

WEIGHTED JACKKNIFE-AFTER-BOOTSTRAP: A HEURISTIC APPROACH

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ABSTRACT

We investigate the problem of deriving precision estimates for bootstrap quantities. The one major stipulation is that no further bootstrapping will be allowed. In 1992, Efron derived the method of jackknife-after-bootstrap (JAB) and showed how this problem can potentially be solved. However, the applicability of JAB was questioned in situations where the number of bootstrap samples was not large. The JAB estimates were inflated and performed poorly. We provide a simple correction to the JAB method using a weighted form where the weights are derived from the original bootstrap samples. Our Monte Carlo experiments show that the weighted jackknife-after-bootstrap (WJAB) performs very well.

1 INTRODUCTION

The bootstrap method is a computer-based technique that has become very popular in recent years for estimating such things as standard errors, confidence intervals, biases, and prediction errors. Its automatic nature and applicability to complicated problems have contributed to this popularity. As with any estimated quantities, measures of precision for bootstrap estimates are often required or are at least desirable. The iterated bootstrap has been proposed; however the computation involved can become prohibitive. A simple approach that uses the information in the original bootstrap samples without further resampling was sought. Efron [1992] derived the JAB in an attempt to provide a solution to this problem. The JAB usually requires 100–1000 times less com-

putation than bootstrap-after-bootstrap.

Although the JAB is theoretically justified, situations arise in practice where it performs poorly. These situations occur when a large number of bootstrap samples are not able to be drawn (Tibshirani [1992]). The JAB estimates in these situations have a tendency to be over-inflated and don't reflect the true variability in the bootstrap statistic but more the limitations of using a small number of bootstrap samples. This paper will outline an approach to rectify this situation through a weighted form of JAB where the weights are themselves derived from the original bootstrap samples. In Section 2, we outline the jackknife and bootstrap methods. In Section 3, we review the method of JAB. In Section 4, we introduce the method of WJAB and compare the performance of different estimates through Monte Carlo results. In Section 5, we discuss our conclusions. Rao [1995] is an early work of this paper.

2 The JACKKNIFE AND BOOTSTRAP

We briefly review the jackknife and bootstrap methods (see Efron [1982], Efron and Tibshirani [1993], Hall [1992] and Shao and Tu [1995] for more details). It is assumed that observed data $\mathbf{x} = (x_1, \dots, x_n)$ are obtained by independent and identically distributed (i.i.d.) sampling from an unknown distribution F

$$F \xrightarrow{\text{i.i.d.}} (x_1, \dots, x_n) = \mathbf{x}.$$

Let $\mathbf{x}_{(i)}$ indicate the data set remaining after deletion of the i th point,

$$\mathbf{x}_{(i)} = (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n).$$

Suppose that $s(\mathbf{x})$ is a real-valued statistic of interest and let $s_{(i)} = s(\mathbf{x}_{(i)})$ present the corresponding deleted point value of the statistic of interest. The jackknife estimate for the standard error of $s(\mathbf{x})$ is

$$\hat{se}_{\text{jack}}\{s\} = \left[\frac{n-1}{n} \sum_{i=1}^n (s_{(i)} - s_{(\cdot)})^2 \right]^{1/2}, \quad (1)$$

where $s_{(\cdot)} = \sum_{i=1}^n s_{(i)}/n$.

The usual estimate of F is \hat{F} , the empirical probability distribution, putting probability $1/n$ on each point x_i ,

$$\hat{F}: \text{probability } 1/n \text{ on } x_i, \quad i = 1, \dots, n.$$

A bootstrap sample $\mathbf{x}^* = (x_1^*, \dots, x_n^*)$ is a random sample of size n drawn from \hat{F} ,

$$\hat{F} \xrightarrow{\text{i.i.d.}} (x_1^*, \dots, x_n^*) = \mathbf{x}^*.$$

Then $s^* = s(\mathbf{x}^*)$, the statistic of interest evaluated for data set \mathbf{x}^* , is a bootstrap replication of s . A typical bootstrap analysis consists of independently drawing a large number B of independent bootstrap samples, evaluating the bootstrap replicates $s^{*b} = s(\mathbf{x}^{*b})$ for $b = 1, \dots, B$ and using summary statistics of the s^{*b} values to assess the accuracy of the original statistic $s(\mathbf{x})$. The bootstrap estimate of standard error for s is

$$\hat{se}_B\{s\} = \left[\sum_{b=1}^B \frac{(s^{*b} - s^*)^2}{B-1} \right]^{1/2}, \quad (2)$$

where $s^* = \sum_{b=1}^B s^{*b}/B$.

3 The JACKKNIFE-AFTER-BOOTSTRAP

The method of JAB was proposed by Efron [1992]. Suppose we have drawn B bootstrap samples and calculated $\hat{se}_B \equiv \hat{se}_B\{s\}$, a bootstrap estimate of the standard error of $s(\mathbf{x})$. We would like to have a measure of the uncertainty in \hat{se}_B . The JAB method provides a way of estimating $se(\hat{se}_B)$ using only information in our B bootstrap samples. The jackknife estimate of standard error of \hat{se}_B involves two steps:

1. For $i = 1, \dots, n$, leave out data point i and recompute \hat{se}_B and called the result $\hat{se}_{B(i)}$.
2. Define $\hat{se}_{\text{jack}}(\hat{se}_B) = \{[(n-1)/n] \sum_{i=1}^n (\hat{se}_{B(i)} - \hat{se}_{B(\cdot)})^2\}^{1/2}$, where $\hat{se}_{B(\cdot)} = \sum_{i=1}^n \hat{se}_{B(i)}/n$.

For each i , there are some bootstrap samples in which that the data point x_i does not appear, and we can use those samples to estimate $\hat{se}_{B(i)}$. Formally, if we let C_i denote the indices of the bootstrap samples

that don't contain data point x_i , and there are B_i such samples, then

$$\hat{se}_{B(i)} = \left[\sum_{b \in C_i} \frac{(s(\mathbf{x}^{*b}) - \bar{s}_i)^2}{B_i} \right]^{1/2}, \quad (3)$$

where $\bar{s}_i = \sum_{b \in C_i} s(\mathbf{x}^{*b})/B_i$. The JAB estimate of standard error of \hat{se}_B is

$$\hat{se}_{\text{jab}}(\hat{se}_B) = \left[\frac{n-1}{n} \sum_{i=1}^n (\hat{se}_{B(i)} - \hat{se}_{B(\cdot)})^2 \right]^{1/2} \quad (4)$$

where $\hat{se}_{B(\cdot)} = \sum_{i=1}^n \hat{se}_{B(i)}/n$.

4 The WEIGHTED JACKKNIFE-AFTER-BOOTSTRAP

Efron [1992] points out that the JAB method is only reliable when B is some large number like 1000. The example of Tibshirani [1992] shows that small values of B can terribly inflate the JAB estimate of errors. We propose a modification to the JAB method which incorporates a weighting scheme for the deleted point jackknife quantities. The weights are derived directly from the original bootstrap samples and no further bootstrap computations are required. Comparing with the JAB, true jackknife, and Tibshirani's approximation (Tibshirani [1992]), our Monte Carlo experiments show that the WJAB performs very well.

Tibshirani [1992] introduces a simple formula to estimate the standard error of the bootstrap quantity,

$$\hat{se}_{\text{tib}}(\hat{se}_B) = \left[\left(1 + \frac{1}{B}\right) \tilde{\sigma}^2 \right]^{1/2} \quad (5)$$

where $\tilde{\sigma}^2 = \sum_{b=1}^B (s^{*b} - s^*)^2 / (B-1)$ is the bootstrap variance. This method performs reasonable well in his example (Tibshirani [1992]).

In the computation of the JAB, the sample size B_i is involved in computing $\hat{se}_{B(i)}$. Here B_i is random and depends on the B bootstrap samples. But for $i = 1, \dots, n$, each $\hat{se}_{B(i)}$ was treated equally likely in computing $\hat{se}_{\text{jab}}(\hat{se}_B)$. Thus for large B_i , $\hat{se}_{B(i)}$ may contribute more information to $\hat{se}_{\text{jab}}(\hat{se}_B)$. The heuristic approach we propose is to assign a weight w_i to each $\hat{se}_{B(i)}$ that is proportional to B_i . As mentioned, the JAB performs well when B is large (Efron [1992]) so in order to keep consistent with the JAB method, w_i should converge to 1 as B goes to infinity.

We define $\tilde{se}_{B(i)} = w_i \hat{se}_{B(i)}$, then the WJAB estimate of the standard error of \hat{se}_B is

$$\hat{se}_{\text{wjab}}(\hat{se}_B) = \left[\frac{n-1}{n} \sum_{i=1}^n (\tilde{se}_{B(i)} - \tilde{se}_{B(\cdot)})^2 \right]^{1/2} \quad (6)$$

where $\hat{s}e_{B(\cdot)} = \sum_{i=1}^n \hat{s}e_{B(i)}/n$.

A natural candidate for w_i is

$$w_i = \frac{B_i}{\sum_{i=1}^n B_i/n}, \quad i = 1, \dots, n. \quad (7)$$

Thus, w_i is proportional to B_i . From DiCiccio and Martin [1992], w_i converges to 1 as B goes to infinity since B_i/B converges to 1/2 as B goes to infinity.

Next, we consider a series of Monte Carlo experiments where we assume that the statistic of interest, $s(\mathbf{x})$ is the sample mean, $\bar{x} = \sum_{i=1}^n x_i/n$, and the observed data $\mathbf{x} = (x_1, \dots, x_n)$ are i.i.d. from the standard normal distribution. All Monte Carlo simulation results are averaged over thirty independent replications. The method of common random numbers was used in the Monte Carlo design for comparison. In order to compare the WJAB and the JAB we consider the ratio of squared error of the JAB to the WJAB using the true jackknife estimate $\hat{s}e_{tj}(\hat{s}e_B)$ as the standard,

$$R = \frac{\sum (\hat{s}e_{jab}(\hat{s}e_B) - \hat{s}e_{tj}(\hat{s}e_B))^2}{\sum (\hat{s}e_{wjab}(\hat{s}e_B) - \hat{s}e_{tj}(\hat{s}e_B))^2}. \quad (8)$$

The most obvious way to implement the true jackknife estimate would be to delete one point out at a time from the observed data \mathbf{x} and then carry out the bootstrap sampling for each deleted point sample. For each i , the bootstrap sample size, which was used in Monte Carlo experiments for computing $\hat{s}e_{B(i)}$ of the true jackknife estimate, is 10000.

With the natural weight $w_i = B_i/(\sum_{i=1}^n B_i/n)$, Tables 1 - 4 compare $\hat{s}e_{jab}(\hat{s}e_B)$ and $\hat{s}e_{wjab}(\hat{s}e_B)$ with $\hat{s}e_{tj}(\hat{s}e_B)$. The Monte Carlo results show that

1. $\hat{s}e_{jab}(\hat{s}e_B) \geq \hat{s}e_{wjab}(\hat{s}e_B) \geq \hat{s}e_{tj}(\hat{s}e_B)$,
2. $\hat{s}e_{jab}(\hat{s}e_B)$ goes to $\hat{s}e_{tj}(\hat{s}e_B)$ as B goes to infinity,
3. $\hat{s}e_{jab}(\hat{s}e_B)$ increases in n and
4. $\hat{s}e_{wjab}(\hat{s}e_B)$ seems to overestimate the standard error when B is small, which is consistent with Tibshirani's result (Tibshirani [1992]).

Comparing with $\hat{s}e_{jab}(\hat{s}e_B)$, $\hat{s}e_{tj}(\hat{s}e_B)$, and R values, $\hat{s}e_{wjab}(\hat{s}e_B)$ is better than $\hat{s}e_{jab}(\hat{s}e_B)$ and closer to $\hat{s}e_{tj}(\hat{s}e_B)$. But, $\hat{s}e_{wjab}(\hat{s}e_B)$ does not improve much. From Tables 1 - 4, the Monte Carlo results using $w_i = B_i/(\sum_{i=1}^n B_i/n)$ are not exciting. Besides converging to 1 as B goes to infinity and being proportional to B_i , the weight w_i should contain the information of B bootstrap samples and the observed data size n . according to Tables 1 - 4, the weight w_i should

Table 1: For $n = 20$ and $w_i = B_i/(\sum_{i=1}^n B_i/n)$

B	$\hat{s}e_{jab}(\hat{s}e_B)$	$\hat{s}e_{wjab}(\hat{s}e_B)$	$\hat{s}e_{tj}(\hat{s}e_B)$	R
10	0.2202	0.1938	0.0357	1.3594
20	0.1538	0.1344	0.0348	1.4062
40	0.0982	0.0952	0.0382	1.1097
60	0.0887	0.0866	0.0363	1.0829
100	0.0645	0.0638	0.0326	1.1115
500	0.0415	0.0413	0.0318	1.0122
1000	0.0328	0.0327	0.0284	1.0164

Table 2: For $n = 50$ and $w_i = B_i/(\sum_{i=1}^n B_i/n)$

B	$\hat{s}e_{jab}(\hat{s}e_B)$	$\hat{s}e_{wjab}(\hat{s}e_B)$	$\hat{s}e_{tj}(\hat{s}e_B)$	R
10	0.2553	0.2198	0.0184	1.3867
20	0.1487	0.1345	0.0147	1.2493
40	0.1074	0.1024	0.0198	1.1063
60	0.0806	0.0787	0.0160	1.0652
100	0.0646	0.0635	0.0143	1.0400
500	0.0309	0.0307	0.0152	1.0150
1000	0.0251	0.0251	0.0161	0.9959

decrease in B and n . After large amount of Monte Carlo experiments, a better weight was obtained,

$$w_i = \frac{B_i}{\sum_{i=1}^n B_i/n + n}, \quad (9)$$

which satisfies all the basic requirement we mentioned before.

With the better weight $w_i = B_i/(\sum_{i=1}^n B_i/n + n)$, Tables 5 - 9 compare $\hat{s}e_{jab}(\hat{s}e_B)$, $\hat{s}e_{tib}(\hat{s}e_B)$, and $\hat{s}e_{wjab}(\hat{s}e_B)$ with $\hat{s}e_{tj}(\hat{s}e_B)$. The Monte Carlo results show that $\hat{s}e_{wjab}(\hat{s}e_B)$ performs extremely well and is always the best estimate. The improvement of $\hat{s}e_{wjab}(\hat{s}e_B)$ is great. Tibshirani's estimate $\hat{s}e_{tib}(\hat{s}e_B)$ performs poorly when the observed data size n is less than 40.

5 DISCUSSION

Efron [1992] points out that the bootstrap-after-bootstrap seems to be too computationally intensive for routine use. The JAB method, a clever idea, introduces a simple way of estimating the standard error of the bootstrap estimates without the need to do a second level of bootstrap replication. However, Tibshirani's example (Tibshirani [1992]) and our Monte Carlo experiment show that the JAB method is not

Table 5: For $n = 20$ and $w_i = B_i / (\sum_{i=1}^n B_i / n + n)$

B	$\hat{s}e_{jab}(\hat{s}e_B)$	$\hat{s}e_{tib}(\hat{s}e_B)$	$\hat{s}e_{wjab}(\hat{s}e_B)$	$\hat{s}e_{tj}(\hat{s}e_B)$	R
10	0.2238	0.1508	0.0304	0.0342	80.690
20	0.1461	0.1471	0.0350	0.0368	59.908
30	0.1107	0.1484	0.0374	0.0395	12.680
50	0.0850	0.1417	0.0390	0.0281	13.246
100	0.0761	0.1550	0.0489	0.0408	5.7174
500	0.0476	0.1521	0.0432	0.0383	1.4917
1000	0.0318	0.1272	0.0300	0.0272	1.6175

Table 6: For $n = 50$ and $w_i = B_i / (\sum_{i=1}^n B_i / n + n)$

B	$\hat{s}e_{jab}(\hat{s}e_B)$	$\hat{s}e_{tib}(\hat{s}e_B)$	$\hat{s}e_{wjab}(\hat{s}e_B)$	$\hat{s}e_{tj}(\hat{s}e_B)$	R
10	0.2470	0.1011	0.0143	0.0167	735.63
20	0.1534	0.0977	0.0176	0.0172	227.04
30	0.1116	0.0969	0.0191	0.0136	154.79
50	0.0842	0.0942	0.0218	0.0138	53.274
100	0.0702	0.1033	0.0292	0.0169	15.126
500	0.0324	0.0970	0.0253	0.0169	2.9229
1000	0.0240	0.0963	0.0211	0.0141	1.9017

Table 7: For $B = 10$ and $w_i = B_i / (\sum_{i=1}^n B_i / n + n)$

n	$\hat{s}e_{jab}(\hat{s}e_B)$	$\hat{s}e_{tib}(\hat{s}e_B)$	$\hat{s}e_{wjab}(\hat{s}e_B)$	$\hat{s}e_{tj}(\hat{s}e_B)$	R
10	0.2096	0.2019	0.0484	0.0549	46.565
20	0.2238	0.1508	0.0304	0.0342	80.690
30	0.2543	0.1405	0.0238	0.0306	248.97
40	0.2405	0.1123	0.0173	0.0219	260.37
50	0.2470	0.1011	0.0143	0.0167	735.63
60	0.2470	0.0950	0.0121	0.0140	1858.1
80	0.2382	0.0755	0.0090	0.0103	4698.8

Table 8: For $B = 20$ and $w_i = B_i / (\sum_{i=1}^n B_i / n + n)$

n	$\hat{s}e_{jab}(\hat{s}e_B)$	$\hat{s}e_{tib}(\hat{s}e_B)$	$\hat{s}e_{wjab}(\hat{s}e_B)$	$\hat{s}e_{tj}(\hat{s}e_B)$	R
10	0.1585	0.2158	0.0628	0.0837	4.7462
20	0.1461	0.1470	0.0350	0.0368	59.908
30	0.1430	0.1191	0.0250	0.0243	96.942
40	0.1395	0.1030	0.0194	0.0203	69.405
50	0.1534	0.0977	0.0176	0.0172	227.04
60	0.1507	0.0850	0.0147	0.0146	300.58
80	0.1554	0.0792	0.0119	0.0131	481.04

Table 9: For $B = 30$ and $w_i = B_i / (\sum_{i=1}^n B_i / n + n)$

n	$\hat{s}e_{jab}(\hat{s}e_B)$	$\hat{s}e_{tib}(\hat{s}e_B)$	$\hat{s}e_{wjab}(\hat{s}e_B)$	$\hat{s}e_{tj}(\hat{s}e_B)$	R
10	0.1228	0.0231	0.0621	0.0784	1.5929
20	0.1107	0.1484	0.0374	0.0395	12.680
30	0.1212	0.1266	0.0306	0.0254	44.964
40	0.1177	0.1031	0.0237	0.0184	136.90
50	0.1116	0.0969	0.0191	0.0136	154.79
60	0.1127	0.0859	0.0164	0.0125	279.81
80	0.1184	0.0793	0.0133	0.0113	462.66

Table 3: For $B = 10$ and $w_i = B_i / (\sum_{i=1}^n B_i / n)$

n	$\hat{s}e_{jab}(\hat{s}e_B)$	$\hat{s}e_{wjab}(\hat{s}e_B)$	$\hat{s}e_{tj}(\hat{s}e_B)$	R
10	0.2072	0.1952	0.0657	1.1658
20	0.2202	0.1938	0.0357	1.3594
30	0.2297	0.1970	0.0228	1.3617
40	0.2399	0.2125	0.0211	1.2770
50	0.2338	0.2035	0.0162	1.3413
60	0.2303	0.1972	0.0142	1.3614
80	0.2561	0.2504	0.0112	1.3772

Table 4: For $B = 20$ and $w_i = B_i / (\sum_{i=1}^n B_i / n)$

n	$\hat{s}e_{jab}(\hat{s}e_B)$	$\hat{s}e_{wjab}(\hat{s}e_B)$	$\hat{s}e_{tj}(\hat{s}e_B)$	R
10	0.1422	0.1321	0.0656	1.3358
20	0.1538	0.1344	0.0348	1.4062
30	0.1475	0.1311	0.0244	1.3301
40	0.1467	0.1342	0.0179	1.2300
50	0.1487	0.1342	0.0147	1.2493
60	0.1518	0.1362	0.0152	1.2594
80	0.1507	0.1374	0.0136	1.2164

very accurate when B is small which restricts its usefulness in application.

The proposed weighted version of the JAB method overcomes this problem by weighting the deleted point values ($\hat{s}e_{B_{(i)}}$). In terms of computation, this just requires some extra bookkeeping for computing the weights. The Monte Carlo experiments considered indicate the WJAB method produces estimates of standard error that are nearly identical to the true jackknife estimates even when B is small. This method can potentially be used for any bootstrap estimates.

The WJAB method performs very well with our weights. What is the theoretical background behind

this method? What are the optimal weights? Those problems are currently under investigation.

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