

Chapter 4

Bootstrap

4.1 Introduction

The estimation of parameters in probability distributions is a basic problem in statistics that one tends to encounter already during the very first course on the subject. Along with the estimate itself we are usually interested in its accuracy, which is can be described in terms of the bias and the variance of the estimator, as well as confidence intervals around it. Sometimes, such measures of accuracy can be derived analytically. Often, they can not. Bootstrap is a technique that can be used to estimate them numerically from a single data set¹.

4.2 The general idea

Let X_1, \dots, X_n be a i.i.d. sample from distribution F , that is $\mathbf{P}(X_i \leq x) = F(x)$, and let $X_{(1)}, \dots, X_{(n)}$ be the corresponding ordered sample. We are interested in some parameter θ which is associated with this distribution (mean, median, variance etc). There is also an estimator $\hat{\theta} = t(\{X_1, \dots, X_n\})$, with t denoting some function, that we can use to estimate θ from data. In this setting, it is the deviation of $\hat{\theta}$ from θ that is most interesting.

Ideally, to get an approximation of the estimator distribution we would like to repeat the data-generating experiment, say, N times, calculating $\hat{\theta}$ for each of the N data sets. That is, we would draw N samples of size n from the true distribution F (with replacement, if F is discrete). In practice, this is impossible.

The bootstrap method is based on the following simple idea: *Even if we do not know F we can approximate it from data and use this approximation, \hat{F} , instead of F itself.*

This idea leads to several flavours of bootstrap that deviate in how, exactly, the approximation \hat{F} is obtained. Two broad areas are the *parametric* and *non-parametric* bootstrap.

The non-parametric estimate is the so called empirical distribution (you will see the

¹More generally, bootstrap is a method of approximating the distribution of functions of the data (statistics), which can serve different purposes, among others the construction of CI and hypothesis testing.

corresponding pdf if you simply do a histogram of the data), that can be formally defined as follows:

Definition 4.1. With $\#$ denoting the number of members of a set, the empirical distribution function \tilde{F} is given by

$$\tilde{F}(x) = \frac{\#\{i : X_i \leq x\}}{n} = \begin{cases} 0 & \text{if } x \in (-\infty, X_{(1)}), \\ i/n & \text{if } x \in [X_{(i)}, X_{(i+1)}) \text{ for } i \in \{1, \dots, n-1\}, \\ 1 & \text{if } x \in [X_{(n)}, \infty). \end{cases}$$

That is, it is a discrete distribution that puts mass $1/n$ on each data point in your sample.

The parametric estimate assumes that the data comes from a certain distribution family (Normal, Gamma etc). That is, we say that we know the general functional form of the pdf, but not the exact parameters. Those parameters can then be estimated from the data (typically with Maximum Likelihood) and plugged in the pdf to get \hat{F} . This estimation method leads to more accurate inference if we guessed the distribution family correctly but, on the other hand, \hat{F} may be quite far from F if the family assumption is wrong.

4.2.1 Algorithms

The two algorithms below describe how the bootstrap can be implemented.

Non-parametric bootstrap

Assuming a data set $x = (x_1, \dots, x_n)$ is available.

1. Fix the number of bootstrap re-samples N . Often $N \in [1000, 2000]$.
2. Sample a new data set x^* set of size n from x *with replacement* (this is equivalent to sampling from the empirical cdf \hat{F}).
3. Estimate θ from x^* . Call the estimate $\hat{\theta}_i^*$, for $i = 1, \dots, N$. Store.
4. Repeat step 2 and 3 N times.
5. Consider the empirical distribution of $(\hat{\theta}_1^*, \dots, \hat{\theta}_N^*)$ as an approximation of the true distribution of $\hat{\theta}$.

Parametric bootstrap

Assuming a data set $x = (x_1, \dots, x_n)$ is available.

1. Assume that the data comes from a known distribution family F_ψ described by a set of parameters ψ (for a Normal distribution $\psi = (\mu, \sigma)$ with μ being the expected value and σ the standard deviation).
2. Estimate ψ with, for example, Maximum likelihood, obtaining the estimate $\hat{\psi}$.
3. Fix the number of bootstrap re-samples N . Often $N \in [1000, 2000]$.
4. Sample a new data set x^* set of size n from $F_{\hat{\psi}}$.
5. Estimate θ from x^* . Call the estimate $\hat{\theta}_i^*$, for $i = 1, \dots, N$. Store.
6. Repeat 4 and 5 N times.
7. Consider the empirical distribution of $(\hat{\theta}_1^*, \dots, \hat{\theta}_N^*)$ as an approximation of the true distribution of $\hat{\theta}$.

Concretely,, let us say that $X_i \sim N(0,1)$, θ is the median and it is estimated by $\hat{\theta} = X_{(n/2)}$. In the Figure 4.1 the distribution of $\hat{\theta}$ approximated with the non-parametric and parametric bootstrap is plotted. Note that the parametric distribution is smoother than the non-parametric one, since the samples were drawn from a continuous distribution. As stated earlier, the parametric version could be more accurate, but also potentially more difficult to set up. In particular, we have to sample from $F_{\hat{\psi}}$ which is not easily done if F is not one of the common distributions (such as Normal) for which a pre-programmed sample function is usually available.

4.3 Bias and variance estimation

The theoretical bias and variance of an estimator $\hat{\theta}$ are defined as

$$\mathbf{Bias}(\hat{\theta}) = \mathbf{E}[\hat{\theta} - \theta] = \mathbf{E}[\hat{\theta}] - \theta$$

$$\mathbf{Var}(\hat{\theta}) = \mathbf{E} \left[(\hat{\theta} - \mathbf{E}[\hat{\theta}])^2 \right]$$

In words, the bias is a measure of a systematic error ($\hat{\theta}$ tends to be either smaller or larger than θ) while the variance is a measure of random error.

In order to obtain the bootstrap estimates of bias and variance we plug in the original estimate $\hat{\theta}$ (which is a constant given data) in place of θ and $\hat{\theta}^*$ (the distribution of which

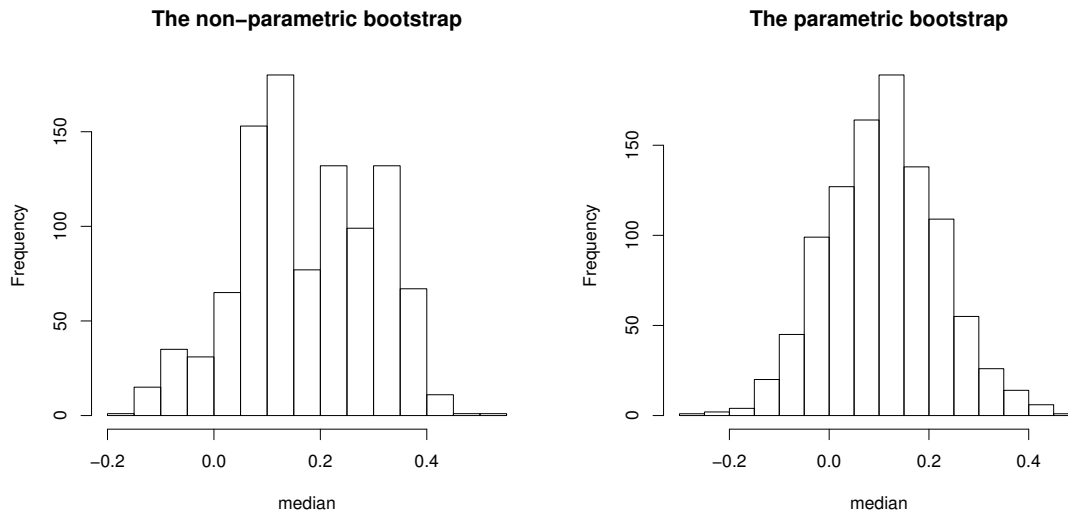


Figure 4.1: The non-parametric and the parametric bootstrap distribution of the median, $N = 1000$.

we get from bootstrap) in place of $\hat{\theta}$. This leads us to the following approximations:

$$\mathbf{Bias}(\hat{\theta}) \approx \frac{1}{N} \sum_i \hat{\theta}_i^* - \hat{\theta} = \hat{\theta}^* - \hat{\theta}$$

$$\mathbf{Var}(\hat{\theta}) \approx \frac{1}{N-1} \sum_i (\hat{\theta}_i^* - \hat{\theta}^*)^2$$

That is, the variance is, as usual, estimated by the sample variance (but for the bootstrap sample of $\hat{\theta}$) and bias is estimated by how much the original $\hat{\theta}$ deviates from the average of the bootstrap sample.

4.4 Confidence intervals

There are several methods for CI construction with Bootstrap, the most popular being "normal", "basic" and "percentile". Let $\hat{\theta}_{(i)}^*$ be the ordered bootstrap estimates, with $i = 1, \dots, N$ indicating the different samples. Let α be the significance level. In all that follows, $\hat{\theta}_\alpha^*$ will denote the α -quantile of the distribution of $\hat{\theta}^*$. You can approximate this quantile with $\hat{\theta}_{\lfloor (N+1)\alpha \rfloor}^*$ with the $\lfloor x \rfloor$ indicating the integer part of x or through interpolation.

Basic	$[2\hat{\theta} - \hat{\theta}_{1-\alpha/2}^*, 2\hat{\theta} - \hat{\theta}_{\alpha/2}^*]$
Normal	$[\hat{\theta} - z_{1-\alpha/2}\hat{s}e, \hat{\theta} - z_{\alpha/2}\hat{s}e]$
Percentile	$[\hat{\theta}_{\alpha/2}^*, \hat{\theta}_{1-\alpha/2}^*]$

with z_α denoting an α quantile from a Normal distribution and $\hat{s}e$ the estimated standard deviation of $\hat{\theta}$ calculated from the bootstrap sample.

Basic CI

To obtain this confidence interval we start with $W = \hat{\theta} - \theta$ (compare to the classic CI that correspond to a t -test). If the distribution of W was known, then a two-sided CI could be obtained by considering $\mathbf{P}(w_{\alpha/2} \leq W \leq w_{1-\alpha/2}) = 1 - \alpha$, which leads to $\text{CI} = [l_{low}, l_{up}] = [\hat{\theta} - w_{1-\alpha/2}, \hat{\theta} - w_{\alpha/2}]$. However, the distribution of W is not known, and is approximated with the distribution for $W^* = \hat{\theta}^* - \hat{\theta}$, with w_α^* denoting the corresponding α -quantile. The CI becomes $[\hat{\theta} - w_{1-\alpha/2}^*, \hat{\theta} - w_{\alpha/2}^*]$. Noting that $w_\alpha^* = \hat{\theta}_\alpha^* - \hat{\theta}$ and substituting this expression in the CI formulation leads to the definition given in the box.

This interval construction relies on an assumption about the distribution of $\hat{\theta} - \theta$, namely that it is independent of θ . This assumption, called *pivotality*, does not necessarily hold in most cases. However, the interval gives acceptable results even if $\hat{\theta} - \theta$ is close to pivotal.

Normal CI

This confidence interval probably looks familiar since it is almost an exact replica of the commonly used confidence interval for a population mean. Indeed, similarly to that familiar CI, we can get it if we have reasons to believe that $Z = (\hat{\theta} - \theta)/\hat{s}e \sim N(0, 1)$ (often true asymptotically). Alternatively, we can again consider $W = \hat{\theta} - \theta$, place the restriction that it should be normal and estimate its variance with bootstrap. Observe that the normal CI also implicitly assumes *pivotality*.

Percentile CI

These type of CI may seem natural and obvious but actually requires a quite convoluted argument to motivate. Without going into details, you get this CI by assuming that there exists a transformation h such that the distribution of $h(\hat{\theta}) - h(\theta)$ is pivotal, symmetric and centered around 0. You then construct a Basic CI for $h(\theta)$ rather than θ itself, get the α quantiles and transform those back to the original scale by applying h^{-1} . Observe that although we do not need to know h explicitly, the existence of such a transformation is a must, which is not always the case.

4.5 Limitations of bootstrap

Yes, those do exist. Bootstrap tends to give results easily (too much so, in fact), but it is possible that those results are completely wrong. More than that, they can be completely wrong without being obvious about it. The following are some such situations.

4.5.1 Infinite variance

In the "general idea" of bootstrapping we plugged in an estimate \hat{F} of the density F , and then sampled from it. This works only if \hat{F} actually is a good estimate of F , that is it captures the essential features of F despite being based on a finite sample. This may not be the case if F is very heavy tailed, i.e. has infinite variance. The intuition is that in this case extremely large or small values can occur, and when they do they have a great effect on the bootstrap estimate of the distribution of $\hat{\theta}$, making it unstable. As a consequence, the measures of accuracy of $\hat{\theta}$, such as CI, will be unreliable.

The classic example of this is the mean estimator $\hat{\theta} = \bar{X}$ with the data generated from a Cauchy distribution. For it, both the first and the second moments (e.g. mean and variance) are infinite, leading to nonsensical confidence intervals even for large sample sizes. A less obvious example is a non-central Student t distribution with 2 degrees of freedom. This distribution has pdf

$$f_X(x) = \frac{1}{2(1 + (x - \mu)^2)^{3/2}} \quad \text{for } x \in \mathbb{R}.$$

where μ is the location parameter, defined as $\mathbf{E}[X]$. So, the first moment is finite and its estimator \bar{X} is consistent. The second moment, however, is infinite, and the right tail of the distribution grows heavier with increasing μ . This leads to the 95% CI coverage probabilities that are quite far from the supposed 95% even when the sample size is as large as 500.

4.5.2 Parameter on the boundary

The classical example here is the $Uni(0, \theta)$ distribution. The maximum likelihood estimate $\hat{\theta}$ is simply $\max(x_1, \dots, x_n)$, which will always be biased ($\hat{\theta} < \theta$). In this case the non-parametric bootstrap leads to a very discrete distribution, with more than half of the bootstrap estimates $\hat{\theta}^*$ equal to the original $\hat{\theta}$ (Figure 4.2). Clearly, if the quantiles used in CIs are taken from this distribution the results will be far from accurate. However, the parametric bootstrap will give a much smoother distribution and more reliable results.

4.5.3 Lack of pivotality

In all the CI descriptions above the word "pivotality" shows up. So we can guess that it is a bad thing not to have (see Lab, assignment 3). To circumvent this, something called "studentized bootstrap" can be used.

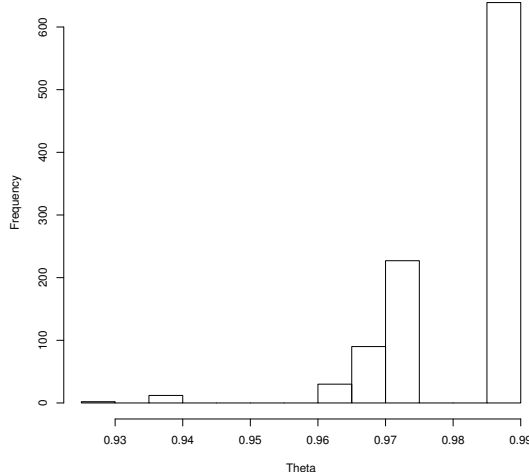


Figure 4.2: Histogram of 1000 non-parametric bootstrap samples of $\hat{\theta}^*$, the data from $Uni(0, \theta)$ distribution. $\theta = 1$.

The idea behind the method is simple and can be seen as an extrapolation of the basic bootstrap CI. There, we looked at $W = \hat{\theta} - \theta$. Now, we instead consider the standardized version $W = (\hat{\theta} - \theta)/\sigma$, with σ denoting the standard deviation of $\hat{\theta}$. The confidence interval will then be calculated through

$$\mathbf{P}(w_{\alpha/2} \leq W \leq w_{1-\alpha/2}) = \mathbf{P}(\hat{\theta} - w_{1-\alpha/2}\sigma \leq \theta \leq \hat{\theta} - w_{\alpha/2}\sigma) = 1 - \alpha$$

As with the basic CI, the distribution of W is not known and has to be approximated, this time with the distribution of $W^* = (\hat{\theta}^* - \hat{\theta})/\hat{s}e^*$. Here, $\hat{s}e^*$ denotes the standard deviation corresponding to *each bootstrap sample*.

This CI is considered to be more reliable than the ones described earlier. However, there is a catch, and this catch is the estimate of the standard deviation of $\hat{\theta}^*$, $\hat{s}e^*$. This estimate is not easily obtained. You can get it either parametrically (but then you need a model which you probably don't have) or through re-sampling. This means that you have to do an extra bootstrap for each of the original bootstrap samples. That is, you will have a loop within a loop, and it can become very heavy computationally.

4.6 Computer assignment: Bootstrap re-sampling.

The aim of this assignment is to study the performance of bootstrap estimates, as well as corresponding variance, bias and CI, using different bootstrap techniques. The total amount of points is 14 and you need 6 points to pass the lab. Details about what your report should

contain and how the points are divided between different tasks can be found in the document "Instructions for report writing, lab 4". The lab is to be done in R.

In the assignment you are mainly going to work with the statistic sample mean, as an estimator for the theoretical mean. We are going to simulate the sample data from a known gamma distribution. In this case you will be able to know the distribution of the estimator, and hence also the bias and the variance. We are however going to use different bootstrap techniques to approximate these things, to have a setting where you know "the truth" and can compare your results to this.

4.6.1 Assignment 1, The gamma distribution and the estimator sample mean

First, we will generate some data to work with. Let us say that the data comes from a definitely non-normal, highly skewed distribution. Such as, for example, the gamma distribution.

- Generate a data set of size $n = 100$ from a $Gamma(k, \gamma)$ distribution, where $k = 2$ is the shape parameter and $\gamma = 2$ the scale parameter (see hint in section 4.6.5). Do a histogram of the data. What are the theoretical mean and variance of this $Gamma$ distribution?
- Let us say that our parameter of interest θ is the mean and that we will use the sample mean as estimator ($\hat{\theta}$) for it. What are the theoretical mean and variance of the estimator sample mean, when using $n = 100$ and knowing that the data comes from the distribution above? Distribution for sample mean?

4.6.2 Assignment 2, Non-parametric bootstrap

We start with the easier task of setting up a non-parametric bootstrap. The parameter of interest θ is the mean and we will use the sample mean as estimator ($\hat{\theta}$). We will use a dataset with observations generated in the way described in Assignment 1.

Assignment 2.1

Write your own function that approximates the distribution of $\hat{\theta}$ with non-parametric bootstrap. Present the distribution in a histogram. What are the estimated bias and variance of $\hat{\theta}$?

Assignment 2.2

As with many other things nowadays, there already exists a package that does bootstrap for you. In R this package is **boot**. Use it to get the distribution of θ and the estimates of its bias and variance.

Assignment 2.3

Construct CI for θ (normal, basic, percentile). Check your results with the pre-programmed function `boot.ci`.

Assignment 2.4

Bootstrap is known to give less reliable results if the sample size n is small. Study this by doing the following. Fix an $n = 10$. Draw 1000 samples of this size. For each sample, calculate a bootstrap CI (choose one of the three methods above) and record whether it covers the true value of θ (the theoretical mean, that is). Repeat this for $n = 20, 30, \dots, 100$. For each n , does the CI have the correct coverage probability? Present the results in a graph. You can use either your own code or `boot.ci` to get the bootstrap CIs.

4.6.3 Assignment 3, Parametric bootstrap

Now, we are going to repeat most of the tasks in Assignment 2, but instead using parametric bootstrap instead of non-parametric.

Assignment 3.1

In order to do parametric bootstrap (we will use the assumption that the data comes from a gamma distribution), you have to estimate the k and γ parameters in the Gamma distribution through, for example, maximum-likelihood estimation. A nice, closed form MLE solution for the parameters does not exist, so you will have to write a function that finds the maximum of the likelihood function L numerically. Do this, and test your function on a simulated sample from a gamma distribution.

Assignment 3.2

Write your own function that approximates the distribution of $\hat{\theta}$ with parametric bootstrap. Present the distribution in a histogram. What are the estimated bias and variance of $\hat{\theta}$?

Assignment 3.3

Use the R package `boot` to get the distribution of $\hat{\theta}$ and the estimates of its bias and variance.

Assignment 3.4

Repeat Assignment 2.4, but now using parametric bootstrap.

4.6.4 Assignment 4, Studentized CI

Our parameter of interest θ is no longer the true mean, but the true variance.

- Repeat Assignment 2.4 (using the basic CI), but now for the variance instead of mean. What can be said about the performance of this confidence interval? What do you think is the reason?
- Construct studentized confidence intervals for the variance. Check the coverage for different sample sizes as in the above. Any improvement?

4.6.5 Software - some hints on useful commands/routines

- Functions you may find useful: **rgamma**, **sample**, **apply**, **replicate**, **boot**, **boot.ci**, **gamma**, **nlm**
- Observe that the *Gamma* distribution can be defined both through γ and $1/\gamma$. Look out for which definition R uses as default and how to choose the other version.
- When working with Assignment 3, note that most optimization packages look for minimum and not maximum, so work with $-\log(L)$ instead of L itself.
- To construct studentized confidence intervals will require much computing power, so to reduce the running time you can use the following values: for the loop (or its alternative) that counts the number of CI that cover the true value, construct 100-200 CIs. For the inner bootstrap, the one estimating the variance for each sample, draw 50 samples. For the outer bootstrap, don't draw more than 1000 samples.
- You can construct the studentized CI both from scratch with your own code or using **boot** and **boot.ci**. If you choose to do the latter, make sure that the "statistic" function that you have to specify in **boot** returns two values: $\hat{\theta}^*$ and $\text{Var}(\hat{\theta}^*)$. It is recommended, but not mandatory, that you solve Assignment 4 without using the function **boot**.
- Computations may be sped up by giving **boot** the arguments `parallel="multicore"` and `ncpus=x` where x is the number of CPUs on the computer you are using.

4.6.6 Further reading

For a wider and deeper treatment of the bootstrap see chapters 10 and 11 in Computer Age Statistical Inference by Bradley Efron and Trevor Hastie.