Simulation and the bootstrap

packages

```r
library(tidyverse)
```

Simulation

- Sometimes you know the exact mathematical answer to a problem, eg:
  - $X_1, \ldots X_n \sim N(\mu, \sigma^2)$, what is distribution of $\bar{X}$? (Ans: $N(\mu, \sigma^2/n)$.)
- More often, though, you don't:
  - if $X \sim Bin(2, 0.5), Y \sim Bin(3, 0.2)$, what is dist of $Z = X + Y$?
- Simulation: generate random X and Y, calculate sum, repeat many times. Gives you (approx) dist of $X + Y$ without any mathematics!

Random numbers in R

- R knows about a lot of distributions, eg: `norm` `binom` `pois` `exp` `gamma` `t` `chisq` (type `?distributions` in Console to see more)
- to generate random numbers from a distribution, put `r` on front of these; inputs are number of random values to generate, and parameters of distribution to simulate from.
- Examples:

```
rnorm(5, 100, 15)
```

```
[1] 111.96072  89.80331 113.74231  90.74167  89.86461
```

and

```
rpois(10, 3.5)
```

```
 [1] 5 2 5 5 3 5 1 3 4 0
```

Our problem: simulating once

- if $X \sim Bin(2, 0.5), Y \sim Bin(3, 0.2)$, what is dist of $Z = X + Y$?

```
x <- rbinom(1, 2, 0.5)
y <- rbinom(1, 3, 0.2)
x
```

```
[1] 1
```

```
y
```

```
[1] 1
```

```
x + y
```

```
[1] 2
```

To simulate many times: - set up dataframe with space for each simulated value - work rowwise - do one simulation per row

Simulating many times

```
tibble(sim = 1:10000) %>%
  rowwise() %>%
  mutate(x = rbinom(1, 2, 0.5),
         y = rbinom(1, 3, 0.2),
         z = x + y) -> d
```

Results

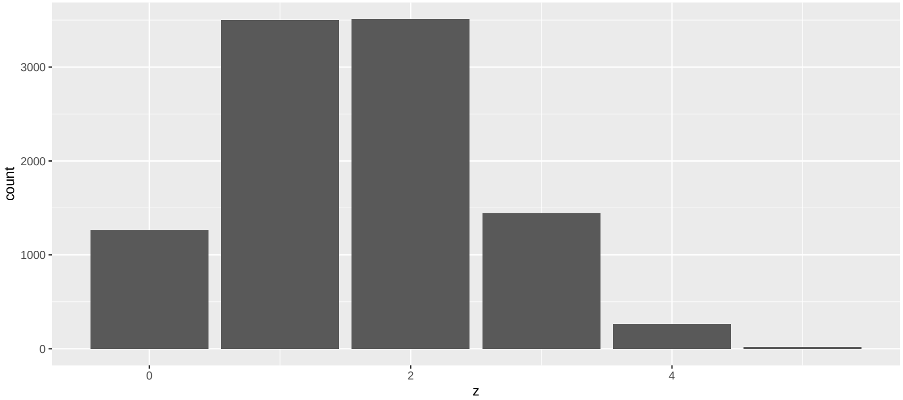
```
d
```

```
# A tibble: 10,000 x 4
# Rowwise:
     sim     x     y     z
   <int> <int> <int> <int>
 1     1     1     0     1
 2     2     2     1     3
 3     3     1     0     1
 4     4     0     0     0
 5     5     1     0     1
 6     6     2     0     2
 7     7     1     0     1
 8     8     0     0     0
 9     9     0     2     2
10    10     0     1     1
# i 9,990 more rows
```

Distribution of sum

Make a bar chart rather than a histogram because distribution of Z is discrete:

```r
ggplot(d, aes(x = z)) + geom_bar()
```



(Simulated) probability that the sum is at least 4:

```
d %>% count(z >= 4)
```

```
# A tibble: 2 x 2
# Rowwise:
  `z >= 4`      n
  <lgl>     <int>
1 FALSE      9715
2 TRUE        285
```

Only this much:

```
285/10000
```

```
[1] 0.0285
```

A sum of 5 is possible though very unlikely.

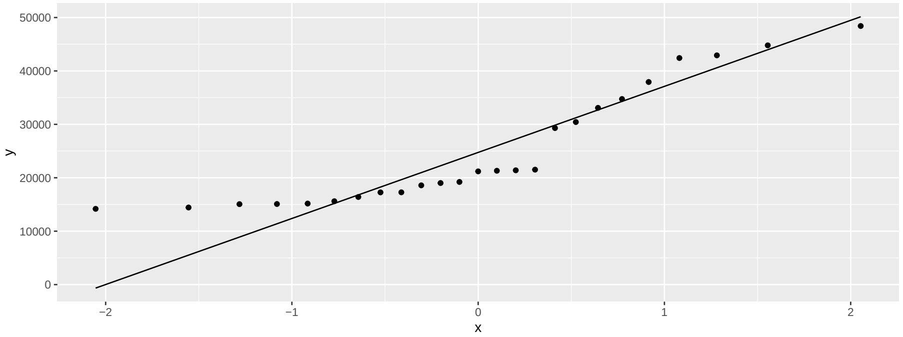
The bootstrap

Source: Hesterberg et al

- Sampling distribution of a statistic is distribution of that statistic over "all possible samples" from population of interest.
- "Plug-in principle": sample mean estimates population mean, sample variance estimates population variance, etc.
- Also, sample is estimate of population (precisely, proportion of sample values $\leq x$ estimates probability of drawing value $\leq x$ from population, for any x).
- As long as your sample is representative, sampling *from the sample* (!) is an estimate of sampling from the population. Called a *bootstrap sample*.
- Sample from sample *with* replacement, or else you get original sample back.

Blue Jays attendances:

```
ggplot(jays, aes(sample = attendance)) +
  stat_qq() + stat_qq_line()
```



- t procedure for the mean may not be a good idea because the distribution is skewed.
- Previously: hand-waving with sample size.

What *actually* matters

- It's not the distribution of the *data* that has to be approx normal (for a t procedure).
- What matters is the *sampling distribution of the sample mean*.
- If the sample size is large enough, the sampling distribution will be normal enough even if the data distribution is not.
  - This is why we had to consider the sample size as well as the shape.
- But how do we know whether this is the case or not? We only have *one* sample.
- Use the bootstrap to simulate sampling distribution.

Simulating the sampling distribution of sample statistic

- Sample from our sample *with replacement*.
- Calculate statistic
- Repeat many times (simulation).
- This gives an idea of how our statistic might vary in repeated samples: that is, its sampling distribution.
- Called the **bootstrap distribution** of the statistic.
- If the bootstrap distribution is approx normal, infer that the true sampling distribution also approx normal, therefore inference about the mean such as t is good enough.
- If not, we should be more careful.

Bootstrapping the Blue Jays attendances

- Sampling with replacement is done like this (the default sample size is as long as the original data):

```r
boot <- sample(jays$attendance, replace=TRUE)
mean(boot)
```

```
[1] 23764.76
```

- That's one bootstrapped mean. We need a whole bunch.

Comparing the actual sample with the bootstrapped one

```r
sort(jays$attendance)
```

```
 [1] 14184 14433 15062 15086 15168 15606 16402 17264 17276 18581
[11] 19014 19217 21195 21312 21397 21519 29306 30430 33086 34743
[21] 37929 42419 42917 44794 48414
```

```r
sort(boot)
```

```
 [1] 14184 14433 14433 15086 15086 15168 15168 16402 17264 17264
[11] 17276 17276 17276 17276 18581 19014 21312 21519 33086 37929
[21] 42419 42419 42917 42917 48414
```

Bootstrap sample has repeats plus missing values from original sample.

A whole bunch

- We are now doing a simulation. I like 10,000 samples when testing for normality:

```
tibble(sim = 1:10000) %>%
  rowwise() %>%
  mutate(boot_sample = list(sample(jays$attendance, replace =
  mutate(my_mean = mean(boot_sample)) -> samples
```

- for each row:
  - obtain a bootstrap sample (`list` because we are saving the whole sample in one cell of the dataframe)
  - work out the mean of that bootstrap sample.

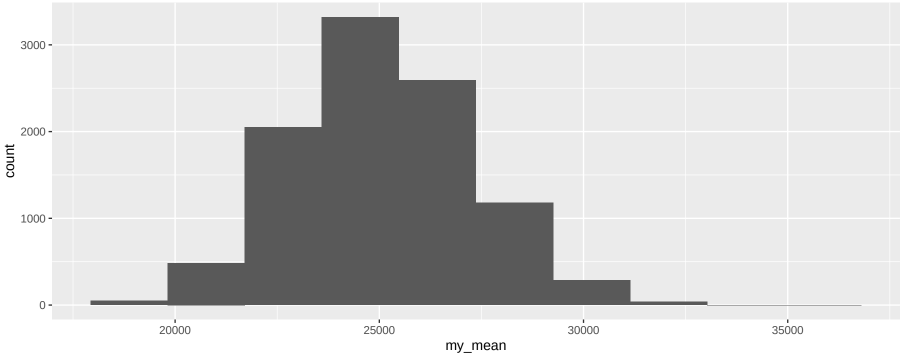
Bootstrap sample means

```
samples
```

```
# A tibble: 10,000 x 3
# Rowwise:
     sim boot_sample my_mean
   <int> <list>        <dbl>
 1     1 <dbl [25]>   23055.
 2     2 <dbl [25]>   25513.
 3     3 <dbl [25]>   25563.
 4     4 <dbl [25]>   29198.
 5     5 <dbl [25]>   23615.
 6     6 <dbl [25]>   28472.
 7     7 <dbl [25]>   28648.
 8     8 <dbl [25]>   23329.
 9     9 <dbl [25]>   24808.
10    10 <dbl [25]>   24665.
# i 9,990 more rows
```

Sampling distribution of sample mean

```
ggplot(samples, aes(x=my_mean)) + geom_histogram(bins=10)
```

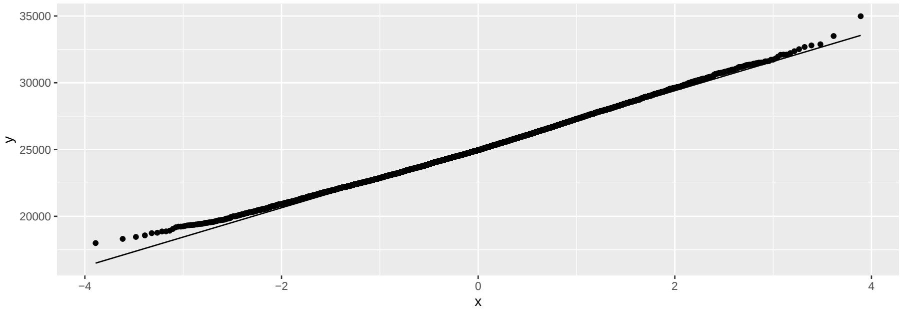


- Is that a slightly long right tail?

Normal quantile plot

might be better than a histogram:

```
ggplot(samples, aes(sample = my_mean)) +
  stat_qq()+stat_qq_line()
```

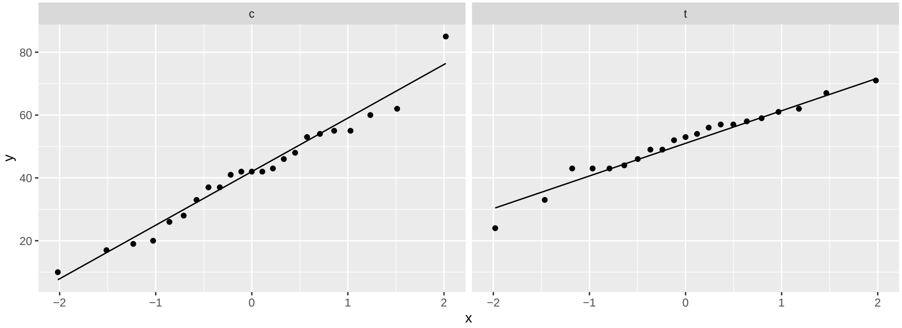


- a very very slight right-skewness, but very close to normal.
- hence the t-test is fine for the Blue Jays attendances.

Kids learning to read

- Normal quantile plots, one for each sample:

```
ggplot(kids, aes(sample = score)) +
  stat_qq() + stat_qq_line() +
  facet_wrap(~ group)
```



- These both look close to normal.

Control group

- Pull out control group children
- Obtain bootstrap sampling distribution of scores

```
kids %>% filter(group == "c") -> controls
tibble(sim = 1:10000) %>%
  rowwise() %>%
  mutate(my_sample = list(sample(controls$score,
                                 replace = TRUE))) %>%
  mutate(my_mean = mean(my_sample)) -> samples1
```

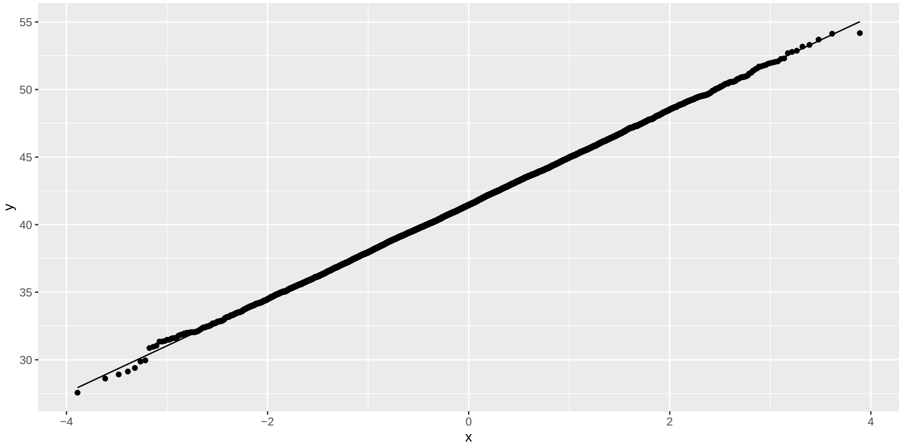
Bootstrap sample means

```
samples1
```

```
# A tibble: 10,000 x 3
# Rowwise:
     sim my_sample  my_mean
   <int> <list>       <dbl>
 1     1 <dbl [23]>    43.7
 2     2 <dbl [23]>    38.9
 3     3 <dbl [23]>    44.3
 4     4 <dbl [23]>    40.8
 5     5 <dbl [23]>    42.9
 6     6 <dbl [23]>    37.3
 7     7 <dbl [23]>    42.2
 8     8 <dbl [23]>    46.7
 9     9 <dbl [23]>    40.5
10    10 <dbl [23]>    39.2
# i 9,990 more rows
```

The bootstrap sampling distribution

```
ggplot(samples1, aes(sample = my_mean)) +
  stat_qq() + stat_qq_line()
```



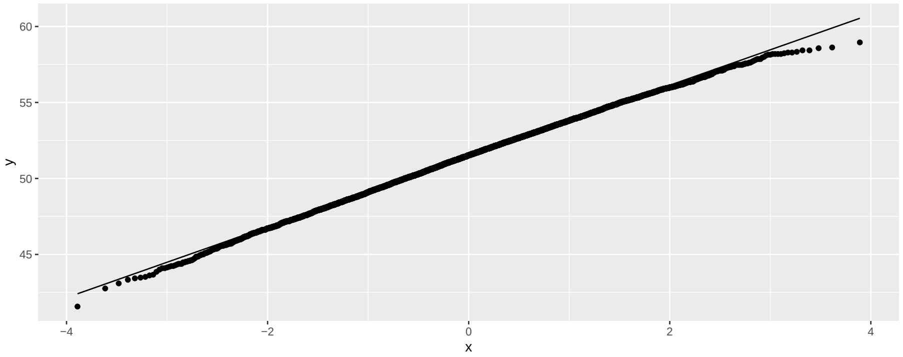
- Very close to normal.

Same, for treatment group

```
kids %>% filter(group == "t") -> treated
tibble(sim = 1:10000) %>%
  rowwise() %>%
  mutate(my_sample = list(sample(treated$score,
                                 replace = TRUE))) %>%
  mutate(my_mean = mean(my_sample)) -> samples2
```

The bootstrap sampling distribution

```
ggplot(samples2, aes(sample = my_mean)) +
  stat_qq() + stat_qq_line()
```



- Very slightly left-skewed, but close to normal. Not a problem.

Pain relief

- With matched pairs, assumption is of normality of *differences*:

```
pain %>% mutate(diff = druga - drugb) -> pain
pain
```

```
# A tibble: 12 x 4
   subject druga drugb    diff
     <dbl> <dbl> <dbl>   <dbl>
 1       1   2     3.5  -1.5
 2       2   3.6   5.7  -2.1
 3       3   2.6   2.9  -0.300
 4       4   2.6   2.4   0.200
 5       5   7.3   9.9  -2.6
 6       6   3.4   3.3   0.100
 7       7  14.9  16.7  -1.80
 8       8   6.6   6     0.600
 9       9   2.3   3.8  -1.5
10      10   2     4    -2
11      11   6.8   9.1  -2.3
12      12   8.5  20.9 -12.4
```

Bootstrap sampling distribution of differences

```
tibble(sim = 1:10000) %>%
  rowwise() %>%
  mutate(my_sample = list(sample(pain$diff, replace = TRUE)))
  mutate(my_mean = mean(my_sample)) -> samples
```

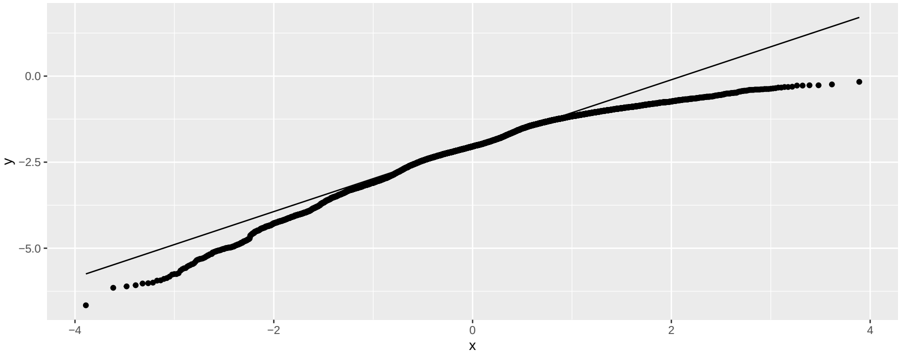
Result

```
samples
```

```
# A tibble: 10,000 x 3
# Rowwise:
     sim my_sample  my_mean
   <int> <list>       <dbl>
 1     1 <dbl [12]>  -1.82
 2     2 <dbl [12]>  -3.58
 3     3 <dbl [12]>  -2.66
 4     4 <dbl [12]>  -2.9
 5     5 <dbl [12]>  -0.975
 6     6 <dbl [12]>  -2.25
 7     7 <dbl [12]>  -2.32
 8     8 <dbl [12]>  -1.84
 9     9 <dbl [12]>  -4.77
10    10 <dbl [12]>  -2.42
# i 9,990 more rows
```

Assess it for normality

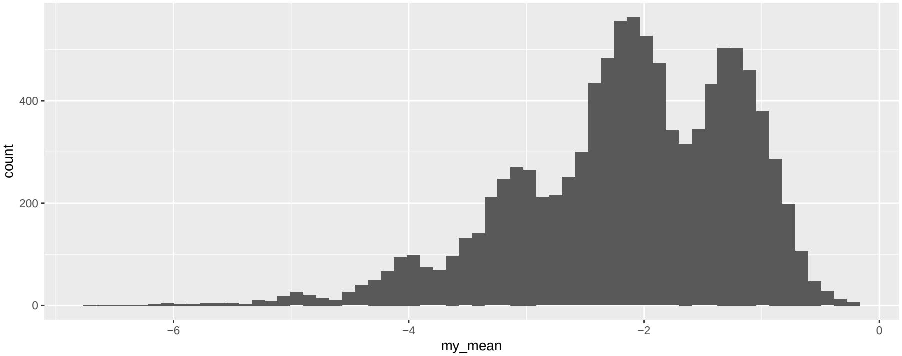
```
ggplot(samples, aes(sample = my_mean)) +
  stat_qq() + stat_qq_line()
```



- Very skewed to the left (because of low outlier)
- Matched pairs t not to be trusted at all.

Histogram with many bins

```
ggplot(samples, aes(x = my_mean)) + geom_histogram(bins = 60)
```



- actually a very multimodal distribution: one mode for each time the low outlier appears in the bootstrap sampling distribution (can be none at all up to several times).