Bootstrap Methods in R

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Abstract

We present a variety of bootstrap methods in R. SAY MORE

1 Introduction

Short intro to all three bootstraps. SAY MORE.

We have developed a package, Bootstrap, with functions to implement the bootstrap, Bayesian bootstrap and bag of little bootstraps. The package can be obtained from GitHub,

```
devtools::install_github("EllaKaye/Module1")
```

and loaded.

```
library(Bootstrap)
```

2 The Bootstrap

The bootstrap (Efron 1979), is a statistical tool which gives measures of accuracy of estimators, and can therefore be used draw inference about the parameters of the sampling distribution. It is a powerful and widely applicable tool.

Suppose we observe a sample of n iid realisations $x_1, \ldots, x_n \sim P$, for some probability measure P. Let θ be a parameter of the distribution, and $\hat{\theta}_n$ be an estimator of θ. The goal of the bootstrap is to obtain an assessment, ξ, of the quality of the estimator. For example, θ_n could be the median, and ξ the standard error. To obtain a bootstrap estimate, we procede as follows:

1. Repeatedly (B times) sample n points with replacement from the original dataset, giving bootstrap replications (resamples) $(x_1^{*(i)}, \ldots, x_n^{*(i)}), i = 1, \ldots, B$
2. Compute $\hat{\theta}_n^{*(i)}$ on each of the B resamples.

3. Compute $\xi^* = \xi(\hat{\theta}_n^{*(1)}, \ldots, \hat{\theta}_n^{*(B)})$ as our estimate of ξ.

The Bootstrap library contains a function, bootstrap, which automates the above procedure. It takes as inputs a data set (which can be a vector, matrix or dataframe), a function, FUN, which is used to obtain the statistic of interest, and the number, B, of bootstrap resamples required. Note that the data must be passed to FUN in one object.

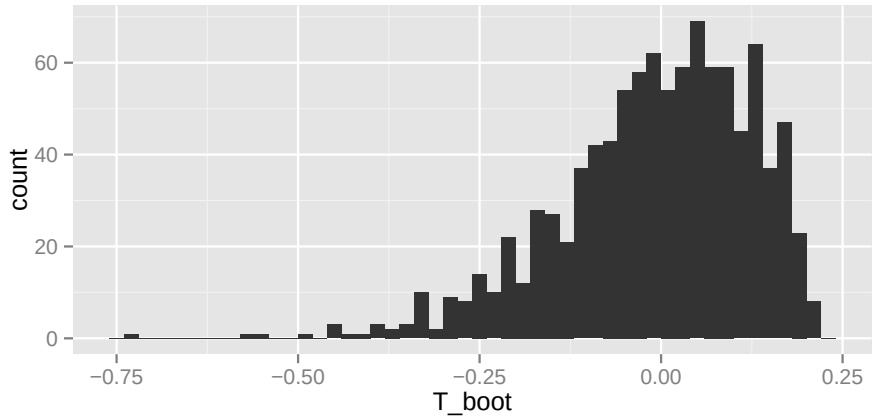
We now show how to use this function to replicate the example on page 37-38 of Efron and Gong (1983), where we are interested in obtaining the bootstrap estimate of the standard error of the Pearson correlation coefficient. The Bootstrap library contains a function, `cor_df`, which calculates the Pearson correlation coefficient between the first and second columns of a matrix or dataframe.

```
law_school <- data.frame(
  LSAT=c(576,635,558,578,666,580,555,
         661,651,605,653,575,545,572,594),
  GPA=c(3.39,3.30,2.81,3.03,3.44,3.07,3.00,
        3.43,3.36,3.13,3.12,2.74,2.76,2.88,2.96))

set.seed(1)
bootstrap_law <- bootstrap(law_school, cor_df, B=1000)
bootstrap_law$se

## [1] 0.1334911

library(ggplot2)
bootstrap_law_df <- data.frame(
  T_boot = bootstrap_law$T_boot - cor_df(law_school))
qplot(T_boot, data=bootstrap_law_df, geom="histogram",
      binwidth=0.02)
```



3 Bayesian Bootstrap

Rubin introduced the Bayesian bootstrap (BB) as the natural Bayesian analogue of the bootstrap. Each BB replication generates a posterior probability for each x_i, which is centered at $1/n$, but has variability. To obtain a BB replication, first generate a set of weights by drawing $(n-1)$ uniform(0,1) random variates, $u_1, \ldots, u_(n-1)$, ordering them and calculating the gaps $g_t = u_{(t)} - u_{(t-1)}, t = 1, \ldots, n$, where $u_{(0)} = 0$ and $u_{(n)} = 1$. These gaps, $g = (g_1, \ldots, g_n)$ form the weights to attach to the data values in that replication. Considering all the BB replications gives the BB distribution of X, and thus of any parameter of this distibution.

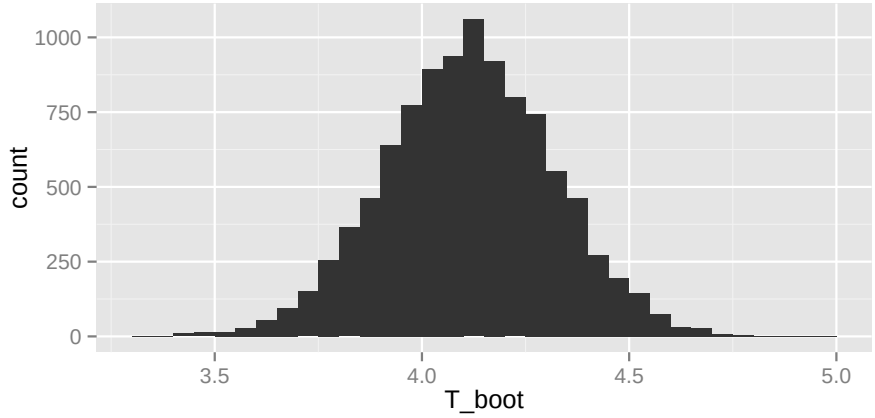
Our function BB gives a BB distribution. It takes as its inputs a dataset (as a vector, matrix or dataframe), a function for calculating the statistic $\hat{\theta}$ (this function must take two arguments - one for data and one for weights), and B, the number of replications required. It returns a list, the first item of which is the standard error of the replicates. The second item is a dataframe with $\theta^*_1, \ldots, \theta^*_B$.

The following code gives the BB distribution when the parameter of interest is the mean. Here the function weighted.mean is in the R base package.

```
X <- rnorm(100, 4, 2)
BB_mean <- BB(X, weighted.mean, B=10000)
BB_mean$se

## [1] 0.2037395

qplot(T_boot, data=BB_mean$replicates, geom="histogram", binwidth=0.05)
```



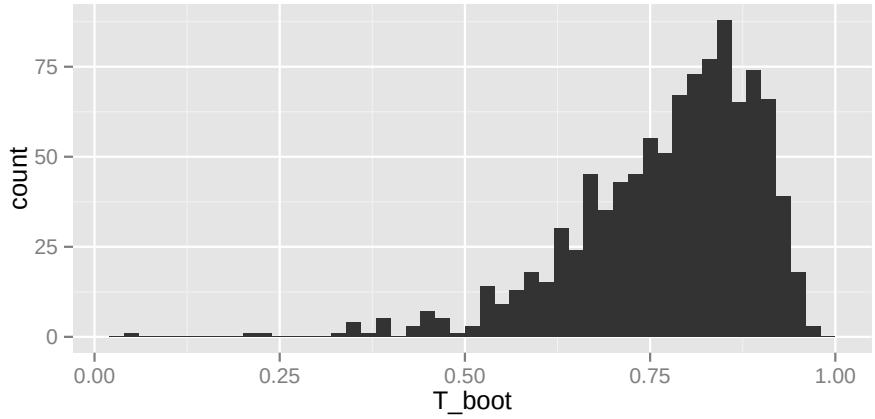
It may be necessary to define your own function for the statistic of interest that can take weights as an argument. By way of example, we show the BB equivalent of the correlation example from the previous section. The function

`cor` in the R base package cannot take weights; the fuction `weighted.cor` in our Bootstrap package does.

```
set.seed(1)
BB_law <- BB(law_school, weighted.cor, B=1000)
BB_law$se

## [1] 0.1224361

qplot(T_boot, data=BB_law$replicates, geom="histogram",
      binwidth=0.02)
```



Note the similarity of the distributions obtained for the law school data using bootstrap and Bayesian bootstrap resamples. Indeed Rubin (1981) points out the inferential similarities between these two methods. As a result, whenever the applicability of the Bayesian bootstrap is called into question, we should also be weary of using the standard bootstrap. Typically, the standard bootstrap is seen as widely applicable, because it is completely non-parametric and does not seem to involve any model assumptions. However, both the bootstrap and Bayesian bootstrap operate under the assumption that all possible values of X have been observed. In any application, the researcher will need to ask themselves whether such an assumption is reasonable. Furthermore, the BB and the bootstrap make the assumption that there are no relationships between the parameters, which may not be realistic. In such cases, smoothing the parameters may be appropriate. Although there exist models that incorporate smoothing, inference on the parameters will not be the same and neither the bootstrap nor BB can avoid this.

DISCRETE. LARGEST VALUE.

4 Bag of Little Bootstraps

The original bootstrap arose around the time when increases in computing power allowed the development of statistical tools that had previously been too computationally expensive. In recent years, there has been an influx of 'big data', alongside the development of parallel computing architectures. Kleiner et al. (2014) have developed a scalable bootstrap for massive data, known as the Bag of Little Bootstraps (BLB). With massive datasets, the bootstrap's need for recomputation on resamples of the same size as the original dataset is problematic. Rather than obtain bootstrap samples from the whole dataset, the BLB breaks down the process as follows:

1. Repeatedly (s times) subsample $b(n) < n$ points *without replacement* from the original dataset of size n.
2. For each of the s subsamples, do the following:
   (a) Repeatedly (r times) resample n point *with replacement* from the subsample.
   (b) Compute $\hat{\theta}_n^*$ on each resample.
   (c) Compute an estimate of ξ based on these r realisations of $\hat{\theta}_n^*$.
3. We now have one estimate of ξ per subsample. Output their average as the final estimate of ξ for $\hat{\theta}_n$.

Kleiner et al. (2014) recommends taking $b(n) = n^\gamma$, where $\gamma \in [0.5, 1]$. This procedure dramatically reduces the size of each resample. For example, if $n =$ 1 million and $\gamma = 0.6$, the size of the original dataset may be around 1TB, with a bootstrap resample typically occupying approximately 632GB, and a BLB subsample or resample occupying just 4GB.

The Bootstrap package contains three functions which implement BLB in different cases, `BLB.1d, BLB.multi` and `BLB.adapt`. The function `BLB.1d` implements the simplest version of BLB. It takes as input a 1-dimensional dataset in a vector, γ, which controls the value of b, and a function FUN, which computes the parameter estimate, $\hat{\theta}_n$. It also takes as arguments s and r, which default to 20 and 100 respectively (Kleiner et al. (2014) demonstates that these values are likely as large as they'll need to be to obtain convergence). The function returns a BLB estimate of ξ, which is set as the standard error.

```
X <- rnorm(5000)
BLB.1d(X, mean, gamma=0.5)

## [1] 0.01390571
```

INCREASE DIM AND SAY SOMETHING ABOUT TIME.

In their paper, Kleiner et al. (2014) conduct a simulation study. They generate data from the true underlying distribution, a linear model $Y_i = \tilde{X}_i^\top \mathbf{1}_d + \epsilon_i$,

with iid $\tilde{X}_i \sim MVN(0, \mathbb{I}_d)$ and $\epsilon_i \sim N(0, 10)$. The estimator $\hat{\theta}_n$ consists of a linear least squares regression coefficients, with a small L_2 penalty of $\lambda = 10^{-5}$. To replicate their results, we created the function `BLB.multi`, which accepts as input an $n \times (d + 1)$ dataframe or matrix, where each row is an observation, combining the d-dimensional x observation and, in the right-most column, the response, y. The tuning parameters for BLB γ, r and s can all be set, as can the tuning parameter λ for the penalised regression, and α, which controls the width of the confidence intervals. The function returns a list containing the BLB estimate of three quality measures, ξ^*: the confidence intervals for each dimension of the estimator, a vector with the width of those intervals, and the standard error of the estimator. As in the paper, we tested the function with $n = 20,000$, though we reduced the dimension d from 100 to 10. We chose $\gamma = 0.7$, kept $r = 100$, and set $s = 15$ (which is ample for convergence). This took under under 90 seconds to evaluate.

```
# generate the data
n=1000
d=10
library(MASS)
set.seed(1)
X <- mvrnorm(n, mu=rep(0,d), Sigma=diag(d))
epsilon <- rnorm(n, mean=0, sd=sqrt(10))
t_theta <- as.matrix(rep(1,d))
Y <- X %*% t_theta + epsilon
data <- cbind(X,Y)

# apply the function and look at the results
system.time(
  BLB.multi_out <- BLB.multi(data, gamma=0.7, s=15, r=100)
)

##    user  system elapsed
##   4.824   0.203   5.028

BLB.multi_out

## $CI
##             [,1]      [,2]
##  [1,] 0.7447234 1.1395386
##  [2,] 0.9159413 1.3041599
##  [3,] 0.6395992 0.9924294
##  [4,] 1.0650250 1.4445697
##  [5,] 0.8533737 1.2363316
##  [6,] 0.8669677 1.2089213
##  [7,] 0.9434961 1.3085097
##  [8,] 0.9358243 1.2996644
```

```
##  [9,] 0.7688616 1.1419913
## [10,] 0.8700360 1.2583149
##
## $CI_width
##  [1] 0.3948153 0.3882186 0.3528302 0.3795447 0.3829580 0.3419536 0.3650136
##  [8] 0.3638402 0.3731297 0.3882788
##
## $se
##  [1] 0.10072004 0.09903717 0.09000936 0.09682440 0.09769515 0.08723466
##  [7] 0.09311742 0.09281807 0.09518789 0.09905254
```

As Kleiner et al. (2014) point out, when $n = 20,000$ the true average (across dimensions) marginal confidence interval width for the estimated parameter vector is approximately 0.1, so our function gives the expected results.

4.1 Adaptive tuning parameter selection

In `BLB.multi`, we need to specify values for s, the number of subsamples and r, the number of bootstrap replicates per subsample. As Kleiner et al. (2014) discuss, in practice fairly modest values for these tuning parameters often suffice for convergence, though they will vary depending on the value of γ, as well as on the parameter θ being estimated and the choice of quality assessment ξ. We wish to use the smallest values of r and s which have sufficiently good statistical properties. In order to minimise the computational cost, we can select r and s adaptively. Kleiner et al. (2014) suggest the following scheme. Suppose we are currenlty processing subsample j. We repeatedly produce resamples, compute the parameter $\theta_n^\star$ and evaluate $\xi_n^\star$, until convergence. Convergence is said to occurred when $\xi_n^\star$ no longer changes significantly after being updated from a new resample.

The exact measure of convergence is given by the following algorithm: Given a series of realisations of ξ_n^*, $z^{(1)}, ..., z^{(t)} \in \mathbb{R}^d$; a window $w \in \mathbb{N}$ $(w < t)$; and a target relative error ϵ, we keep on producing subsamples until the following condition holds: $\forall j \in [1, w]$, $1/d \sum_{i=1}^{d} |(z_{(i)}^{t-i} - z_i^t|/|z_{(i)}^{(t)}| \leq \epsilon$.

The same condition can be used for the selection of s. Therefore, both parameters can be selected adaptively and in this case r is chosen independently for each subsample. The function `BLB.adapt` implements BLB with adaptive selection of both r and s. It takes data in the same format as `BLB.multi`, and likewise the parameter of interest is the coefficients of a penalised linear regression. Kleiner et al. (2014) suggest the values of $w = 3$ for the selection of s, $w = 20$ for the selection of r and $\epsilon = 0.05$ for both adaptive procedures. The values of γ, λ and ϵ can also be set as arguments, as well as α, which controls the width of the confidence intervals. It returns the width of the marginal confidence intervals, along with the final value of s, and a vector of the values of r used in each subsample. Here we apply `BLB.adapt` to the same data as we used above with `BLB.multi`. Most arguments are set to the default values suggested above.

```
system.time(
  BLB.adapt_out <- BLB.adapt(data, gamma=0.7)
)

##    user  system elapsed
##   1.393   0.094   1.488

BLB.adapt_out

## $s
## [1] 7
##
## $r
## [1] 47 57 61 46 61 62 47
##
## $mean_width
## [1] 0.400683
##
## $mean_se
## [1] 0.1022169
```

COMPARE TIMES
DISCUSSION OF BLB
Not run in parallel

References

Efron, Bradley (1979). "Bootstrap methods: another look at the jackknife". In: *Annals of Statistics* 7, pp. 1–26.

Efron, Bradley and Gail Gong (1983). "A Leisurely Look at the Bootstrap, the Jackknife, and Cross-Validation". In: *The American Statistician* 37.1, pp. 36–48.

Kleiner, Ariel et al. (2014). "A scalable bootstrap for massive data". In: *Journal of the Royal Statistical Society (Series B)* 76.4, pp. 795–816.

Rubin, Donald B (1981). "The Bayesian Bootstrap". In: *The Annals of Statistics* 9.1, pp. 130–134.