A PARAMETRIC VERSION OF JACKKNIFE-AFTER-BOOTSTRAP

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ABSTRACT

In this paper, we investigate the problem of deriving precision estimates for bootstrap quantities within parametric families. Efron’s [1992] jackknife-after-bootstrap is a simple approach that only uses the information in the original bootstrap samples via the importance sampling technique, with no further resampling required. This method can be applied to many Monte Carlo experiments, especially, to the parametric input modeling problems. Variance analysis of the parametric jackknife-after-bootstrap is discussed. Under some reasonable conditions, the parametric jackknife-after-bootstrap method is as good as the true jackknife method. A generalized parametric jackknife-after-bootstrap method is introduced.

1 INTRODUCTION

Monte Carlo simulation is a powerful method for studying complex real-world systems when models of these systems are virtually impossible to solve mathematically. The bootstrap method is a computer-based Monte Carlo technique that has become very popular in recent years for estimating standard errors, confidence intervals, biases, and prediction errors. But the parametric bootstrap method has received less attention in both theory and practice of Monte Carlo simulation. The number of applications of the parametric bootstrap technique in Monte Carlo simulation is limited. Cheng [1995] points out the importance of parametric bootstrap which has been playing an important role in parametric input modeling problems. Many Monte Carlo experiments can be considered as an application of the parametric bootstrap. Sometimes, people just don’t realize that they are using parametric bootstrap.

As with any estimated quantities, measures of precision for bootstrap estimates are often desirable or required. To assess the accuracy of the variation for the simulation from the first stage requires the second stage of simulation. Bootstrap-after-bootstrap, true jackknife, and some other methods are often used to deal with this problem. But all of them need further samples. Sometimes the involved computation can become prohibitive, as Nelson [1990] points out that bootstrap methods are computationally expensive. The jackknife-after-bootstrap (JAB) proposed by Efron [1992] is in an attempt to provide a solution to this problem. It uses only the information from the original bootstrap samples without further resampling. Comparing with bootstrap-after-bootstrap, JAB usually requires 100–1000 times less computation (Efron [1992]).

The parametric version of JAB is an application of the importance sampling method (Hammersley and Handscomb [1964]). It is an efficient Monte Carlo simulation method. Only the information from the first stage bootstrap samples is used to construct jackknife estimates of the second level accuracy of the variation-estimate. No further samples are required. In this paper, we mainly study the variance properties of the parametric JAB comparing with the true jackknife method. In Section 2, we review the parametric Bootstrap and jackknife techniques. In Section 3, we outline the parametric version of JAB. In Section 4, we study the variance properties of the parametric JAB. In Section 5, we introduce a generalized version of parametric JAB. In Section 6, we discuss our conclusions. Detailed discussions of non-parametric JAB can be found in Efron [1992], Efron and Tibshirani [1993], Tibshirani [1992], DiCiccio and Martin [1992], and Wang, Rao, and Shao [1997].

2 PARAMETRIC BOOTSTRAP AND JACKKNIFE

We briefly review the parametric bootstrap and jackknife methods (see Efron [1982], Efron and Tibshirani [1993], Hall [1992] and Shao and Tu [1995] for more details).

Suppose that \( \mathcal{F} = \{ f_\eta(x), \eta \in \mathbb{N} \} \) is a parametric family of density functions indexed by a parametric vector \( \eta \) and the observed data \( x = (x_1, \ldots, x_n) \) is an independent
and identically distributed (i.i.d.) sample from a member of \( \mathcal{F} \),
\[ f_\eta \overset{\text{i.i.d.}}{\longrightarrow} (x_1, \ldots, x_n) = x. \]
Let \( f_\eta(x) = \prod_{j=1}^n f_\eta(x_j) \) indicate the density of whole sample. The parameter space \( N \) is a subset of \( k \)-dimensional Euclidean space.

Given \( x \), we estimate \( \eta \) according to some rule \( \hat{\eta} = \hat{\eta}(x) \), such as the maximum likelihood estimator method. A parametric bootstrap sample is an i.i.d. sample from \( f_\hat{\eta} \),
\[ f_\hat{\eta} \overset{\text{i.i.d.}}{\longrightarrow} (x_1^*, \ldots, x_n^*) = x^*. \]

Suppose that \( s(x) \) is a real-valued statistic of interest. Then \( s^* = s(x^*) \), the statistic of interest evaluated for data set \( x^* \), 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 \( s^b = s(x^{*b}) \) for \( b = 1, \ldots, B \) and using summary statistics of the \( s^b \) values to assess the accuracy of the original statistic \( s(x) \). The bootstrap estimate of standard error for \( s \) is
\[ \hat{\text{se}}_B(s) = \left( \frac{B}{B-1} \sum_{b=1}^B (s^b - s^*)^2 \right)^{1/2}, \]
where \( s^* = \frac{\sum_{b=1}^B s^b}{B} \).

Let \( x_{(i)} \) indicate the data set remaining after deletion of the \( i \)th point,
\[ x_{(i)} = (x_1, \ldots, \hat{x}_i, \ldots, x_n). \]
Let \( s_{(i)} = s(x_{(i)}) \) present the corresponding deleted point value of the statistic of interest, and let \( \hat{\eta}_{(i)} = \hat{\eta}(x_{(i)}) \) be the estimate of \( \eta \) based on the deleted point data set \( x_{(i)} \). The jackknife estimate for the standard error of \( s(x) \) is
\[ \hat{\text{se}}_{\text{jack}}(s) = \left( \frac{n-1}{n} \sum_{i=1}^{n} (s_{(i)} - \bar{s})^2 \right)^{1/2}, \]
where \( \bar{s} = \frac{\sum_{i=1}^{n} s_{(i)}}{n} \).

3 PARAMETRIC JACKKNIFE-AFTER-BOOTSTRAP

The method of JAB was proposed by Efron [1992]. Suppose we have drawn \( B \) bootstrap samples and calculated \( \hat{\text{se}}_B(s) \), a bootstrap estimate of the standard error of \( s(x) \). We would like to have a measure of the uncertainty in \( \hat{\text{se}}_B \). The JAB method provides a way of estimating \( \hat{\text{se}}(\hat{\text{se}}_B) \) using only information in our \( B \) bootstrap samples. The true parametric jackknife estimate of standard error of \( \hat{\text{se}}_B \) involves two steps. In the first step, for \( i = 1, \ldots, n \), let \( \hat{\eta}_{(i)} = \hat{\eta}(x_{(i)}) \) be the estimate of \( \eta \) based on the deleted point data set \( x_{(i)} \). Under deleted point bootstrap sampling, we draw an i.i.d. sample from \( f_{\hat{\eta}_{(i)}} \),
\[ f_{\hat{\eta}_{(i)}} \overset{\text{i.i.d.}}{\longrightarrow} (x_1^*, \ldots, x_n^*) = x^*. \]
and recompute \( \hat{\text{se}}_B \) and called the result \( \hat{\text{se}}_{B(i)} \). In the second step, we define
\[ \hat{\text{se}}_{\text{jack}}(\hat{\text{se}}_B) = \left[ \frac{n-1}{n} \sum_{i=1}^{n} (\hat{\text{se}}_{B(i)} - \hat{\text{se}}_B) \right]^{1/2}, \]
where \( \hat{\text{se}}_{B(i)} = \frac{\sum_{b=1}^{n} \hat{\eta}_{(i)}(x_{(i)})}{n} \). Here \( \hat{\text{se}}_{\text{jack}}(\hat{\text{se}}_B) \) is the true parametric jackknife estimate of standard error of \( \hat{\text{se}}_B \).

The bootstrap density ratio
\[ R_i(x^*) = \frac{f_{\hat{\eta}_{(i)}}(x^*)}{f_\eta(x^*)} \]
is assumed to be finite with probability 1 when sampling from \( f_{\hat{\eta}_{(i)}}(x^*) \). Then we have a standard importance sampling result from Lemma 2 of Efron [1992]. The following two expectations of \( s(x^*)R_i(x^*) \) and \( s(x^*) \) are the same under the two different probability measures.

**Theorem 3.1** For \( i = 1, \ldots, n \),
\[ E_{f_\eta} [s(x^*)R_i(x^*)] = E_{f_{\hat{\eta}_{(i)}}} [s(x^*)]. \]

**Proof:** For \( i = 1, \ldots, n \),
\[ E_{f_{\hat{\eta}_{(i)}}} [s(x^*)R_i(x^*)]\]
\[ = \int \cdots \int s(x_1^*, \ldots, x_n^*) \prod_{j=1}^{n} \frac{f_{\hat{\eta}_{(i)}}(x_j^*)}{f_\eta(x_j^*)} \times \prod_{j=1}^{n} f_\eta(x_j^*) \, dx_1^* \cdots dx_n^* \]
\[ = \int \cdots \int s(x_1^*, \ldots, x_n^*) \prod_{j=1}^{n} f_{\hat{\eta}_{(i)}}(x_j^*) \, dx_1^* \cdots dx_n^* \]
\[ = E_{f_{\hat{\eta}_{(i)}}} [s(x^*)]. \]

\( \square \)

Based on the suggestion of Theorem 3.1, we reuse the original \( B \) bootstrap samples without further resampling from \( f_{\hat{\eta}_{(i)}} \) \( i = 1, \ldots, n \). Define
\[ s_{(i)}^b = s(x^{*b})R_i(x^{*b}), \quad b = 1, \ldots, B, \quad i = 1, \ldots, n \]
and
\[ \hat{\text{se}}_{B(i)} = \left[ \frac{B}{B-1} \sum_{b=1}^{B} (s_{(i)}^b - s_{(i)}^*) \right]^{1/2}, \]
(6)
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where \( s^B_{(i)} = \sum_{b=1}^B s^b_{(i)} / B \). We use \( \hat{s}B_{(i)} \) to replace \( \hat{s}B_{(i)} \) in Equation 5. Then the parametric IAB is defined as

\[
\hat{s}_{\text{IAB}} (\hat{s}B) = \left[ \frac{n - 1}{n} \sum_{i=1}^n (\hat{s}B_{(i)} - \hat{s}B_{(i)})^2 \right]^{1/2} \tag{7}
\]

where \( \hat{s}B_{(i)} = \sum_{i=1}^n \hat{s}B_{(i)} / n \).

4 VARIANCE ANALYSIS

Importance sampling has long been recognized as a useful technique for increasing the efficiency of Monte Carlo simulation. Hammersley and Handscomb [1964], Sigmund [1976], Wilson [1984], Therneau, [1983], Hesterberg [1988], Johns [1988], Glynn and Iglehart [1989] discuss different applications of importance sampling. The usual situation where importance sampling may be helpful involves estimating the expected value of some random variable with known distribution, by simulation. The simulation size required for a given accuracy may be substantially reduced by sampling from a suitably chosen alternative distribution and correcting the estimate using the appropriate likelihood ratio. The object in importance sampling is to concentrate the distribution of the sample point in the parts of the interval that are of the most importance instead of spreading them out evenly. Good results in importance sampling require good sampling distributions. A bad sampling distribution can result in variance increase.

For the parametric IAB, importance sampling is used not as a classical variance reduction technique. Instead, it is used to construct jackknife estimates of the second level accuracy of variation. Therefore, variance reductions in importance sampling are not guaranteed even though the parametric IAB is an efficient simulation method. Variance may decrease or increase. It depends on the given parametric family of density functions \( \mathcal{F} = \{ f_\eta (x), \eta \in N \} \), the observed data \( x = (x_1, \ldots, x_n) \) which is an i.i.d. sample from some member of \( \mathcal{F} \), and the rule for estimating \( \eta \).

The following lemma is very useful for variance analysis of the parametric IAB.

**Lemma 4.1** For \( i = 1, \ldots, n \), if

\[
\lim_{n \to \infty} \hat{\eta} = \eta \quad \text{a.s.}
\]

and \( f_\eta (x) \) is continuous in \( \eta \), then

\[
\lim_{n \to \infty} \hat{\eta}_{(i)} = \eta \quad \text{a.s.}
\]

and

\[
\lim_{n \to \infty} R_i (x) = 1 \quad \text{a.s.}.
\]

**Proof:** For \( i = 1, \ldots, n \), if

\[
\lim_{n \to \infty} \hat{\eta} = \eta \quad \text{a.s.}
\]

then

\[
\lim_{n \to \infty} \hat{\eta}_{(i)} = \eta \quad \text{a.s.}
\]

Since \( f_\eta (x) \) is continuous in \( \eta \), by the Corollary 2 [Chow and Teicher [1978], page 67], we have

\[
\lim_{n \to \infty} f_{\hat{\eta}_{(i)}} = f_\eta (x) \quad \text{a.s.}
\]

and

\[
\lim_{n \to \infty} f_{\hat{\eta}_{(i)}} = f_\eta (x) \quad \text{a.s.}
\]

Therefore

\[
\lim_{n \to \infty} R_i (x) = \lim_{n \to \infty} \frac{f_{\hat{\eta}_{(i)}} (x)}{f_\eta (x)} = \frac{f_\eta (x)}{f_\eta (x)} = 1 \quad \text{a.s.}
\]

For \( i = 1, \ldots, n \), we define the difference between the two variances of \( s(x^*) R_i (x^*) \) and \( s(x^*) \) under two different probability measures, respectively,

\[
D_i = \text{Var}_{f_\eta} [s(x^*) R_i (x^*)] - \text{Var}_{f_{\hat{\eta}_{(i)}}} [s(x^*)].
\]

Based on the result of Theorem 3.1, we define

\[
\mu_i = E_{f_\eta} [s(x^*) R_i (x^*)] = E_{f_{\hat{\eta}_{(i)}}} [s(x^*)].
\]

We are now introducing the main results for variance analysis of the parametric IAB.

**Theorem 4.1** For \( i = 1, \ldots, n \),

\[
D_i = E_{f_\eta} [s^2(x^*) R_i (x^*) (R_i (x^*) - 1)].
\]

**Proof:** For \( i = 1, \ldots, n \),

\[
D_i = \text{Var}_{f_\eta} [s(x^*) R_i (x^*)] - \text{Var}_{f_{\hat{\eta}_{(i)}}} [s(x^*)]
\]

\[
= E_{f_\eta} [s^2(x^*) R_i^2 (x^*)] - \mu_i^2
\]

\[
- \left( E_{f_{\hat{\eta}_{(i)}}} [s^2(x^*)] - \mu_i^2 \right)
\]

\[
= E_{f_\eta} [s^2(x^*) R_i^2 (x^*)] - E_{f_{\hat{\eta}_{(i)}}} [s^2(x^*)]
\]

\[
= E_{f_\eta} [s^2(x^*) R_i^2 (x^*)] - E_{f_\eta} [s^2(x^*) R_i (x^*)]
\]

\[
= E_{f_\eta} [s^2(x^*) R_i (x^*) (R_i (x^*) - 1)]
\]

In Theorem 4.1, both \( s^2(x^*) \) and \( R_i (x^*) \) are nonnegative. We hope that \( D_i \) is as small as possible. Here \( D_i \) depends on the expectation and the variance of \( R_i (x^*) - 1 \).
Theorem 4.2 For \( i = 1, \ldots, n \),
\[
E_{f_q} \left[ R_i(x^*) - 1 \right] = 0.
\]

Proof: For \( i = 1, \ldots, n \),
\[
E_{f_q} \left[ R_i(x^*) - 1 \right] = E_{f_q} R_i(x^*).
\]
\[
= \int \cdots \int \prod_{j=1}^{n} \frac{f_{\hat{\eta}(x_j)}}{f_{\eta}(x_j)} \prod_{j=1}^{n} f_{\hat{\eta}}(x_j^*) \, dx_1^* \cdots dx_n^* - 1
\]
\[
= \int \cdots \int \prod_{j=1}^{n} f_{\hat{\eta}(x_j)} \, dx_1^* \cdots dx_n^* - 1 = 0.
\]

Theorem 4.1 indicates that the factor \( R_i(x^*) - 1 \), in the average sense, is zero. But we still don't know how good the \( D_i \) is and what the variance of \( R_i(x^*) - 1 \) is.

Theorem 4.3 For \( i = 1, \ldots, n \),
\[
\text{Var}_{f_q} \left[ R_i(x^*) - 1 \right] = E_{f_{\hat{\eta}(x)}} R_i(x^*) - 1.
\]

Proof: For \( i = 1, \ldots, n \),
\[
\text{Var}_{f_q} \left[ R_i(x^*) - 1 \right] = E_{f_q} \left[ R_i(x^*) - 1 \right]^2
\]
\[
= E_{f_q} R_i^2(x^*) - 1
\]
\[
= \int \cdots \int R_i^2(x^*) \prod_{j=1}^{n} f_{\hat{\eta}}(x_j^*) \, dx_1^* \cdots dx_n^* - 1
\]
\[
= \int \cdots \int R_i(x^*) \prod_{j=1}^{n} \frac{f_{\hat{\eta}}(x_j^*)}{f_{\eta}(x_j^*)} \prod_{j=1}^{n} f_{\hat{\eta}}(x_j^*) \, dx_1^* \cdots dx_n^* - 1
\]
\[
= \int \cdots \int R_i(x^*) \prod_{j=1}^{n} f_{\hat{\eta}(x_j^*)} \, dx_1^* \cdots dx_n^* - 1
\]
\[
= E_{f_{\hat{\eta}(x)}} R_i(x^*) - 1.
\]

If the sample size \( n \) of the observed data is large enough and \( \hat{\eta} \) is a consistent estimate of \( \eta \), from Lemma 4.1, \( \hat{f}_q \) is almost as the same as \( f_{\hat{\eta}(x)} \). In other words, the two densities are almost the same in the same density family if the density family is insensitive with respect to the parameter \( \eta \). From Theorem 4.3, \( E_{f_{\hat{\eta}(x)}} R_i(x^*) - 1 \) is almost zero. It indicates that the variance of \( R_i(x^*) - 1 \) is almost zero. From both Theorems 4.2 and 4.3, the expectation and variance of \( R_i(x^*) - 1 \) are almost zeros. Therefore, from Theorem 4.1, \( D_i \) is almost zero.

As another view of \( D_i \), we consider the ratio of the two variances of \( s(x^*) R_i(x^*) \) and \( s(x^*) \).

Theorem 4.4 For \( i = 1, \ldots, n \),
\[
\frac{\text{Var}_{f_q} \left[ s(x^*) R_i(x^*) \right]}{\text{Var}_{f_{\hat{\eta}(x)}} \left[ s(x^*) \right]} = \frac{E_{f_{\hat{\eta}(x)}} \left[ s^2(x^*) R_i(x^*) \right] - \mu_i}{E_{f_q} \left[ s^2(x^*) R_i(x^*) \right] - \mu_i}.
\]

Proof: For \( i = 1, \ldots, n \),
\[
\frac{\text{Var}_{f_q} \left[ s(x^*) R_i(x^*) \right]}{\text{Var}_{f_{\hat{\eta}(x)}} \left[ s(x^*) \right]} = \frac{E_{f_q} \left[ s^2(x^*) R_i(x^*) \right]}{E_{f_{\hat{\eta}(x)}} \left[ s^2(x^*) \right] - \mu_i}
\]
\[
= \frac{\int \cdots \int s^2(x^*) \prod_{j=1}^{n} f_{\hat{\eta}(x_j)}(x_j^*) \prod_{j=1}^{n} f_{\hat{\eta}}(x_j^*) \, dx_1^* \cdots dx_n^* - \mu_i}{\int \cdots \int s^2(x^*) \prod_{j=1}^{n} f_{\hat{\eta}(x_j)}(x_j^*) \prod_{j=1}^{n} f_{\hat{\eta}}(x_j^*) \, dx_1^* \cdots dx_n^* - \mu_i}
\]
\[
= \frac{\int \cdots \int R_i(x^*) \prod_{j=1}^{n} \frac{f_{\hat{\eta}(x_j)}(x_j^*)}{f_{\eta}(x_j)} \prod_{j=1}^{n} f_{\hat{\eta}}(x_j^*) \, dx_1^* \cdots dx_n^* - \mu_i}{\int \cdots \int R_i(x^*) \prod_{j=1}^{n} \frac{f_{\hat{\eta}(x_j)}(x_j^*)}{f_{\eta}(x_j)} \prod_{j=1}^{n} f_{\hat{\eta}}(x_j^*) \, dx_1^* \cdots dx_n^* - \mu_i}
\]
\[
= \frac{E_{f_{\hat{\eta}(x)}} \left[ s^2(x^*) R_i(x^*) \right] - \mu_i}{E_{f_q} \left[ s^2(x^*) R_i(x^*) \right] - \mu_i}.
\]

Similar to the discussion of Theorem 4.3, we assume that the sample size \( n \) of the observed data is large enough and \( \hat{\eta} \) is a consistent estimate of \( \eta \). From Theorem 4.4, the ratio of the two variances of \( s(x^*) R_i(x^*) \) and \( s(x^*) \) is almost 1. In other words, The variance of \( s(x^*) R_i(x^*) \) and the variance of \( s(x^*) \) are nearly identical.

Theoretically speaking, the parametric JAB should be as good as the true jackknife method under the two basic conditions, which are not difficult to meet in general. In practice, the sample size \( n \) of the observed data is large enough when \( n \geq 30 \). To find a consistent estimate \( \hat{\eta} \) of \( \eta \) is not difficult either. In many cases, for example, the maximum likelihood estimator method will solve this problem.

5 GENERALIZATION

In this section, we introduce a generalized version of the parametric JAB, which is more applicable to the parametric input modeling problems. In both formulas 1 and 4 of the parametric JAB, the number \( n \) is required to be as the same as the size of the observed data. A generalized parametric JAB is to relax this condition. We allow \( n \) to be any number \( m \), which may not be the same number as \( n \). Both formulas 1 and 4 become
\[
f_{\hat{i}, \text{i.d.}}(x_1^*, \ldots, x_m^*) = x^*
\]
and
\[ f_{\theta_i} \overset{\text{i.i.d.}}{\longrightarrow} (x_1, \ldots, x_m) = x^* . \]

For the generalized parametric JAB, all discussions and results of previous sections stay the same.

6 CONCLUSIONS

The parametric JAB method, a clever idea, introduces a simple way of estimating the standard error of the bootstrap estimates within parametric families, without the need to do a second level of bootstrap replication. It is an efficient method. Under some reasonable conditions, the quality of the parametric JAB is almost as good as the true jackknife method. The bootstrap-after-bootstrap and true jackknife methods are too computationally intensive for routine use.

As pointed out by Cheng [1995], it should be realized that bootstrapping methods are an alternative to, rather than a replacement for, more standard statistical procedures. The parametric JAB method can be applied to many Monte Carlo experiments, especially, to the parametric input modeling problems.

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