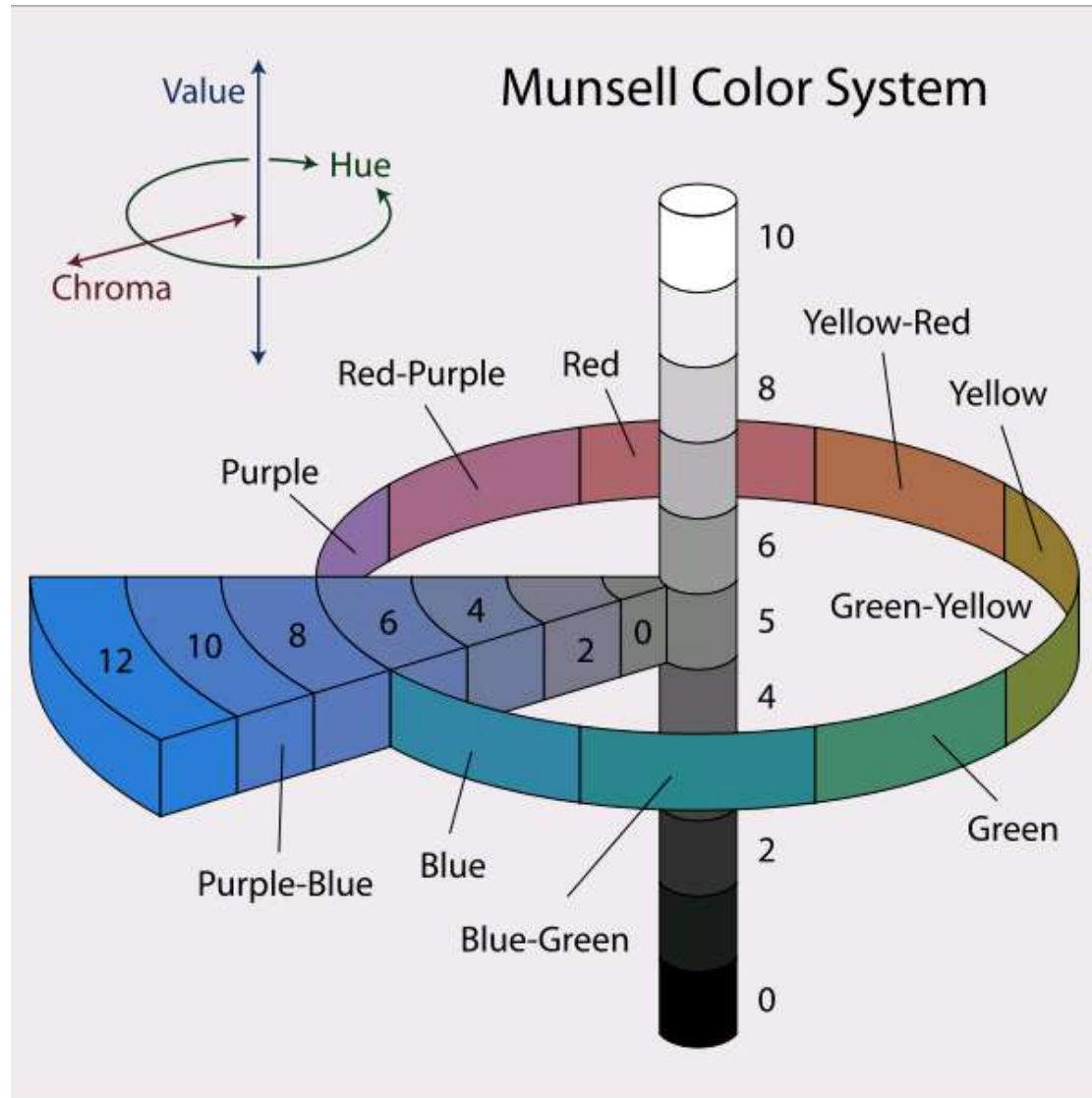


From A. Zeileis, Reensburg 2007

Albert Munsell (1858-1918) divided the circle of hues into 5 main hues — R, Y, G, B, P (red, yellow, green, blue and purple).

Value, Chroma: ranges divided into 10 equal steps.

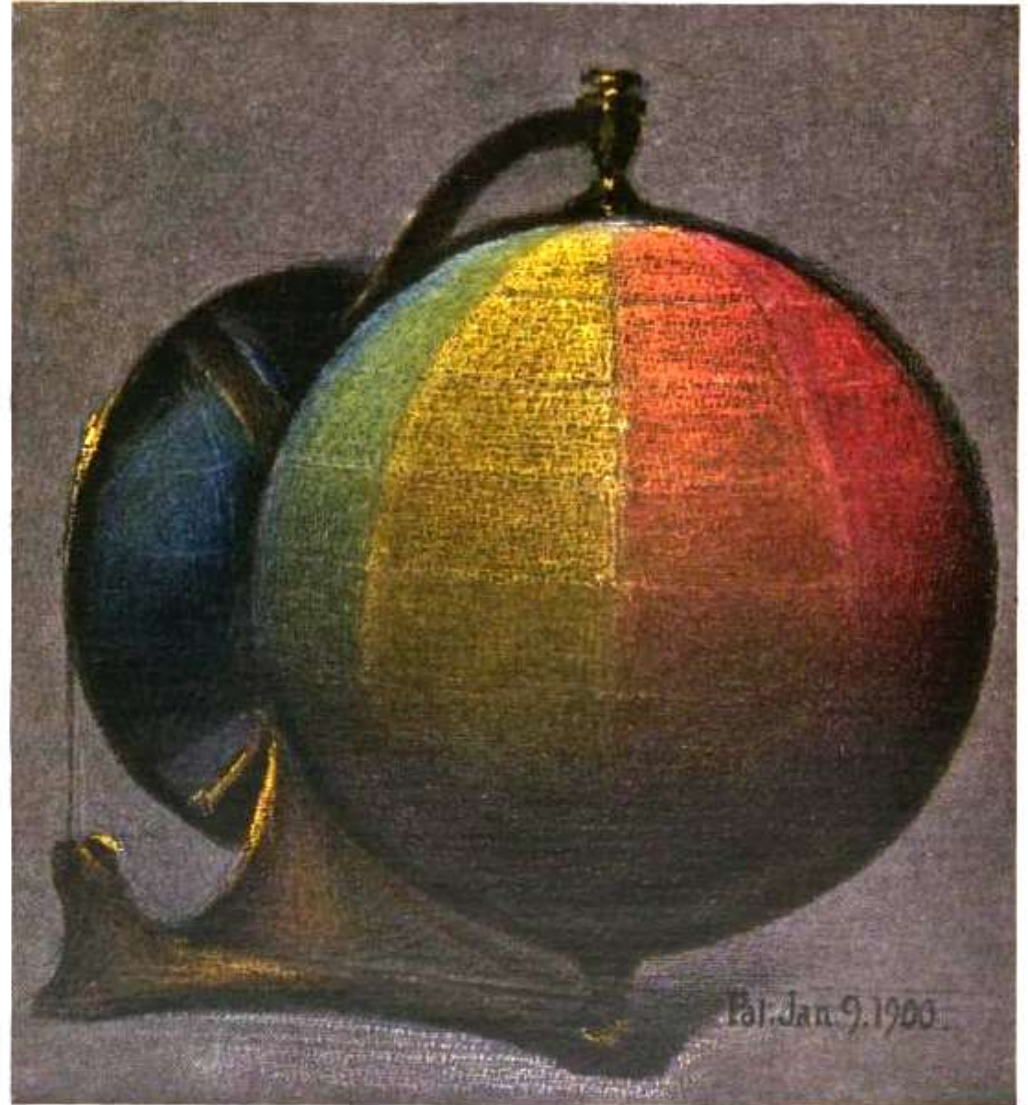
E.g. R 4/5 = hue of red with a value of 4 and a chroma of 5.



Albert Munsell
(1858-1918) divided the
circle of hues into 5 main
hues — R, Y, G, B, P (red,
yellow, green, blue and
purple).

Value, Chroma: ranges
divided into 10 equal
steps.

E.g. R 4/5 = hue of red
with a value of 4 and a
chroma of 5.



A BALANCED COLOR SPHERE

Colour Harmony



Figure 3: The principal Munsell 5/5 colours. From the top these are R 5/5, Y 5/5, G 5/5, B 5/5 and P 5/5. This figure is redrawn from Birren (1969).

Figure 4: The same images as Figure 3, but drawn with full saturation HSV colours.

Balance

The intensity of colour which should be used is dependent on the area that that colour is to occupy. Small areas need to be more colourful than larger ones.

Choose colours centered on a mid-range or neutral value, or;

Choose colours at equally spaced points along smooth paths through (perceptually uniform) colour space: equal luminance and chroma and correspond to set of evenly spaced hues.

Acknowledgements

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