

# Bootstrap confidence intervals

## Class 24, 18.05, Spring 2014

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## 1 Learning Goals

1. Be able to construct and sample from the empirical distribution of data.
2. Be able to explain the bootstrap principle.
3. Be able to design and run an empirical bootstrap to compute confidence intervals.
4. Be able to design and run a parametric bootstrap to compute confidence intervals.

## 2 Introduction

The *empirical bootstrap* is a statistical technique popularized by Bradley Efron in 1979. Though remarkably simple to implement, the bootstrap would not be feasible without modern computing power. The key idea is to perform computations on the data itself to estimate the variation of statistics that are themselves computed from the same data. That is, the data is ‘pulling itself up by its own bootstrap.’ (A google search of ‘by ones own bootstraps’ will give you the etymology of this metaphor.) Such techniques existed before 1979, but Efron widened their applicability and demonstrated how to implement the bootstrap effectively using computers. He also coined the term ‘bootstrap’ <sup>1</sup>.

Our main application of the bootstrap will be to estimate the variation of point estimates; that is, to estimate confidence intervals. An example will make our goal clear.

**Example 1.** Suppose we have data

$$x_1, x_2, \dots, x_n$$

If we knew the data was drawn from  $N(\mu, \sigma^2)$  with the unknown mean  $\mu$  and known variance  $\sigma^2$  then we have seen that

$$\left[ \bar{x} - 1.96 \frac{\sigma}{\sqrt{n}}, \bar{x} + 1.96 \frac{\sigma}{\sqrt{n}} \right]$$

is a 95% confidence interval for  $\mu$ .

Now suppose the data is drawn from some completely unknown distribution. To have a name we’ll call this distribution  $F$  and its (unknown) mean  $\mu$ . We can still use the sample mean  $\bar{x}$  as a *point estimate* of  $\mu$ . But how can we find a confidence interval for  $\mu$  around  $\bar{x}$ ? Our answer will be to use the bootstrap!

In fact, we’ll see that the bootstrap handles other statistics as easily as it handles the mean. For example: the median, other percentiles or the trimmed mean. These are statistics where, even for normal distributions, it can be difficult to compute a confidence interval from theory alone.

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<sup>1</sup>Paraphrased from Dekking et al. *A Modern Introduction to Probability and Statistics*, Springer, 2005, page 275.

### 3 Sampling

In statistics to *sample* from a set is to choose elements from that set. In a random sample the elements are chosen randomly. There are two common methods for random sampling.

#### Sampling without replacement

Suppose we draw 10 cards at random from a deck of 52 cards without putting any of the cards back into the deck between draws. This is called *sampling without replacement* or *simple random sampling*. With this method of sampling our 10 card sample will have no duplicate cards.

#### Sampling with replacement

Now suppose we draw 10 cards at random from the deck, but after each draw we put the card back in the deck and shuffle the cards. This is called *sampling with replacement*. With this method, the 10 card sample might have duplicates. It's even possible that we would draw the 6 of hearts all 10 times.

**Think:** What's the probability of drawing the 6 of hearts 10 times in a row?

**Example 2.** We can view rolling an 8-sided die repeatedly as sampling with replacement from the set  $\{1,2,3,4,5,6,7,8\}$ . Since each number is equally likely, we say we are sampling uniformly from the data. There is a subtlety here: each data point is equally probable, but if there are repeated values within the data those values will have a higher probability of being chosen. The next example illustrates this.

### 4 The empirical distribution of data

The empirical distribution of data is simply the distribution that you see in the data. Let's illustrate this with an example.

**Example 3.** Suppose we roll an 8-sided die 10 times and get the following data, written in increasing order:

1, 1, 2, 3, 3, 3, 3, 4, 7, 7.

Imagine writing these values on 10 slips of paper, putting them in a hat and drawing one at random. Then, for example, the probability of drawing a 3 is  $4/10$  and the probability of drawing a 4 is  $1/10$ . The full empirical distribution can be put in a probability table

|           |        |        |        |        |        |
|-----------|--------|--------|--------|--------|--------|
| value $x$ | 1      | 2      | 3      | 4      | 7      |
| $p(x)$    | $2/10$ | $1/10$ | $4/10$ | $1/10$ | $2/10$ |

**Notation.** If we label the true distribution the data is drawn from as  $F$ , then we'll label the empirical distribution of the data as  $F^*$ . If we have enough data then the law of large numbers tells us that  $F^*$  should be a good approximation of  $F$ .

**Example 4.** In the dice example just above, the true and empirical distributions are:

|           |       |       |       |       |       |       |       |       |
|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| value $x$ | 1     | 2     | 3     | 4     | 5     | 5     | 7     | 8     |
| $p(x)$    | $1/8$ | $1/8$ | $1/8$ | $1/8$ | $1/8$ | $1/8$ | $1/8$ | $1/8$ |

The true distribution  $F$  of the 8-sided die.

|           |      |      |      |      |      |
|-----------|------|------|------|------|------|
| value $x$ | 1    | 2    | 3    | 4    | 7    |
| $p(x)$    | 2/10 | 1/10 | 4/10 | 1/10 | 2/10 |

The empirical distribution  $F^*$  of the sample data drawn from  $F$ .

Because  $F^*$  is derived strictly from data we call it the *empirical distribution* of the data. We will also call it the *resampling distribution*. Notice that we always know  $F^*$  explicitly. In particular the expected value of  $F^*$  is just the sample mean  $\bar{x}$ .

## 5 Resampling

The empirical bootstrap proceeds by resampling from the data. We continue the dice example above.

**Example 5.** Suppose we have 10 data points, given in increasing order:

$$1, 1, 2, 3, 3, 3, 3, 4, 7, 7$$

We view this as a *sample* taken from some underlying distribution. To *resample* is to sample from the empirical distribution, e.g. put these 10 numbers in a hat and draw one at random. To resample again, we put the number back in the hat and draw again. (We called this *sampling with replacement*.)

To get us a little closer to implementing this on a computer we rephrase this in the following way. Label the 10 data points  $x_1, x_2, \dots, x_{10}$ . To resample is to draw a number  $j$  from the uniform distribution on  $\{1, 2, \dots, 10\}$  and take  $x_j$  as our resampled value. In this case we could do so by rolling a 10-sided die. For example, if we roll a 6 then our resampled value is 3, the 6<sup>th</sup> element in our list.

If we want a resampled data set of size 5, then we roll the 10-sided die 5 times and choose the corresponding elements from the list of data. If the 5 rolls are

$$5, 3, 6, 6, 1$$

then the resample is

$$3, 2, 3, 3, 1.$$

Notes: 1. Because we are sampling with replacement, the same data point can appear multiple times when we resample.

2. Also because we are sampling with replacement, we can have a resample data set of any size we want, e.g. we could resample 1000 times.

Of course, in practice one uses a software package like R to do the resampling.

### 5.1 Star notation

If we have sample data of size  $n$

$$x_1, x_2, \dots, x_n$$

then we denote a resample of size  $m$  by

$$x_1^*, x_2^*, \dots, x_m^*$$

Just as  $\bar{x}$  is the mean of the original data, we write  $\bar{x}^*$  for the mean of the resampled data.

## 6 The empirical bootstrap

Suppose we have  $n$  data points

$$x_1, x_2, \dots, x_n$$

drawn from a distribution  $F$ . An *empirical bootstrap sample* is a resample of the *same size*  $n$ :

$$x_1^*, x_2^*, \dots, x_n^*.$$

You should think of the latter as a sample of size  $n$  drawn from the empirical distribution  $F^*$ . For any statistic  $v$  computed from the original sample data, we can define a statistic  $v^*$  by the same formula but computed instead using the resampled data. With this notation we can state the **bootstrap principle**:

1.  $F^* \approx F$ .
2. The distribution of  $v^*$  approximates the distribution of  $v$ .

It turns out that in practice the approximation of  $v$  by  $v^*$  may not be very good. However, the variation of  $v$  is usually well-approximated by the variation of  $v^*$ , and this is what we will exploit in examples.

### Example 6. Toy example of an empirical bootstrap confidence interval

We start with a made-up set of data that is small enough to show each step explicitly. The sample data is

$$30, 37, 36, 43, 42, 43, 43, 46, 41, 42$$

Problem: Estimate the mean  $\mu$  of the underlying distribution and give an 80% confidence interval.

**answer:** We use  $\bar{x} = 40.3$  to estimate the true mean  $\mu$  of the underlying distribution. As in Example 1, to make the confidence interval we need to know how much the distribution of  $\bar{x}$  varies around  $\mu$ . That is, we'd like to know the distribution of

$$\delta = \bar{x} - \mu.$$

If we knew this distribution we could find  $\delta_{.1}$  and  $\delta_{.9}$ , the .1 and .9 critical values of  $\delta$ . Then we'd have

$$P(\delta_{.9} \leq \bar{x} - \mu \leq \delta_{.1} \mid \mu) = .8 \Leftrightarrow P(\bar{x} - \delta_{.9} \geq \mu \geq \bar{x} - \delta_{.1} \mid \mu) = .8$$

which gives an 80% confidence interval of

$$[\bar{x} - \delta_{.1}, \bar{x} - \delta_{.9}].$$

As always with confidence intervals, we hasten to point out that the probabilities computed above are probabilities concerning the statistic  $\bar{x}$  *given that the true mean is*  $\mu$ .

The bootstrap principle offers a practical approach to estimating the distribution of  $\delta = \bar{x} - \mu$ . It says that we can approximate it by the distribution of

$$\delta^* = \bar{x}^* - \bar{x}$$

where  $\bar{x}^*$  is the mean of an empirical bootstrap sample.

Here's the beautiful key to this: since  $\delta^*$  is computed by resampling the original data, we can have a computer simulate  $\delta^*$  as many times as we'd like. Hence, by the law of large numbers, we can estimate the distribution of  $\delta^*$  with high precision.

Now let's return to the sample data with 10 points. We used R to generate 20 bootstrap samples, each of size 10. Each of the 20 columns in the following array is one bootstrap sample.

```

43 36 46 30 43 43 43 37 42 42 43 37 36 42 43 43 42 43 42 43
43 41 37 37 43 43 46 36 41 43 43 42 41 43 46 36 43 43 43 42
42 43 37 43 46 37 36 41 36 43 41 36 37 30 46 46 42 36 36 43
37 42 43 41 41 42 36 42 42 43 42 43 41 43 36 43 43 41 42 46
42 36 43 43 42 37 42 42 46 30 43 36 43 43 42 37 36 42 30
36 36 42 42 36 36 43 41 30 42 37 43 41 41 43 43 42 46 43 37
43 37 41 43 41 42 43 46 46 36 43 42 43 30 41 46 43 46 30 43
41 42 30 42 37 43 43 42 43 43 46 43 30 42 30 42 30 43 43 42
46 42 42 43 41 42 30 37 30 42 43 42 43 37 37 37 42 43 43 46
42 43 43 41 42 36 43 30 37 43 42 43 41 36 37 41 43 42 43 43

```

Next we compute  $\delta^* = \bar{x}^* - \bar{x}$  for each bootstrap sample (i.e. each column) and sort them from smallest to biggest:

```

-1.6 -1.4 -1.4 -0.9 -0.5 -0.2 -0.1 0.1 0.2 0.2
0.4 0.4 0.7 0.9 1.1 1.2 1.2 1.6 1.6 2.0

```

We will approximate the critical values  $\delta_{.1}$  and  $\delta_{.9}$  by  $\delta_{.1}^*$  and  $\delta_{.9}^*$ . The only difficulty here is deciding exactly which entries in our list are  $\delta_{.1}^*$  and  $\delta_{.9}^*$ . Since  $\delta_{.1}^*$  is at the 90th percentile we choose the 18th element in the list, i.e. 1.6. Likewise, since  $\delta_{.9}^*$  is at the 10th percentile we choose the 2nd element in the list, i.e. -1.4.

Therefore our bootstrap 80% confidence interval for  $\mu$  is

$$[\bar{x} - \delta_{.1}^*, \bar{x} - \delta_{.9}^*] = [40.3 - 1.6, 40.3 + 1.4] = [38.7, 41.7]$$

We explain below how to use R for bootstrapping and include the code for this example. Using R, we would generate 1000 or more bootstrap samples in order to obtain a very accurate estimate of  $\delta_{.1}^*$  and  $\delta_{.9}^*$ .

## 6.1 Justification for the bootstrap principle

The bootstrap is remarkable because resampling gives us a decent estimate on how the point estimate might vary. We can only give you a 'hand-waving' explanation of this, but it's worth a try. The bootstrap is based roughly on the law of large numbers, which says, in short, that with enough data the empirical distribution will be a good approximation of the true distribution. Visually it says that the histogram of the data should approximate the density of the true distribution.

First let's note what resampling can't do for us: it can't improve our point estimate. For example, if we estimate the mean  $\mu$  by  $\bar{x}$  then in the bootstrap we would compute  $\bar{x}^*$  for many resamples of the data. If we took the average of all the  $\bar{x}^*$  we would expect it to be very close to  $\bar{x}$ . This wouldn't tell us anything new about the true value of  $\mu$ .

Even with a fair amount of data the match between the true and empirical distributions is not perfect, so there will be error in estimating the mean (or any other value). But

the amount of variation in the estimates is much less sensitive to differences between the density and the histogram. As long as they are reasonably close both the empirical and true distributions will exhibit the similar amounts of variation. So, in general the bootstrap principle is more robust when approximating the distribution of relative variation than when approximating absolute distributions.

What we have in mind is the scenario of our examples. The distribution (over different sets of experimental data) of  $\bar{x}$  is ‘centered’ at  $\mu$  and the distribution of  $\bar{x}^*$  is centered at  $\bar{x}$ . If there is a significant separation between  $\bar{x}$  and  $\mu$  then these two distributions will also differ significantly. On the other hand the distribution of  $\delta = \bar{x} - \mu$  describes the variation of  $\bar{x}$  about its center. Likewise the distribution of  $\delta^* = \bar{x}^* - \bar{x}$  describes the variation of  $\bar{x}^*$  about its center. So even if the centers are quite different the two variations about the centers can be approximately equal.

## 7 Other statistics

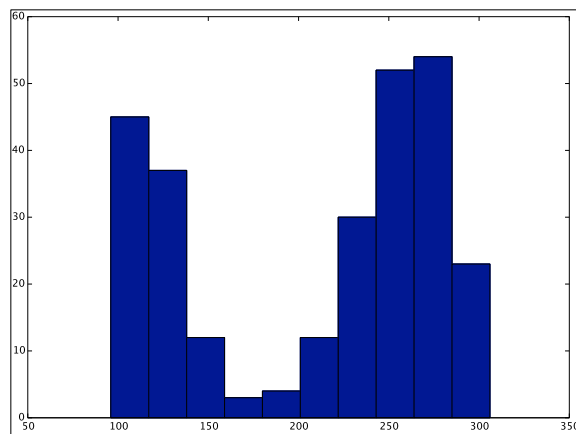
So far in this class we’ve avoided confidence intervals for the median and other statistics because their sample distributions are hard to describe theoretically. The bootstrap has no such problem. In fact, to handle the median all we have to do is change ‘mean’ to ‘median’ in the R code from Example 6.

### Example 7. Old Faithful: confidence intervals for the median

Old Faithful is a geyser in Yellowstone National Park in Wyoming:

[http://en.wikipedia.org/wiki/Old\\_Faithful](http://en.wikipedia.org/wiki/Old_Faithful)

There is a publicly available data set which gives the durations of 272 consecutive eruptions. Here is a histogram of the data.



**Question:** Estimate the median length of an eruption and give a 90% confidence interval for the median.

**answer:** The R file `oldfaithful_simple.r` and the Old Faithful data set are posted at

[http://ocw.mit.edu/ans7870/18/18.05/s14/r-code/oldfaithful\\_simple.r](http://ocw.mit.edu/ans7870/18/18.05/s14/r-code/oldfaithful_simple.r)

<http://ocw.mit.edu/ans7870/18/18.05/s14/r-code/oldfaithful.txt>

Note: the code in `oldfaithful_simple.r` assumes that the data `oldfaithful.txt` is in

the current working directory. You can modify the code to point directly at this url for the data..

Let's walk through a summary of the steps needed to answer the question.

1. Data:  $x_1, \dots, x_{272}$
2. Data median:  $x_{\text{median}} = 240$
3. Find the median  $x_{\text{median}}^*$  of a bootstrap sample  $x_1^*, \dots, x_{272}^*$ . Repeat 1000 times.
4. Compute the bootstrap differences

$$\delta^* = x_{\text{median}}^* - x_{\text{median}}$$

Put these 1000 values in order and pick out the .95 and .05 critical values, i.e. the 50th and 950th biggest values. Call these  $\delta_{.95}^*$  and  $\delta_{.05}^*$ .

5. The bootstrap principle says that we can use  $\delta_{.95}^*$  and  $\delta_{.05}^*$  as estimates of  $\delta_{.95}$  and  $\delta_{.05}$ . So our estimated 90% bootstrap confidence interval for the median is

$$[x_{\text{median}} - \delta_{.05}^*, x_{\text{median}} - \delta_{.95}^*]$$

The bootstrap 90% CI we found for the Old Faithful data was [235, 250]. Since we used 1000 bootstrap samples a new simulation starting from the same sample data should produce a similar interval. If in Step 3 we increase the number of bootstrap samples to 10000, then the intervals produced by simulation would vary even less. One common strategy is to increase the number of bootstrap samples until the resulting simulations produce intervals that vary less than some acceptable level.

**Example 8.** Using the Old Faithful data, estimate  $P(|\bar{x} - \mu| > 5 \mid \mu)$ .

**answer:** We proceed exactly as in the previous example except using the mean instead of the median.

1. Data:  $x_1, \dots, x_{272}$
2. Data mean:  $\bar{x} = 209.27$
3. Find the mean  $\bar{x}^*$  of 1000 empirical bootstrap samples:  $x_1^*, \dots, x_{272}^*$ .
4. Compute the bootstrap differences

$$\delta^* = \bar{x}^* - \bar{x}$$

5. The bootstrap principle says that we can use the distribution of  $\delta^*$  as an approximation for the distribution  $\delta = \bar{x} - \mu$ . Thus,

$$P(|\bar{x} - \mu| > 5 \mid \mu) = P(|\delta| > 5 \mid \mu) \approx P(|\delta^*| > 5)$$

Our bootstrap simulation for the Old Faithful data gave 0.225 for this probability.

## 8 Parametric bootstrap

The examples in the previous sections all used the empirical bootstrap, which makes no assumptions at all about the underlying distribution and draws bootstrap samples by resampling the data. In this section we will look at the *parametric bootstrap*. The only difference

between the parametric and empirical bootstrap is the source of the bootstrap sample. For the parametric bootstrap, we generate the bootstrap sample from a parametrized distribution.

Here are the elements of using the parametric bootstrap to estimate a confidence interval for a parameter.

0. Data:  $x_1, \dots, x_n$  drawn from a distribution  $F(\theta)$  with unknown parameter  $\theta$ .
1. A statistic  $\hat{\theta}$  that estimates  $\theta$ .
2. Our bootstrap samples are drawn from  $F(\hat{\theta})$ .
3. For each bootstrap sample

$$x_1^*, \dots, x_n^*$$

we compute  $\hat{\theta}^*$  and the bootstrap difference  $\delta^* = \hat{\theta}^* - \hat{\theta}$ .

4. The bootstrap principle says that the distribution of  $\delta^*$  approximates the distribution of  $\delta = \hat{\theta} - \theta$ .
5. Use the bootstrap differences to make a bootstrap confidence interval for  $\theta$ .

**Example 9.** Suppose the data  $x_1, \dots, x_{300}$  is drawn from an  $\exp(\lambda)$  distribution. Estimate  $\lambda$  and give a 95% parametric bootstrap confidence interval for  $\lambda$ .

**answer:** This is implemented in the R script `parametric_bs_class24.r` which is posted alongside with our other R code in

<http://ocw.mit.edu/ans7870/18/18.05/s14/r-code/rstuff.html>.

It's easiest to explain the solution using commented code.

```
# Parametric bootstrap
# Given 300 data points with mean 2.
# Assume the data is exp(lambda)
# PROBLEM: Compute a 95% parametric bootstrap confidence interval for lambda
# We are given the number of data points and mean
n = 300
xbar = 2

# The MLE for lambda is 1/xbar
lambda_hat = 1/xbar

# Generate the bootstrap samples
# Each column is one bootstrap sample (of 300 resampled values)
nboot = 1000

# Here's the key difference with the empirical
# bootstrap. We draw the bootstrap sample from Exponential(lambda_hat)
x = rexp(n*nboot, lambda_hat)
bootstrap_sample = matrix(x, nrow=n, ncol=nboot)

# Compute the bootstrap lambda_star
lambda_star = 1./colMeans(bootstrap_sample);

# Compute the differences
deltastar = lambda_star - lambda_hat;
```



```
# Find the .05 and .95 quantile for delta_star
d = quantile(deltastar, c(.05,.95))
# Calculate the 95% confidence interval for lambda.
ci = lambda.hat - c(d[2], d[1])
# This line of code is just one way to format the output text.
# sprintf is an old C function for doing this. R has many other
# ways to do the same thing.
s = sprintf("Confidence interval for lambda:  [%.3f, %.3f]", ci[1], ci[2])
cat(s)
```

## 9 The bootstrap percentile method

Instead of computing the differences  $\delta^*$ , the bootstrap percentile method uses the distribution of the bootstrap sample statistic as a direct approximation of the data sample statistic.

**Example 10.** Let's redo Example 6 using the bootstrap percentile method.

We first compute  $\bar{x}^*$  from the bootstrap samples given in Example 6. After sorting we get

```
35.7 37.4 38.0 39.5 39.7 39.8 39.8 40.1 40.1 40.6 40.7 40.8 41.1 41.1 41.7 42.0
42.1 42.4 42.4 42.4
```

The percentile method says to use the distribution of  $\bar{x}^*$  as an approximation to the distribution of  $\bar{x}$ . The .9 and .1 critical values are given by the 2nd and 18th elements. Therefore the 80% confidence interval is [37.4, 42.4]. This is a bit wider than our answer to Example 6.

The bootstrap percentile method is appealing due to its simplicity. However it depends on the bootstrap distribution of  $\bar{x}^*$  based on a *particular* sample being a good approximation to the true distribution of  $\bar{x}$ . Rice says of the percentile method, "Although this direct equation of quantiles of the bootstrap sampling distribution with confidence limits may seem initially appealing, it's rationale is somewhat obscure."<sup>2</sup> In short, **don't use it**. Use the empirical bootstrap instead (we have explained both in the hopes that you won't confuse the empirical bootstrap for the percentile bootstrap).

## 10 R annotated transcripts

### 10.1 Using R to generate a random sample from an array

```
# Data for the example 6
x = c(30,37,36,43,42,43,43,46,41,42)
n = length(x)
# sample mean
xbar = mean(x)
nboot = 20
# Generate 20 bootstrap samples, i.e. an n x 20 array of
```

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<sup>2</sup>\*John Rice, *Mathematical Statistics and Data Analysis*, 2nd edition, p. 272

```
# random resamples from x
tmpdata = sample(x,n*nboot, replace=TRUE)
bootstrap_sample = matrix(tmpdata, nrow=n, ncol=nboot)

# Compute the means  $\bar{x}^*$ 
bsmeans = colMeans(bootstrap_sample)

# Compute  $\delta^*$  for each bootstrap sample
deltastar = bsmeans - xbar

# Sort the results
sorteddeltastar = sort(deltastar)

# Look at the sorted results
hist(sorteddeltastar, nclass=6)
sorteddeltastar

# Find the .1 and .9 critical values of  $\delta^*$ 
d9 = sorteddeltastar[2]
d1 = sorteddeltastar[18]

# Find and print the 80% confidence interval for the mean
CI = xbar - c(d1,d9)
print(CI)
```

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