Simulation and the bootstrap

packages

library(tidyverse)

Simulation

- Sometimes you know the exact mathematical answer to a problem, eg:
 - $\blacktriangleright~X_1, \dots X_n \sim N(\mu, \sigma^2)$, 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:

rpois(10, 3.5)

```
rnorm(5, 100, 15)
[1] 111.96072 89.80331 113.74231 90.74167 89.86461
and
```

```
[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
```

Γ1 1

9

[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

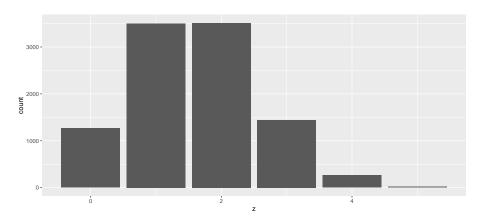
d

```
# A tibble: 10,000 x 4
# Rowwise:
     sim
           X
   <int> <int> <int> <int>
       2
       3
       4
       5
       6
10
      10
    9,990 more rows
```

Distribution of sum

Make a bar chart rather than a histogram because distribution of ${\cal Z}$ is discrete:

$$ggplot(d, aes(x = z)) + geom_bar()$$



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

$$d \%>\% count(z >= 4)$$

Only this much:

285/10000

[1] 0.0285

A sum of 5 is possible though very unlikely.

The bootstrap

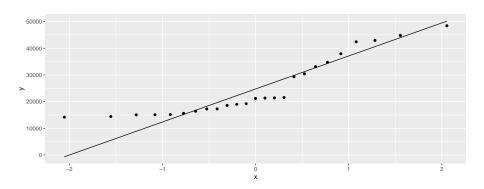
Source: Hesterberg et al

- 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):

```
boot <- sample(jays$attendance, replace=TRUE)
mean(boot)</pre>
```

```
[1] 23764.76
```

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

Comparing the actual sample with the bootstrapped one

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
```

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.

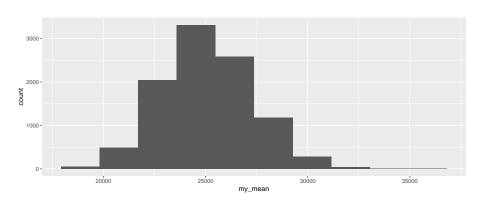
Bootstrap sample means

samples

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

Sampling distribution of sample mean

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

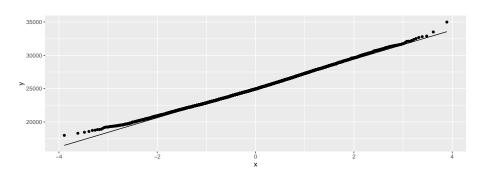


• Is that a slightly long right tail?

Normal quantile plot

might be better than a histogram:

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

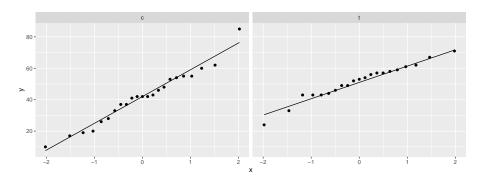


- a very very slight right-skewness, but very close to normal.
- hence the *t*-test is fine for the Blue Jays attendances.

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

Bootstrap sample means

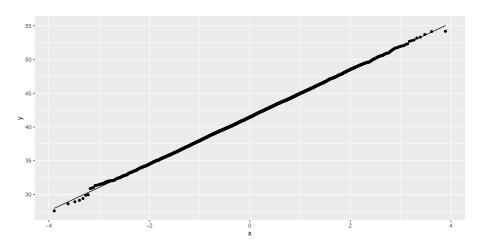
samples1

```
A tibble: 10,000 x 3
 Rowwise:
    sim my_sample my_mean
  <int> <list>
                    <dbl>
      1 <dbl [23]> 43.7
1
      2 <dbl [23]> 38.9
      3 <dbl [23]> 44.3
4
      4 <dbl [23]> 40.8
5
      5 <dbl [23]> 42.9
6
      6 <dbl [23]> 37.3
      7 <db1 [23]> 42.2
8
      8 <dbl [23]> 46.7
9
      9 <dbl [23]> 40.5
     10 <dbl [23]>
10
                     39.2
   9,990 more rows
```

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The bootstrap sampling distribution

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

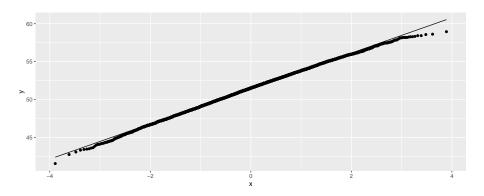


Very close to normal.

Same, for treatment group

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>
            2 	 3.5 - 1.5
         2 \quad 3.6 \quad 5.7 \quad -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
            2.3 \quad 3.8 \quad -1.5
10
        10
            2
                  4
                        -2
11
        11
            6.8
                  9.1 - 2.3
                 20.9 - 12.4
12
        12
            8.5
```

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
```

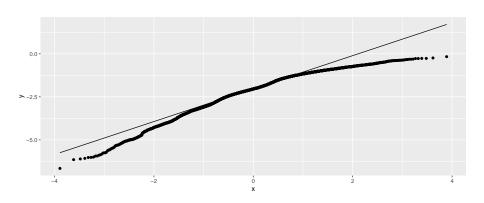
Result

samples

```
# A tibble: 10,000 x 3
 Rowwise:
    sim my_sample my_mean
  <int> <dbl>
      1 <dbl [12]> -1.82
      2 <dbl [12]> -3.58
      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 <dbl [12]> -1.84
8
 9
      9 <dbl [12]> -4.77
     10 <dbl [12]> -2.42
10
# i 9,990 more rows
```

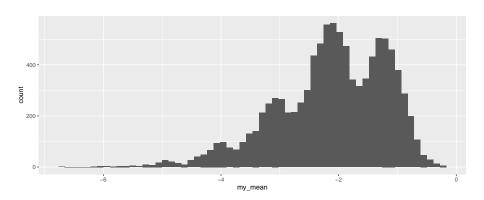
Assess it for normality

```
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



 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).