Elegant Graphics for Data Analysis with ggplot2

Yann Abraham

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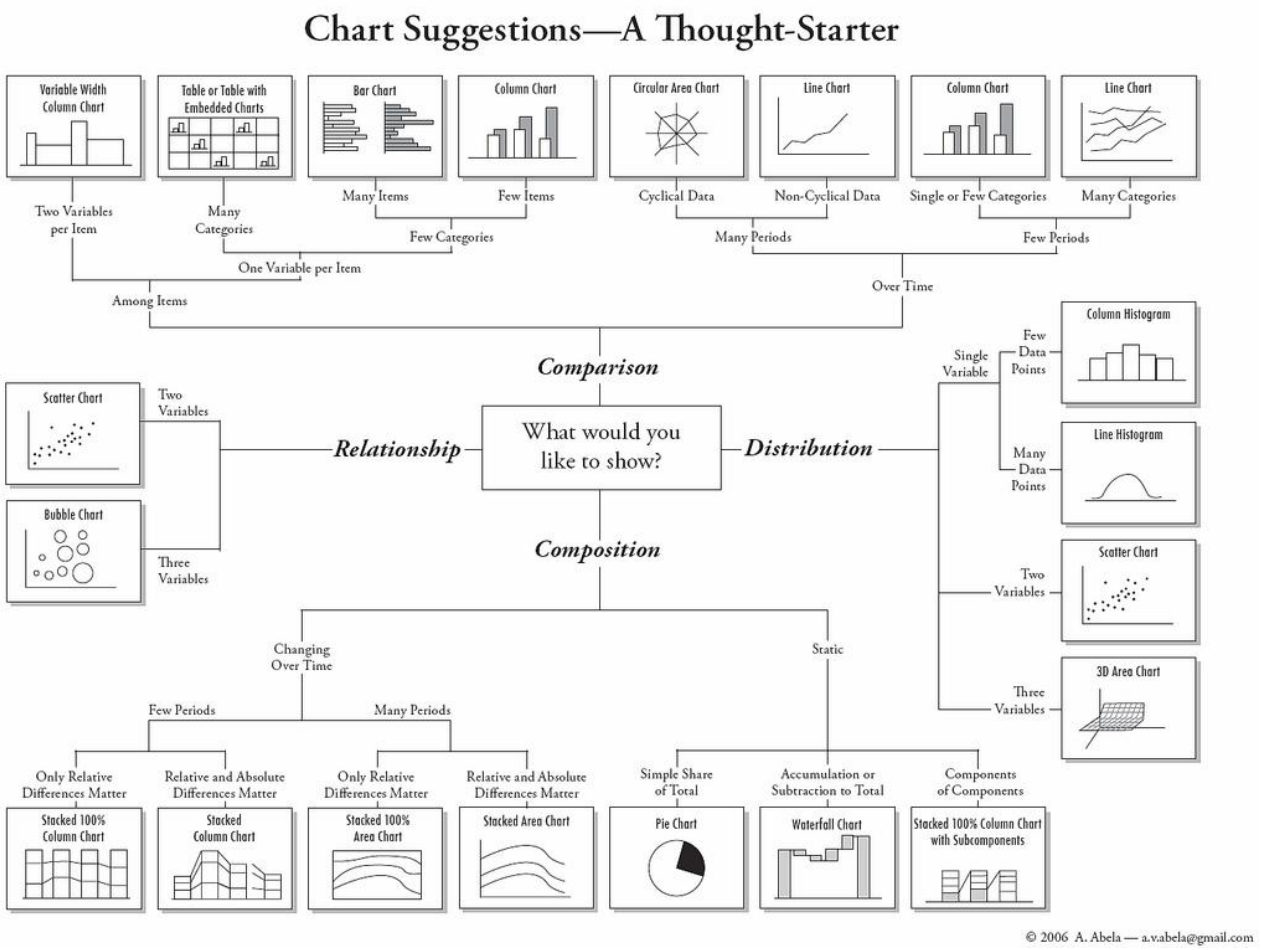
Who is Yann Abraham

- Biochemist by training
- Bioinformatician by trade
- Pharma/Biotech
  - Cellzome AG
  - Novartis Pharma AG

- http://ch.linkedin.com/in/yannabraham

How to Represent Data



“A Picture is Worth a Thousand Words”

- Visualization is a critical component of data analysis
- Graphics are the most efficient way to digest large volumes of data & identify trends
- Graphical design is a mixture of mathematical and perceptual science

A Straightforward Way to Create Visualizations

- Grammar of Graphics provides a framework to streamline the description and creation of graphics
- For a given dataset to be displayed:
  - Map variables to aesthetics
  - Define Layers
    - A representation (a 'geom') ie line, boxplot, histogram,…
    - Associated statistical transformation ie counts, model,…
  - Define Scales
    - Color, Shape, axes,…
  - Define Coordinates
  - Define Facets

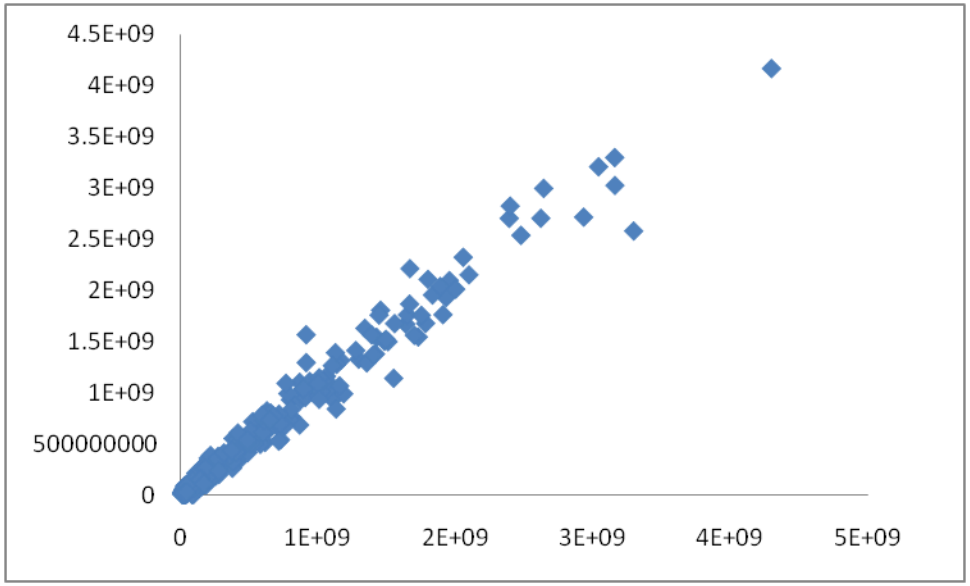
Why Use *ggplot2*?

- Simple yet powerful syntax
- Provides a framework for creating any type of graphics
- Implements basic graphical design rules by default

An Example

- 4 cell lines where treated with a compound active against a class of enzymes
- Proteins where extracted and quantified using mass spectrometry
- Is there anything interesting?!?

Excel…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4E+09
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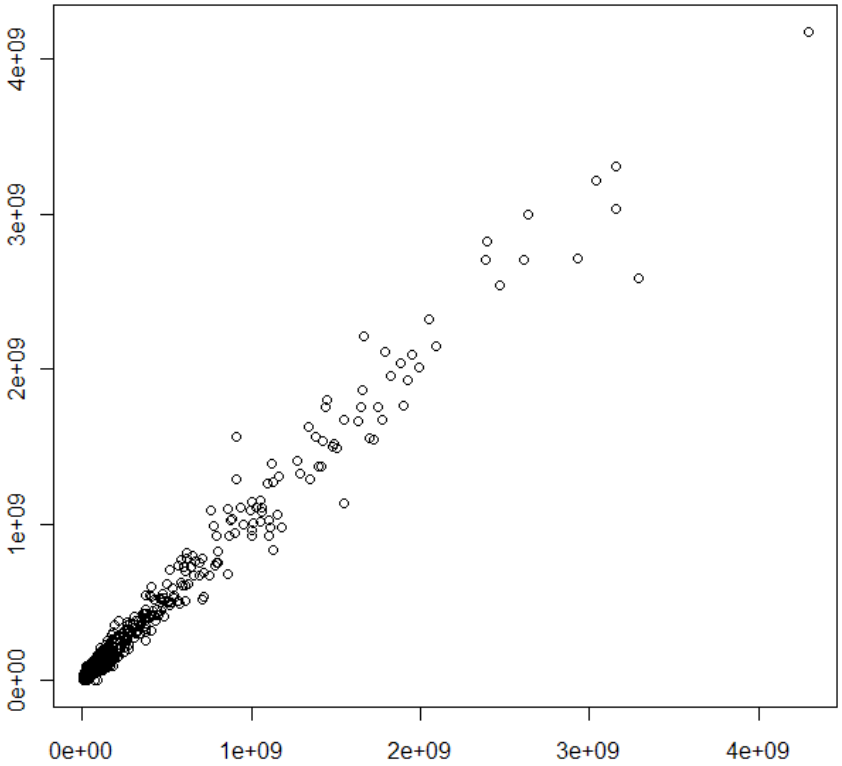
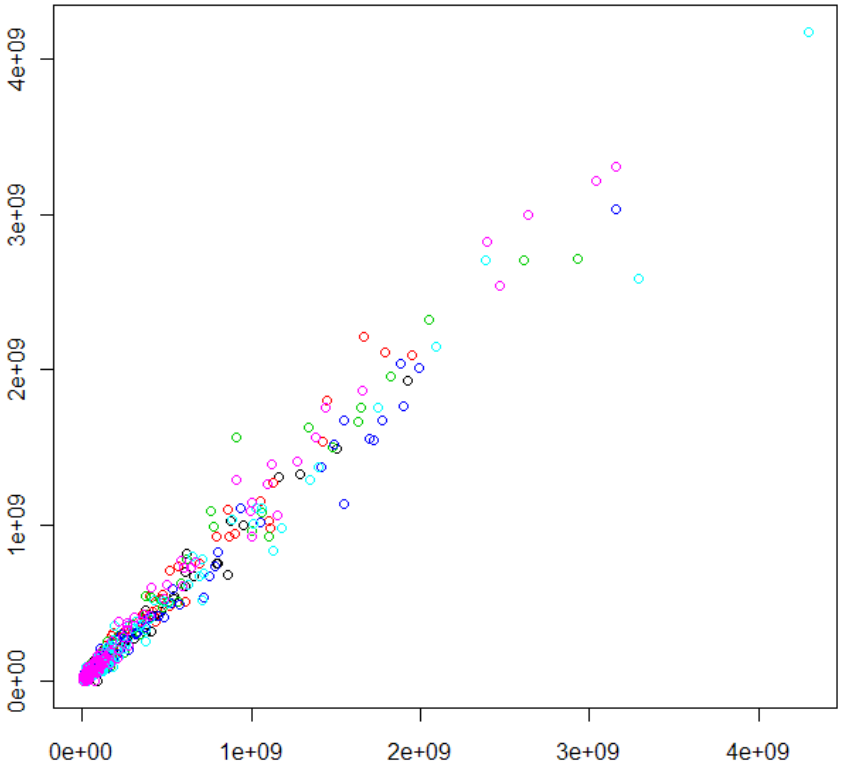
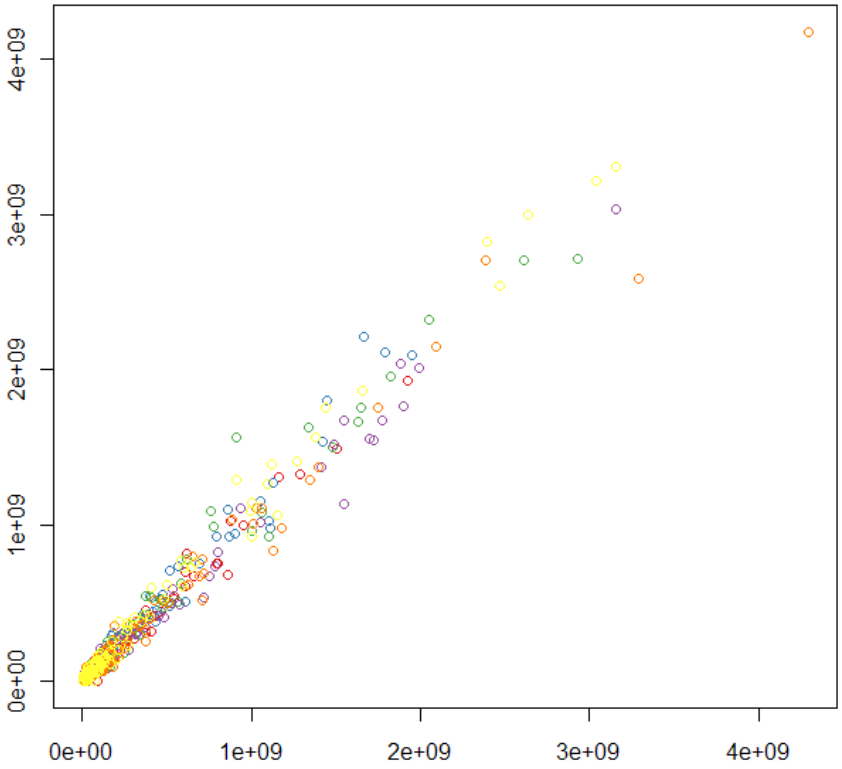
R…



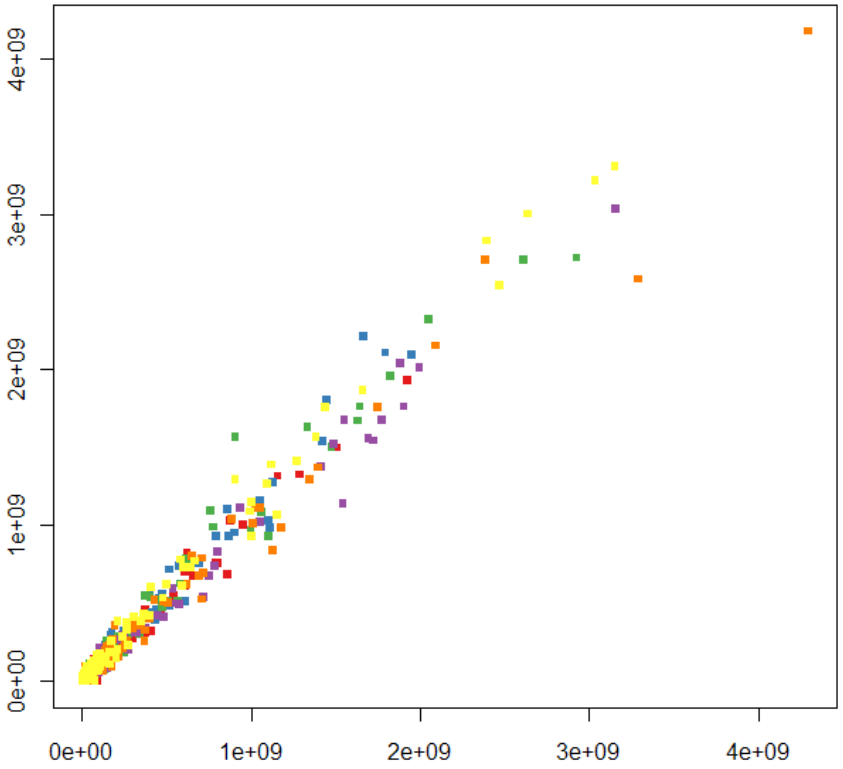
R…



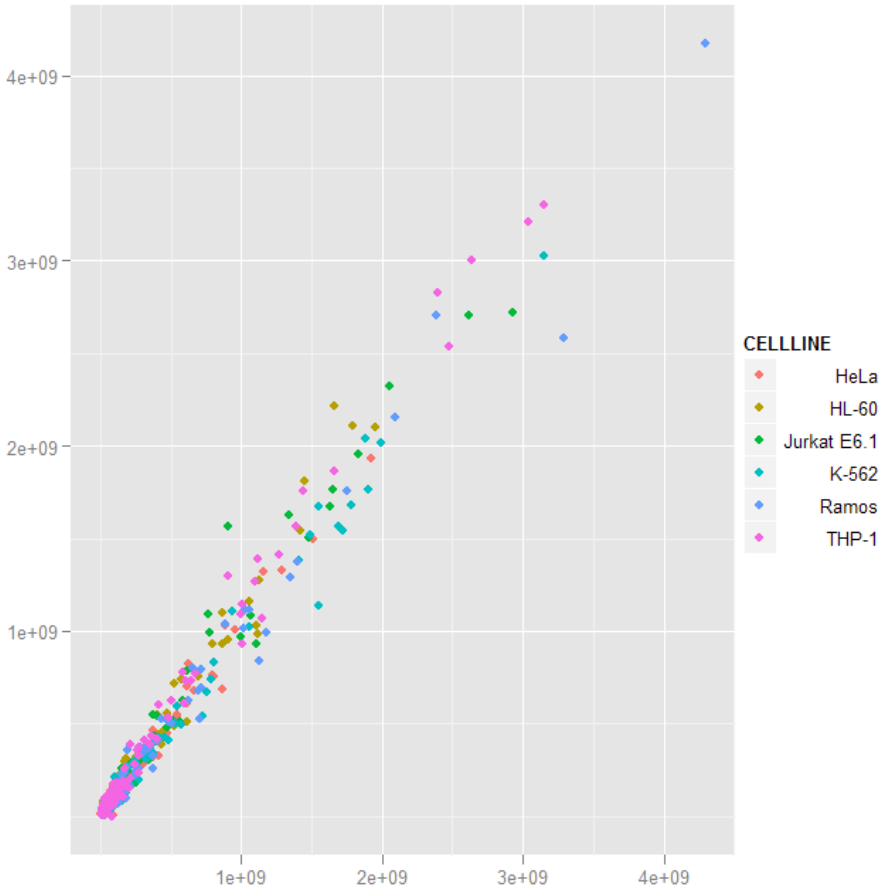
R…



R… (this could go on for hours)



…ggplot2!


4e+09
3e+09
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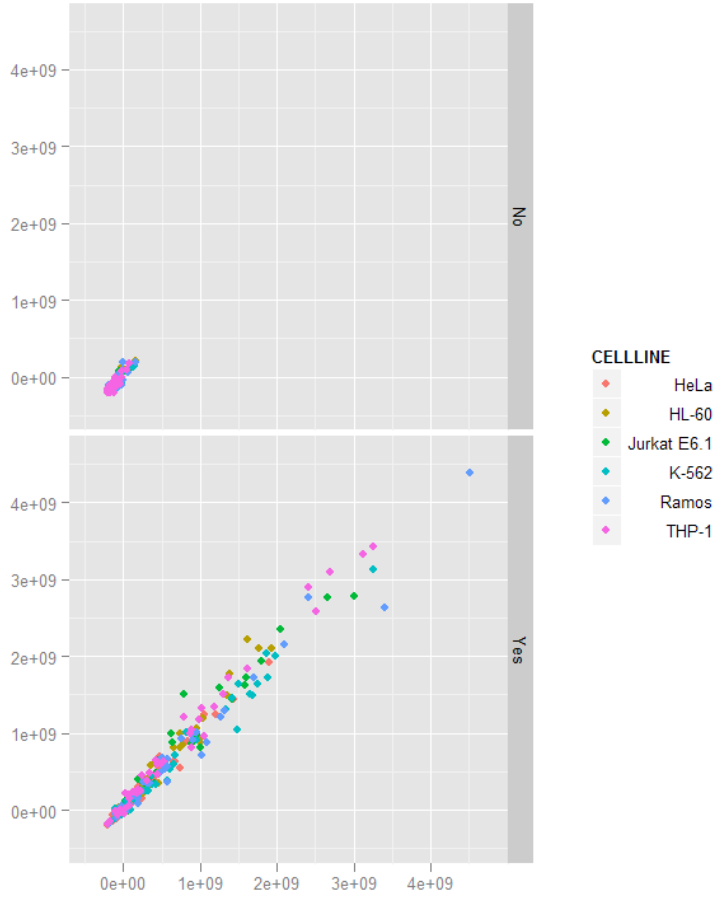
CELLLINE
HeLa
HL-60
Jurkat E6.1
K-562
Ramos
THP-1

ggplot2!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3e+09
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K-562
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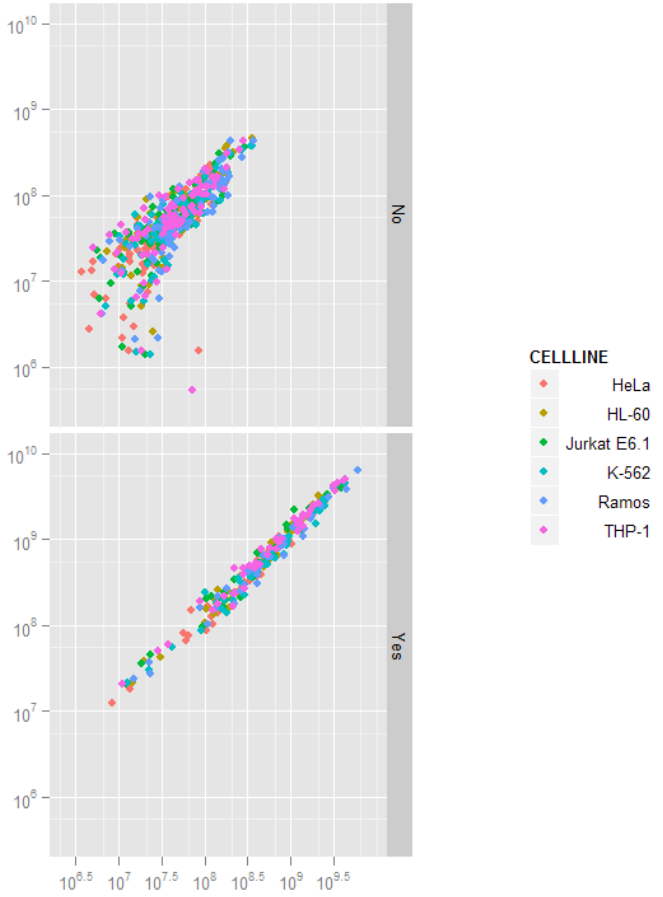
ggplot2!


10^{10}
10^{9}
10^{8}
10^{7}
10^{6}
No
Yes
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Jurkat E6.1
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ggplot2!


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Yes
CELLLINE
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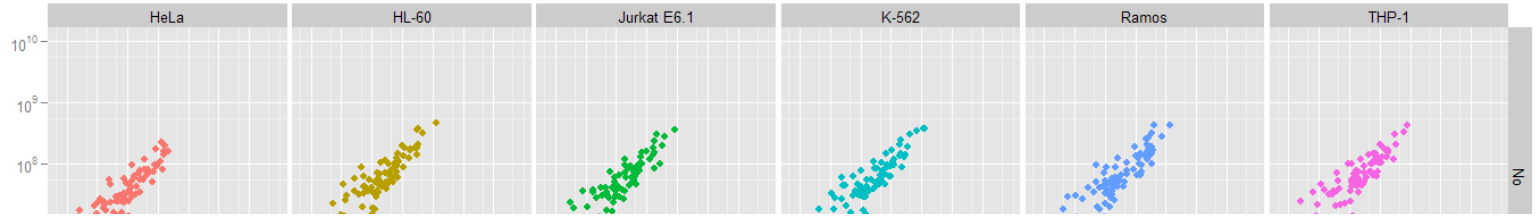
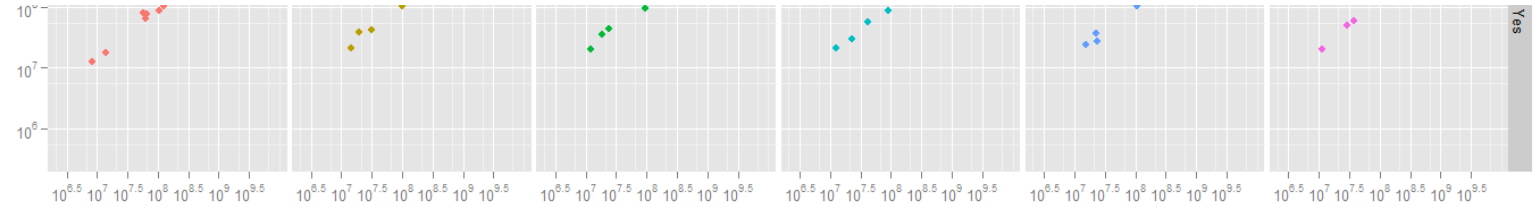
ggplot2!




```
qplot(Experiment_1,Experiment_2,data=comp,color=CELLLINE,facets=ISTARGET~CELLLINE)+
      coord_equal()+
      scale_x_log10()+
      scale_y_log10()
```



When Visualization Alone is Not Enough

- Some datasets are large multidimensional data structures
- Representing data from such structure requires data transformation
- R is good at handling large sets
- R functions for handling multidimensional sets are complex to use

Easy Data Transformation With *plyr*

- *plyr* provides wrappers around typical R operations
  - Split
  - Apply
  - Combine
- *plyr* functions are similar to the *by()* function

Why use *plyr*?

- Simple syntax
- Predictable output
- Tightly integrated into *ggplot2*

- This comes at a price – somewhat slower than *apply*

An Example

- Given a set of raw data from a High Throughput Screen, compute the plate-normalized effect

The standard R way

```
plate.mean <- aggregate(hts.data$RAW,
list(hts.data$PLATE_ID),mean)

names(plate.mean) <- c('PLATE_ID','PLATE_MEAN')

hts.data <- merge(hts.data,plate.mean)

hts.data$NORM<-
hts.data$RAW/hts.data$PLATE_MEAN
```

The *plyr* way

```
hts.data <-
ddply(hts.data,.(PLATE_ID),function(df) {
    df$NORM<-df$RAW/mean(df$RAW)
    return(df) }
)
```

Benefits of Using *plyr* & *ggplot2*

- Compact, straightforward syntax
  - Good basic output, complex options only required for polishing
- Shifts focus from plotting to exploring
  - Presentation graphics can be created from there at minimal cost
  - Data transformation is intuitive
- Powerful statistics available
  - It's R!

Some links…

- The Grammar of Graphics book by Leland Wilkinson
- The *ggplot2* book by Hadley Wickham
  - And the corresponding website
- A presentation about *plyr* by JD Long
  - And his initial blog post

THANK YOU FOR YOUR ATTENTION!