

# Bootstrap Confidence Intervals

Patrick Breheny

September 18

## Introduction

- So far, we have discussed the idea behind the bootstrap and how it can be used to estimate standard errors
- Standard errors are often used to construct confidence intervals based on the estimate having a normal sampling distribution:

$$\hat{\theta} \pm z_{1-\alpha/2}SE;$$

alternatively, the interval could be based on the  $t$  distribution

- The bootstrap SE can be used in this way as well

# Introduction

- However, recall that the bootstrap can also be used to estimate the CDF  $G$  of  $\hat{\theta}$
- Thus, with the bootstrap, we do not need to make assumptions/approximations concerning the sampling distribution of  $\hat{\theta}$  – we can estimate it as part of the confidence interval procedure
- This has been an active area of theoretical research into the bootstrap

# The bootstrap- $t$ interval

- For example, suppose that the standard error of an estimate varies with the size of the estimate
- If this is so, then our confidence interval should be wider on the right side than it is on the left
- One way to implement this idea is to estimate the SE separately for each bootstrap replication — this is the idea behind the *bootstrap- $t$  interval*

## The bootstrap- $t$ interval: Procedure

The procedure of the *bootstrap- $t$*  interval is as follows:

- (1) For each bootstrap sample, compute

$$z_b^* = \frac{\hat{\theta}_b^* - \hat{\theta}}{\widehat{SE}_b^*}$$

where  $\widehat{SE}_b^*$  is an estimate of the standard error of  $\hat{\theta}^*$  based on the data in the  $b$ th bootstrap sample

- (2) Estimate the  $\alpha$ th percentile of  $z^*$  by the value  $\hat{t}_\alpha$  such that

$$B^{-1} \sum_b I(z_b^* \leq \hat{t}_\alpha) = \alpha$$

- (3) A  $1 - \alpha$  confidence interval for  $\theta$  is then

$$(\hat{\theta} - \hat{t}_{1-\alpha/2} \widehat{SE}, \hat{\theta} - \hat{t}_{\alpha/2} \widehat{SE})$$

## The bootstrap- $t$ interval: Example

- As a small example, the survival times of 9 rats were 10, 27, 30, 40, 46, 51, 52, 104, and 146 days
- Consider estimating the mean; the point estimates are  $\hat{\theta} = 56.2$  and  $\widehat{SE} = 14.1$
- The percentile points for a 95% confidence interval:

Normal	-1.96	1.96
$t$	-2.31	2.31
Bootstrap- $t$	-4.86	1.61

- This translates into the following confidence intervals:

Normal	28.5	84.0
$t$	23.6	88.9
Bootstrap- $t$	33.4	125.1

## The bootstrap- $t$ interval: R

- If you want to implement this confidence interval in R, your function that you pass to `boot` will need to return two things:  $\hat{\theta}_b^*$  and  $\hat{V}(\hat{\theta}_b^*)$

- For example:

```
mean.boot <- function(x, ind) {
  c(mean(x[ind]), var(x[ind])/length(x))
}
out <- boot(x, mean.boot, 999)
boot.ci(out)
```

- The function `boot.ci` returns the bootstrap- $t$  interval (which it calls the “studentized” interval) along with the normal interval and some other intervals which we will talk about next

## Double bootstrap

- Estimation of  $\widehat{SE}_b^*$  is straightforward for the mean (and a few other statistics), but what about in general?
- Once again, the functional delta method and jackknife are options
- The bootstrap is also an option – here we use the bootstrap within a bootstrap replication to estimate the standard error of a bootstrap replication – and is called the *double bootstrap*
- The obvious drawback to the double bootstrap is that it requires  $B^2$  bootstrap replications, and is therefore time-consuming to compute

## Confidence intervals and sampling distributions

- The next interval we will discuss is not based on the usual pivoting ideas we encounter when constructing confidence intervals
- Instead, it is based on the observation that, if  $\hat{\theta}^* \sim N(\hat{\theta}, \widehat{SE}^2)$ ,

$$\hat{\theta} \pm \widehat{SE} z_{1-\alpha/2} = (\hat{\theta}_{\alpha/2}^*, \hat{\theta}_{1-\alpha/2}^*)$$

is a  $1 - \alpha$  level confidence interval for  $\theta$ , where  $\hat{\theta}_\alpha^*$  is the  $\alpha$ th percentile of the distribution of  $\hat{\theta}^*$

- Letting  $\hat{G}$  the empirical CDF of  $\hat{\theta}^*$ , another way of writing the above interval is  $[\hat{G}^{-1}(\alpha/2), \hat{G}^{-1}(1 - \alpha/2)]$
- Thus, there is a connection (at least, if  $\hat{\theta}^* \sim \text{Normal}$ ) between the resampling distribution of  $\hat{\theta}^*$  and confidence intervals for  $\theta$

## The percentile interval

- This interval – called the *percentile interval* – is much simpler to construct than the bootstrap- $t$ , and turns out to work surprisingly well in a wide range of examples
- The percentile interval has an additional justification beyond approximation to the normal: it is invariant to transformations of  $\theta$
- For example, suppose we wish to construct a confidence interval for  $\phi = m(\theta)$ , where  $m$  is a monotone transformation
- We do not need to generate new bootstrap replications:  $\hat{\phi}_b^* = m(\hat{\theta}_b^*)$ , because

$$\left( \hat{\phi}_{\alpha/2}, \hat{\phi}_{1-\alpha/2} \right) = \left[ m(\hat{\theta}_{\alpha/2}), m(\hat{\theta}_{1-\alpha/2}) \right]$$

## Percentile interval theorem

- In the 20th century, statisticians explored dozens of transformations of various statistics designed to make the sampling distribution of the statistic more normal, from simple ones like the log-odds to more complex ones like the Fisher and Anscombe transformations
- One compelling justification for the percentile interval is that, if such a transformation exists, the percentile interval will find it automatically
- **Theorem:** Suppose there exists  $\phi = m(\theta)$  such that

$$\hat{\phi}^* \sim N(\hat{\phi}, \tau^2)$$

for some  $\tau$ . Then the percentile interval  $(\hat{\theta}_{\alpha/2}^*, \hat{\theta}_{1-\alpha/2}^*)$  is equivalent to the optimal pivot-based interval based on the above relationship.

## Example: Automatic transformation

- As an example, suppose  $X_1, \dots, X_{10} \stackrel{\text{iid}}{\sim} N(0, 1)$ , and we are interested in estimating  $\theta = e^\mu$
- In this case, there does exist a normalizing transformation  $\phi = \log(\theta)$  such that  $\hat{\phi} \sim N(\phi, \tau^2)$
- Suppose, however, that we didn't know any of this and applied the ordinary nonparametric bootstrap:

	$\hat{\theta}_L$	$\hat{\theta}_U$
Exact	0.49	2.29
Normal bootstrap	0.15	1.81
Percentile interval	0.50	2.10

## Percentile intervals in R

- Percentile intervals are also returned by `boot.ci`
- They can also be obtained by applying `quantile` to the output of `boot`
- For the mouse survival data from earlier,

Normal	28.5	84.0
$t$	23.6	88.9
Bootstrap- $t$	33.4	125.1
Percentile	32.1	87.7

## Standard vs. bootstrap approach

- The standard approach is based on taking literally the following asymptotic relationship

$$\frac{\hat{\theta} - \theta}{\sigma} \sim N(0, 1)$$

- The bootstrap percentile interval relaxes that assumption; instead of requiring normality of  $\hat{\theta}$ , it requires only that  $\exists m : \phi = m(\theta)$  satisfies

$$\frac{\hat{\phi} - \phi}{\tau} \sim N(0, 1)$$

- However, this still requires that there exists a single transformation that is both normalizing and variance-stabilizing – often, such a transformation does not exist

## Generalizing the bootstrap assumptions

- Thus, in a brilliant 1987 paper, Efron considers a generalization of the bootstrap assumptions
- Suppose that for some monotone increasing transformation  $m$ , some bias constant  $z_0$ , and some acceleration constant  $a$ , the following relationship holds for  $\phi = m(\theta)$ :

$$\frac{\hat{\phi} - \phi}{\sigma} \sim N(-z_0, 1), \quad \sigma = 1 + a\phi$$

- Efron named the confidence interval based on this assumption the  $BC_\alpha$  interval, because it corrects for both bias and “acceleration” of the variance

## The BC $_{\alpha}$ interval

- **Theorem:** If the relationship on the previous slide holds, then the following interval is “correct,” in the sense of being the optimal pivot-based interval:

$$\theta \in \left[ \hat{G}^{-1}\{\Phi(z[\alpha])\}, \hat{G}^{-1}\{\Phi(z[1 - \alpha])\} \right]$$

where

$$z[\alpha] = z_0 + \frac{z_0 + z^{(\alpha)}}{1 - a(z_0 + z^{(\alpha)})}.$$

- Note that, in order to construct the BC $_{\alpha}$  interval, one has to estimate  $z_0$  and  $a$ , but, like the percentile interval, it is not necessary to know  $m$

## Example revisited

- Unfortunately, we don't have time to cover in detail the derivation of this interval and the estimation of  $z_0$  and  $a$ , but it is available from `boot.ci`
- When applied to our mouse survival data, we have  $\hat{z}_0 = -0.026$  and  $\hat{a} = 0.066$ , which gives us the adjusted percentage points  $(0.037, 0.986)$  and the resulting interval

Normal	28.5	84.0
$t$	23.6	88.9
Bootstrap- $t$	33.4	125.1
Percentile	32.1	87.7
$BC_a$	37.3	90.9

## Asymptotic accuracy of confidence intervals

- Let us denote a confidence interval procedure by its confidence points  $\hat{\theta}[\alpha]$ , where ideally,  $\mathbb{P}(\theta \leq \hat{\theta}[\alpha]) = \alpha$
- A confidence point is called *first-order accurate* if

$$\mathbb{P}(\theta \leq \hat{\theta}[\alpha]) = \alpha + O(n^{-1/2})$$

and *second-order accurate* if

$$\mathbb{P}(\theta \leq \hat{\theta}[\alpha]) = \alpha + O(n^{-1})$$

## Second-order accuracy of bootstrap confidence intervals

- It can be shown (our textbook has some details on this and the regularity conditions that are required) that the standard interval and the percentile interval are first-order accurate, while the bootstrap- $t$  and  $BC_a$  intervals are second-order accurate – regardless of the true distribution,  $F$
- This is a powerful theoretical justification for the bootstrap- $t$  and  $BC_a$  intervals
- Arguments can be made for either interval in different situations
- The  $BC_a$  interval is also transformation-invariant and *range-preserving*, meaning that, if it is not possible for a statistic or a function of a statistic to lie outside a certain range  $[a, b]$ , then the  $BC_a$  interval will be contained in  $[a, b]$  (the bootstrap- $t$  intervals are neither transformation-invariant nor range-preserving)

## Bootstrap failure #1

- Bootstrap confidence intervals are unquestionably a tremendous methodological advance, and the  $BC_\alpha$  interval represents the “state of the art” as far as nonparametric confidence intervals goes
- However, bootstrap intervals are limited by the accuracy of  $\hat{F}$
- The empirical CDF is generally poorly estimated at the tails of a distribution
- Consequently, it is difficult to produce nonparametric confidence intervals for statistics that are highly influenced by distribution tails

## Bootstrap failure #2

- Furthermore, the bootstrap still requires conditions such as Hadamard differentiability and can fail to produce accurate intervals when those conditions do not hold
- We have already encountered the example of density estimation
- As an additional example, consider  $\hat{\theta} = \max(x_i)$
- The  $BC_\alpha$  interval can never exceed  $\hat{G}^{-1}(1) = \max(x_i)$ , and therefore provides a 0% confidence interval for any continuous distribution

# Homework

- In an earlier homework, we examined the coverage probabilities of parametric and nonparametric confidence intervals for the variance
- Your assignment now is to compare three nonparametric methods: the functional delta method, the bootstrap percentile interval, and the  $BC_a$  interval
- **Homework:** Conduct a simulation study to determine how the coverage probability and average interval width of these two intervals varies with the sample size  $n$ , when (i) the data is truly normally distributed, and (ii) the data follows an exponential distribution. For each distribution, produce a plot of coverage probability versus sample size, with lines representing the various methods, as well as a corresponding plot for interval width.