

# **Resampling methods: Bootstrap and Permutation tests**

---

Julia Wrobel

# Overview

```
library(tidyverse)
```

Today, we cover:

- Resampling methods
  - Bootstrap
  - Permutation tests

## Announcements:

- HW2 posted and due 2/11 at 10:00AM
- Final project due 5/1 at midnight

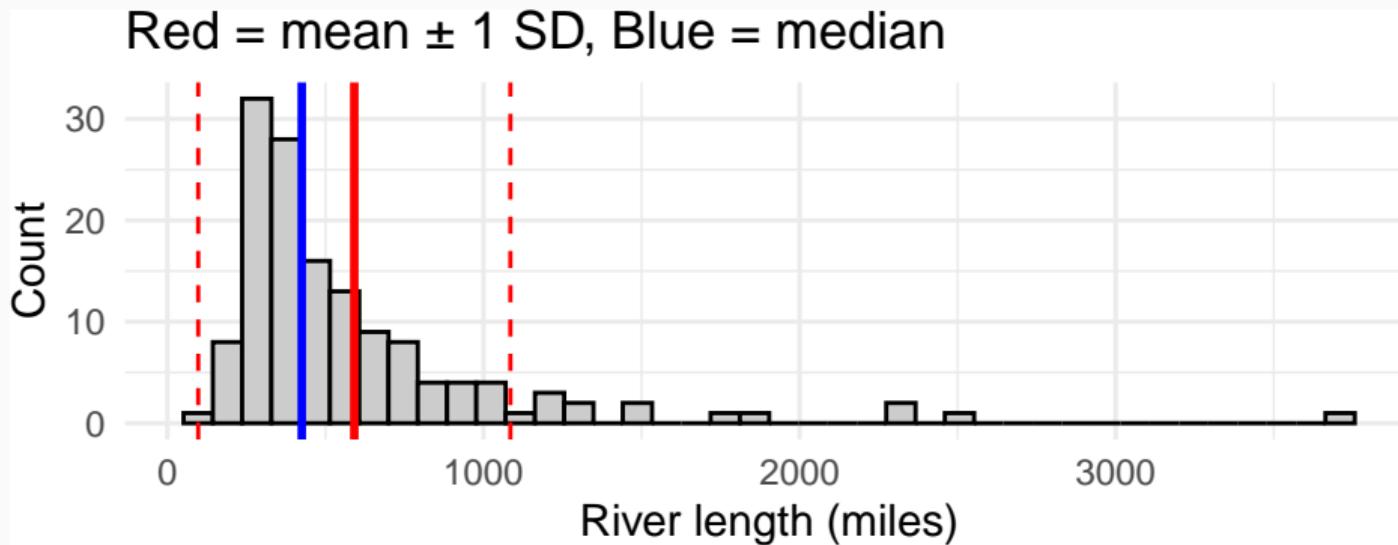
# Why do we need resampling methods?

- Inference requires understanding the **sampling distribution** of a statistic
- Classical tools rely on:
  - Known parametric models
  - Large sample (CLT-based) approximations
- In many modern settings:
  - Sampling distributions are unknown
  - Asymptotics may be inaccurate or hard to obtain
  - Deriving standard errors is difficult or impossible

# Rivers t-test example

- rivers data: length (in miles) of 141 major North American Rivers

Red = mean  $\pm$  1 SD, Blue = median



# Rivers t-test example

Is the mean length of rivers in North America equal to 1000 miles?

- $H_0 : \mu = 1000$

One Sample t-test

```
data: rivers
t = -9.8293, df = 140, p-value < 2.2e-16
alternative hypothesis: true mean is not equal to 1000
95 percent confidence interval:
 508.9559 673.4129
sample estimates:
mean of x
591.1844
```

# Rivers t-test example

## T-test assumptions

- Observations are independent
- CLT holds: sampling distribution of  $\bar{Y}$  will be approximately normal even if the population isn't
- $\bar{Y}$  and  $s$  are approximately independent

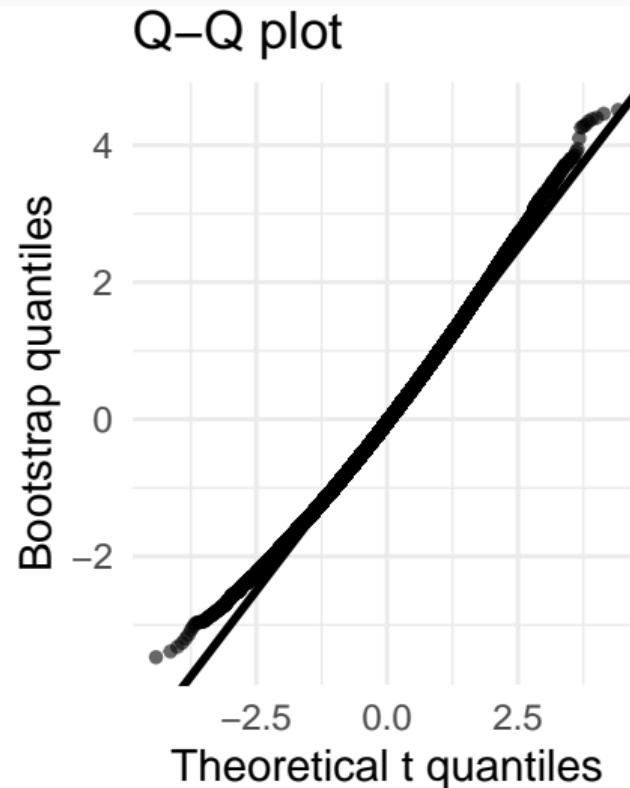
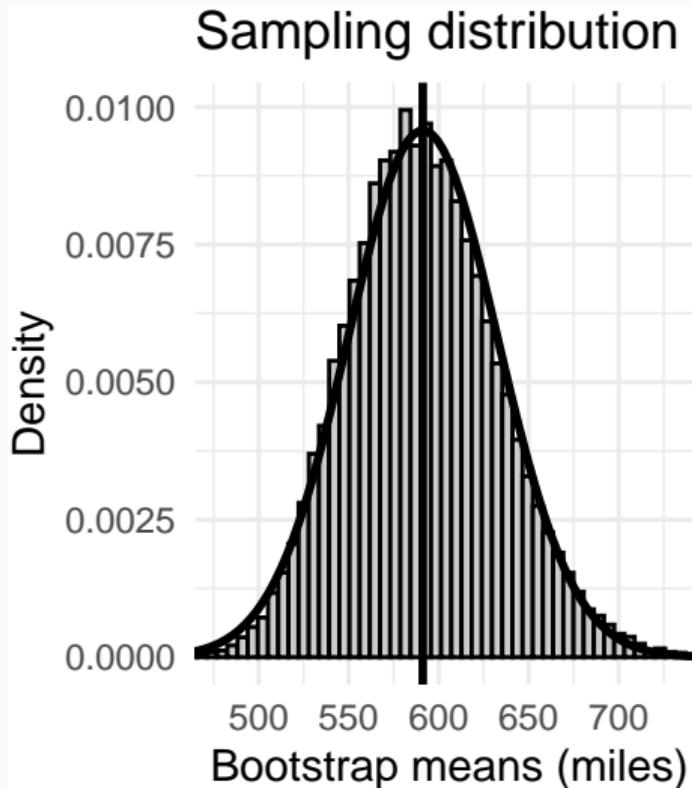
$$t = \frac{\bar{Y} - \mu}{s/\sqrt{n}}$$

- $t \sim t_{n-1}$  or  $t \approx N(0, 1)$

Highly skewed data violates these assumptions

- Mean and variance are correlated
- Skewness is a property of the underlying distribution, not  $n$ , so increasing sample size won't necessarily fix the problem
  - Poor t-test coverage

# Rivers t-test sampling distribution



# Bootstrap: motivation

Suppose we observe data  $Y_1 \dots Y_n \sim F$  and we want to compute a statistic  $T(Y_1, \dots Y_n)$ .

We want:

- Standard errors
- Confidence intervals
- But  $F$  is unknown
- The distribution of  $T$  depends on  $F$

**How can we approximate the sampling distribution of  $T$  without knowing  $F$ ?**

# Why classical asymptotics can fail

CLT-based inference assumes approximate normality of the test statistic. This can fail, even as  $n \rightarrow \infty$  when:

- Data is skewed or heavy-tailed
- For nonlinear or non-smooth statistics (i.e. sample median vs. sample mean)

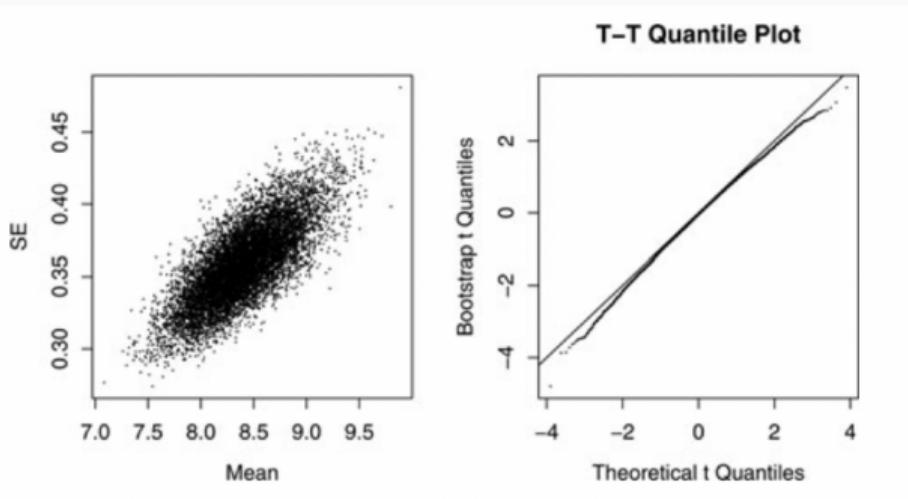
When these assumptions fail, asymptotics-based confidence intervals can have poor coverage.

- Also great for more complicated statistics where asymptotics can be hard to calculate

# When t is not t

When  $Y_i$  come from a skewed distribution, the sample mean and its SE are correlated and their correlation does not decrease as  $n \rightarrow \infty$

- $\Rightarrow$  t-statistic is not t-distributed



- If your test or CI assumes your statistic has a normal or t sampling distribution, **any deviation** from the diagonal implies your test/interval will perform poorly

# When t is not t

Idea: confidence intervals for parameter estimates provide no robustness against non-normality!

- Coverage does not improve as  $n \rightarrow \infty$ !

Bootstrapping can be very useful for constructing better confidence intervals for these parameters.

# A computational workaround

- We cannot repeatedly sample from the true population distribution  $F$
- But, we *do* have data sampled from  $F$

**Idea:** use the observed data to approximate  $F$  through simulation

# Parameters as functionals

For some cumulative distribution function  $F$ , suppose we are interested in a parameter,  $\theta \stackrel{\triangle}{=} T(F)$ , written as a functional of  $F$

- A **functional** is a function of a function
  - Mean of  $F$ :  $T(F) = \int y dF(y)$
  - Median of  $F$ :  $T(F) = \inf\{y : F(y) \geq 0.5\}$
- The statistic  $T(Y_1, \dots, Y_n)$  is an estimate of  $T(F)$

Inference about a statistic is inference about a **functional of an unknown distribution**.

# Estimating the data-generating distribution

- The true distribution of  $F$  is unknown, so we have to estimate it
- A natural estimator is the **empirical distribution**:

$$\hat{F}_n(y) = \frac{1}{n} \sum_{i=1}^n I\{Y_i \leq y\}$$

- $\hat{F}_n$  places  $1/n$  mass at each observed data point
- To estimate a functional  $T(F)$ , we plug in the empirical distribution,  $\hat{F}_n(y)$ , for  $F(y)$ :

# The Bootstrap Principle

- Replace the unknown distribution  $F$  with its estimate  $\hat{F}_n$
- Approximate the sampling distribution of  $T(Y_n, \dots, Y_n)$  by:
  - Repeatedly sampling from  $\hat{F}_n$
  - Recomputing the statistic

**Idea:** Bootstrap principle is used to estimate the sampling distribution of a *statistic* without relying on strong parametric assumptions about the underlying population distribution

# What the bootstrap gives us

- Approximate sampling distribution
- Standard error estimates
- Confidence intervals

# The Bootstrap Principle

- Nonparametric bootstrap
- Parametric bootstrap
- Wild bootstrap
- Smooth bootstrap
- Bag of little bootstraps

# Nonparameteric bootstrap

A **bootstrap sample** is a random sample of size drawn **with replacement** from  $\hat{F}_n$

- Bootstrap sample denoted  $y^* = (y_1^*, y_2^*, \dots, y_n^*)$
- $\hat{\theta}^* \stackrel{\triangle}{=} T(\hat{F}_n(y^*))$  is the corresponding bootstrap estimate using the sample  $y^*$ 
  - We'll call this  $T(\hat{F}_n^*)$  to simplify notation

Draw  $B$  bootstrap samples and calculate  $\hat{\theta}_i^*, i = 1, \dots, B$ .

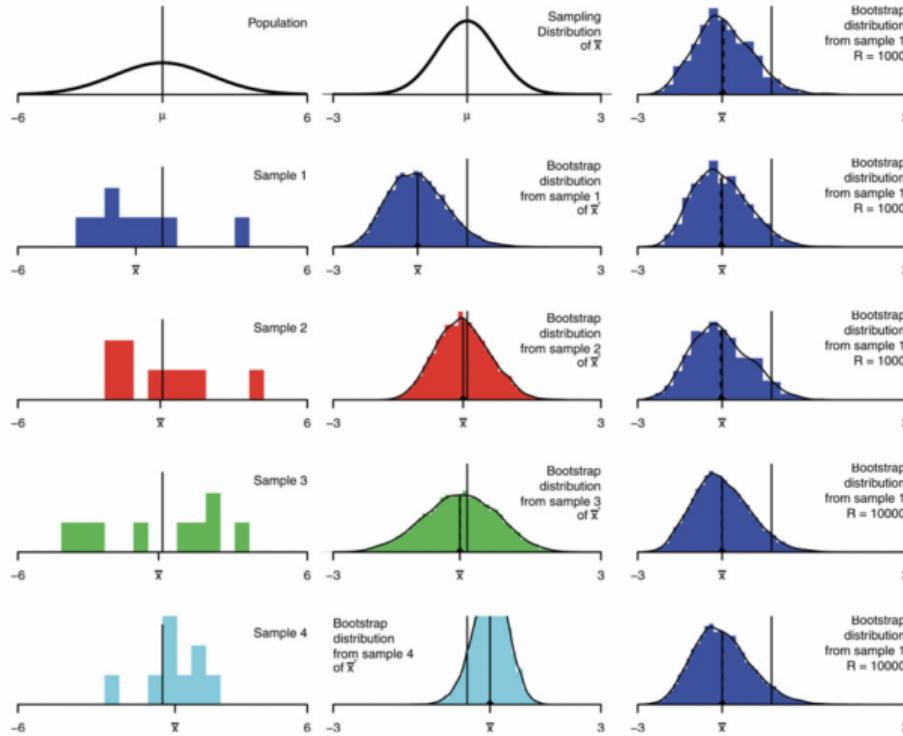
- Then, SE of  $\hat{\theta}$  can be estimated using the standard deviation of the  $B$  replications:

$$\widehat{SE}(\hat{\theta}) = \sqrt{\frac{\sum_{i=1}^B (\hat{\theta}_i^* - \bar{\theta}^*)^2}{B - 1}}$$

# Why does it work?

- $\hat{F}_n \rightarrow F$  uniformly by Glivenko-Cantelli
- $\implies$  when  $n$  is large, sampling from  $\hat{F}_n$  resembles sampling from  $F$
- Potential sources of error:
  - Finite sample bias
  - Bootstrap distribution contains Monte Carlo error when exhaustive resampling is infeasible
    - For fixed  $n$ , number of possible bootstrap samples is  $\binom{2n-1}{n}$

# Sources of error



# Example: nonparameteric bootstrap

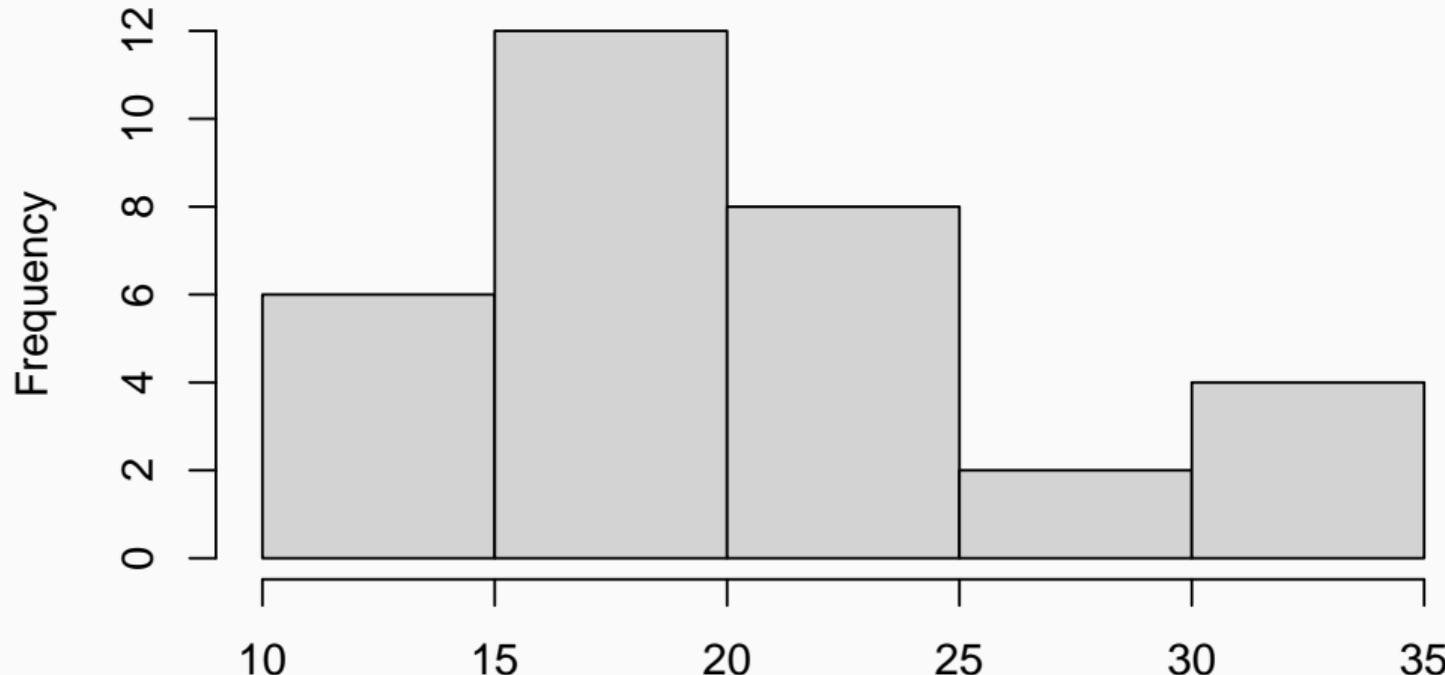
Using mtcars dataset, we will look at the mean mpg for different cars

```
data(mtcars)  
str(mtcars)
```

```
'data.frame': 32 obs. of 11 variables:  
 $ mpg : num 21 21 22.8 21.4 18.7 18.1 14.3 24.4 22.8 19.2 ...  
 $ cyl : num 6 6 4 6 8 6 8 4 4 6 ...  
 $ disp: num 160 160 108 258 360 ...  
 $ hp  : num 110 110 93 110 175 105 245 62 95 123 ...  
 $ drat: num 3.9 3.9 3.85 3.08 3.15 2.76 3.21 3.69 3.92 3.92 ...  
 $ wt  : num 2.62 2.88 2.32 3.21 3.44 ...  
 $ qsec: num 16.5 17 18.6 19.4 17 ...  
 $ vs  : num 0 0 1 1 0 1 0 1 1 1 ...  
 $ am  : num 1 1 1 0 0 0 0 0 0 0 ...  
 $ gear: num 4 4 4 3 3 3 3 4 4 4 ...  
 $ carb: num 4 4 1 1 2 1 4 2 2 4 ...
```

# Example: nonparameteric bootstrap

Histogram of mtcars\$mpg



# Example: nonparameteric bootstrap

```
B = 10000
mpg = mtcars$mpg
boot_mean = rep(NA, B)
set.seed(222)
for(i in 1:B){
  ystar = sample(mpg, size = length(mpg), replace = TRUE)
  boot_mean[i] = mean(ystar)
}

paste0("mean: ", round(mean(mpg),3),
      "; bootstrapped mean: ", round(mean(boot_mean),3))
```

```
[1] "mean: 20.091; bootstrapped mean: 20.096"
```

## Example: nonparameteric bootstrap

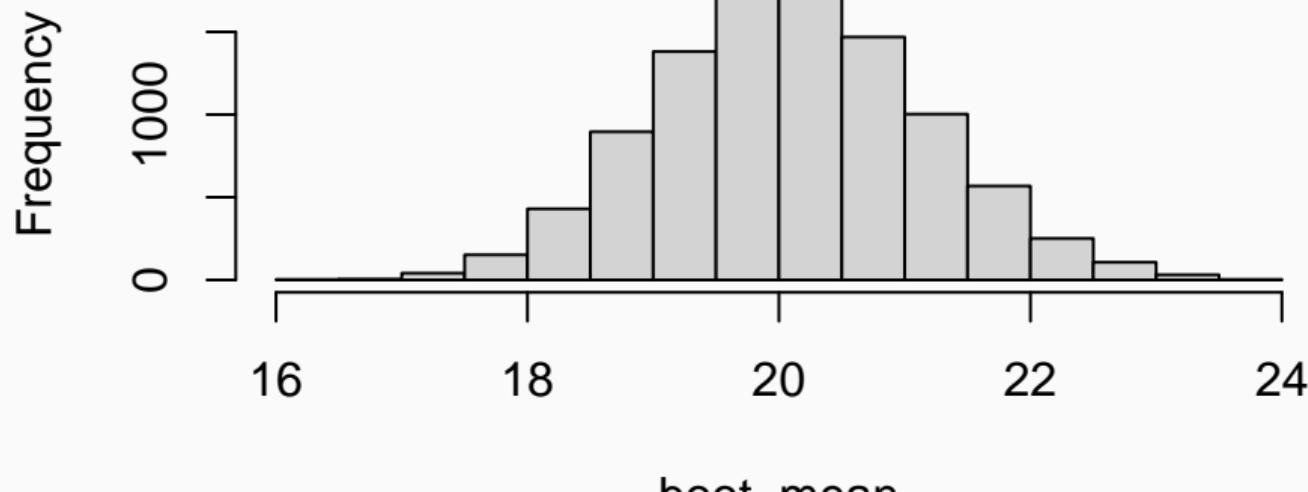
```
se_mean = sd(mpg)/sqrt(length(mpg))
paste0("sd: ", round(se_mean,3),
      "; bootstrapped sd: ", round(sd(boot_mean),3))
```

```
[1] "sd: 1.065; bootstrapped sd: 1.056"
```

## Example: nonparameteric bootstrap

```
hist(boot_mean)
```

Histogram of boot\_mean



# Bootstrap confidence intervals

- When it works, the bootstrap can be very useful for constructing confidence intervals (CIs) for a parameter  $\theta$
- Multiple methods for constructing bootstrap CIs exist!
  - Percentile intervals
  - $t$  intervals with bootstrap SE (also called Wald-type)
  - bootstrap  $t$
  - BCa intervals
- Quality of different approaches generally depends on  $n$  and the skewness of the original data

# Order of accuracy

- Recall “big-O” notation for non-negative functions  $f, g$ :
  - $f(x) \in O(g(x))$  iff  $f(x) \leq hg(x) \forall x \geq x_0$  and some  $h > 0$
- A confidence interval is **first-order accurate** if the non-coverage probability differs from the nominal value by  $O(n^{-1/2})$ :
  - $Pr(\theta < \theta_{lb}) + P(\theta > \theta_{ub}) = \alpha + O(n^{-1/2})$
- A confidence interval is second-order accurate if the non-coverage probability differs from the nominal value by  $O(n^{-1})$ :
  - $Pr(\theta < \theta_{lb}) + P(\theta > \theta_{ub}) = \alpha + O(n^{-1})$

# Percentile method

The simplest approach to constructing a bootstrap CI is the **percentile method**.

- Let  $\hat{\theta}_1^*, \dots, \hat{\theta}_B^*$  be a bootstrap sample of point estimators
- Then, a two-sided  $100 \times (1 - \alpha)\%$  bootstrap percentile CI is

$$(\xi_{\alpha/2}^*, \xi_{1-\alpha/2}^*)$$

- where  $\xi_p^*$  is the  $p^{th}$  percentile of the bootstrap samples

# Percentile method

## Pros:

- Simple to implement and easy to understand
- It is **transformation invariant**: the percentile method confidence interval for a monotone transformation of  $\theta$  can be obtained by transforming the endpoints of the interval for  $\theta$
- Works better than some other methods when data are skewed

## Cons:

- Tends to be too narrow with small sample sizes
- The percentile method is only first-order accurate

## *t* intervals with bootstrap SE

Recall that if  $(\hat{\theta} - \theta) / \hat{se}(\hat{\theta}) \rightarrow N(0, 1)$ , then the (Wald) approximate CI for  $\theta$  is

$$\hat{\theta} \pm Z_{1-\alpha/2} \times \hat{se}(\hat{\theta})$$

- This interval will closely agree with the percentile bootstrap CI when  $\hat{\theta}$  is approximately normal
- What if we don't know  $se(\hat{\theta})$  or  $se(\hat{\theta})$  is difficult to calculate?

## $t$ intervals with bootstrap SE

When  $se(\hat{\theta})$  is unknown or cumbersome, we can use a bootstrap estimate of the standard error of  $\hat{\theta}$  instead:

$$\hat{\theta} \pm Z_{1-\alpha/2} \times \hat{se}_b(\hat{\theta})$$

- For smaller samples, replace the  $Z$  quantile by a  $t$  quantile:

$$\hat{\theta} \pm t_{1-\alpha/2, n-1} \times \hat{se}_b(\hat{\theta})$$

- If you can estimate  $se(\hat{\theta})$  directly, there is no real benefit of using  $\hat{se}_b(\hat{\theta})$

# *t* intervals with bootstrap SE

## Pros:

- Simple to implement and easy to understand
- Can be applied to situations where  $se(\hat{\theta})$  is difficult to derive

## Cons:

- **Biased:** comparable to using the MLE  $\sqrt{\frac{1}{n} \sum_i (x_i - \bar{x})^2}$  instead of the unbiased estimate  $\sqrt{\frac{1}{n-1} \sum_i (x_i - \bar{x})^2}$
- Can perform poorly if distribution is skewed
- Tends to be too narrow with small sample sizes
- Only first-order accurate

# Bootstrap $t$ method

The **bootstrap-t** method uses simulation to estimate the  $t$  quantile for the interval.

- For each bootstrap sample, calculate  $t_b^*$ , where:
  - $t_b^* = \frac{\hat{\theta}_b^* - \hat{\theta}}{se(\hat{\theta}_b^*)}$
  - $\hat{\theta}$  is estimated from the original sample
  - $\hat{\theta}_b^*$  is estimated from the  $b^{th}$  bootstrap sample
  - $se(\hat{\theta}_b^*)$  is the SE of the  $b^{th}$  estimate

# Bootstrap $t$ method

The **bootstrap-t** method uses simulation to estimate the  $t$  quantile for the interval.

- For **each** bootstrap sample, calculate  $t_b^*$ , where:
  - $t_b^* = \frac{\hat{\theta}_b^* - \hat{\theta}}{se(\hat{\theta}_b^*)}$
  - $\hat{\theta}$  is estimated from the original sample
  - $\hat{\theta}_b^*$  is estimated from the  $b^{th}$  bootstrap sample
  - $se(\hat{\theta}_b^*)$  is the SE of the  $b^{th}$  estimate
- Since  $se(\hat{\theta}_b^*)$  is unknown, must estimate it...

# Bootstrap $t$ method

Note that calculating  $\hat{se}(\hat{\theta}_b^*)$  for each bootstrap estimate requires (nested) bootstrapping!

- Obtain a bootstrap estimate of  $se(\hat{\theta}_b^*)$  for **each**  $b = 1, \dots, B$ 
  - For each bootstrap sample  $b$ , run  $k = 1, \dots, K$  bootstrap simulations to obtain  $\hat{\theta}_{b,k}^*$  and use these to estimate  $se(\hat{\theta}_b^*)$  for calculating  $t_b^*$
- Calculate lower and upper quantiles of the *bootstrap t distribution*,  $t_{1-\alpha/2}^*$  and  $t^*\alpha/2$  and construct the CI:

$$(\hat{\theta} - t_{1-\alpha/2}^* \times se(\hat{\theta}), \hat{\theta} - t_{\alpha/2}^* \times se(\hat{\theta}))$$

- $se(\hat{\theta})$  is the SE of the estimate from the original sample, or can be estimated using the top-level bootstrap

# Bootstrap $t$ method

## Pros:

- Second-order accurate
- Usually outperforms the other methods discussed so far, especially for non-normal populations.
- For skewed data, much more asymmetric than the percentile bootstrap interval which corrects for the possibility that we observed too few observations from the tail

## Cons:

- Requires an iterated bootstrap
- The bootstrap-t interval is not transformation invariant. Must reconstruct the CI for a function of the parameter  $g(\theta)$

# BCa Bootstrap

The bias-corrected accelerated (BCa) method is an improvement over the percentile method, though still does not work well in small sample sizes.

- BCa intervals use percentiles of the bootstrap distribution, but not necessarily the  $100 \times \alpha$ -th and  $100 \times (1 - \alpha)$ -th percentiles
- Adjusts for **bias** in the bootstrap distribution and variability in the precision of the estimate (aka **acceleration**)

First, estimate a bias correction factor  $\hat{z}_0$ :

$$\hat{z}_0 = \Phi^{-1} \left( \frac{\#\{\hat{\theta}^* < \hat{\theta}\}}{B} \right)$$

- The acceleration parameter measures how the estimator's variability changes with the true parameter

# BCa Bootstrap

Next, estimate the acceleration parameter  $\hat{a}$ :

$$\hat{a} = \frac{\sum_{i=1}^n (\hat{\theta}_{(.)} - \hat{\theta}_{(i)})^3}{6 \left( \sum_{i=1}^n (\hat{\theta}_{(.)} - \hat{\theta}_{(i)})^2 \right)^{3/2}}$$

- $\hat{\theta}_{(i)}$  is the value of the statistic with the  $i^{th}$  observation removed (i.e. the  $i^{th}$  jackknife estimate)
- $\hat{\theta}_{(.)}$  is the mean of the  $n$  jackknife estimates
- adjusts for the rate of change in the standard error as the estimate changes

# BCa Bootstrap

After estimating the bias correction  $\hat{z}_0$  and acceleration  $\hat{a}$ , compute:

$$\alpha_1 = \Phi \left( \hat{z}_0 + \frac{\hat{z}_0 + z_{\alpha/2}}{1 - \hat{a}(\hat{z}_0 + z_{\alpha/2})} \right)$$

$$\alpha_2 = \Phi \left( \hat{z}_0 + \frac{\hat{z}_0 + z_{1-\alpha/2}}{1 - \hat{a}(\hat{z}_0 + z_{1-\alpha/2})} \right)$$

- $\Phi$  is the standard normal CDF (`pnorm`)
- $z_\alpha$  is the  $100 \times \alpha$ -th percentile of the standard normal
- Use these new percentiles to construct a CI
  - The BCa interval is the same as the percentile interval when  $\hat{a} = \hat{z}_0 = 0$

# BCa Bootstrap

## Pros:

- Second-order accurate and transformation invariant
- Works well for a variety parameters
- For skewed data, the percentile bootstrap is not asymmetric enough and the BCa bootstrap addresses this limitation
- Implemented in the `bcanon()` function in the `bootstrap` R library

## Cons:

- Estimation of the acceleration parameter requires the jackknife
- Less intuitive than other methods
- Still doesn't work great for small sample sizes

# Parametric bootstrap

If we have information about the population distribution, this can be used in resampling for bootstrap inference

- If the assumption about the population distribution is correct then the parametric bootstrap will perform better than the nonparametric bootstrap
- If the assumption not correct, then the nonparametric bootstrap should perform better.

# Parametric bootstrap example

Suppose we have data from a  $N(\mu, \sigma^2)$  distribution,  $Y = \{y_1, \dots, y_n\}$

- Interested in obtaining an estimate of the standard error of the trimmed mean with 10% trimmed from each tail
- To employ the parametric bootstrap, we would start by generating  $n$  values from a  $N(\hat{\mu}, \hat{\sigma}^2)$ 
  - $\hat{\mu}, \hat{\sigma}^2$  are the ML estimates
- Then, compute trimmed mean using the simulated sample
  - repeat B times

Only difference between parametric and non-parametric bootstrap is the way to generate data!

# Bootstrapping regression models

Regression model:

$$E(Y_i | \mathbf{X}_i) = f(\cdot, \mathbf{X}_i), i = 1, \dots, n$$

- $f$  is a known function,  $\mathbf{X}_i$  a vector of parameters
- Interested in estimating a SE or CI for a function of parameters

# Bootstrapping regression models

Three common methods:

1. Bootstrap the pairs  $(Y_i, \mathbf{X}_i)$  and generate bootstrap parameter estimates that can be used to obtain bootstrap CIs
2. Bootstrap the **residuals** of the original model
3. Estimate the residual variance and simulate residuals

# Bootstrapping regression models: residuals

Let's take linear regression as an example,

$$Y_i = \mathbf{X}_i^T + \epsilon_i; \epsilon_i \sim N(0, \sigma^2)$$

To fit a bootstrap on the residuals:

- Fit a model on the original data to obtain residuals  $\hat{\epsilon}_i$ 
  - $\hat{\epsilon}_i = Y_i - \mathbf{X}_i^T$
- Resample residuals  $\hat{\epsilon}_i$  with replacement and repeat  $B$  times:
  - Compute  $Y_i^b = \mathbf{X}_i^T + \hat{\epsilon}_i^b$  for all  $i$
  - Refit model using  $Y_i^b, i = 1, \dots, n$  to estimate  $\hat{\beta}^b$
- This approach assumes errors are **identically distributed**

# Bootstrapping regression models: residual variance

- Estimate residual variance from sample,  $\hat{\sigma}^2$
- Repeat  $B$  times:
  - Generate a residual  $\epsilon_i^b \sim N(0, \hat{\sigma}^2)$  and associated outcome  $Y_i^b = \mathbf{X}_i^T + \epsilon_i^b$  for  $i = 1, \dots, n$
  - Refit model using  $Y_i^b$ ,  $i = 1, \dots, n$  to estimate  $\hat{\beta}^b$

This approach assumes the residual errors are **normally distributed**

# Wild bootstrap

$$Y_i = \mathbf{X}_i^T + \epsilon_i$$

The models previously discussed fail if there is **heteroskedasticity** - i.e., if  $\epsilon_i$  are not identically distributed

The **wild bootstrap** is a modification of the residual bootstrap intended to handle heteroskedasticity.

- Fit a model on the original data to obtain residuals  $\hat{\epsilon}_i$
- Repeat  $B$  times:
  - Multiply residuals by random weights to obtain  $\hat{\epsilon}_i^b$
  - Compute  $Y_i^b = \mathbf{X}_i^T + \hat{\epsilon}_i^b$  for all  $i$
  - Refit model using  $Y_i^b, i = 1, \dots, n$  to estimate  $\hat{\beta}^b$

# Wild bootstrap

Common options for weights:

1. Multiply  $\hat{\epsilon}_i$  by  $-1$  or  $1$  with equal probability
2. Multiply  $\hat{\epsilon}_i$  by a standard normal random variable

# When does the bootstrap fail?

We must assume that the original sample is representative of the population so that  $\hat{F}_n$  is a good estimate of  $F$

The bootstrap may fail when:

- The support of  $F$  depends on the parameter of interest
- The true parameter sits on the boundary of the parameter space
- The parameter of interest is nonregular, i.e., there does not exist an estimator that converges to it uniformly in distribution over the parameter space

# Permutation tests

Typically bootstrap is used for CI rather than hypothesis testing. For hypothesis testing and p-values, we can use a **permutation test**. - Idea: use resampling to generate a **null distribution** for a test statistic, then compare it to the one you observe in the real data

- **Null distribution:** the distribution of a quantity of interest (i.e.  $\hat{\beta}$ ) if the null hypothesis  $H_0$  is true
- The null distribution is available theoretically in some cases. For example, assume  $Y_i \sim N(\mu, \sigma^2), i = 1, \dots, n.$ 
  - Under  $H_0 : \mu = 0$ , we have  $\bar{Y} \sim N(0, \sigma^2/n)$ 
    - Test  $H_0$  by comparing  $\bar{Y}$  with  $N(0, \sigma^2/n)$
  - Use **permutation test** when null distribution cannot be obtained theoretically

# Permutation tests

The basic procedure of permutation test for  $H_0$ :

- Permute data under  $H_0$   $B$  times. Each time recompute the test statistics. The test statistics obtained from the permuted data form the null distribution.
- Compare the observed test statistics with the null distribution to obtain statistical significance.

# Permutation test example

Assume there are two sets of independent normal r.v.'s with the same known variance and different means:

- $X_i \sim N(\mu_1, \sigma^2)$
- $Y_i \sim N(\mu_2, \sigma^2)$

Our goal is to test  $H_0 : \mu_1 = \mu_2$ . Define test statistic:  $t = \bar{X} - \bar{Y}$ . Permutation test steps:

1. Randomly shuffle labels of  $X$  and  $Y$
2. Compute  $t^* = \bar{X}^* - \bar{Y}^*$
3. Repeat `nperm` times. Resulting  $t^*$  values form the **empirical null distribution** of  $t$ .
4. To compute p-values calculate  $Pr(|t^*| > |t|)$