Week 2: Reproducibility, Ethics, Data Exploration

MATH-517 Statistical Computation and Visualization

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Section 1

Last Week's Leftovers

Our Workflow

- open RStudio (specifically your `StatComp-123456.Rproj` project)
- load some packages
- work in a (R Markdown) script
- save your progress
- push your changes to GitHub

Bookdown – a lot of interesting books written in R Markdown, including one of the references for this course, the R for Data Science book co-authored by Hadley Wickham.

Good Coding Practices

- consistency (following a certain style)
- indentation
- naming conventions – short but informative variable/function names
  - `camelCase`
  - `snake_case` – my personal preference
  - `dot.case` – not bad, but some languages will not allow it
  - others such as `PascalCase` or `kebab-case` are inferior
- simplicity
- comments (more the merrier!)
- load packages at the top
- loading data comes next (possibly in a separate script)
- functions come next (possibly in a separate script)
- use `set.seed()` if RNG present
- re-run with empty environment

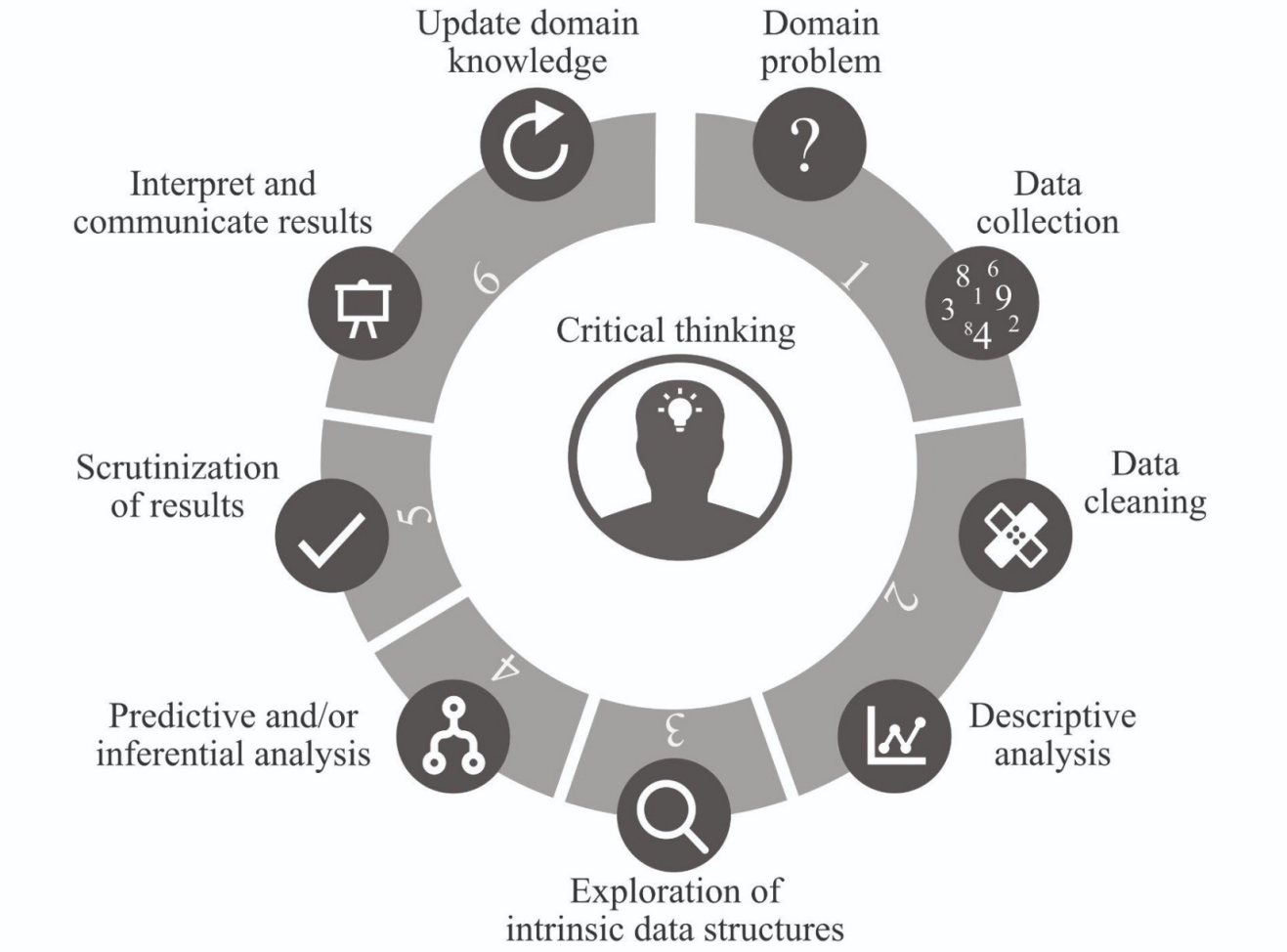
Section 2

Reproducibility

Job of a Statistician

- think about uncertainty
- estimate variation ($\Rightarrow$ confidence intervals, significance)
- avoid bias (not entirely possible, but anticipate and reduce it)
- build models emulating nature
  - inference about the models leads to conclusions about nature – but what if the model is a poor emulation of nature?
- provide *interpretable* models allowing for rational conclusions
  - prediction vs. information extraction
  - all models are wrong $\Rightarrow$ critical model validation
- draw conclusions from data
  - this is rather vague since almost everything is data
- traditional role: statisticians invited to analyze existing data
  - problems such as: does the existing data set contain the desired information?
- modern role: collaborative step-by-step
  - from acquisition of data to presentation of results
  - interdisciplinary communication
- exploratory vs. confirmatory analysis

Cycle of (Data-driven) Science



credit: Bin Yu, Rebecca Barter

Domains of Application

- actuarial science
- biostatistics (medicine, pharma, genetics, etc.)
- business
- chemometrics
- econometrics
- epidemiology
- finance
- geostatistics
- machine learning and AI
- official statistics (demography, surveys, etc.)
- psychology
- quality control
- reliability
- physics
- signal processing
- ...

Statistics in Science

An overwhelming portion of contemporary scientific conclusions is based on the concept of *statistical significance*:

- there is a hypothesis (e.g. drug A is better than drug B)
- data is collected (e.g. patients are split, some are given drug A, others drug B, and some relevant response Y‘ is collected)
- null hypothesis is formed (e.g. “effect A on $Y >$ effect B on Y”)
  - this usually requires a model
- if p-value < 5 %, conclusion is reached

Problems:

- was there really a hypothesis at the beginning?
- how exactly were data collected?
- is the model good? (confounders?)
- the “if” above

Shady Practices I

- from chapter titled "Writing the Empirical Journal Article" a popular career guide in psychology:

  "There are two possible articles you can write: (1) the article you planned to write when you designed your study or (2) the article that makes the most sense now that you have seen the results. They are rarely the same, and the correct answer is (2). [...] If you see dim traces, try to reorganize [...] Go on a fishing expediction for something, anything..."

- this is called *p*-hacking and should be avoided!

Shady Practices II

- Carney, Cuddy & Yap (2010) Power Posing: ...
  - ... has positive effects on your mind
- Cuddy (2012) Your body language may shape who you are, TED talk
  - 2nd most viewed TED talk of all time
- 2015 first reproducibility issues
- 2016 Carney withdraws her name
  - she no longer believes in the effect, because

We ran subjects in chunks and checked the effect along the way. It was something like 25 subjects run, then 10, then 7, then 5. Back then, this did not seem like p-hacking. It seemed like saving money.

- this is called peeking (at p-values) and should be avoided! (or admitted and corrected for)

Example of Peeking

```
peeking <- function(a=25,b=10){
  x <- rnorm(25)
  Tstat <- mean(x)/sd(x)*sqrt(length(x))
  if(abs(Tstat) > qt(0.975,length(x)-1)){
    return(Tstat)
  }else{
    x <- append(x, rnorm(b))
    Tstat <- mean(x)/sd(x)*sqrt(length(x))
    return(Tstat)
  }
}
set.seed(517)
Tstats <- sapply(1:10000,peeking)
mean(I(abs(Tstats) > qnorm(0.975)))
```

```
## [1] 0.0851
```

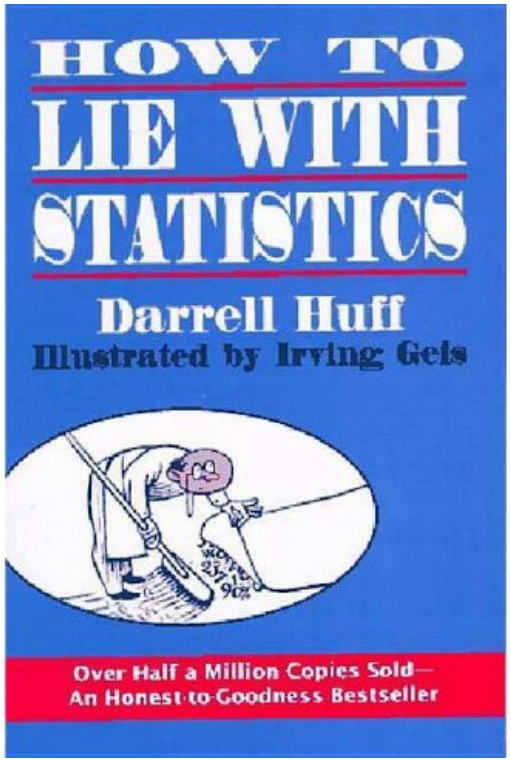
R code explained

- `<-` is the preferred assignment operator
  - while `<-` $\equiv$ `=`, assignment is such a crucial operation it should not be confused with a mathematical/logical operator
- function is an object, like a variable, just of a different class
  - `f_name <- function(params){ f_body }` defines your own function
- univariate distributions are defined by functions named as `[x][distr_name]` where
  - `x` $\in$ { `d`, `p`, `q`, `r` }, standing for density, probability distribution function, quantile function, `r`undom number generation
  - `distr_name` specifying distribution such as `unif`, `norm` (Gaussian), `t` (Student's t), `exp`, `binom`, `gamma`, `beta`, `cauchy`
  - e.g. `rnorm()` is random number generation from a Gaussian, `qt()` is a quantile function of the t distribution
- other pre-defined functions used on the previous slide include
  - `mean()` and `sd()` are the empirical mean and standard deviation of a vector
  - `length()` gives length of a vector
  - `I()` a bit special and actually useless on the previous slide, I just like to think of it as an indicator: `I(a > b)` $\equiv$ `a > b` and it returns `TRUE` iff `a` is greater than `b` (when `a` and `b` are vectors, it returns a vector of `T/F`)
- `?f_name` shows help for a function
- `return()` is not a function, it is part of the function syntax, specifying what should the function return upon call

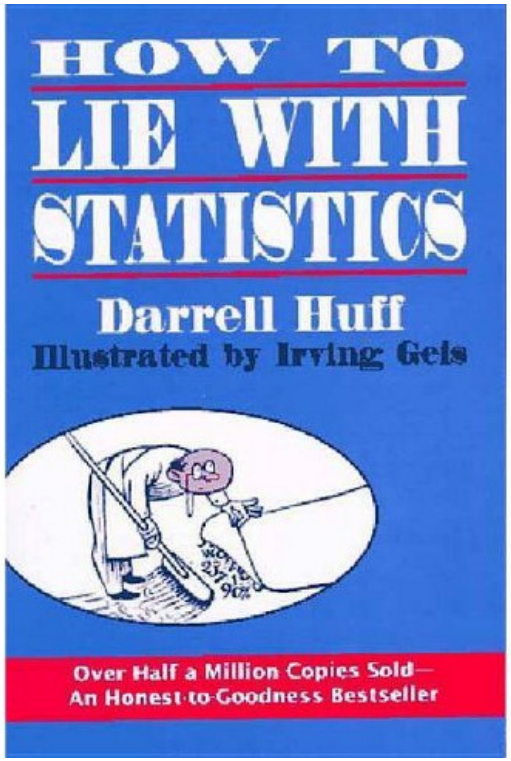
Reproducibility Crisis

- a meta-analysis confirms only 37 % out of 97 % significant results published in psychology
  – Open Science Collaboration (2015) Estimating the Reproducibility of psychological science. *Science*
- similar issues in other fields, e.g. biology, chemistry, economics, social sciences, or nutrition (Is everything we eat cancer?)
  - we are talking even about *Nature* and *Science* publications not being reproducible!
- it is *not* the fault of *p*-values

More on Shady Practices



More on Shady Practices



"Ironically, written by a journalist with little knowledge of statistics who later accepted thousands of dollars from cigarette companies and told a congressional hearing in 1965 that inferences in the Surgeon General's report on the dangers of smoking were fallacious."
– Andrew Gelman

Reproducible Research

- sharing data (and code)
- documenting data collection/cleaning and analyses
  - in particular any judgement calls (mostly data cleaning and modeling choices, but sometimes also tuning parameter selection, etc.)
- encapsulation
- pre-registration
- publishing negative results

Reproducible Data Analysis

Levels of Research Reproducibility

Trying things out in the R Console pane, saving tables and figures to named files.

Writing code in an RScript or Rmarkdown file, generating saved tables, figures, and manuscripts that can be re-run if needed.

Using Projects and {here} , sharing code, documenting with README and comments, doing code review,
and sharing code publicly on GitHub

All of the above, plus public sharing of code and data, and preserving your local package environment with {renv}

All of the above plus encapsulating the entire computing environment (R, packages, code) in a Docker image.

Section 3

Ethics

Ethical Guidelines for Statistical Practice

- Professional Integrity and Accountability
  - expose yourself to (self-)criticism
- Integrity of Data and Methods
  - aim for reproducibility
- Responsibilities to Stakeholders
- Responsibilities to Research Subjects
  - research on living beings must be supervised
  - privacy for human subjects
- Multidisciplinary Teams
  - profession-specific ethical guidelines
- Responsibilities to the Statistical Profession, Mentoring, etc.
  - the career guide above fails big here

Section 4

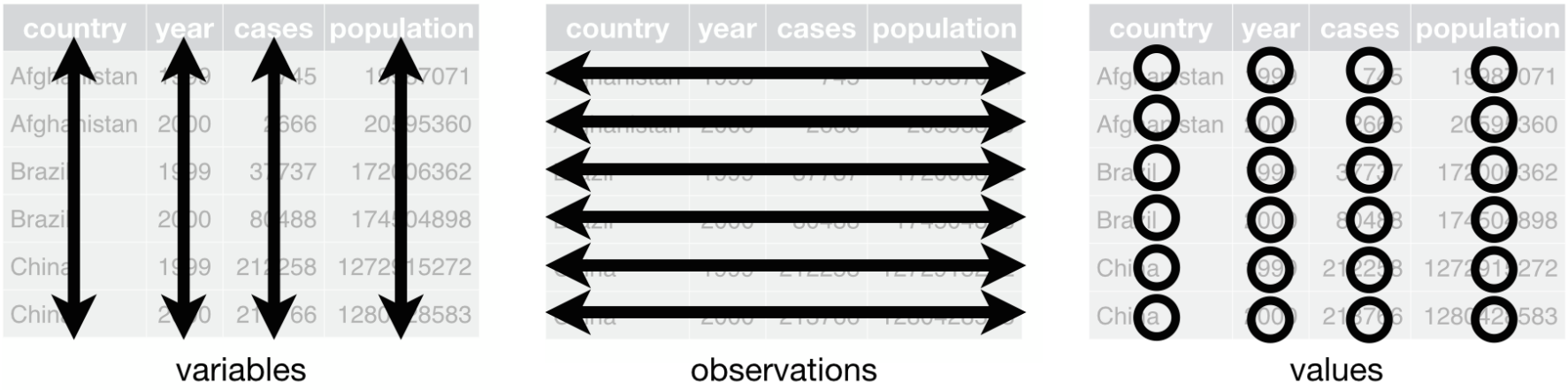
Data Exploration

Data Set I

```
library(faraway)
data(chredlin) # attaches the data into the global env
head(chredlin)
```

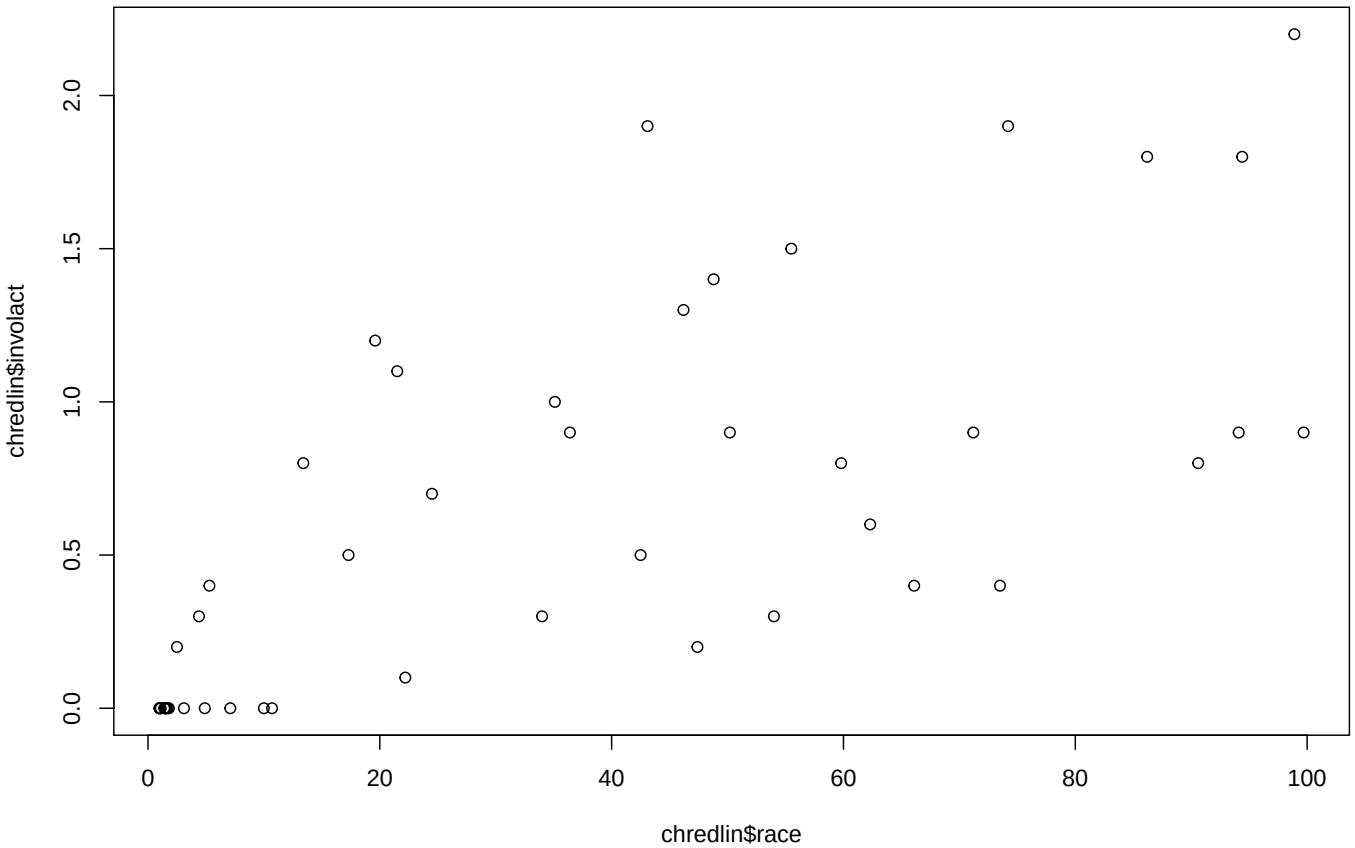
```
##       race fire theft  age involact income side
## 60626 10.0  6.2    29 60.4      0.0 11.744    n
## 60640 22.2  9.5    44 76.5      0.1  9.323    n
## 60613 19.6 10.5    36 73.5      1.2  9.948    n
## 60657 17.3  7.7    37 66.9      0.5 10.656    n
## 60614 24.5  8.6    53 81.4      0.7  9.730    n
## 60610 54.0 34.1    68 52.6      0.3  8.231    n
```

Data Frame


country
year
cases
population
variables
observations
values

Base R

```
plot(x = chredlin$race, y = chredlin$involact)
```



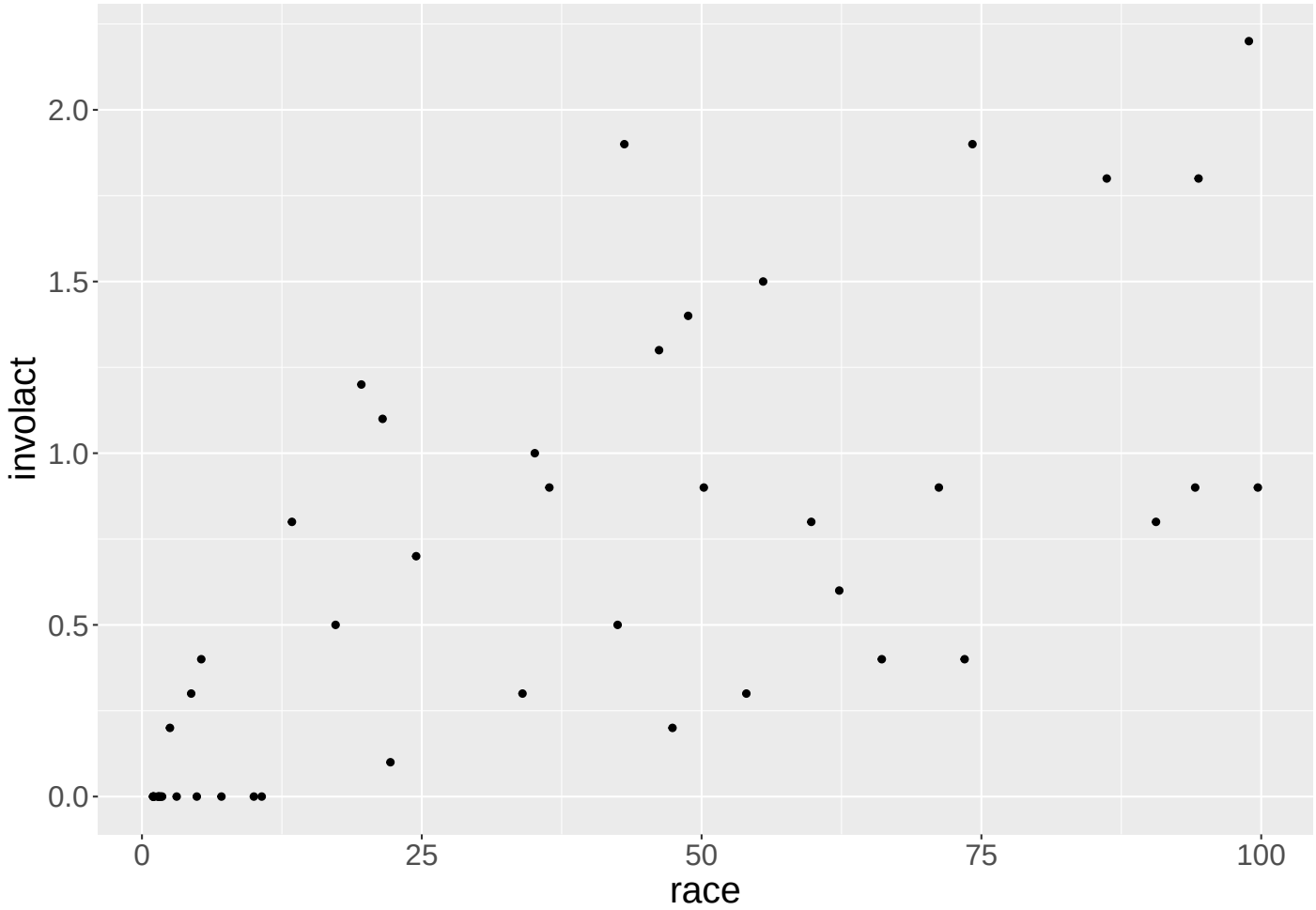
tidyverse

`tidyverse` is a bundle of R packages (itself a package) that allow for modern data manipulation and visualization

```
library(tidyverse)
```

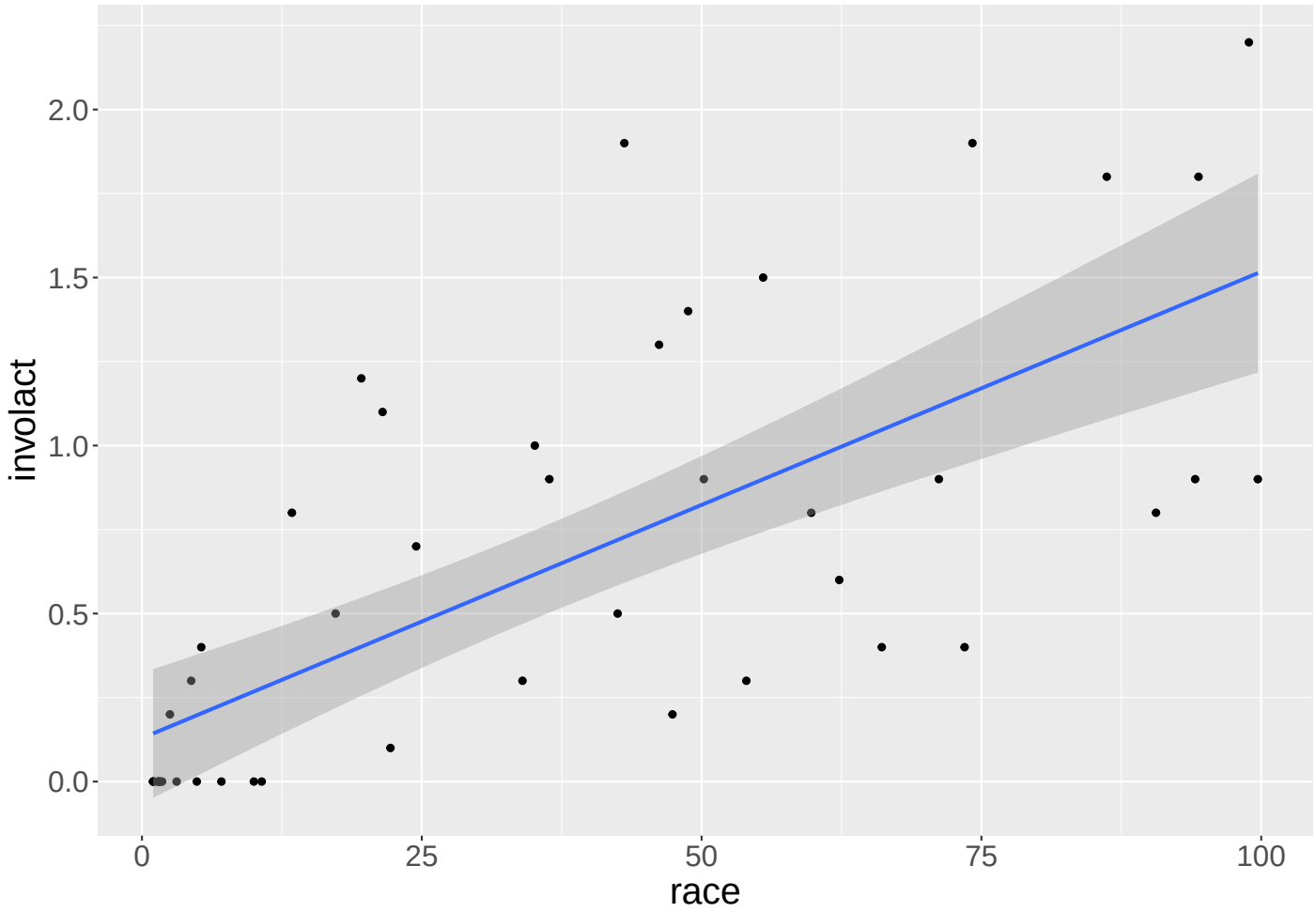
ggplot2

```
ggplot(data = chredlin, mapping = aes(x = race, y = involact)) +
  geom_point() # adds a layer to the empty plot above
```



ggplot2

```
ggplot(data = chredlin, mapping = aes(x = race, y = involact)) +
  geom_point() + # adds a layer to the empty plot above
  stat_smooth(method="lm") # adds a regression line too
```



`tidyverse` verbs

The basic verbs (functions) which will allow us to do most of the data manipulation tasks are

- `filter()` picks observations by chosen values
  - `select()` picks variables (by their names), hence is a poor "transpose" of `filter()`
- `mutate()` creates new variables as functions of existing ones
- `arrange()` orders the observations
- `group_by()` allows all of the above to work locally
  - `summarize()` collapses values down to a single summary – only useful together with `group_by()`

Data Set II

```
library(data.table)
```

```
flights <- fread("https://raw.githubusercontent.com/Rdatatable/data.table/master/vignettes/flights14.csv")
### flights have 1/4 million rows, so subsample
# flights <- flights[sample(1:dim(flights)[1], 5000),] # base R version of sub-sampling
flights <- flights %>%
  slice_sample(n=5000)                                  # tidyverse version of sub-sampling
head(flights)
```

```
##    year month day dep_delay arr_delay carrier origin dest air_time distance
## 1: 2014     7   6        -6       -34      AA    JFK  SFO      321     2586
## 2: 2014     3  26        71        66      WN    LGA  BNA      108      764
## 3: 2014     3  22        -7       -10      AA    LGA  ORD      121      733
## 4: 2014     1  31        -1       -13      MQ    JFK  CLE       85      425
## 5: 2014     5  30        -4       -15      EV    EWR  IAD       47      212
## 6: 2014    10  12        -4        -6      EV    EWR  BNA      118      748
##    hour
## 1:    7
## 2:   18
## 3:    8
## 4:   14
## 5:    6
## 6:   15
```

Drop (Non-numerical) Variables

```
flights <- select(flights, -carrier, -origin, -dest)
head(flights)
```

```
##    year month day dep_delay arr_delay air_time distance hour
## 1: 2014     7   6        -6       -34      321     2586    7
## 2: 2014     3  26        71        66      108      764   18
## 3: 2014     3  22        -7       -10      121      733    8
## 4: 2014     1  31        -1       -13       85      425   14
## 5: 2014     5  30        -4       -15       47      212    6
## 6: 2014    10  12        -4        -6      118      748   15
```

- above is `tidyverse` function/verb `select`, but used in a base R syntax
- `tidyverse` pairs well with **piping** operator `%>%` defined by to make the following equivalent:
  - `f(x,y)` ... `select(flights, -carrier)`
  - `x %>% f(y)` ... `flights %>% select(-carrier)`
- piping can be chained – we are always operating on the data!
  - `g(f(x,y),z)` is equivalent to
  - `x %>% f(y) %>% g(z)`

Example

Say the goal is

- to look at some flights that took place on 1st April
- having the variables that should be factors transformed into factors

```
flights <- fread("https://raw.githubusercontent.com/Rdatatable/data.table/m
flights %>%
  filter(month ==4, day == 1) %>%
  mutate(carrier = as.factor(carrier),
         origin = as.factor(origin),
           dest = as.factor(dest)) %>%
  head()
```

```
##    year month day dep_delay arr_delay carrier origin dest air_time dista
## 1: 2014     4   1        -8       -23      MQ    LGA  BNA      113
## 2: 2014     4   1        -8       -11      MQ    LGA  RDU       71
## 3: 2014     4   1        -4        -2      MQ    LGA  BNA      113
## 4: 2014     4   1        -6       -13      MQ    LGA  CMH       77
## 5: 2014     4   1        -9       -28      MQ    LGA  DTW       83
## 6: 2014     4   1        -6        -2      MQ    LGA  RDU       66
##    hour
## 1:   12
```

Variable Types

5 basic data types:

- numeric
- integer
- character
- logical
- complex

5 basic data structures:

- array
  - vector ... `c(1,2,3)` ≡ `1:3`
  - matrix ... `matrix(some_vector, ncol=2)`
- data frame – `tidyverse` has instead `tibble`
- factor
- list

```
c(1,"me","you","me",2,3,1,1) %>%
  as.factor() %>% levels() %>% length()
```

Common Variable Transformations

- `log(x, base)` and `exp(x,base)`
- `x^power` or `sqrt(x)`
- `sin(x)`, `cos(x)` and other trigonometric functions
- `sign(x)`
- Box-Cox transform $y_n^{(\lambda)} = \begin{cases} \frac{y_n^\lambda - 1}{\lambda} & \text{if } \lambda \neq 0 \\ \log(y_n) & \text{if } \lambda = 0 \end{cases}$
  - only used for the response variable in a linear model (good λ estimated by profile likelihood)
  - `boxcox(model)` in R, where `model <- lm(...)`

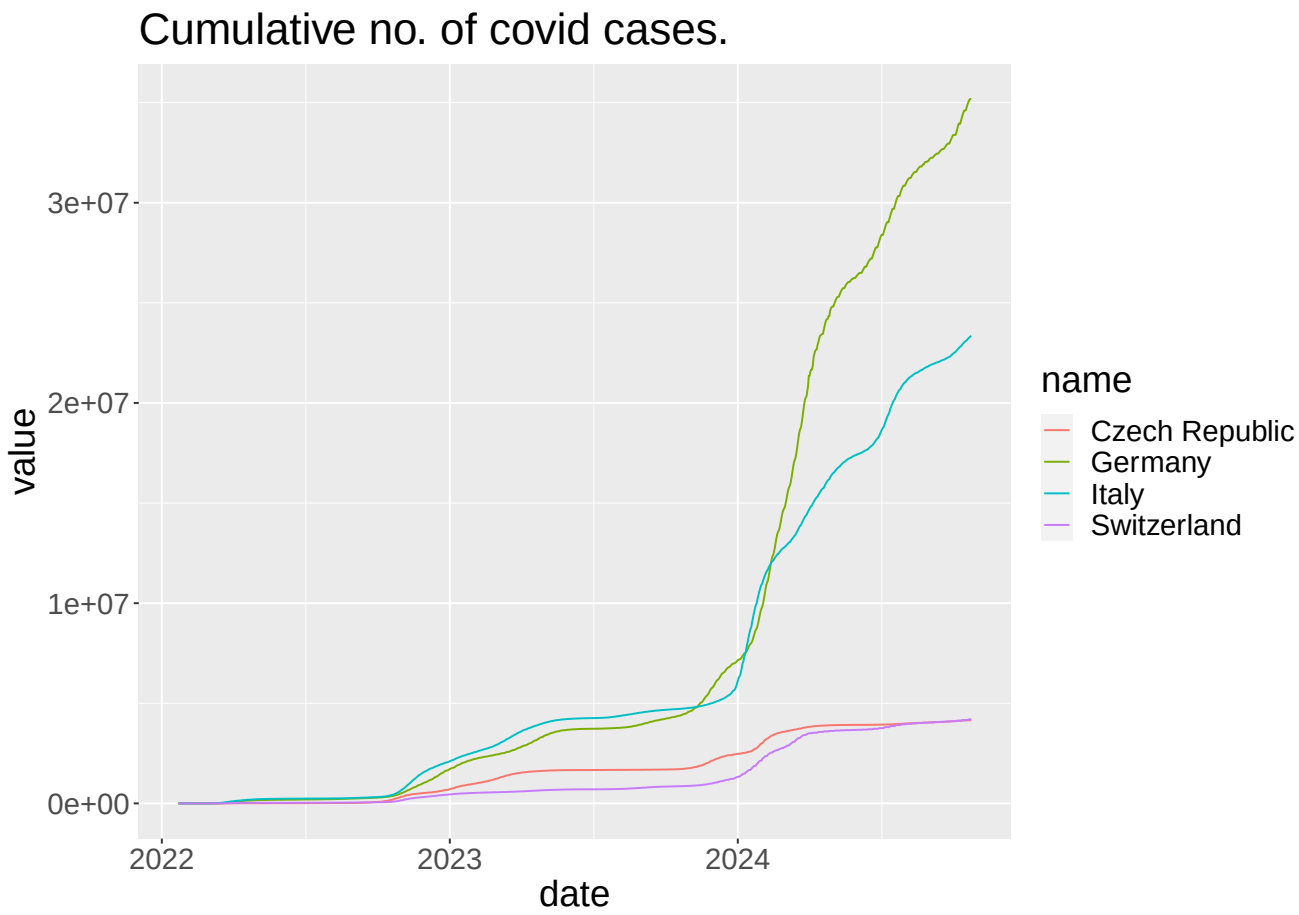
Examples of Transformations

```
flights <- flights %>%
  mutate(late_flag = as.factor(sign(arr_delay)),
         arr_delay_sqrt = sqrt(abs(arr_delay)),
         arr_delay_log = log(1+abs(arr_delay)))
flights %>%
  select(late_flag,arr_delay_sqrt,arr_delay_log)%>%
  str()
```

```
## Classes 'data.table' and 'data.frame':   253316 obs. of  3
##  $ late_flag     : Factor w/ 3 levels "-1","0","1": 3 3 3 1
##  $ arr_delay_sqrt: num  3.61 3.61 3 5.1 1 ...
##  $ arr_delay_log : num  2.639 2.639 2.303 3.296 0.693 ...
##  - attr(*, ".internal.selfref")=<externalptr>
```

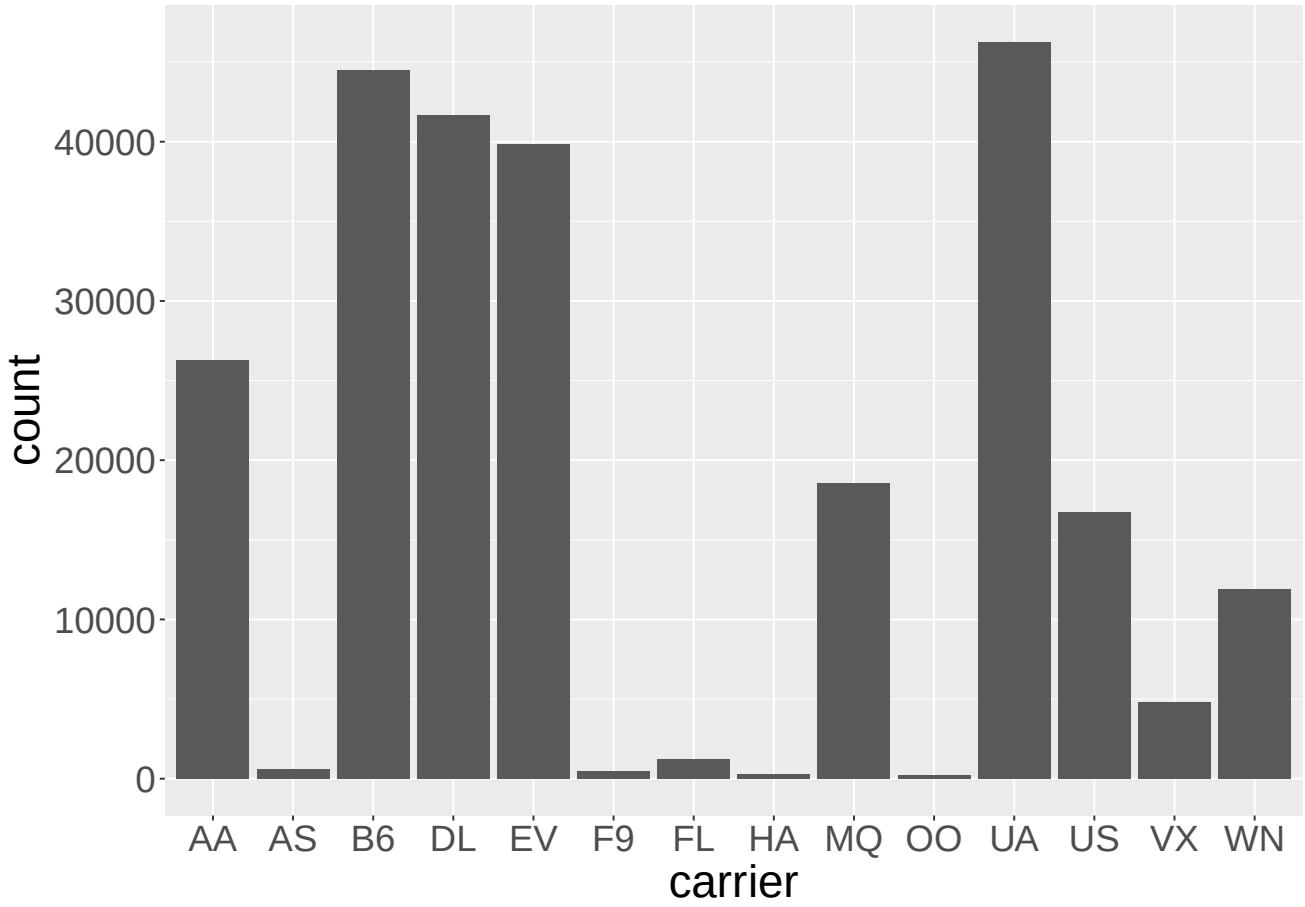
Line Plot

- there needs to be a linearly ordered variable, typically time



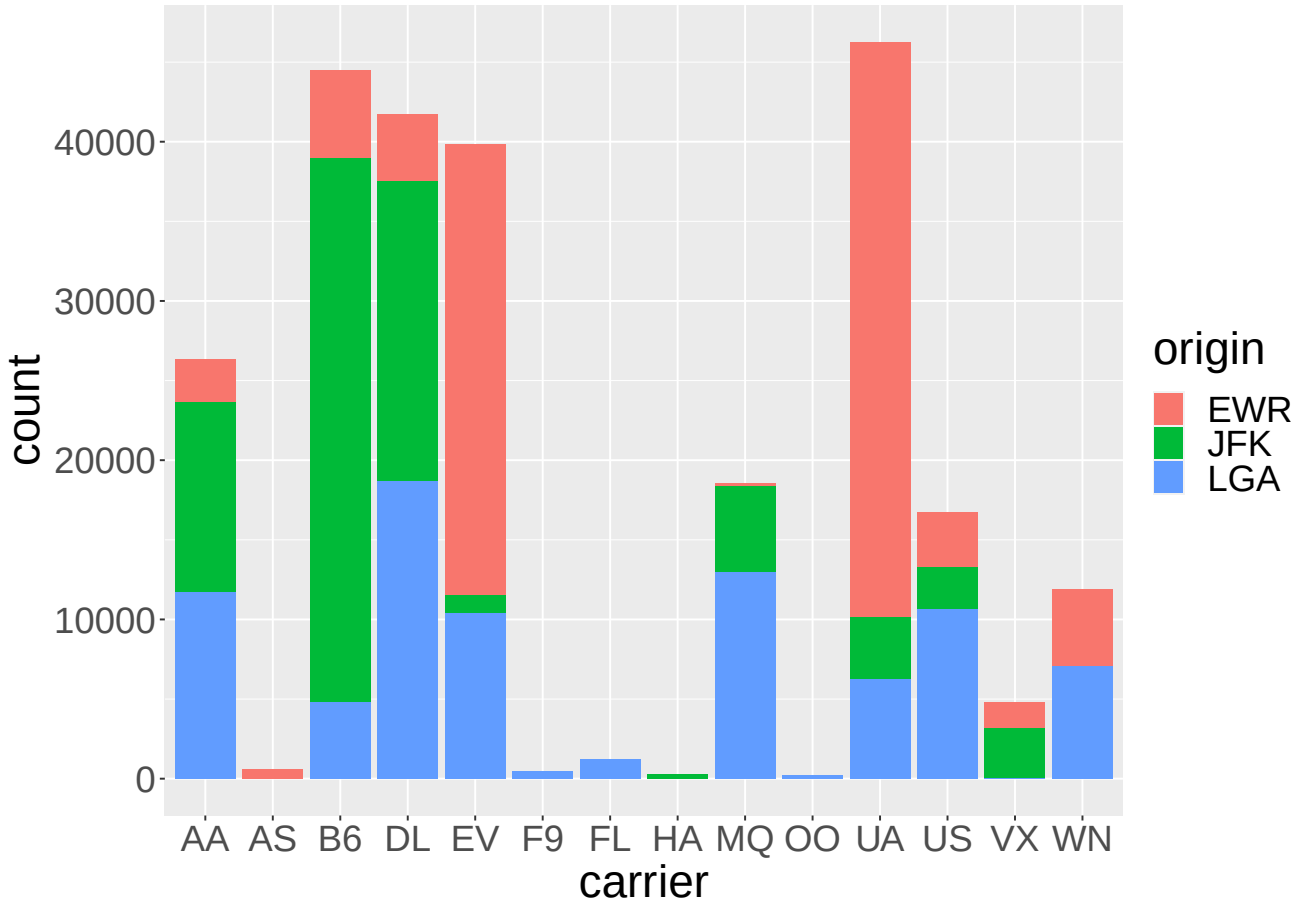
Bar Plot

```
ggplot(data = flights) +
  geom_bar(mapping = aes(x = carrier)) +
  theme(text = element_text(size = 25))
```



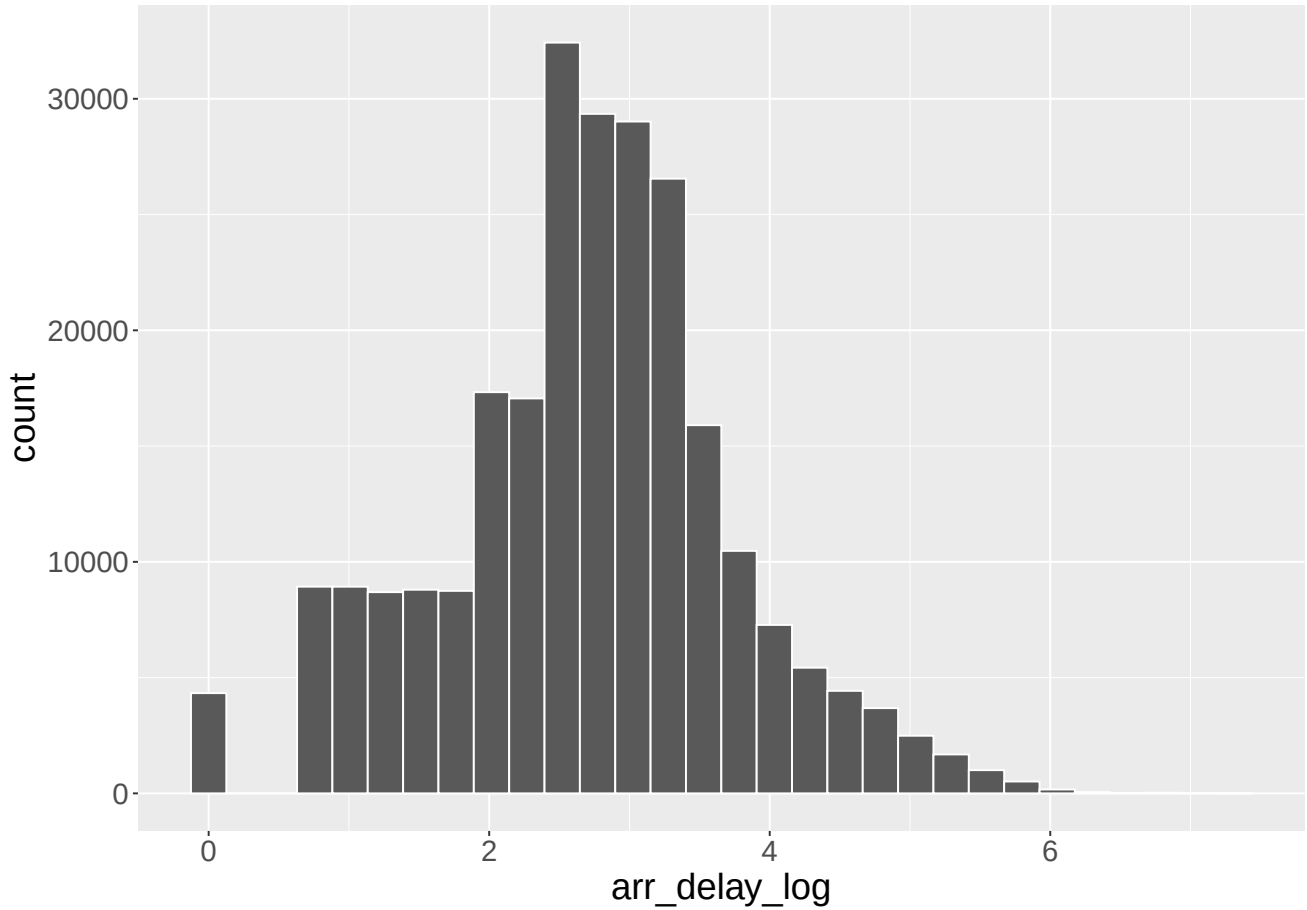
Bar Plot

```
ggplot(data = flights) +
  geom_bar(mapping = aes(x = carrier, fill = origin)) +
  theme(text = element_text(size = 25))
```



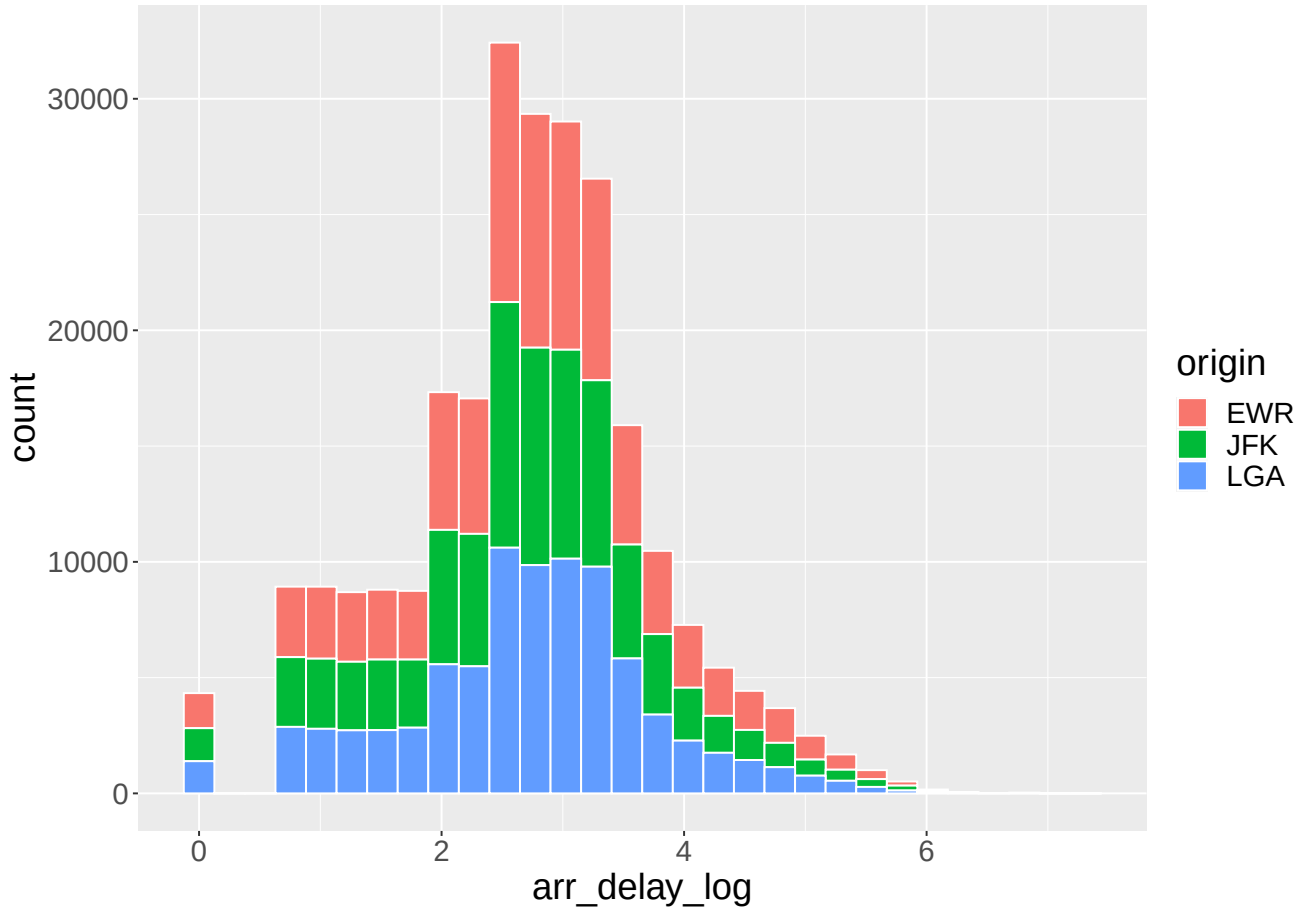
Histogram

```
ggplot(data = flights) +
  geom_histogram(mapping = aes(x = arr_delay_log),
                 color="white")
```



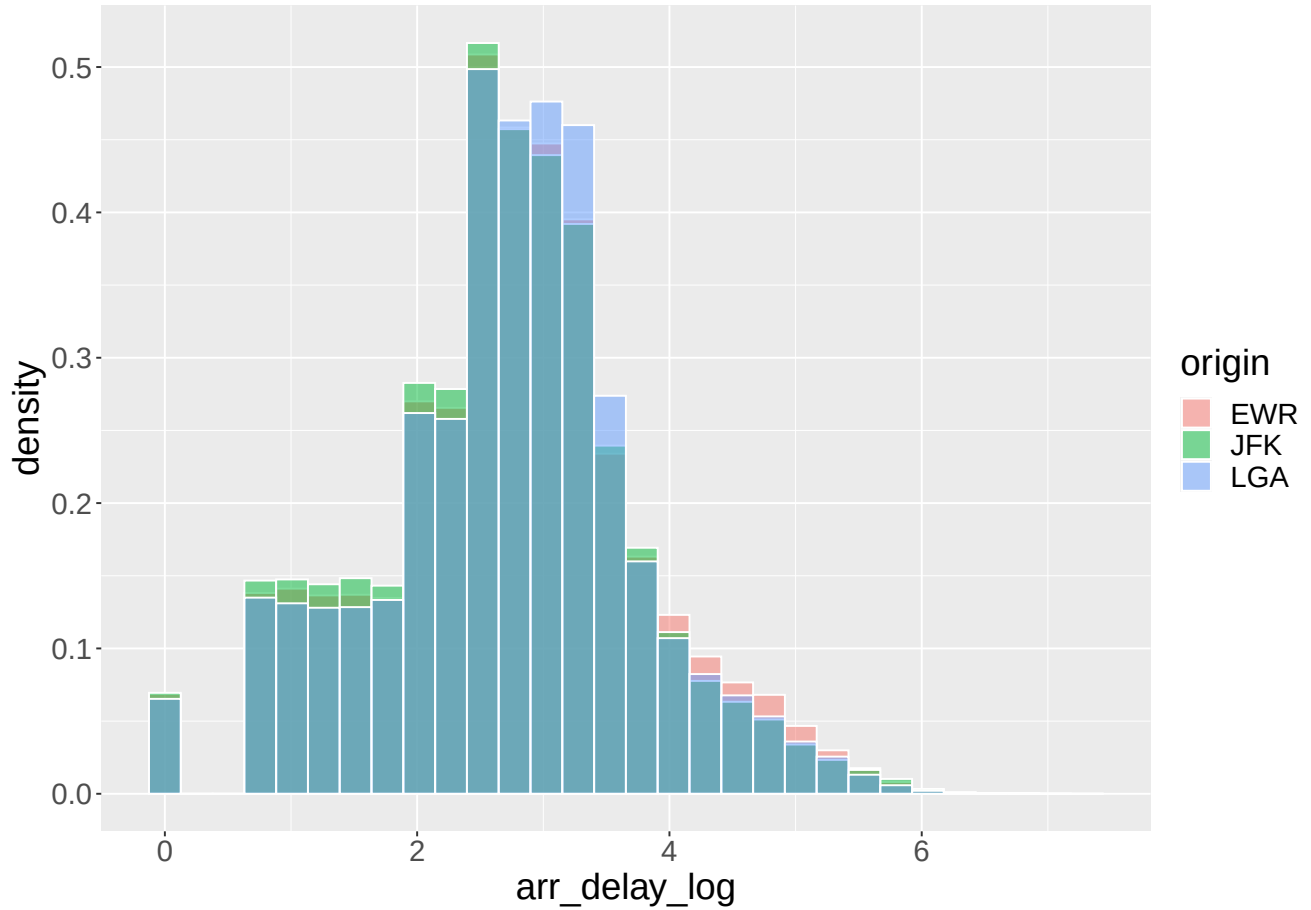
Histogram

```
ggplot(data = flights) +
  geom_histogram(aes(x = arr_delay_log, fill=origin),
                 color="white")
```



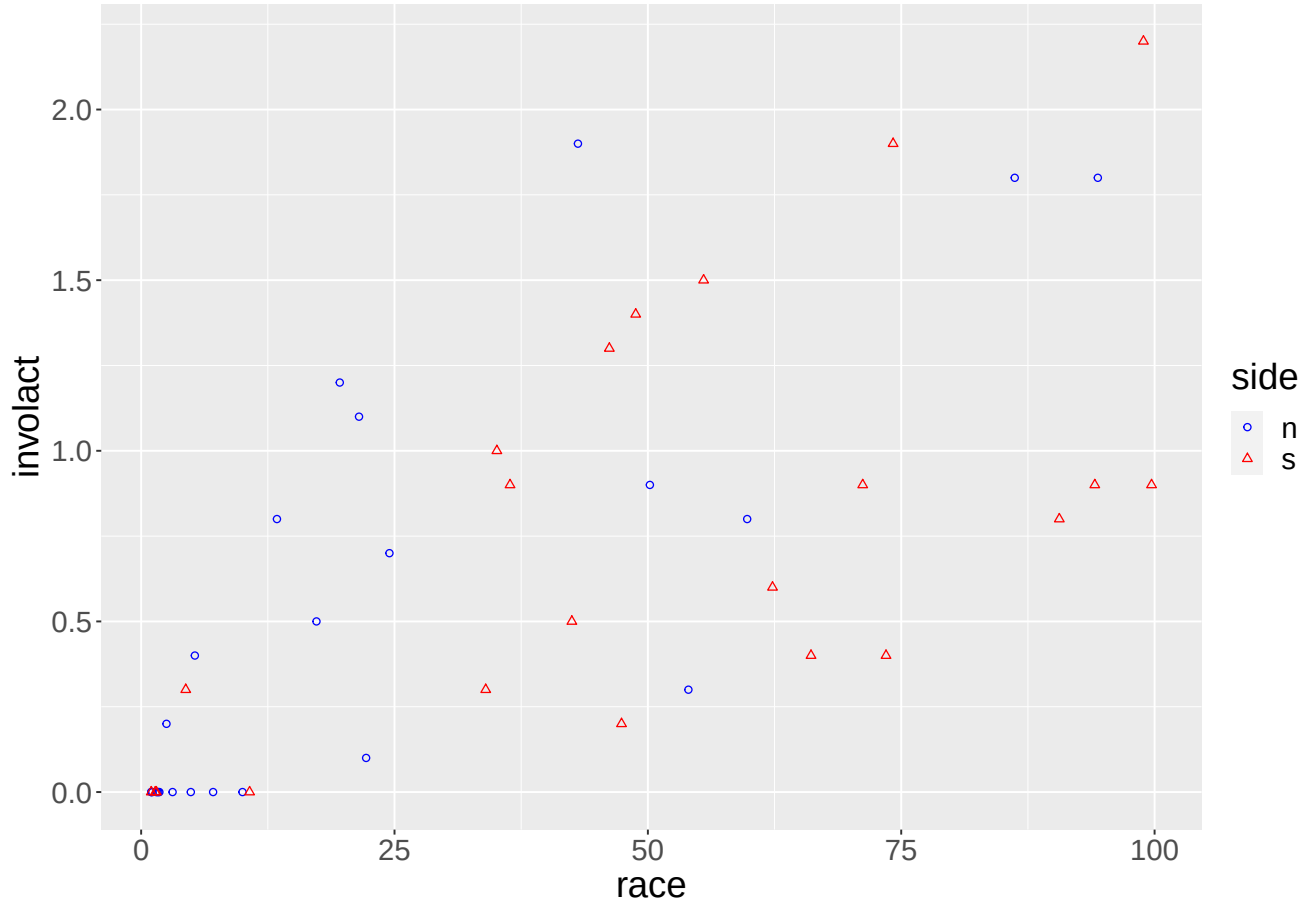
Histogram

```
ggplot(data = flights) +
  geom_histogram(aes(x = arr_delay_log, y=..density.., fill=origin),
                 position='identity', alpha=0.5, color="white")
```



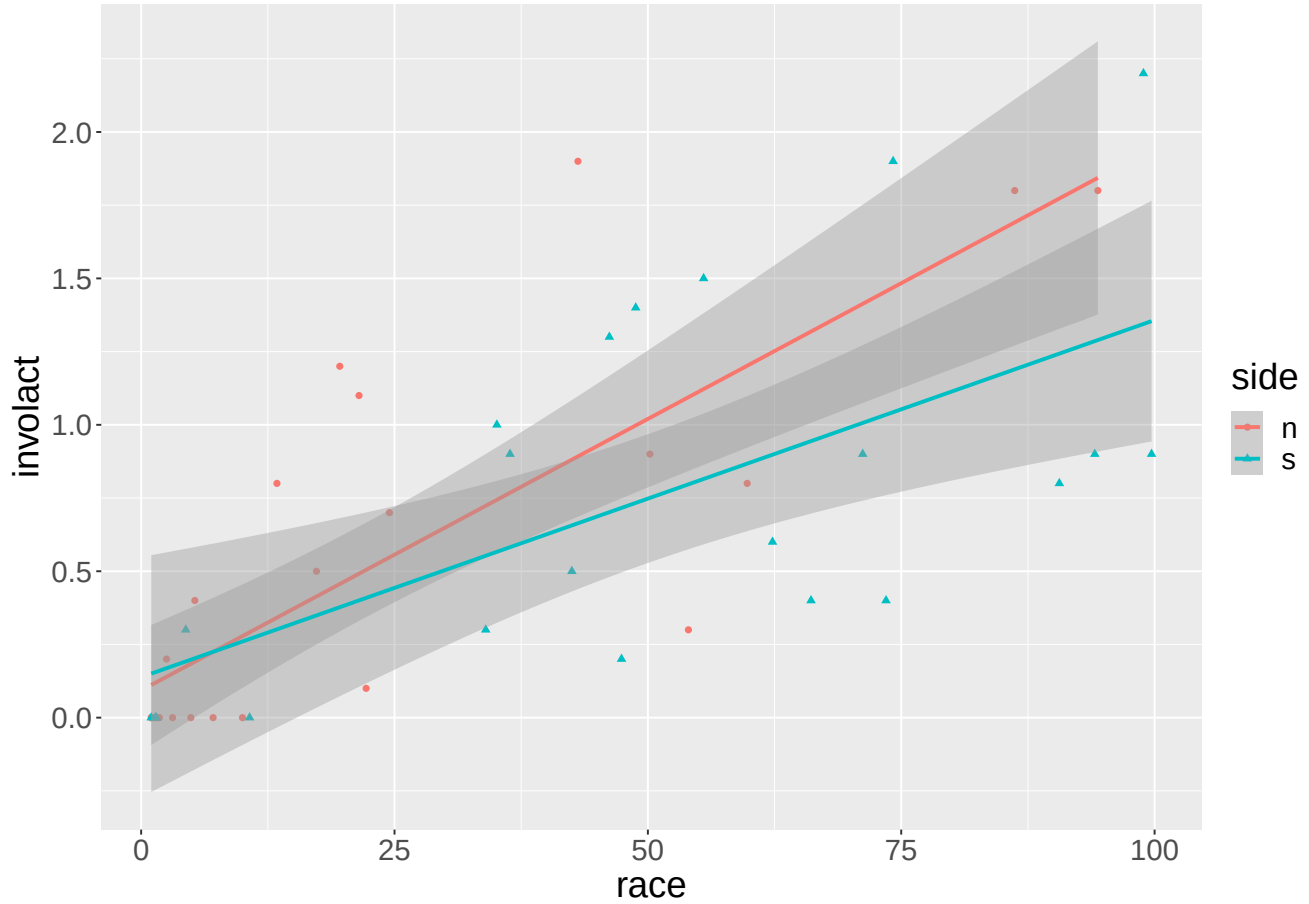
Scatterplot

```
ggplot(data = chredlin,
       mapping = aes(x = race, y = involact, color = side, shape = side)) +
  geom_point() + scale_color_manual(values = c("blue","red")) +
  scale_shape_manual(values = c(1,2))
```



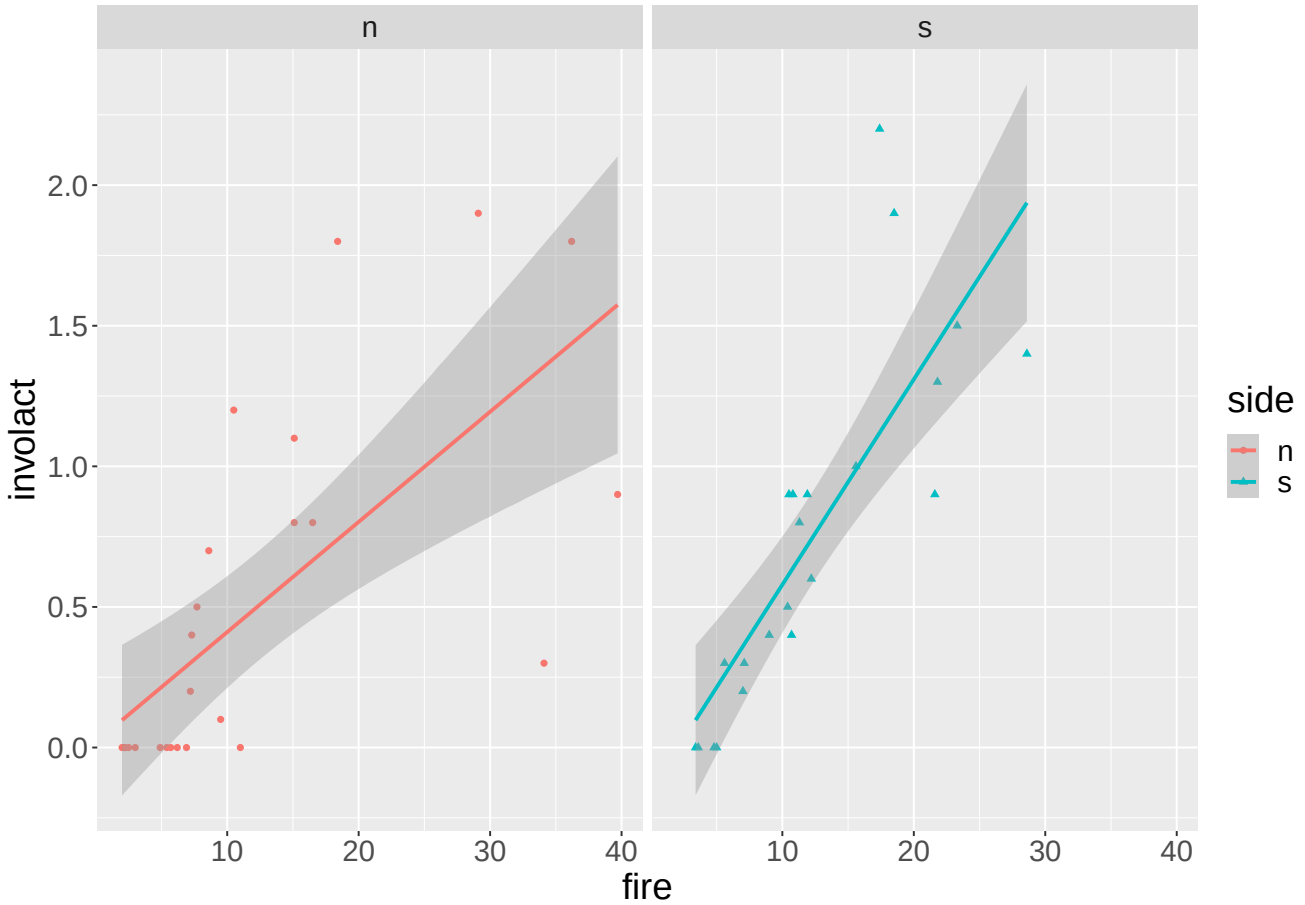
Scatterplot with Regression Lines

```
ggplot(data = chredlin, mapping = aes(x = race, y = involact,
                                      shape = side, color = side)) +
  geom_point() + # adds a layer to the empty plot above
  stat_smooth(method=lm) # adds a regression line too
```



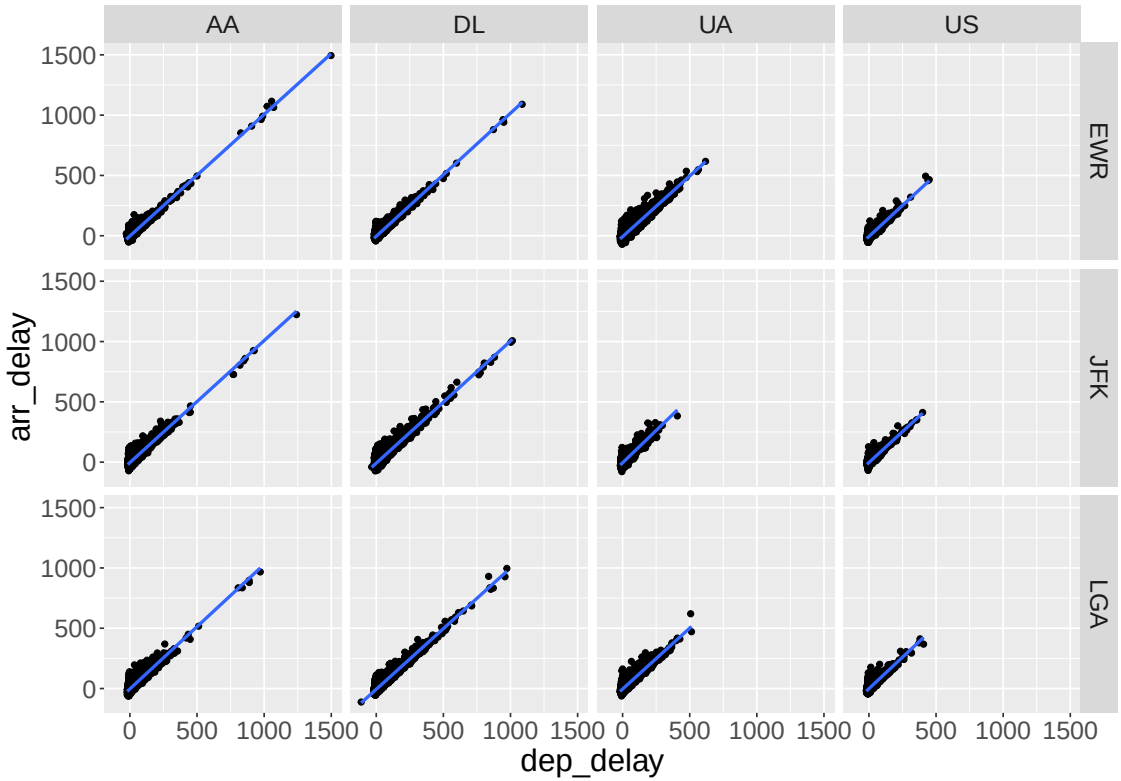
Plot by Factor

```
ggplot(data = chredlin, mapping = aes(x = fire, y = involact,
                                      shape = side, color = side)) +
  geom_point() +
  stat_smooth(method=lm) +
  facet_wrap(~ side) # split by a value of a factor
```



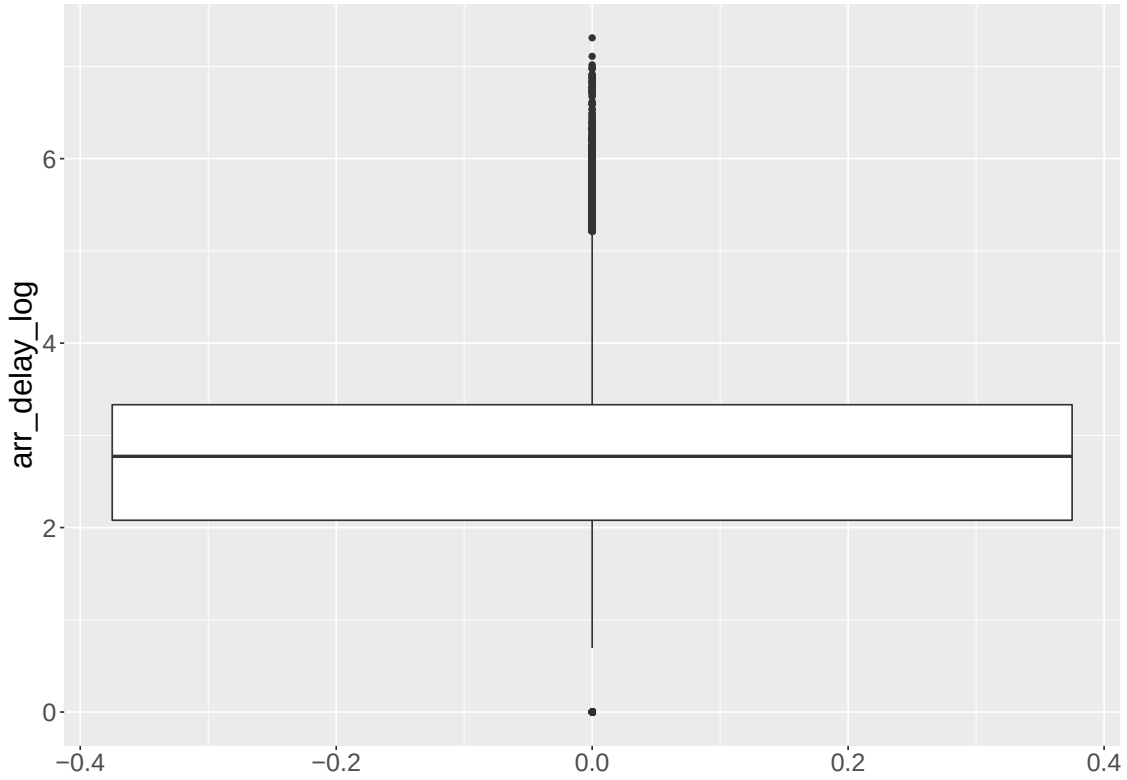
Plot by Two Factors

```
flights %>%
  filter(carrier %in% c("AA", "UA", "DL", "US")) %>%
  ggplot(mapping = aes(x = dep_delay, y = arr_delay)) +
  geom_point() + stat_smooth(method=lm) +
  facet_grid(origin ~ carrier)
```



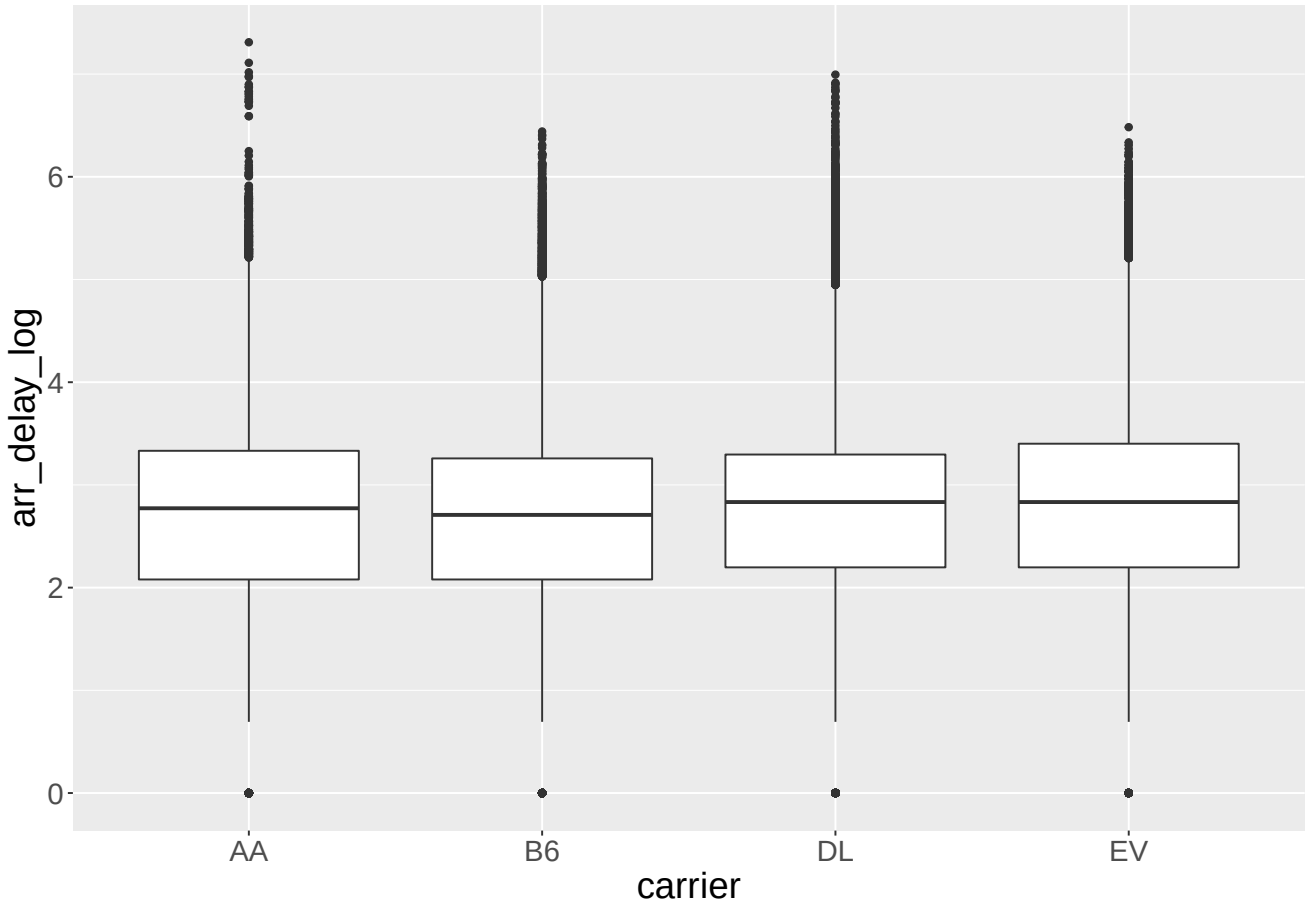
Boxplot

```
flights %>%
  filter(carrier %in% c("AA", "B6", "DL", "EV")) %>%
  ggplot(mapping = aes(y = arr_delay_log)) +
  geom_boxplot()
```



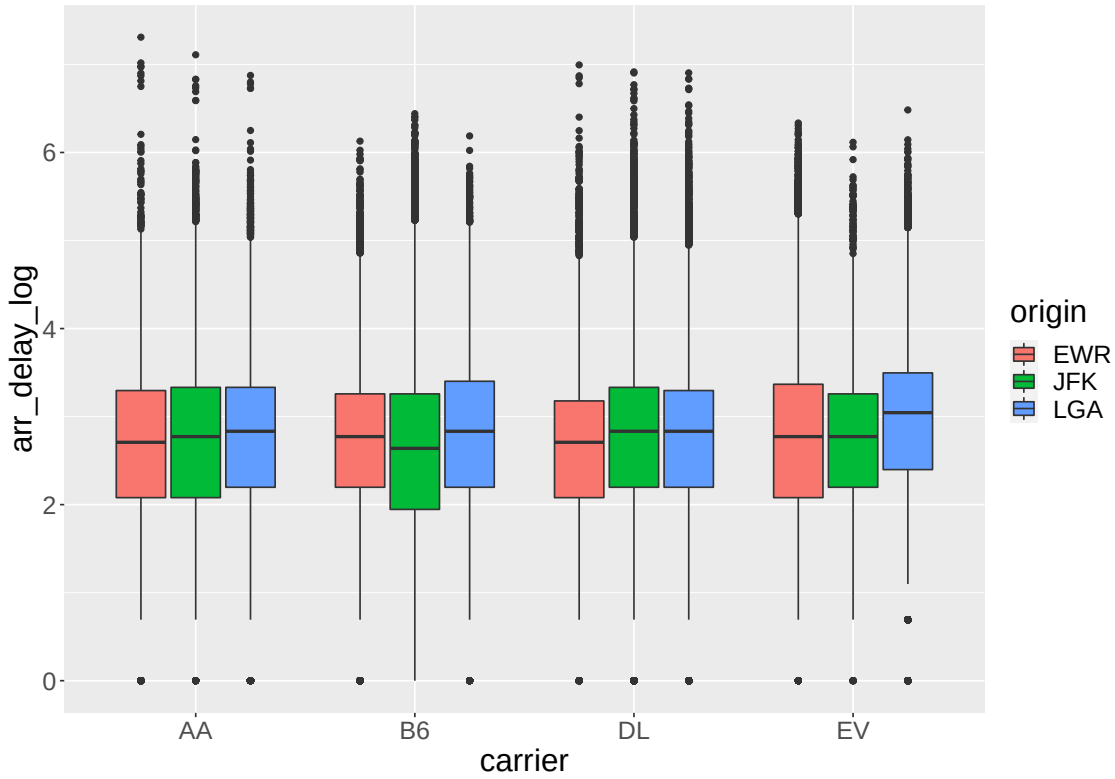
Boxplot by Factor

```
flights %>%
  filter(carrier %in% c("AA", "B6", "DL", "EV")) %>%
  ggplot(mapping = aes(x = carrier, y = arr_delay_log)) +
  geom_boxplot()
```



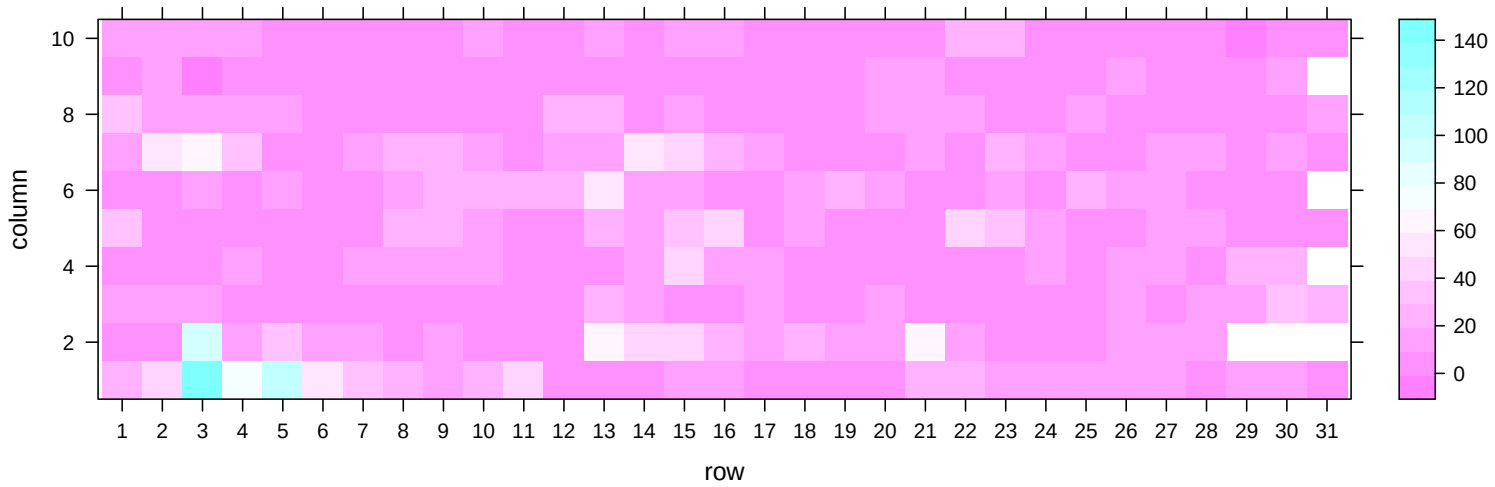
Boxplot by Two Factors

```
flights %>%
  filter(carrier %in% c("AA", "B6", "DL", "EV")) %>%
  ggplot(mapping = aes(x = carrier, y = arr_delay_log,
                       fill = origin)) +
  geom_boxplot()
```



Heatmaps

```
new_dat <- flights %>%
  group_by(month, day) %>%
  summarize(count = mean(dep_delay)) %>%
  pivot_wider(names_from = day, values_from = count) %>%
  ungroup() %>% select(-month)
library(lattice)
levelplot(t(as.matrix(new_dat)))
```

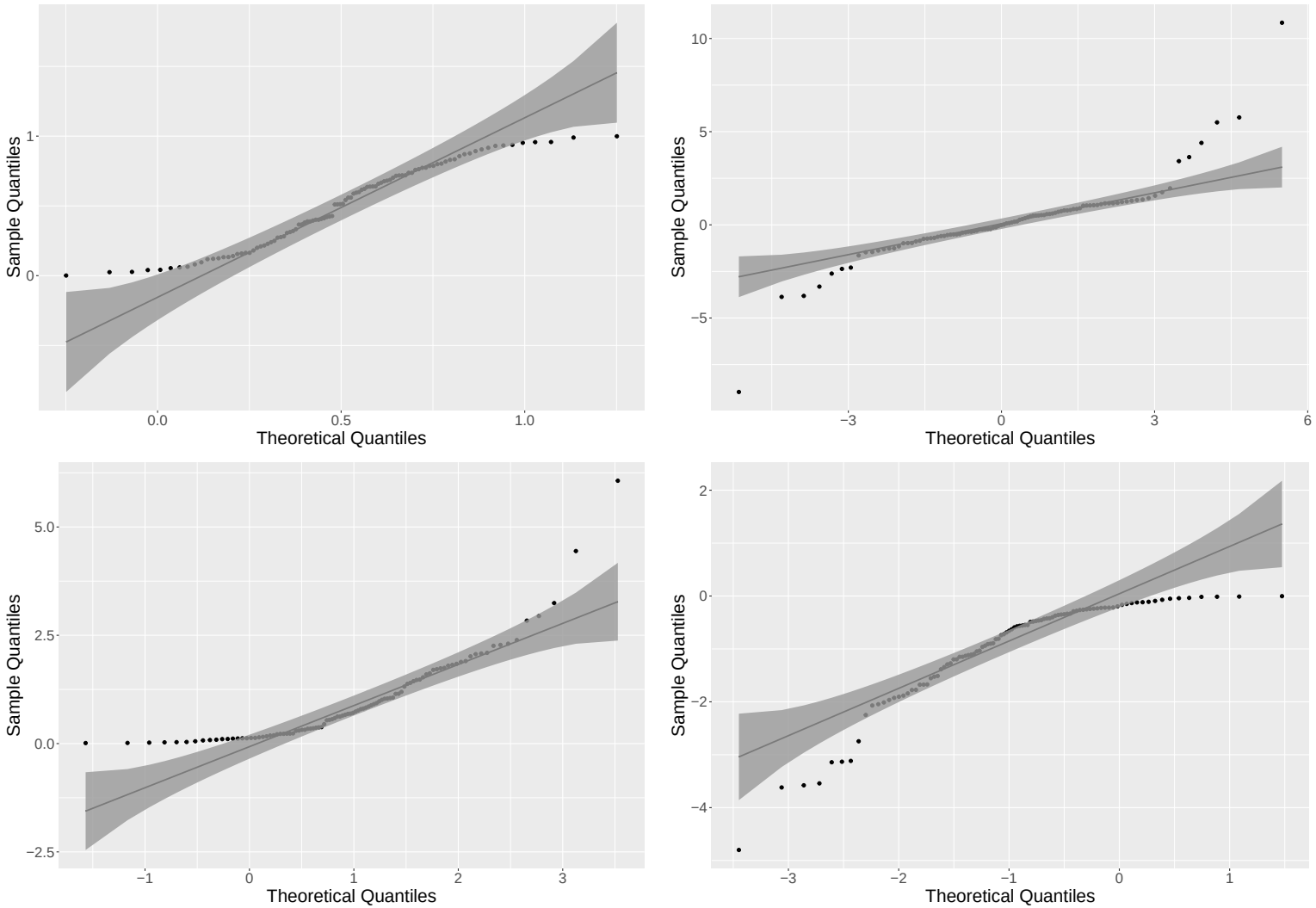


QQ plot

```
library(qqplotr)
set.seed(517)
mydat <- data.frame(light_tail = runif(100),
                    heavy_tail = rt(100,df=3),
                    skewed_right = rexp(100),
                    skewed_left = -rexp(100))
myqqplot <- function(myvar){
  mydat %>%
    ggplot(mapping = aes_string(sample = myvar)) +
    stat_qq_point() + # reference Gaussian by default
    stat_qq_line() +
    stat_qq_band() +
    labs(x = "Theoretical Quantiles", y = "Sample Quantiles")
}
```

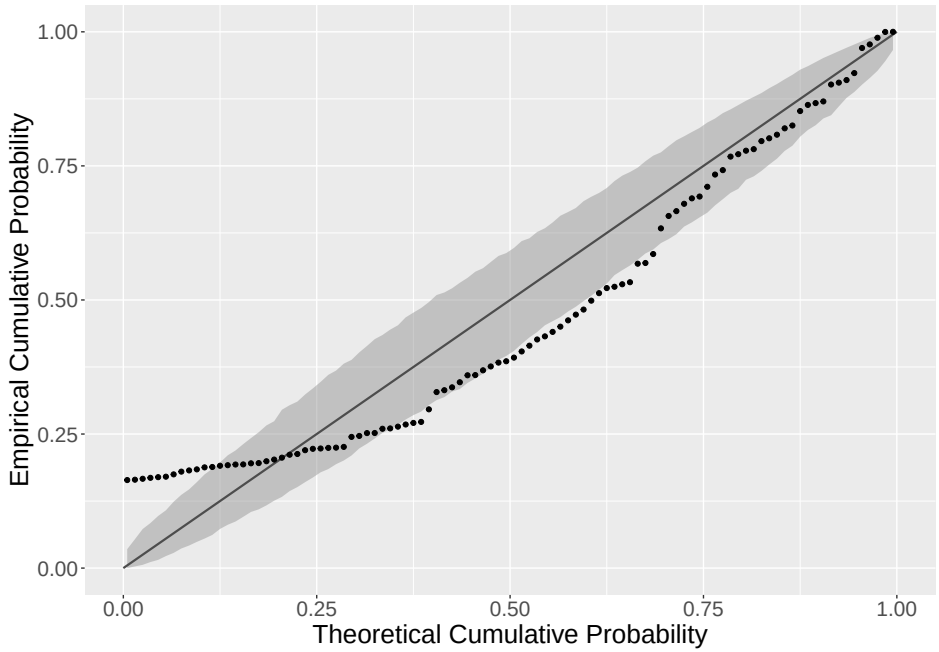
QQ Plot

```
myqqplot("light_tail"); myqqplot("heavy_tail")
myqqplot("skewed_right"); myqqplot("skewed_left")
```



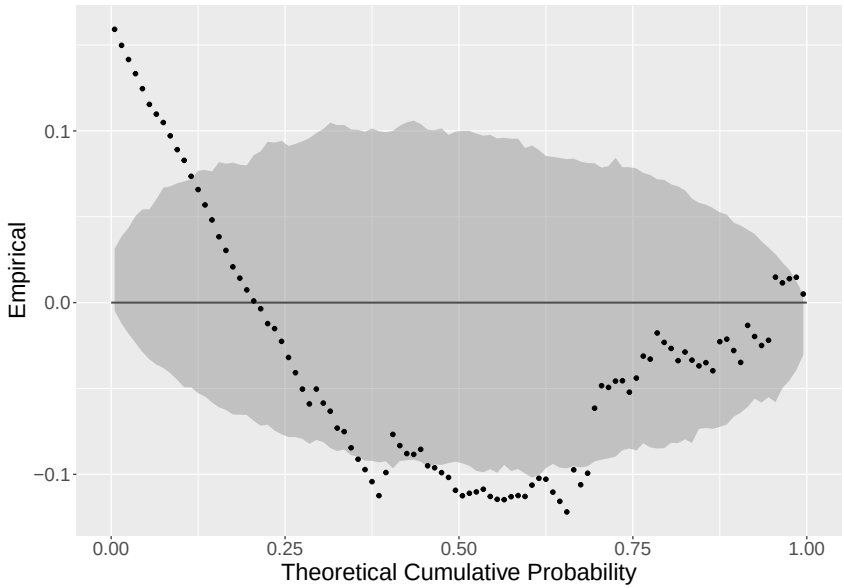
PP plot

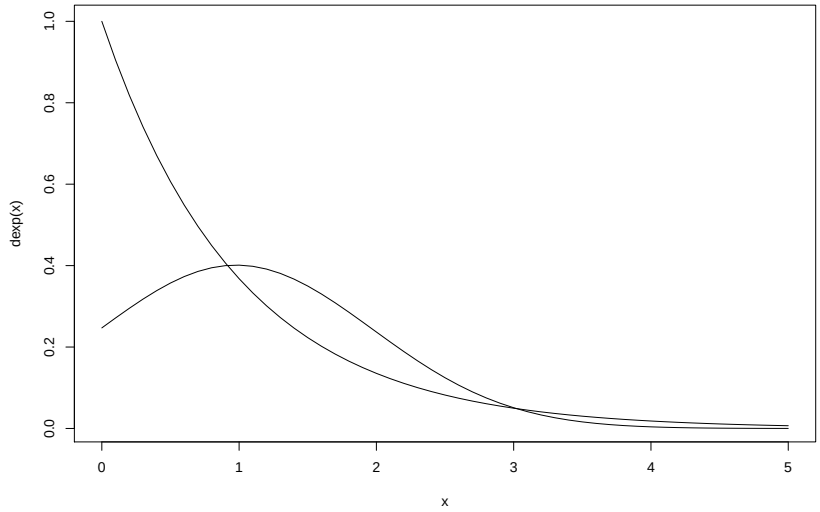
```
mydat %>%
    ggplot(mapping = aes(sample = skewed_right)) +
    stat_pp_band() +
    stat_pp_line() +
    stat_pp_point() +
    labs(x = "Theoretical Cumulative Probability",
         y = "Empirical Cumulative Probability")
```



PP plot

```
mydat %>%
    ggplot(mapping = aes(sample = skewed_right)) +
    stat_pp_band(detrend=T) +
    stat_pp_line(detrend=T) +
    stat_pp_point(detrend=T) +
    labs(x = "Theoretical Cumulative Probability", y = "Empirical")
x <- seq(0,5,by=0.1)
plot(x,dexp(x),type="l")
points(x,dnorm(x,mean(mydat$skewed_right),sd(mydat$skewed_right)),type="l")
```





Final Remarks

- principal component analysis (PCA) and clustering can be helpful for exploration
  - both PCA and clustering part of the MATH-444 Multivariate Statistics class
- exploratory vs. explanatory analysis/graphics
  - exploratory . . . helps you understand the patterns
  - explanatory . . . designed to communicate your understanding

Exercises

1. Freedman (2009) Statistical Models, Example 4, p. 75:
   Suppose Y consists of 100 independent $\mathcal{N}(0,1)$ random variables. This is pure noise. Let $X \in \mathbb{R}^{100\times 50}$ be the design matrix with independent $\mathcal{N}(0,1)$ variables (just more noise). We regress Y on X (i.e. no intercept). The coefficient of determination R^2 will be about 50/100=0.5. Suppose we test each of the 50 coefficients at the 10 % level and keep only the "significant" variables. There will be about $50 \times 0.1 = 5$ keepers (just by chance). Running the regression on the keepers only (again, without intercept), we are likely to get a decent R^2 (like 0.2 – decent by the social-science standards) and dazzling t-statistics. Run a couple of simulations and see for yourself.

2. The "Example of Peeking" above is an example of a small simulation study, checking whether a designed test strategy respects the nominal level $\alpha = 0.05$ or not. Incorporate further levels of peeking in order to mimic the power-posing study. Write your results using Markdown and push them to your GitHub repository.

References

- Poldrack (2019) Statistical Thinking for the 21st Century
- JASA Ethical Guidelines for Statistical Practice
- Gelman (2018) Ethics in statistical practice and communication
- Wickham & Grolemund (2017) R for Data Science