

Bootstrap Notes

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Objectives

- 1) Use the bootstrap to estimate the standard error, the standard deviation, of the sample statistic.
- 2) Using bootstrap methods, obtain and interpret a confidence interval for an unknown parameter, based on a random sample.
- 3) Describe the advantages, disadvantages, and assumptions behind using bootstrapping for confidence intervals.

Confidence intervals

In the last lesson, we introduced the concept of confidence intervals. As a reminder, confidence intervals are used to describe uncertainty around an estimate of a parameter. A confidence interval can be interpreted as a range of feasible values for an unknown parameter, given a representative sample of the population.

Recall the four general steps of building a confidence interval:

- 1) Identify the parameter you would like to estimate.
- 2) Identify a good estimate for that parameter.
- 3) Determine the distribution of your estimate or a function of your estimate.
- 4) Use this distribution to obtain a range of feasible values (confidence interval) for the parameter.

We previously used the central limit theorem to determine the distribution of our estimate. This lesson, we will build *bootstrap distribution* of sample estimates.

Bootstrapping

In many contexts, the sampling distribution of a sample statistic is either unknown or subject to assumptions. For example, suppose we wanted to obtain a 95% confidence interval on the *median* of a population. The central limit theorem does not apply to the median; we don't know its distribution.

The theory required to quantify the uncertainty of the sample median is complex. In an ideal world, we would sample data from the population again and recompute the median with this new sample. Then we could do it again. And again. And so on until we get enough median estimates that we have a good sense of the precision of our original estimate. This is an ideal world where sampling data is free or extremely cheap. That is rarely the case, which poses a challenge to this “resample from the population” approach.

However, we can sample from the sample. *Bootstrapping* allows us to simulate the sampling distribution by **resampling** from the sample. Suppose x_1, x_2, \dots, x_n is an iid random sample from the population. First

we define the empirical distribution function of X by assigning an equal probability to each x_i . Then, we sample from this empirical probability mass function. In practice, this simply means sampling from your original sample *with replacement*. Thus we are treating our sample as a discrete uniform random variable.

The general procedure for bootstrapping is to sample with replacement from your original sample, calculate and record the sample statistic for that bootstrapped sample, then repeat the process many times. The collection of sample statistics comprises a *bootstrap distribution* of the sample statistic. Generally, this procedure works quite well, provided that the sample is representative of the population. Otherwise, any bias or misrepresentation is simply amplified throughout the bootstrap process. Further, for very small sample sizes, bootstrap distributions become “choppy” and hard to interpret. Thus in small sample cases, we must use permutation or mathematical methods to determine the sampling distribution.

Once you have completed the procedure, the bootstrap distribution can be used to build a confidence interval for the population parameter or estimate the standard error. We are not using the bootstrap to find p-values.

Bootstrap example

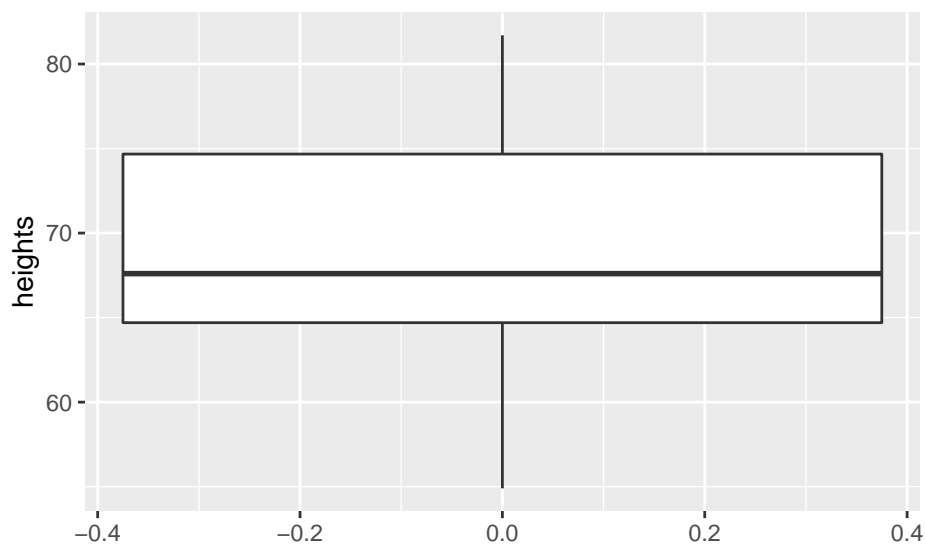
To help us understand the bootstrap, let's use an example of a single mean. We would like to estimate the mean height of students at a local college. We collect a sample of size 50 (stored in vector `heights` below).

Exercise Using both an asymptotic method, via the CLT, and the bootstrap method, find 95% confidence intervals for μ . Compare the two intervals.

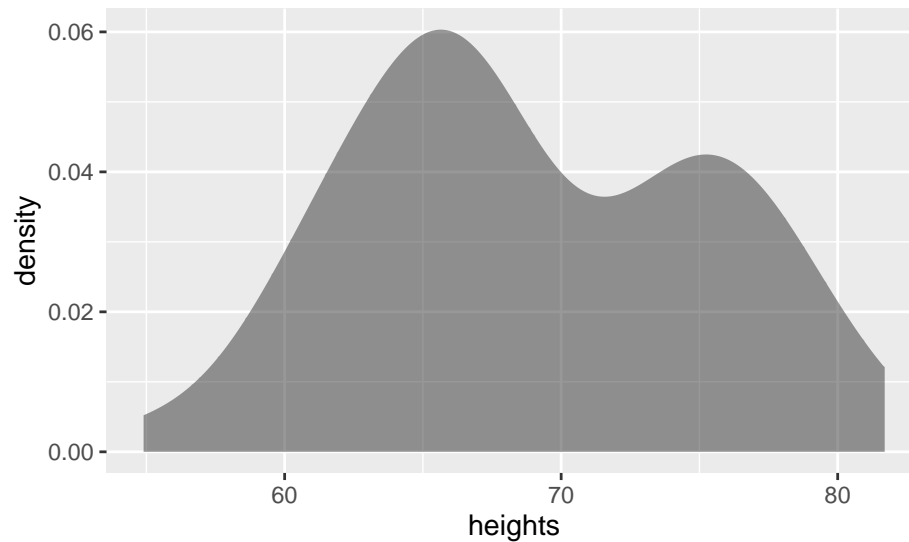
```
heights<-c(62.0,73.8,59.8,66.9,75.6,63.3,64.0,63.1,65.0,67.2,73.0,  
62.3,60.8,65.7,60.8,65.8,63.3,54.9,67.8,65.1,74.8,75.0,  
77.8,73.7,74.3,68.4,77.5,77.9,66.5,65.5,71.7,75.9,81.7,  
76.5,77.8,75.0,64.6,59.4,60.7,69.2,78.2,65.7,69.6,80.0,  
67.6,73.0,65.3,67.6,66.2,69.6)
```

Let's look at the data.

```
gf_boxplot(~heights)
```



```
gf_density(~heights)
```



It looks bimodal since there are probably both men and women in this sample and thus we have two different population distributions of heights.

```
favstats(~heights)
```

```
##   min   Q1 median    Q3  max  mean    sd  n missing
##  54.9 64.7  67.6 74.675 81.7 68.938 6.345588 50      0
```

Using CLT

The data comes from less than 10% of the population so we feel good about the assumption of independence. However, the data is bimodal and clearly does not come from a normal distribution. The sample size is larger, so this may help us. Let's continue and generate a confidence interval using the CLT and then compare with the bootstrap.

```
confint(t_test(~heights))
```

```
##   mean of x  lower  upper level
## 1    68.938 67.1346 70.7414  0.95
```

We can also calculate by hand.

```
##Asymptotically
xbar<-mean(heights)
sd<-sd(heights)
n<-length(heights)
tval<-qt(0.975,n-1)
xbar+c(-1,1)*tval*sd/sqrt(n)
```

```
## [1] 67.1346 70.7414
```

If we want to use the `tidyverse`, we must convert to a `dataframe`.

```
heights <- tibble(height=heights)
```

```
head(heights)
```

```
## # A tibble: 6 x 1
##   height
##   <dbl>
## 1    62
## 2   73.8
## 3   59.8
## 4   66.9
## 5   75.6
## 6   63.3
```

```
heights %>%
  summarise(mean=mean(height),stand_dev=sd(height),n=n(),
            ci=mean+c(-1,1)*qt(0.975,n-1)*stand_dev/sqrt(n))
```

```
## # A tibble: 2 x 4
##   mean stand_dev    n    ci
##   <dbl>    <dbl> <int> <dbl>
## 1  68.9     6.35    50  67.1
## 2  68.9     6.35    50  70.7
```

Bootstrap

The idea behind the bootstrap is that we will get an estimate of the distribution of the statistic of interest by sampling the original data with replacement. We must sample under the same regime as the original data was collected. In R, we will use the `resample()` function from the `mosaic` package. There are entire packages dedicated to resampling and you will learn more about them in Math 378.

When applied to a data frame, the `resample()` function samples rows with replacement to produce a new data frame with the same number of rows as the original, but some rows will be duplicated and others missing.

To illustrate, let's use `resample()` on the first 10 positive integers.

```
set.seed(305)
resample(1:10)
```

```
## [1] 8 7 8 1 4 4 2 2 6 9
```

Notice that 8, 4 and 2 appeared at least twice. The number 3 did not appear. This is a single bootstrap replicate of the data.

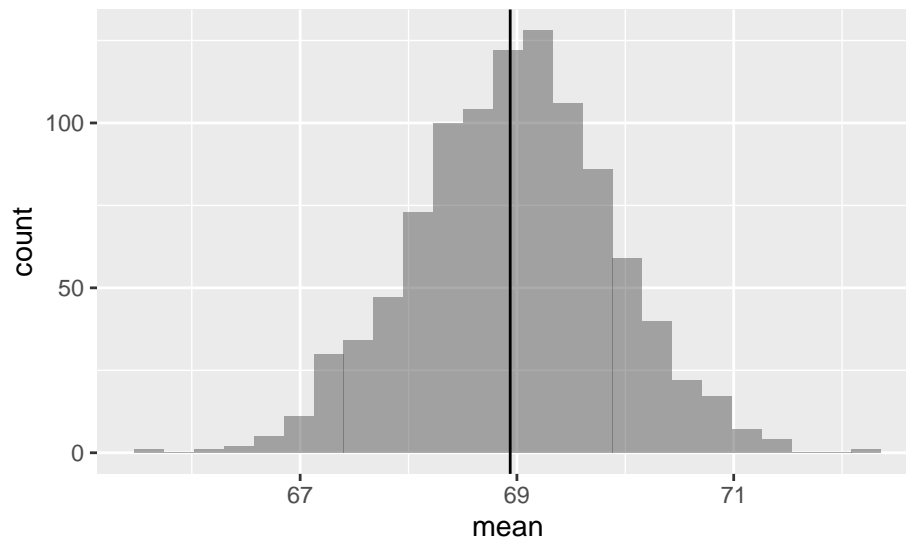
We then calculate a point estimate of the result. We repeat a large number of times, 1000 or maybe even 10000. The collection of the point estimates is called the bootstrap distribution. For the sample mean, ideally, the bootstrap distribution should be unimodal, roughly symmetric, and centered at the original estimate

Here we go with our problem.

```
set.seed(2115)
boot_results<-do(1000)*mean(~height,data=resample(heights))
```

```
boot_results %>%
  gf_histogram(~mean) %>%
  gf_vline(xintercept = 68.938)
```

Warning: geom_vline(): Ignoring 'mapping' because 'xintercept' was provided.



And a summary of the bootstrap distribution:

```
favstats(~mean,data=boot_results)
```

```
##      min      Q1 median   Q3  max    mean      sd    n missing
## 65.684 68.3915 68.976 69.55 72.3 68.96724 0.9040555 1000      0
```

Now there are two ways we could go from here to calculate a confidence interval. The first is called the percentile method where we go into the bootstrap distribution and find the appropriate quantiles. The second is called the t interval with bootstrap error. In this second method you construct a confidence interval like you would using the CLT except you use the bootstrap estimate of standard error.

Bootstrap percentile The function `cdata()` makes this easy for us.

```
cdata(~mean,data=boot_results,p=0.95)
```

```
##      lower  upper central.p
## 2.5% 67.2197 70.7964      0.95
```

Or we can use the `qdata()`.

```
qdata(~mean,data=boot_results,p=c(0.025,0.975))
```

```
##      2.5%   97.5%
## 67.2197 70.7964
```

t interval with bootstrap standard error Since the bootstrap distribution looks like a t distribution, we can use a t interval with the bootstrap standard error. The standard deviation of the bootstrap distribution is the standard error of the sample mean. We will not have to divide by \sqrt{n} since we are dealing with the distribution of the mean directly.

```
xbar<-mean(boot_results$mean)
SE<-sd(boot_results$mean)
xbar+c(-1,1)*qt(.975,49)*SE
```

```
## [1] 67.15047 70.78401
```

You could of course use tidyverse but we must change the column name.

```
boot_results %>%
  mutate(stat=mean) %>%
  summarise(mean=mean(stat),stand_dev=sd(stat),ci=mean+c(-1,1)*qt(0.975,49)*stand_dev)
```

```
##      mean stand_dev      ci
## 1 68.96724 0.9040555 67.15047
## 2 68.96724 0.9040555 70.78401
```

Of course there is a function to make this easier for us.

```
confint(boot_results, method = c("percentile", "stderr"))
```

```
##   name    lower    upper level    method estimate margin.of.error df
## 1 mean 67.21970 70.79640 0.95 percentile  68.938             NA NA
## 2 mean 67.15047 70.78401 0.95      stderr  68.938          1.816768 49
```

The three intervals are very similar.

Non-standard sample statistics

One of the huge advantages of simulation-based methods is the ability to build confidence intervals on parameters whose estimates don't have nice tidy distributions.

Example median

Consider the height data again, we would like to know the median student height and use a confidence interval for the estimate. However, we have no idea of the sampling distribution of the median. We can use bootstrapping to obtain an empirical distribution of the median.

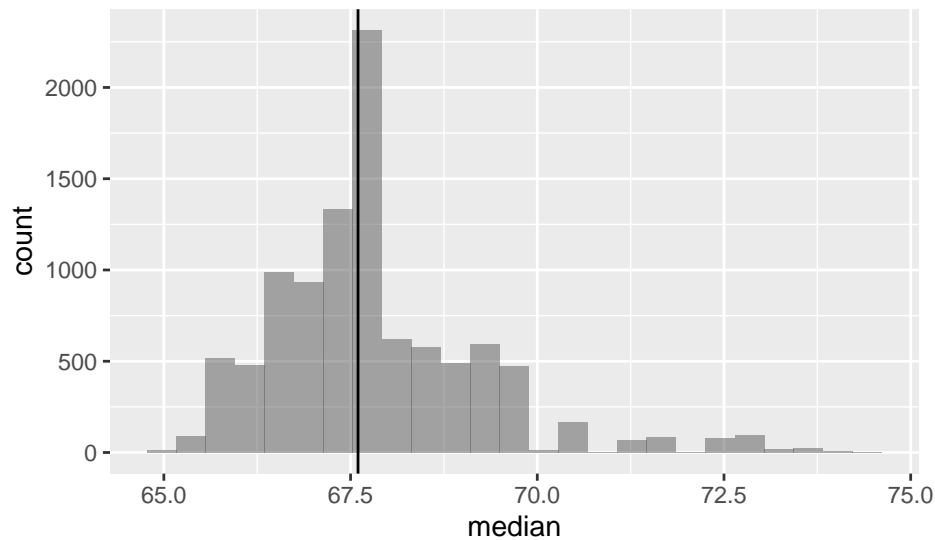
Exercise:

Find a 90% confidence interval for the median height of the students at a local college.

```
set.seed(427)
boot_results<-do(10000)*median(~height,data=resample(heights))
```

```
boot_results %>%
  gf_histogram(~median) %>%
  gf_vline(xintercept = 67.6)
```

```
## Warning: geom_vline(): Ignoring 'mapping' because 'xintercept' was provided.
```



The bootstrap sampling distribution is not symmetrical so we would not want to use the t interval approach. We will still calculate the confidence interval based on the assumption of symmetry.

```
cdata(~median,data=boot_results,p=0.90)
```

```
##      lower upper central.p
## 5%  65.8  70.65      0.9
```

```
confint(boot_results, method = c("percentile", "stderr"),level=0.9)
```

```
## Warning: confint: Using df = Inf.
```

```
##      name  lower  upper level  method estimate margin.of.error
## 1 median 65.8000 70.6500  0.9 percentile      67.6              NA
## 2 median 65.4648 70.1297  0.9      stderr      67.6      2.332455
```

Summary bootstrap

The key idea behind the bootstrap is that we estimate the population with the sample, this is called the *plug in principle*. We can then generate new samples from this population estimate. The bootstrap does not improve the accuracy of the original estimate, in fact the bootstrap distribution is centered on the original sample estimate. Instead we only get information about the variability of the sample estimate. Some people

are suspicious that we are using the data over and over. But remember we are just getting estimates of variability. In traditional statistics, when we calculate the sample standard deviation, we are using sample mean. Thus we are using the data twice. Always think of the bootstrap as providing a way to find the variability in an estimate.

Confidence interval for difference in means

To bring all the ideas we have learned so far in this block, we will work an example of testing for a difference of two means. In our opinion, the easiest method to understand is the permutation test and the most difficult is the one based on the CLT, because of the assumptions necessary to get a mathematical solution for the sampling distribution. We will also introduce the bootstrap to get a confidence interval.

Health evaluation and linkage of primary care

The HELP study was a clinical trial for adult inpatients recruited from a detoxification unit. Patients with no primary care physician were randomized to receive a multidisciplinary assessment and a brief motivational intervention or usual care, with the goal of linking them to primary medical care.

We are interested if there is a difference between male and female ages.

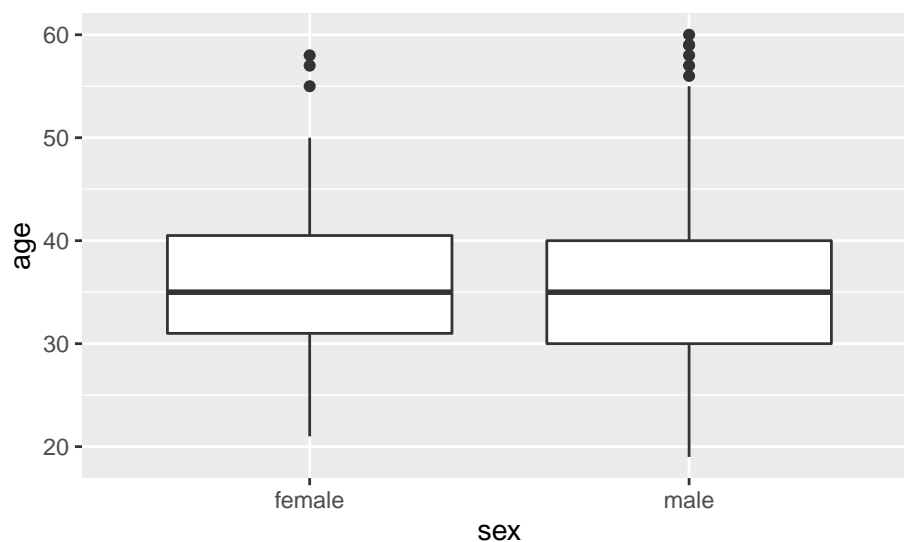
```
data("HELPrct")
```

```
HELP_sub <- HELPrct %>%  
  select(age,sex)
```

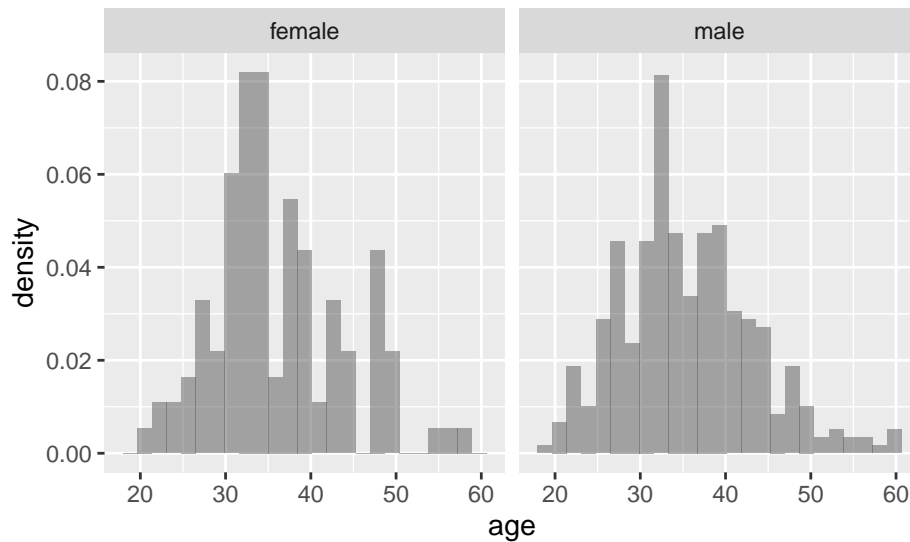
```
favstats(age~sex,data=HELP_sub)
```

##	sex	min	Q1	median	Q3	max	mean	sd	n	missing
## 1	female	21	31	35	40.5	58	36.25234	7.584858	107	0
## 2	male	19	30	35	40.0	60	35.46821	7.750110	346	0

```
HELP_sub %>%  
  gf_boxplot(age~sex)
```




```
HELP_sub %>%
  gf_dhistogram(~age|sex)
```



There might be a slight difference in the means, but is it statistically significant?

Permutation test

The permutation test is ideally suited for a hypothesis test so we will conduct that first and then see if we can generate a confidence interval.

The hypothesis for

H_0 : There is no difference in average age for men and women in the detoxification unit. In statistical notation: $\mu_{male} - \mu_{female} = 0$, where μ_{female} represents female inpatients and μ_{male} represents the male inpatients.

H_A : There is some difference in average age for men and women in the detoxification unit ($\mu_{male} - \mu_{female} \neq 0$).

Let's perform a randomization, permutation, test.

```
favstats(age~sex,data=HELP_sub)
```

```
##      sex min Q1 median   Q3 max   mean      sd   n missing
## 1 female 21 31   35 40.5  58 36.25234 7.584858 107      0
## 2  male 19 30   35 40.0  60 35.46821 7.750110 346      0
```

```
obs_stat<-diffmean(age~sex,data=HELP_sub)
obs_stat
```

```
## diffmean
## -0.7841284
```

```
set.seed(345)
results <- do(10000)*diffmean(age~shuffle(sex),data=HELP_sub)
```

```
favstats(~diffmean,data=results)
```

```
##      min      Q1    median     Q3     max      mean      sd     n
## -3.378154 -0.5638809 0.01120955 0.5863 3.486224 0.009350908 0.8492454 10000
## missing
##      0
```

The sampling distribution is centered on the null value of 0, more or less, and the standard deviation is 0.849. This is an estimate of the variability of the difference in mean ages.

```
results %>%
  gf_histogram(~diffmean) %>%
  gf_vline(xintercept=obs_stat,color="red") %>%
  gf_labs(x="Difference of means",title="Sampling distribution of difference of two means",
  subtitle="Null assumes equal means")
```

```
## Warning: geom_vline(): Ignoring 'mapping' because 'xintercept' was provided.
```



Our test statistic does not appear to be too extreme.

```
2*prop1(~(diffmean <= obs_stat),data=results)
```

```
## prop_TRUE
## 0.3523648
```

Based on this p-value, we would fail to reject the null hypothesis.

Now to construct a confidence interval we have to be careful and think about this. The object **results** has the distribution of difference in means assuming there is no difference. To get a confidence interval, we want to center this difference on the observed difference in means and not on zero.

```
cdata(~(diffmean+obs_stat),data=results)
```

```
##          lower      upper central.p
## 2.5% -2.449246 0.8789368      0.95
```

We are 95% confident that the true difference in mean ages between female and male participants in the study is between -2.45 and 0.88. Since 0 is in the confidence interval, we would fail to reject the null hypothesis.

We are assuming that the test statistic can be transformed. It turns out that the percentile method is transformation invariant so we can do the transform of shifting the null distribution by the observed value.

CLT

Using the CLT becomes difficult because we have to find a way to calculate the standard error. There have been many proposed methods, you are welcome to research them, but we will only present a couple of ideas in this section. Let's summarize the process for both hypothesis testing and confidence intervals in the case of the difference of two means using the CLT.

Hypothesis tests

When applying the t distribution for a hypothesis test, we proceed as follows:

1. Write appropriate hypotheses.
2. Verify conditions for using the t distribution.

For a difference of means when the data are not paired: each sample mean must separately satisfy the one-sample conditions for the t distribution, and the data in each group must also be independent. Just like in the one-sample case, slight skewness will not be a problem for larger sample sizes. We can have moderate skewness and be fine if our sample is 30 or more. We can have extreme skewness if our sample is 60 or more.

3. Compute the point estimate of interest, the standard error, and the degrees of freedom.
4. Compute the T score and p-value.
5. Make a conclusion based on the p-value, and write a conclusion in context and in plain language so anyone can understand the result.

We added the extra step of checking the assumptions.

Confidence intervals

Similarly, the following is how we generally computed a confidence interval using a t distribution: 1. Verify conditions for using the t distribution. (See above.)

2. Compute the point estimate of interest, the standard error, the degrees of freedom, and t_{df}^* .
3. Calculate the confidence interval using the general formula, point estimate $\pm t_{df}^* SE$.
4. Put the conclusions in context and in plain language so even non-statisticians can understand the results.

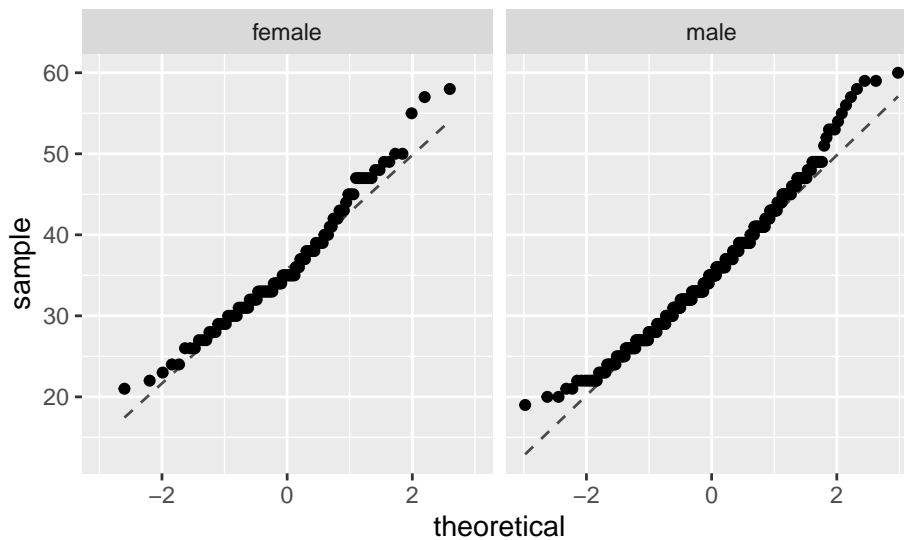
If the assumptions above are met, each sample mean can itself be modeled using a t distribution and if the samples are independent, then the sample difference of two means, $\bar{x}_1 - \bar{x}_2$, can be modeled using the t distribution and the standard error

$$SE_{\bar{x}_1 - \bar{x}_2} = \sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}$$

To calculate the degrees of freedom, use statistical software or the smaller of $n_1 - 1$ and $n_2 - 1$.

Results Back to our study, the men and women were independent of each other. Additionally, the distributions in each population don't show any clear deviations from normality, some slight skewness but the sample size reduces this concern. Finally, within each group we also need independence. If they represent less than 10% of the population, we are good to go on this. This condition might be difficult to verify.

```
HELP_sub %>%
  gf_qq(~age|sex) %>%
  gf_qqline(~age|sex)
```



The distribution of males tends to have longer tails than a normal and the female distribution is skewed to the right. The sample sizes are large enough that this does not worry us.

```
favstats(age~sex,data=HELP_sub)
```

```
##      sex min Q1 median   Q3 max   mean      sd  n missing
## 1 female 21 31    35 40.5  58 36.25234 7.584858 107      0
## 2  male 19 30    35 40.0  60 35.46821 7.750110 346      0
```

Let's find the confidence interval first.

```
(35.47-36.25)+c(-1,1)*qt(.975,106)*sqrt(7.58^2/107+7.75^2/346)
```

```
## [1] -2.4512328  0.8912328
```

This very close to what we got with the permutation test.

Now let's find the p-value for the hypothesis test.

The test statistic is:

$$T = \frac{\text{point estimate} - \text{null value}}{SE}$$

$$= \frac{(35.47 - 36.25) - 0}{\sqrt{\left(\frac{7.58^2}{107} + \frac{7.75^2}{346}\right)}} = -0.92976$$

We use the smaller of $n_1 - 1$ and $n_2 - 1$ as the degrees of freedom: $df = 106$.

The p-value is:

```
2*pt(-0.92976,106)
```

```
## [1] 0.3546079
```

Of course, there is a function that does this for us.

```
t_test(age~sex,data=HELP_sub)
```

```
##
## Welch Two Sample t-test
##
## data: age by sex
## t = 0.92976, df = 179.74, p-value = 0.3537
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
## -0.8800365 2.4482932
## sample estimates:
## mean in group female mean in group male
## 36.25234 35.46821
```

Notice that the degrees of freedom are not an integer, this is because it is a weighted average of the two different samples sizes and standard deviations.

Pooled standard deviation Occasionally, two populations will have standard deviations that are so similar that they can be treated as identical. This is an assumption of equal variance in each group. For example, historical data or a well-understood biological mechanism may justify this strong assumption. In such cases, we can make the t distribution approach slightly more precise by using a pooled standard deviation.

The **pooled standard deviation** of two groups is a way to use data from both samples to better estimate the standard deviation and standard error. If s_1 and s_2 are the standard deviations of groups 1 and 2 and there are good reasons to believe that the population standard deviations are equal, then we can obtain an improved estimate of the group variances by pooling their data:

$$s_{pooled}^2 = \frac{s_1^2 \times (n_1 - 1) + s_2^2 \times (n_2 - 1)}{n_1 + n_2 - 2}$$

where n_1 and n_2 are the sample sizes, as before. To use this new statistic, we substitute s_{pooled}^2 in place of s_1^2 and s_2^2 in the standard error formula, and we use an updated formula for the degrees of freedom:

$$df = n_1 + n_2 - 2$$

The benefits of pooling the standard deviation are realized through obtaining a better estimate of the standard deviation for each group and using a larger degrees of freedom parameter for the t distribution. Both of these changes may permit a more accurate model of the sampling distribution of $\bar{x}_1 - \bar{x}_2$.

Caution

Pooling standard deviations should be done only after careful research

A pooled standard deviation is only appropriate when background research indicates the population standard deviations are nearly equal. When the sample size is large and the condition may be adequately checked with data, the benefits of pooling the standard deviations greatly diminishes.}

In R we can before the difference of two means with equal variance using `var.equal`.

```
t_test(age~sex,data=HELP_sub,var.equal=TRUE)

##
## Two Sample t-test
##
## data: age by sex
## t = 0.91923, df = 451, p-value = 0.3585
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
## -0.8922735 2.4605303
## sample estimates:
## mean in group female mean in group male
## 36.25234 35.46821
```

Since our sample sizes were so large, this did not have a big impact on the results.

Bootstrap

Finally, we will construct a confidence interval through the use of the bootstrap distribution. In this problem we have to be careful and sample within each group. Compare the following two sets of samples.

```
favstats(age ~ sex, data = resample(HELP_sub))

##      sex min Q1 median   Q3 max   mean      sd  n missing
## 1 female 21 30   33 38.75 50 34.64706 6.267387 102      0
## 2  male 19 29   33 39.00 59 34.74359 7.833066 351      0
```

and

```
favstats(age ~ sex, data = resample(HELP_rct,groups=sex))

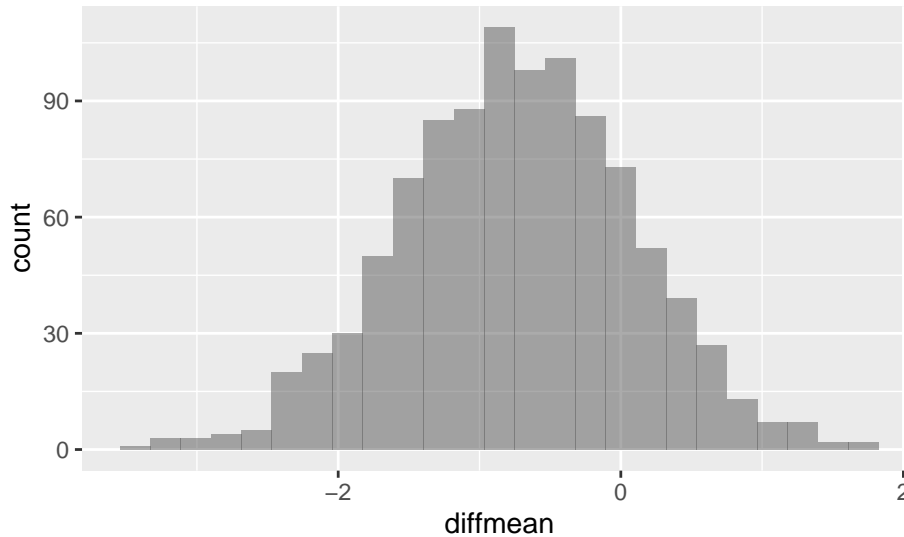
##      sex min Q1 median   Q3 max   mean      sd  n missing
## 1 female 22 31   34 39.5 57 35.60748 6.901951 107      0
## 2  male 20 31   35 41.0 60 35.94798 8.039227 346      0
```

Notice in the second, we are keeping the samples the same size.

Let's get our bootstrap distribution.

```
set.seed(2527)
results <- do(1000) * diffmean(age ~ sex, data = resample(HELP_sub, groups = sex))

results %>%
  gf_histogram(~diffmean)
```



```
cdata( ~ diffmean, p = 0.95, data = results)
```

```
##          lower      upper central.p
## 2.5% -2.394406 0.8563786      0.95
```

Again, similar results.

Frequently asked questions

1. There are more types of bootstrap techniques, right?

Yes! There are many excellent bootstrap techniques. We have only chosen to present two bootstrap techniques that could be explained in a single lesson and is also reasonably reliable. There are many adjustments that can be made to speed up and improve accurate. Packages such as **resample** and **boot** are more appropriate for these situations.

2. I've heard the percentile bootstrap is very robust.

It is a **commonly** held belief that the percentile bootstrap is a robust bootstrap method. That is false. The percentile method is one of the least reliable bootstrap methods. However, it is easy to use and understand and can give a first attempt at a solution before more accurate methods are used.

3. I should use 1000 replicates in my bootstrap and permutation tests.

The randomization and bootstrap distributions involve a random component from the sampling process and thus p-values and confidence intervals computed from the same data will vary. The amount of this **Monte Carlo** variability depends on the number of replicates used to create the randomization or bootstrap distribution. It is important that we not use too few as this will introduce too much random noise into p-value and confidence interval calculations. But each replicate costs time, and the marginal gain for each additional replicate decreases as the number of replicates increases. There is little reason to use millions of replicates (unless the goal is to estimate very small p-values). We generally use roughly 1000 for routine or preliminary work and increase this to 10,000 when we want to reduce the effects of Monte Carlo variability.

File Creation Information

- File creation date: 2020-10-25
- Windows version: Windows 10 x64 (build 18362)
- R version 3.6.3 (2020-02-29)
- `mosaic` package version: 1.7.0
- `tidyverse` package version: 1.3.0