Hyperparameter Selection for Subsampling Bootstraps

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Abstract

Massive data analysis becomes increasingly prevalent, subsampling methods like BLB (Bag of Little Bootstraps) serves as powerful tools for assessing the quality of estimators for massive data. However, the performance of the subsampling methods are highly influenced by the selection of tuning parameters (e.g., the subset size, number of resamples per subset). In this article we develop a hyperparameter selection methodology, which can be used to select tuning parameters for subsampling methods. Specifically, by a careful theoretical analysis, we find an analytically simple and elegant relationship between the asymptotic efficiency of various subsampling estimators and their hyperparameters. This leads to an optimal choice of the hyperparameters. More specifically, for an arbitrarily specified hyperparameter set, we can improve it to be a new set of hyperparameters with no extra CPU time cost but the resulting estimator’s statistical efficiency can be much improved. Both simulation studies and real data analysis demonstrate the superior advantage of our method.

KEY WORDS: Bag of Little Bootstraps, Computational cost, Subsampling
1. INTRODUCTION

Real data analysis often runs into situations, where statistical inference is too complicated to be analytically attractable. This could happen if the target statistics is a complicated function of sample moments (e.g., sample correlation coefficient). In this case, various bootstrap methods (Efron, 1990; Efron and Tibshirani, 1994) become practically appealing for their outstanding ability in automatic inference. Automatic inference refers to the fact that important inference parameters (e.g., standard error) can be computed without knowing its analytical formula. The resulting estimators are generally consistent (Van Der Vaart and Wellner, 1996) and could be more accurate than those based upon asymptotic approximation (Hall, 1994).

Traditional bootstrap (TB) methods are typically applied to datasets of small sizes. In that case, computation is not an issue. This enables bootstrap methods to be used for automatic statistical inference. Unfortunately, such a standard paradigm becomes problematic if the datasets are of massive sizes. In this case, the computational cost is no longer negligible. Instead, it could be rather challenging even if one single point estimate needs to be computed based on the whole sample. Accordingly a straightforward implementation of the traditional bootstrap methods becomes practically infeasible. To mitigate this problem, one possible solution is to utilize the parallel and distributed computing system. However, this might lead to huge communication cost between different computer nodes (Kleiner et al., 2014). Therefore, how to conduct statistically valid and computationally efficient bootstrap inference for massive datasets becomes a problem of great importance.

Motivated by the need for an automatic statistical inference with massive data, Kleiner et al. (2014) introduced a new method called as Bag of Little Bootstraps (BLB). For each bootstrap iteration, a traditional bootstrap method should draw a sample
of the same size as the original data. In case of massive data, this leads to huge computational cost. BLB replaces this procedure by two novel steps. In the first step, BLB obtain a first bootstrap sample with size much smaller than that of the whole data. In the second step, BLB obtains a second bootstrap sample by simple random sampling with replacement from the first bootstrap sample. The size of the second bootstrap sample needs to be the same as that of the whole dataset.

At the first glance, it seems that the BLB method should lead to no less computational cost than the traditional bootstrap because the sample size involved in the second stage is as large as the whole dataset. However, the merit of BLB is that the second bootstrap sample is obtained from the first bootstrap sample. Since the first bootstrap sample size is much smaller than that of the whole dataset, the second bootstrap sample could be done by directly generating the frequency number for each data point in the first bootstrap sample. The frequency number here refers to the number of times for a data point in the first bootstrap sample to be selected by the second step bootstrap sample. Accordingly, the target parameter can be computed in a weighted manner. The computational cost of a BLB method becomes the same order as that of the first bootstrap sample, which is much smaller than that of the TB methods. On the other hand, in theory, the second bootstrap sample is of the same size as the whole data. Consequently, no analytical re-scaling is needed (Kleiner et al., 2014). That makes BLB a fully automatic method for statistical inference.

However, the outstanding performance of BLB relies on three important hyperparameters, which need to be selected. Specifically, the three hyperparameters are, respectively, (1) the size of the first stage bootstrap sample \( n \); (2) for a given first step bootstrap sample, the total number of bootstrap datasets \( B \) needs to be generated in the second step; (3) the total number of overall Monte Carlo iterations \( R \).
With unlimited computational resources, those hyperparameters should be as large as possible, because the larger they are, the more accurate the resulting statistical inference is. With limited computational budget, these three hyperparameters need to be carefully selected. Sengupta et al. (2016) have pointed out that under limited computational cost, it remains unclear how to choose the optimal hyperparameters in BLB that balances statistical accuracy and running time. In the meanwhile, understanding such kind of relationships are important as they can have an empirical guidance for hyperparameter selection.

In this work, we are seeking to find the optimal balance between the statistical efficiency and computational cost. To solve this problem, we start with the simplest statistic sample mean and its standard error (SE). We next move on to more sophisticated statistics. We start with sample mean mainly for its simplicity. It leads to fruitful and insightful theoretical findings. These findings can be easily extended to more sophisticated statistics without much difficulty. We study SE because it is an important parameter that needs to be estimated for many important statistical inference. These important statistical inferences include, but are not limited to confidence interval, hypotheses testing, and others. To estimate SE, one might rely on asymptotic approximation. This is typically done by sophisticated Taylor’s series approximation. Nevertheless, this method becomes challenging if the target statistic is too complicated to have an analytically tractable formula. In this case, automatic inference method (such as bootstrap) becomes practically appealing. This amounts to use a method like BLB to estimate the SE. The resulting estimation accuracy (about SE) should be closely related to various hyperparameters. Its relationship should be theoretically investigated. For theoretical completeness, we have studied the estimation accuracy of four popularly used bootstrap methods. They are, respectively, the traditional boot-
strap (TB, Efron, 1990), the bag of little bootstraps method (BLB, Kleiner et al., 2014), the $m$-out of-$n$ bootstrap (SB, Bickel et al., 1997), and the subsampled double bootstrap (SDB, Sengupta et al., 2016).

By a careful theoretical analysis, we find that the asymptotic efficiency of the subsampling estimate is closely related to its hyperparameters. The relationship is analytically simple and elegant. For illustration purpose, we consider the BLB method, as it involves a total of three hyperparameters (i.e., $n, R, B$). For a given computational platform, the time cost for BLB can be approximate by $\beta_1(nBR) + \beta_2(nR)$ for some positive coefficients $\beta_1$ and $\beta_2$. Both the coefficients are computational platform specific and can be consistently estimated. Our simulation experience suggests that this leads to fairly accurate approximation; see subsection 4.3 for the details. Moreover, the details of the hyperparameter selection approach are to be introduced in subsection 3.2. Once $\beta_1$ and $\beta_2$ are given, we then minimize $\text{MSE}(\hat{\text{SE}}_C^2)$ under the constraint $\beta_1 nBR + \beta_2 nR \leq C_{\text{max}}$, where $C_{\text{max}}$ is the maximum time cost we can bear. This leads to an optimal choice of the hyperparameters. More specifically for an arbitrarily specified hyperparameter set, we can improve it to be a new set of hyperparameters. The consequence is that no extra CPU time is needed but the resulting estimator’s statistical efficiency can be much improved. Extensive numerical studies are conducted to demonstrate its performance.

The rest of this article is organized as follows. We first introduce different bootstrap methods and then study their associated theoretical properties in subsection 3.1. The hyperparameter selection approach is presented in subsection 3.2. Next, more general parameters and statistics are to be introduced in subsection 3.3. Extensive numerical studies are conducted in Section 4. Lastly, the article is concluded with a short discussion in Section 5.
2. BOOTSTRAP METHODS

2.1. Traditional Bootstraps

We start with the traditional bootstrap (TB) method. Let \( X_1, X_2, \ldots, X_N \in \mathbb{R}^1 \) be independent and identically distributed random variables with mean \( \mu \) and variance \( \sigma^2 \). For simplicity purpose, we start with the simple parameter \( \mu \), which can be estimated by \( \bar{X} = N^{-1} \sum_{i=1}^{N} X_i \). More complicated parameters and statistics are to be studied subsequently. The estimation accuracy of \( \bar{X} \) can be reflected by its standard deviation, which is also referred to as a Standard Error (SE). Specifically, the SE of \( \bar{X} \) is \( \sigma/\sqrt{N} \) and it is analytically simple. Consequently, it can be estimated by \( \hat{SE}_\lambda = \hat{\sigma}/\sqrt{N} \), where \( \hat{\sigma}^2 = \sum_{i=1}^{N} (X_i - \bar{X})^2/N \). This is an estimator obtained by analytical formula. We thus refer to it as an AF estimator. In the meanwhile, it can be estimated by a standard bootstrap method as follows. For simplicity, we assume \( X_i \in \mathbb{R}^1 \) is a scalar. However, the theory to be presented hereafter can be readily applied to multivariate \( X_i \)s without any difficulty.

Let \( \mathcal{S} = \{X_1, \ldots, X_N\} \) be the whole sample dataset and \( B \) be the total number of bootstrap datasets. Then, for any \( b = 1, \ldots, B \), the \( b \)th bootstrap dataset is given by \( \mathcal{B}_B^{(b)} = \{X_{1,B}^{(b)}, X_{2,B}^{(b)}, \ldots, X_{N,B}^{(b)}\} \), where \( X_{i,B}^{(b)} \) (for each \( 1 \leq i \leq N \)) are independently generated by the method of simple random sampling with replacement from the whole sample dataset \( \mathcal{S} \). Based on \( \mathcal{B}_B^{(b)} \), the \( b \)th bootstrap sample mean can be calculated as \( \bar{X}_B^{(b)} = N^{-1} \sum_{i=1}^{N} X_{i,B}^{(b)} \). Then, an estimate for \( SE^2 \) is given by

\[
\hat{SE}_B^2 = B^{-1} \sum_{b=1}^{B} \left( \bar{X}_B^{(b)} - \bar{X} \right)^2.
\]

Conditional on the whole sample dataset \( \mathcal{S} \) and assume appropriate regularity conditions, it can be verified that \( \hat{SE}_B^2/\hat{SE}_\lambda^2 \to_p 1 \), as \( B \to \infty \); see Theorem 2 in Section 3.
for the details.

2.2. Bag of Little Bootstraps

We next provide a brief review about the Bag of Little Bootstraps (BLB), which is a novel method proposed by Kleiner et al. (2014). The BLB method should be carried out by a number of random replications. Here, we use $R$ to represent the total number of random replications. For each $1 \leq r \leq R$, we should obtain a little bootstrap sample, which is denoted as $B(r)_{C} = \{X_{1,C}^{(r)}, X_{2,C}^{(r)}, \ldots, X_{n,C}^{(r)}\}$, where $X_{i,C}^{(r)}$s are independently generated by the method of simple random sampling with replacement from the whole sample dataset $S$. It is remarkable that the size of $B(r)_{C}$ is $n$, which is much smaller than the whole dataset $N$.

In theory, we should do a second stage bootstrap sampling of size $N$ from each $B(r)_{C}$. This leads to another $B$ bootstrap samples given by $B(r,b)_{C} = \{X_{i,C}^{(r,b)}: 1 \leq i \leq N\}$, where $X_{i,C}^{(r,b)}$s are independently generated from $B(r)_{C}$ by simple random sampling with replacement. Based on $B(r,b)_{C}$, the target statistic $\overline{X}$ can be computed as

$$\overline{X}^{(r,b)}_{C} = N^{-1} \sum_{i=1}^{N} X_{i,C}^{(r,b)} = N^{-1} \sum_{i=1}^{n} X_{i,C}^{(r)} f^{(r,b)}_{i,C}.$$  \hspace{1cm} (2.1)

Here, $f^{(r,b)}_{i,C}$ is the sampling frequency of $X_{i,C}^{(r)} \in B(r)_{C}$. That is $f^{(r,b)}_{i,C} = \sum_{j=1}^{N} I(X_{j,C}^{(r)} = X_{i,C}^{(r)})$ and $I(\cdot)$ is an indicator function. Obviously, the random vector $f^{(r,b)}_{C} = (f^{(r,b)}_{1,C}, f^{(r,b)}_{2,C}, \ldots, f^{(r,b)}_{n,C})^{T} \in \mathbb{R}^{n}$ follows a multinomial distribution with parameter $N$ and $p$. Here, $p = (1/n, 1/n, \ldots, 1/n)^{T} \in \mathbb{R}^{n}$.

This leads to an interesting observation. In theory, a total of $N$ bootstrap samples in $B(r,b)_{C}$ needs to be generated. However, it is practically infeasible because $N$ is ultra large. In the meanwhile, by (2.1), we find that it is equivalent to generate the frequency vector $f^{(r,b)}_{C}$ directly. The dimension of $f^{(r,b)}_{C}$ is $n$, which is much smaller than $N$. That
makes the computational cost much cheaper. Then, with the help of $\bar{X}_C^{(r,b)}$, the target parameter $\text{SE}^2$ can be estimated by

$$\hat{\text{SE}}^2_C = \frac{1}{BR} \sum_{r=1}^{R} \sum_{b=1}^{B} \left( \bar{X}_C^{(r,b)} - \bar{X}_C^{(r)} \right)^2,$$

where $\bar{X}_C^{(r)} = n^{-1} \sum_{i=1}^{n} X_{i,C}^{(r)}$. Conditional on the whole sample dataset $S$ and assume appropriate regularity conditions, it can be verified that $\hat{\text{SE}}_C^2/\hat{\text{SE}}_A^2 \to_p 1$, as $\min\{B,R\} \to \infty$; see Theorem 3 in Section 3 for the details.

### 2.3. Subsampled Bootstrap

As one can see, the BLB method is closely related to another popularly used bootstrap method. That is so-called “m-out-of-N” bootstrap method (Bickel et al., 1997). For convenience, we refer to it as a method of subsampled bootstrap (SB).

Let $B$ be the total number of bootstrap samples. For any $1 \leq b \leq B$, we use $\mathcal{B}_D^{(b)} = \{X_{i,D}^{(b)} : 1 \leq i \leq n\}$ to denote the $b$th bootstrap sample with size $n$. Here, $X_{i,D}^{(b)}$s are generated independently by the simple random sampling with replacement from the whole sample dataset $S$. Based on $\mathcal{B}_D^{(b)}$, the target statistic $\bar{X}$ can be computed as $\bar{X}_D^{(b)} = n^{-1} \sum_{i=1}^{n} X_{i,D}^{(b)}$. Accordingly, the target inferential parameter $\text{SE}^2$ can be estimated by

$$\hat{\text{SE}}^2_D = \left( \frac{n}{N} \right) B^{-1} \sum_{b=1}^{B} \left( \bar{X}_D^{(b)} - \bar{X} \right)^2.$$

Conditional on the whole sample dataset $S$, one can verify that $\hat{\text{SE}}_D^2/\hat{\text{SE}}_A^2 \to_p 1$, as $B \to \infty$; see Theorem 4 in Section 3 for the details. Comparing the formula of $\hat{\text{SE}}_D^2$ with (for example) that of $\hat{\text{SE}}_B^2$, we can find that a re-scaling factor $(n/N)$ is needed for $\hat{\text{SE}}_D^2$. This re-scaling factor requires the knowledge of the convergence rate of the
target estimator. This makes the SDB method less automatic (Kleiner et al., 2014; Sengupta et al., 2016).

2.4. Subsampled Double Bootstrap

Note that the BLB method is also closely related to another interesting bootstrap method for massive data analysis. That is the subsampled double bootstrap (SDB, Sengupta et al., 2016). The implementation of the SDB method is similar to that of the BLB method.

In the first stage, SDB randomly draw $R$ small subsets of the data. For each $1 \leq r \leq R$, the associated little sample bootstrap subset is denoted as $B_E^{(r)} = \{X_{1,E}^{(r)}, X_{2,E}^{(r)}, \ldots, X_{n,E}^{(r)}\}$, where $X_{i,E}^{(r)}$s are independently generated by the method of simple random sampling with replacement from the whole sample dataset $S$. In the second stage, we only generate one bootstrap sample from each subset $B_E^{(r)}$, which is denoted as $B_E^{(r,1)} = \{X_{1,E}^{(r,1)}, X_{2,E}^{(r,1)}, \ldots, X_{n,E}^{(r,1)}\}$. Here, $X_{i,E}^{(r,1)}$s are independently generated from $B_E^{(r)}$ by simple random sampling with replacement. Based on $B_E^{(r,1)}$, the target statistic $\bar{X}$ can be computed as

$$\bar{X}_E^{(r,1)} = \frac{1}{N} \sum_{i=1}^{N} X_{i,E}^{(r,1)} = \frac{1}{N} \sum_{i=1}^{n} X_{i,E}^{(r)} f_{i,E}^{(r,1)}.$$ (2.2)

Here, $f_{i,E}^{(r,1)}$ is the frequency of $X_{i,E}^{(r)} \in B_E^{(r)}$. That is $f_{i,E}^{(r,1)} = \sum_{j=1}^{N} I(X_{i,E}^{(r,1)} = X_{j,E}^{(r)})$. The random vector $f_E^{(r,1)} = (f_{1,E}^{(r,1)}, f_{2,E}^{(r,1)}, \ldots, f_{n,E}^{(r,1)})^\top \in \mathbb{R}^n$ follows the multinomial distribution with parameter $N$ and $p$, where $p = (1/n, 1/n, \ldots, 1/n)^\top \in \mathbb{R}^n$. Then, with the help of $\bar{X}_E^{(r,1)}$, the target parameter $\text{SE}_E^{2}$ can be estimated by

$$\hat{\text{SE}}_E^{2} = R^{-1} \sum_{r=1}^{R} \left( \bar{X}_E^{(r,1)} - \bar{X}_E^{(r)} \right)^2,$$
where $\overline{X}_E^{(r)} = n^{-1} \sum_{i=1}^{n} X_{i,E}^{(r)}$. Conditional on the whole sample dataset $\mathcal{S}$ and assume appropriate regularity conditions, it can be verified that $\overline{SE}_E^2/\overline{SE}_A^2 \to_p 1$, as $R \to \infty$; see Theorem 5 in Section 3 for the details.

3. THEORETICAL PROPERTIES

3.1. Theoretical Properties

We next study the theoretical properties for $\overline{SE}_A^2$ to $\overline{SE}_E^2$. Recall that $\overline{SE}_A = \hat{\sigma}/\sqrt{N}$, where $\hat{\sigma}^2 = \sum_{i=1}^{N} (X_i - \overline{X})^2/N$. Define $E(X_i - \mu)^4 = \sigma_4$. We then have the following theorem.

Theorem 1. For the AF estimator, we have

$$E(\overline{SE}_A^2) = \frac{\sigma^2}{N} \left(1 - \frac{1}{N}\right) \text{ and } \text{var}(\overline{SE}_A^2) = \frac{\sigma_4 - \sigma^4}{N^3} \left\{1 + o(1)\right\}.$$  

By the above theorem result, we can immediately obtain the MSE for $\overline{SE}_A^2$, which can be expressed as

$$\text{MSE}(\overline{SE}_A^2) = \frac{\sigma_4 - \sigma^4}{N^3} \left\{1 + o(1)\right\}. \quad (3.1)$$

We next consider the theoretical properties for $\overline{SE}_B^2$. It is remarkable that conditional on $\mathcal{S}$, $X_{i,B}^{(b)}$s are independent and identically distributed. Specifically, we should have $P(X_{i,B}^{(b)} = X_j) = 1/N$ for any $1 \leq j \leq N$. Accordingly, we have $E(X_{i,B}^{(b)}|\mathcal{S}) = E(X_{i,B}^{(b)}|\mathcal{S}) = \overline{X}$ and $\text{var}(X_{i,B}^{(b)}|\mathcal{S}) = N^{-1}\text{var}(X_{i,B}^{(b)}|\mathcal{S}) = N^{-1}\hat{\sigma}_B^2$. Recall that $\overline{SE}_B^2 = B^{-1} \sum_{b=1}^{B} (\overline{X}_B^{(b)} - \overline{X})^2$. To study the theoretical properties of $\overline{SE}_B^2$, for each $b = 1 \cdots B$, we define $Y_B^{(b)} = (\overline{X}_B^{(b)} - \overline{X})^2$ for convenience. Conditional on $\mathcal{S}$, $Y_B^{(b)}$s are independent and identically distributed with $E(Y_B^{(b)}|\mathcal{S}) = \text{var}(\overline{X}_B^{(b)}|\mathcal{S}) = \hat{\sigma}_B^2/N$. We then obtain the following theorem.
Theorem 2. For the TB estimator, we have

\[
E(\hat{SE}_B^2) = \frac{\sigma^2}{N} \left(1 - \frac{1}{N}\right) \quad \text{and} \quad \text{var}(\hat{SE}_B^2) = \text{var}(\hat{SE}_A^2) \left(\frac{2\sigma^4}{\sigma_4 - \sigma^4} \cdot \frac{N}{B} + 1\right) \left\{1 + o(1)\right\}.
\]

From the above theorem, we can immediately obtain the MSE for \(\hat{SE}_B^2\), which can be expressed as

\[
\text{MSE}(\hat{SE}_B^2) = \text{var}(\hat{SE}_A^2) \left(\frac{2\sigma^4}{\sigma_4 - \sigma^4} \cdot \frac{1}{N^2 B} + \frac{1}{N^3}\right) \left\{1 + o(1)\right\} + \sigma^4 N 4 = \left(\sigma - \sigma^4\right) \left(\frac{2\sigma^4}{\sigma_4 - \sigma^4} \cdot \frac{1}{N^2 B} + \frac{1}{N^3}\right) \left\{1 + o(1)\right\}.
\]

This suggests that the bootstrap sampling size \(B\) needs to be the same/larger order of \(N\), if \(\text{MSE}(\hat{SE}_B^2)\) wants to achieve the same convergence rate with \(\text{MSE}(\hat{SE}_A^2)\).

Recall that \(X_{(r,b)} = N^{-1} \sum_{i=1}^{N} X_{i,C}^{(r,b)}\), \(X_C^{(r)} = n^{-1} \sum_{i=1}^{n} X_{i,C}^{(r)}\), and \(B_C^{(r)} = \{X_{i,C}^{(r)} : 1 \leq i \leq n\}\). Here, \(B_C^{(r)}\) represent the sampling set in the \(r\)th replication. It is remarkable that conditional on \(S\) and \(B_C^{(r)}\), \(X_{(r,b)}\) are independent and identically distributed for \(1 \leq b \leq B\). Accordingly, we have \(E(X_C^{(r,b)}|S, B_C^{(r)}) = X_C^{(r)}\) and \(\text{var}(X_C^{(r,b)}|S, B_C^{(r)}) = N^{-1} \sigma_C^{2}\), where \(\sigma_C^{2} = n^{-1} \sum_{i=1}^{n} (X_{i,C}^{(r)} - X_C^{(r)})^2\). Since \(\hat{SE}_C^2 = (BR)^{-1} \sum_{r=1}^{R} \sum_{b=1}^{B} (X_C^{(r,b)} - \overline{X}_C^{(r)})^2\), we next define \(Y_C^{(r,b)} = (X_C^{(r,b)} - \overline{X}_C^{(r)})^2\) for \(b = 1 \cdots B\). Then, conditional on \(S\) and \(B_C^{(r)}\), \(Y_C^{(r,b)}\) are independent and identically distributed with

\[
E \left(Y_C^{(r,b)}|S, B_C^{(r)}\right) = \text{var}(\overline{X}_C^{(r,b)}|B_C^{(r)}) = N^{-1} \sigma_C^{2}.
\]

Consequently, we have the following theorem.
Theorem 3. For the BLB estimator, we have

\[
E(\widehat{SE}_C^2) = \frac{\sigma^2}{N}(1 - \frac{1}{n})\left\{1 + o(1)\right\},
\]

\[
\text{var}(\widehat{SE}_C^2) = \text{var}(\widehat{SE}_A^2)\left(\frac{2\sigma^4}{\sigma_4^2 - \sigma^4} \cdot \frac{N}{RB} + \frac{N}{nR} + 1\right)\left\{1 + o(1)\right\}.
\]

From the above theorem, we can immediately obtain the MSE for \(\widehat{SE}_C^2\), which can be expressed as

\[
\text{MSE}(\widehat{SE}_C^2) = \text{var}(\widehat{SE}_A^2)\left(\frac{2\sigma^4}{\sigma_4^2 - \sigma^4} \cdot \frac{N}{RB} + \frac{N}{nR} + 1\right)\left\{1 + o(1)\right\} + \frac{\sigma^4}{N^2n^2}
\]

\[
= \frac{\sigma_4 - \sigma^4}{N^2} \left(\frac{2\sigma^4}{\sigma_4^2 - \sigma^4} \cdot \frac{1}{RB} + \frac{1}{nR} + \frac{\sigma^4}{\sigma_4 - \sigma^4} \cdot \frac{1}{n^2}\right)\left\{1 + o(1)\right\} + \frac{\sigma_4 - \sigma^4}{N^3}\left\{1 + o(1)\right\}.
\]

We further study the theoretical properties for \(\widehat{SE}_D^2\). Recall that conditional on \(S\), \(X_{i,D}^{(b)}\)'s are independent and identically distributed with \(P(X_{i,D}^{(b)} = X_j) = 1/N\) for any \(1 \leq j \leq N\). Accordingly, we have \(E(\overline{X}_{i,D}^{(b)}|S) = E(X_{i,D}^{(b)}|S) = \overline{X}\) and \(\text{var}(\overline{X}_{i,D}^{(b)}|S) = n^{-1}\text{var}(X_{i,D}^{(b)}|S) = n^{-1}\hat{\sigma}^2\). Since \(\widehat{SE}_D^2 = n(NB)^{-1}\sum_{b=1}^{B}(\overline{X}_{i,D}^{(b)} - \overline{X})^2\), we next define \(Y_{D}^{(b)} = (\overline{X}_{D}^{(b)} - \overline{X})^2\) for \(b = 1 \cdots , B\). Conditional on \(S\), \(Y_{D}^{(b)}\)'s are independent and identically distributed with \(E(Y_{D}^{(b)}|S) = \text{var}(\overline{X}_{D}^{(b)}|S) = \hat{\sigma}^2/n\). We further have the following theorem.

Theorem 4. For the SB estimator, We have \(E(\widehat{SE}_D^2) = N^{-1}(1 - n^{-1})\sigma^2\) and

\[
\text{var}(\widehat{SE}_D^2) = \text{var}(\widehat{SE}_A^2)\left(\frac{2\sigma^4}{\sigma_4^2 - \sigma^4} \cdot \frac{N}{B} + 1\right)\left\{1 + o(1)\right\}.
\]
Similarly, we can obtain the MSE for \( \widetilde{SE}_D^2 \), which can be expressed as

\[
\text{MSE}(\widetilde{SE}_D^2) = \text{var}(\widetilde{SE}_A^2) \left( \frac{2\sigma^4}{\sigma_4 - \sigma^4} \cdot \frac{N}{B} + 1 \right) \left\{ 1 + o(1) \right\} + \frac{\sigma^4}{N^2n^2}
\]

\[
= \frac{\sigma^4}{N^2} \left( \frac{2}{B} + \frac{1}{n^2} + \frac{\sigma_4 - \sigma^4}{\sigma^4} \cdot \frac{1}{N} \right) \left\{ 1 + o(1) \right\}. \tag{3.4}
\]

Recall that \( \overline{X}_E^{(r,1)} = N^{-1} \sum_{i=1}^{N} X_{i,E}^{(r,1)} \). It is remarkable that conditional on \( S \), \( \overline{X}_E^{(r,1)} \)'s are independent and identically distributed for \( 1 \leq r \leq R \). Accordingly, we have \( E(\overline{X}_E^{(r,1)} | S, \mathcal{B}_E^{(r)}) = \overline{X}_E^{(r)} \) and \( \text{var}(\overline{X}_E^{(r,1)} | S, \mathcal{B}_E^{(r)}) = N^{-1} \sigma_{r,E}^2 \). Since \( \widetilde{SE}_E^2 = R^{-1} \sum_{r=1}^{R} \left( \overline{X}_E^{(r,1)} - \overline{X}_E^{(r)} \right)^2 \), we next define \( Y_E^{(r,1)} = (\overline{X}_E^{(r,1)} - \overline{X}_E^{(r)})^2 \) for \( r = 1 \cdots R \). Conditional on \( S \) and \( \mathcal{B}_E^{(r)} \), \( Y_E^{(r,1)} \)'s are independent and identically distributed with

\[
E \left( Y_E^{(r,1)} | S, \mathcal{B}_E^{(r)} \right) = \text{var}(\overline{X}_E^{(r,1)} | S, \mathcal{B}_E^{(r)}) = \sigma_{r,E}^2 / N. \tag{3.5}
\]

Consequently, we have the following theorem.

**Theorem 5.** For the SDB estimator, we have

\[
E(\widetilde{SE}_E^2) = \left( \frac{\sigma^2}{N} - \frac{\sigma^2}{Nn} \right) \left\{ 1 + o(1) \right\},
\]

\[
\text{var}(\widetilde{SE}_E^2) = \text{var}(\widetilde{SE}_A^2) \left( \frac{2\sigma^4}{\sigma_4 - \sigma^4} \cdot \frac{N}{R} + 1 \right) \left\{ 1 + o(1) \right\}. \tag{3.5}
\]

From the above theorem, we can immediately obtain the MSE for \( \widetilde{SE}_E^2 \), which can be expressed as

\[
\text{MSE}(\widetilde{SE}_E^2) = \text{var}(\widetilde{SE}_A^2) \left( \frac{2\sigma^4}{\sigma_4 - \sigma^4} \cdot \frac{N}{R} + 1 \right) \left\{ 1 + o(1) \right\} + \frac{\sigma^4}{N^2n^2} \left\{ 1 + o(1) \right\}
\]

\[
= N^{-2}\sigma^4 \left( \frac{2}{\sigma_4 - \sigma^4} \cdot \frac{1}{R} + \frac{1}{n^2} \right) \left\{ 1 + o(1) \right\} + \frac{\sigma_4 - \sigma^4}{N^3} \left\{ 1 + o(1) \right\}. \tag{3.6}
\]
3.2. Hyperparameter Selection for the BLB Method

The fruitful theoretical results obtained in the previous subsections can be used to guide us to search for the optimal hyperparameter specification. The objective here is to find the optimal hyperparameter specification so that the resulting statistical efficiency (in terms of MSE) is minimal. For illustration purpose, we consider the BLB method only, because it represents the most complicated case here, as it involves a total of three hyperparameters (i.e., $n$, $R$, $B$).

The BLB method is mostly useful if the whole dataset is too large to be read into a computer memory as a whole. In that case, the whole dataset has to be placed on a hard drive, but the computation can only happen in the memory. Accordingly, BLB needs to repeatedly sample $n$ data points from the disk to the memory. Consequently, the time cost for BLB mainly involves two parts. The first part is the sampling cost, which occurs while sample data from the disk to the memory. There are a total of $R$ iterations and for each iteration there are $n$ data points need to be sampled. Thus, the associated time cost should be the order of $O(nR)$. This part is referred to as the sampling cost. For a given sampling iteration, once the $n$ data points have been read into the memory, one need to compute $\mathbf{x}^{(r,b)}_C$ and $\mathbf{x}^{(r)}_C$ first, which need $O(n)$ flopping operations. Furthermore, one needs to compute $\mathbf{x}^{(r,b)}_C$ for a total of $BR$ times. This leads to $O(nBR)$ flopping operations. Moreover, one needs to compute $(\mathbf{x}^{(r,b)}_C - \mathbf{x}^{(r)}_C)^2$ for $BR$ times. This cost amounts to $O(BR)$ flopping operations. The total computational cost is given by $O(nBR)$ flopping operations. This leads to the second part time cost, which is referred to as the computational cost. Combing the sampling and computational cost together, this leads to the total time cost as $O(nBR) + O(nR)$. For a given computational platform (e.g., a work station), we use the CPU time as a measure for the time cost. It can be approximate by $\beta_1(nBR) + \beta_2(nR)$ for some positive
coefficients $\beta_1$ and $\beta_2$. Both the coefficients are computational platform specific. Our simulation experience suggests that this leads to fairly accurate approximation. The simulation details are to be given in subsection 4.3.

Once $\beta_1$ and $\beta_2$ are given, we then minimize $\text{MSE}(\widehat{SE}_C^2)$ under the constraint $\beta_1 nBR + \beta_2 nR \leq C_{\text{max}}$, where $C_{\text{max}}$ is the maximum time cost we can bear. Write $c = \sigma^4(\sigma_4 - \sigma^4)^{-1}$. This amounts to find the minimum value of $2c(RB)^{-1} + (nR)^{-1} + c(n)^{-2}$ under the constraint $\beta_1 nBR + \beta_2 nR = C_{\text{max}}$. To this end, let $(n, B, R)$ be an arbitrary specification such that $\beta_1 nBR + \beta_2 nR = C_{\text{max}}$. Then, due to Cauchy's inequality,

$$
\left(\frac{2c}{RB} + \frac{1}{nR}\right)\left(\beta_1 nBR + \beta_2 nR\right) = \left(\frac{2c}{RB} + \frac{1}{nR}\right)\left(\beta_1 nBR + \beta_2 nR\right) + \frac{c}{n^2}\left(\beta_1 nBR + \beta_2 nR\right) \geq \left(\sqrt{2c\beta_1 \sqrt{n} + \sqrt{\beta_2}}\right)^2 + C_{\text{max}}\frac{c}{n^2} = f(n),
$$

(3.7)

where the function $f(n)$ is defined by the last equation in (3.7). The first inequality in (3.7) becomes equality if $2c/(\beta_1 n R^2 B^2) = 1/(\beta_2 n^2 R^2)$. When $n$ is fixed, this leads to $B^* = \lfloor(2c\beta_2/\beta_1)n^{1/2}\rfloor$, $R^* = \lfloor C_{\text{max}}/(\beta_1 n B^* + \beta_2 n)\rfloor$, where $\lfloor s \rfloor$ stands for the largest integer that no larger than $s$. This suggests that the CPU time needed by $(n, B^*, R^*)$ is no more than that of the $(n, B, R)$. However, the statistical efficiency (in terms of MSE) is likely to be better. Thus, $(B^*, R^*)$ can be viewed as the optimal specification when $n$ is fixed.

### 3.3. General Parameters and Statistics

In this subsection, we study parameters (statistics) more general than mean (sample mean). Without loss of generality, we still assume $X_i \in \mathbb{R}^1$ is a scalar with mean $E(X_i) = \mu \in \mathbb{R}^1$. Next, we consider a more general parameter $\theta = g(\mu)$, where $g(\cdot)$ is a known, possibly complicated, but sufficiently smooth function. We can then estimate
\( \theta \) by \( \hat{\theta} = g(\bar{X}) \). Asymptotically, we have \( \hat{\theta} - \theta = \hat{g}(\mu)(\bar{X} - \mu)\{1 + o_p(1)\} \), where \( \hat{g}(\cdot) \) stands for the first order derivative of \( g(\cdot) \). We then have \( \sqrt{N}(\hat{\theta} - \theta) \rightarrow_d N(0, \hat{g}^2(\mu)\sigma^2) \).

This means that the asymptotic \( SE^2 \) of \( \hat{\theta} \) is given by \( SE^* = \hat{g}^2(\mu)\sigma^2 / N \). Accordingly, a natural estimator for \( SE^* \) is given by \( \hat{SE}_A^* = \hat{g}^2(\bar{X})\hat{\sigma}^2 / N \), which can be easily compute if \( \hat{g}^2(\mu) \) is analytically simple. The computational cost needed is about \( O(N) \). However, in many cases, \( \hat{g}(\mu) \) could be rather complicated. In this case, various automatic inference methods could be practically appealing. To this end, we next extend various resampling methods (as defined in Sections 2 and 3) to this case.

We start with the TB method. Accordingly, a natural estimator for \( SE^* \) by TB method is given by

\[
\hat{SE}_B^* = B^{-1} \sum_{b=1}^{B} \left\{ g(\bar{X}_B^{(b)}) - g(\bar{X}) \right\}^2. \tag{3.8}
\]

It can be further expressed as

\[
= B^{-1} \sum_{b=1}^{B} \hat{g}^2(\bar{X})(\bar{X}_B^{(b)} - \bar{X})^2 + o_p(N^{-1}) \\
= \left\{ B^{-1} \sum_{b=1}^{B} \hat{g}^2(\mu)(\bar{X}_B^{(b)} - \bar{X})^2 \right\}\{1 + o_p(1)\} + o_p(N^{-1}) \\
= \hat{g}^2(\mu)\hat{SE}_B^* \{1 + o_p(1)\}.
\]

This suggests that the asymptotic behavior of \( \hat{SE}_B^* \) is largely determined by that of \( \hat{SE}_B^2 \). Under the same computational constraint \( C_{max}N \), the best convergence rate can be achieved by \( \hat{SE}_B^* \) should be the same as that of \( \hat{SE}_B^2 \).

Similar analysis can be conducted for BLB, SB and SDB methods. The associated
estimator for $SE^2$ are given by

$$
\hat{SE}^2_C = (BR)^{-1} \sum_{r=1}^{R} \sum_{b=1}^{B} \left\{ g(\overline{X}^{r,b}_C) - g(\overline{X}^{r}_C) \right\}^2 = \hat{g}^2(\mu)\hat{SE}^2_C \left\{ 1 + o_p(1) \right\}, \quad (3.9)
$$

$$
\hat{SE}^2_D = \left( \frac{n}{N} \right) B^{-1} \sum_{b=1}^{B} \left\{ g(\overline{X}^{(b)}_D) - g(\overline{X}) \right\}^2 = \hat{g}^2(\mu)\hat{SE}^2_D \left\{ 1 + o_p(1) \right\}, \quad (3.10)
$$

$$
\hat{SE}^2_E = R^{-1} \sum_{r=1}^{R} \left\{ g(\overline{X}^{(r,1)}_E) - g(\overline{X}^{(r)}_E) \right\}^2 = \hat{g}^2(\mu)\hat{SE}^2_E \left\{ 1 + o_p(1) \right\}, \quad (3.11)
$$

respectively. We find that the asymptotic behavior of $\hat{SE}^2_C$, $\hat{SE}^2_D$, and $\hat{SE}^2_E$ are largely determined by those of $\hat{SE}^2_C$, $\hat{SE}^2_D$, and $\hat{SE}^2_E$. Under the same computational constraint, the best convergence rate can be achieved by $\hat{SE}^2_C$, $\hat{SE}^2_D$ and $\hat{SE}^2_E$ should be the same as those of $\hat{SE}^2_C$, $\hat{SE}^2_D$ and $\hat{SE}^2_E$.

4. NUMERICAL STUDY

4.1. The consistency for $SE^2$

The objective of this subsection is to numerically confirm whether the various sub-sampling methods (e.g., BLB) studied in this work can indeed estimate the true $SE^2$ consistently. As we discussed before, even though our primary theory is developed for sample mean, it can be readily applied for more complicated statistics. For illustration purpose, we can consider here a slightly more complicated statistic, that is sample correlation coefficient (Ross, 2017). Specifically, we have observations $(X_i, Y_i)s$ identically and independently generated from a bivariate normal distribution with mean 0, covariance $(1, \rho; \rho, 1) \in \mathbb{R}^{2 \times 2}$ and $\rho = 0.5$, where $i = 1, \ldots, N$. Then, the sample correlation coefficient is given by

$$
\hat{\rho} = \frac{\sum_{i=1}^{N}(X_i - \overline{X})(Y_i - \overline{Y})}{\sqrt{\sum_{i=1}^{N}(X_i - \overline{X})^2} \sqrt{\sum_{i=1}^{N}(Y_i - \overline{Y})^2}}, \quad (4.1)
$$
where $X = N^{-1} \sum_{i=1}^{n} X_i$ and $Y = N^{-1} \sum_{i=1}^{N} Y_i$. Let $M$ be the total number of simulation replications. Write $\hat{\rho}^{(m)}$ be the estimator for $\rho$ obtained in the $m$th simulation replication for $1 \leq m \leq M$. Then, its true squared standard error ($SE^2$) can be consistently estimated by $SE^*2 = M^{-1} \sum_{m=1}^{M} (\hat{\rho}^{(m)} - \rho)^2$.

Let $\hat{SE}^{2(m)}$ be one particular $SE^2$ estimate obtained in the $m$th simulation replication. For example, it could be the TB estimator. Next, define $\gamma^{(m)} = \hat{SE}^{2(m)}/SE^*2$. If $\hat{SE}^{2(m)}$ is a consistent estimator for $SE^2 = \text{var}(\hat{\rho})$, we should expect $\gamma^{(m)}$ to be very close to 1. Accordingly, the sample mean (MEAN) and sample standard deviation (SD) are computed and reported in Table 1. Various parameter settings are considered. Specifically, we fix $N = 10^5$, $n \in \{\lfloor N^{0.5} \rfloor, \lfloor N^{0.6} \rfloor, \lfloor N^{0.7} \rfloor\}$. Set $B \times R \in \delta$, where $\delta = \{25, 50, 75, 100, 125, 150, 175, 200, 225, 250, 275, 300\}$. Since for TB and SB methods, they do not involve the hyperparameter $R$, we then set $B \in \delta$ for these two methods. Similarly, for SDR method, we set $R \in \delta$. For each fixed parameter setup, a total of $M = 1,000$ random replications have been conducted. The detailed simulation results are summarized in Table 1.

As we can see from this table, the sample mean of $\gamma^{(m)}$ for $1 \leq m \leq M$ is generally all across to 1 for different bootstrap methods, which suggests the correctness of the $SE^*2$ estimators defined in (3.8) to (3.11). Moreover, when $n$ and $\delta$ are fixed, the associated SD values are more or less the same for different methods. Besides, the SD values are consistently decreasing as either $\delta$ or $n$ increases. Take TB estimator for illustration purpose, the associated SD values for $\gamma$ decrease from 0.291 to 0.085, when $(\delta, n)$ increases from $(25, \lfloor N^{0.5} \rfloor)$ to $(300, \lfloor N^{0.7} \rfloor)$.

### 4.2. The Mean Squared Error

The objective of this subsection is to numerically confirm whether the analytical formula for $\text{MSE}(\hat{SE}^2)$ defined in subsection 3.1 are indeed correct. Here, $\hat{SE}^2$ stands
for one particular estimator for SE\(^2\). For example, it could be the SB or SDB estimator. Accordingly, the analytical formula to be evaluated is given by (3.4) and (3.6). Since the analytical formula are available only for sample mean. Thus, the statistic studied in this subsection is sample mean. Here, two different distributions are considered for \(X_i\)s \((1 \leq i \leq N)\). They are, respectively, standard normal distribution (Normal) or centralized standard exponential distribution (Exp). Let \(\widehat{SE}^{2(m)}\) be one particular SE\(^2\) estimate (e.g., the BLB estimator) obtained in the \(m\) th \((1 \leq m \leq M)\) simulation replication. Its true mean squared error (MSE) can then be estimated as

\[
\widehat{MSE} = M^{-1} \sum_{m=1}^{M} \left( \widehat{SE}^{2(m)} - \text{SE}^{*2} \right)^2
\]

(4.2)

where \(\text{SE}^{*2} = M^{-1} \sum_{m=1}^{M} (\overline{X}^{(m)} - \overline{X})^2\) and \(\overline{X}^{(m)}\) is the \(\overline{X}\) estimator obtained in the \(m\) th \((1 \leq m \leq M)\) simulation replication.

Let MSE\(^*\) be the oriented MSE value computed according to our theory. For example, by (3.1) we should be able to compute the theoretical MSE for \(\widehat{SE}^{2}_{A}\). We then evaluate the difference between \(\widehat{MSE}\) and MSE\(^*\) by a ratio \(\kappa = \text{MSE}^{*}/\widehat{MSE}\). It should be close to 1 if our theory is correct. The detailed simulation results are reported in Table 2. In this table, we fix \(N = 10^5\) and various parameter settings are considered. Specifically, we consider \(n \in \{\lfloor N^{0.4} \rfloor, \lfloor N^{0.5} \rfloor, \lfloor N^{0.6} \rfloor\}, B \in \{25, 50\}, \text{ and } R \in \{25, 50\}\). For each fixed parameter setup, a total of \(M = 1,000\) random replications have been conducted. The detailed simulation results are summarized in Table 2. Note that, the ratio \(\kappa\) for AF estimator does not contain any hyperparameter, thus the value for it would not change. Similarly, the TB estimator only involves the hyperparameter \(B\), thus the values of \(\kappa\) for TB method would not change with \(R\) and \(n\). Overall, we find that the values of \(\kappa\) are very close to one across different simulation scenarios. This result suggests that correctness of the theoretical formula for \(\text{MSE}(\widehat{SE}^{2}_A)\) to \(\text{MSE}(\widehat{SE}^{2}_E)\).
which have been given in subsection 3.1.

4.3. Hyperparameter Selection

The objective of this subsection is to evaluate how the selection of the hyperparameters (e.g., $B, R$) would affect the performance of BLB. The performance of other subsampling methods are similar and less complicated. We then omitted for short. In that subsection, the BLB method is implemented with repeatedly reading dataset from disk, instead of reading from memory. Specifically, consider the sample correlation coefficient defined in (4.1), where $(X_i, Y_i)$s are generated from a bivariate normal distribution with mean 0 and covariate $(1, 0.5; 0.5, 1)$. We fix $N = 5 \times 10^5$, $n = 5000$, and consider $B \times R = \delta \times 10^3$, where $\delta \in \{1, 2, 3, 4\}$. Based on the value of $\delta$, we generate 16 different $(B, R)$ combinations to verify the performance of our hyperparameter selection method while using BLB to estimate $\text{SE}^2$.

We first consider how to estimate the coefficient $\beta_0 = (\beta_1, \beta_2)$, which is used to approximate the actual CPU time and find the optimal specification of $(B^*, R^*)$. Here, the CPU time represents the time to conduct BLB with fixed $(B, R)$. The 16 current $(B, R)$ combinations are used to estimate $\beta_0$. To enlarge the variation of $B$ and $R$, we further generate another 10 combinations of $(B, R)$ from $[10 \times U(2, 100)]$ and $[10 \times U(1, 20)]$, respectively. For each $(B, R)$ combination, a total of 20 random replications have been conducted and we recorded the median CPU time. This leads to a total of 26 time records and they are treated as responses. We then use the corresponding $n \times B \times R$ and $n \times R$ as covariates, which are called as $nBR$ and $nR$ hereafter for short. This leads to the coefficient estimator as $\hat{\beta}_1 = 2.342 \times 10^{-7}$ and $\hat{\beta}_2 = 1.076 \times 10^{-4}$. The resulting R.Squared is as high as 98%, which suggests that the approximation is quite accurate. The demanded CPU time can then be estimated by $C_{\text{max}} = \hat{\beta}_1(nBR) + \hat{\beta}_2(nR)$. Based on $C_{\text{max}}$, we further obtain the optimal specification
as $B^* = [(2c\hat{\beta}_2/\hat{\beta}_1)n]^{1/2}$ and $R^* = [C_{max}/(\hat{\beta}_1 n B^* + \hat{\beta}_2 n)]$.

Next, both $(n, B, R)$ and $(n, B^*, R^*)$ specifications are used to estimate SE$^2$. For each fixed parameter setup, a total of $M = 200$ random replications have been conducted. The resulting estimators’ statistical efficiency are then evaluated in a similar manner as in Section 4.1. The resulting mean squared errors (reported by the median value) are denoted by MSE$_a$ and MSE$_b$, respectively. Their log-transformed form are denoted by log(MSE$_a$) and log(MSE$_b$) accordingly. The associated CPU times are denoted by Time$_a$ and Time$_b$, which are reported in seconds. For comparison purpose, two ratios MSE$_b$/MSE$_a$ and Time$_b$/Time$_a$ are also computed.

The detailed simulation results are summarized in Table 3. We find that the ratio Time$_b$/Time$_a$ are generally close or smaller than 1. This suggests that the CPU time consumed by $(n, B, R)$ and $(n, B^*, R^*)$ are comparable. On the other hand, we find that MSE$_b$/MSE$_a$ are all well below 100%. It could be as small as 10%, e.g., when $(B, R) = (10, 100)$, the associated MSE$_b$/MSE$_a = 9.7\%$. In most cases, it stays well below 80%. This implies that the estimators provided by $(n, B^*, R^*)$ are statistically more efficient that those provided by $(n, B, R)$. The averaged improving margin across all simulation cases is as large as 38.5%.

4.4. Real Data Analysis

In this subsection, we consider a U.S. Airline Dataset for illustration purpose. This is a dataset about detailed flight information. We take the data in the year of 2008 for illustration purpose, which contains $N = 1.01 \times 10^6$ records. It is publicly available at [http://stat-computing.org/dataexpo/2009](http://stat-computing.org/dataexpo/2009). The objective of the study is to evaluate how the selection of the hyperparameters (e.g., $B, R$) would affect the SE performance. Our focus is to estimate the SE$^2$ for sample correlation between distance and airline arrival time. Note that the original sample correlation between distance and airline
arrival time equals to 0.975. To enhance the variability between the two variables, we further add a standard error term $N(0, 1)$ to the airline arrival time, which leads to the sample correlation as 0.574. Because we have no knowledge of the true correlation $\rho$ between distance and airline arrival time. We then report the $\widehat{SE}^2$ instead of MSE for the sample correlation coefficient $\hat{\rho}$.

Since BLB is the most complicated subsampling method, in this subsection, we still use BLB for illustration purpose. Specifically, we generated 16 different $(B, R)$ combinations based on $B \times R = \delta \times 10^3$ with $\delta \in \{1, 2, 3, 4\}$. Using the same coefficient estimation method introduced in subsection 4.3. We further obtained the specified optimal $(B^*, R^*)$ accordingly. For each hyperparameter setup, the experiment is randomly replicated for $M = 200$ times. In each replication, the associated $\widehat{SE}^2$ for $\hat{\rho}$ can be calculated via BLB accordingly. Specifically, in the $m$th random replication, it is denoted as $\widehat{SE}^2_{C(m)}$ for each $1 \leq m \leq M$. The resulting median value of $\widehat{SE}^2$ for $(n, B, R)$ and $(n, B^*, R^*)$ are denoted by MedSE$_a$ and MedSE$_b$, respectively. To measure the stability of $\widehat{SE}^2$, we further calculate the standard deviation of it under the $M$ random replications. Let SD$_a$ and SD$_b$ be the standard deviation of $\widehat{SE}^2$ for $(n, B, R)$ and $(n, B^*, R^*)$, respectively. Similar with subsection 4.3, the CPU times are recorded to control the time cost budget. Specifically, let Time$_a$ and Time$_b$ be the associated CPU time for $(n, B, R)$ and $(n, B^*, R^*)$, respectively. For comparison purpose, we then report the ratios MedSE$_b$/MedSE$_a$, SD$_b$/SD$_a$, and Time$_b$/Time$_a$ in Table 4.

The detailed results are summarized in Table 4. First, we find that the ratio Time$_b$/Time$_a$ are generally close or smaller than 1. This suggests that the CPU time consumed by $(n, B, R)$ and $(n, B^*, R^*)$ are comparable. Second, we find that MedSE$_b$/MedSE$_a$ are all very close to 1 for all cases. This implies that both MedSE$_a$ and MedSE$_b$ are consistent with each other. On the other hand, we find that SD$_b$/SD$_a$
are all well below 100%. It could be as small as 20%, e.g., when \((B, R) = (10, 100)\), the associated \(SD_b/SD_a = 19.9\%\). In all cases, it stays well below 80%. This implies that the estimators provided by \((n, B^*, R^*)\) are more stable that those provided by \((n, B, R)\).

5. CONCLUDING REMARKS

In this article we propose a hyperparameter selection approach which can be applied for subsampling methods. These sampling methods are first applied to estimate the standard error (SE) for sample mean. We study SE because it is an important parameter that needs to be estimated for many important statistical inference. It then move on to more sophisticated statistics in subsection 3.3. For theoretical completeness, we have studied the associated theoretical properties of the SE estimators for AF, TB, BLB, SB, and SDB, respectively. Given these theoretical findings, we then proposed a methodology to do hyperparameter selection. Since BLB is the most complicated subsampling method, we have used it for illustration purpose. Similar approaches can be readily applied to other subsampling methods, e.g., SB and SDB.

6. Acknowledgments

Yingying Ma’s research is partially supported by National Natural Science Foundation of China (No.11801022). Hansheng Wang’s research is partially supported by National Natural Science Foundation of China (No.11831008, 11525101, 71532001). It is also supported in part by China’s National Key Research Special Program (No. 2016YFC0207704).
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Table 1: Detailed simulation results are reported for $\gamma$ in Section 4.1 with $N = 10^5$. The SD for $\gamma$ are also recorded in parentheses.

| Parameter | TB          | BLB          | SB          | SDB          |
|-----------|-------------|--------------|-------------|--------------|
|           | Parameter   | MEAN( SD)    | Parameter   | MEAN( SD)    | Parameter   | MEAN( SD)    | Parameter   | MEAN( SD)    |
| $n = \lceil N^{0.5} \rceil$ | B=25        | 1.038 (0.291)| B=5, R=5    | 1.005 (0.290)| B=25        | 1.042 (0.308)| R=25        | 1.013 (0.287)|
|           | B=50        | 1.023 (0.207)| B=5, R=10   | 1.026 (0.206)| B=50        | 1.048 (0.206)| R=50        | 1.023 (0.218)|
|           | B=75        | 1.029 (0.170)| B=15, R=5   | 1.016 (0.184)| B=75        | 1.035 (0.166)| R= 75       | 1.019 (0.167)|
|           | B=100       | 1.027 (0.140)| B=10, R=10  | 1.021 (0.155)| B=100       | 1.034 (0.146)| R=100       | 1.022 (0.147)|
|           | B=125       | 1.022 (0.134)| B=5, R=25   | 1.032 (0.130)| B=125       | 1.028 (0.134)| R=125       | 1.024 (0.131)|
|           | B=150       | 1.021 (0.118)| B=15, R=10  | 1.031 (0.128)| B=150       | 1.022 (0.112)| R=150       | 1.027 (0.115)|
|           | B=175       | 1.024 (0.111)| B=25, R=7   | 1.025 (0.118)| B=175       | 1.031 (0.111)| R=175       | 1.029 (0.105)|
|           | B=200       | 1.028 (0.105)| B=10, R=20  | 1.020 (0.102)| B=200       | 1.030 (0.107)| R=200       | 1.026 (0.107)|
| $n = \lceil N^{0.6} \rceil$ | B=225       | 1.022 (0.098)| B=15, R=15  | 1.032 (0.099)| B=225       | 1.030 (0.098)| R=225       | 1.024 (0.096)|
|           | B=250       | 1.026 (0.090)| B=10, R=25  | 1.029 (0.098)| B=250       | 1.032 (0.093)| R=250       | 1.027 (0.092)|
|           | B=275       | 1.028 (0.087)| B=25, R=11  | 1.026 (0.093)| B=275       | 1.024 (0.088)| R=275       | 1.026 (0.092)|
|           | B=300       | 1.029 (0.085)| B=10, R=30  | 1.026 (0.086)| B=300       | 1.032 (0.083)| R=300       | 1.027 (0.086)|
Table 2: Detailed simulation results are reported for $\kappa$ in Section 4.2 with $N = 10^5$.

| Parameter | Normal | Exp |
|-----------|--------|-----|
| $n$ | $B$ | $R$ | AF | TB | BLB | SB | SDB | AF | TB | BLB | SB | SDB |
| $[N^{0.4}]$ | 25 | 25 | 1.007 | 0.982 | 0.979 | 1.004 | 1.002 | 1.055 | 1.003 | 0.969 | 0.944 | 1.116 |
| | 25 | 50 | 1.007 | 0.982 | 0.914 | 1.004 | 1.101 | 1.055 | 1.003 | 1.001 | 0.944 | 1.061 |
| | 50 | 25 | 1.007 | 0.927 | 0.975 | 1.020 | 1.002 | 1.055 | 1.006 | 0.929 | 0.976 | 1.116 |
| | 50 | 50 | 1.007 | 0.927 | 0.987 | 1.020 | 1.010 | 1.055 | 1.006 | 1.023 | 0.976 | 1.061 |
| $[N^{0.5}]$ | 25 | 25 | 1.007 | 0.982 | 1.042 | 1.075 | 1.000 | 1.055 | 1.003 | 0.991 | 0.964 | 1.069 |
| | 25 | 50 | 1.007 | 0.982 | 0.982 | 1.075 | 1.014 | 1.055 | 1.003 | 1.028 | 0.964 | 1.032 |
| | 50 | 25 | 1.007 | 0.927 | 0.937 | 1.014 | 1.000 | 1.055 | 1.006 | 0.962 | 1.013 | 1.069 |
| | 50 | 50 | 1.007 | 0.927 | 0.950 | 1.014 | 1.014 | 1.055 | 1.006 | 0.946 | 1.013 | 1.032 |
| $[N^{0.6}]$ | 25 | 25 | 1.007 | 0.982 | 0.946 | 0.877 | 0.932 | 1.055 | 1.003 | 1.044 | 0.967 | 0.951 |
| | 25 | 50 | 1.007 | 0.982 | 1.003 | 0.877 | 1.030 | 1.055 | 1.003 | 0.975 | 0.967 | 0.977 |
| | 50 | 25 | 1.007 | 0.927 | 1.059 | 0.991 | 0.932 | 1.055 | 1.006 | 0.965 | 1.121 | 0.951 |
| | 50 | 50 | 1.007 | 0.927 | 1.082 | 0.991 | 1.030 | 1.055 | 1.006 | 1.049 | 1.121 | 0.977 |
Table 3: Detailed simulation results are reported for Section 4.3 with $N = 5 \times 10^5$ and $n = 5000$.

| Setting I | Setting II | MSE Performance | CPU Time |
|-----------|------------|-----------------|----------|
|            |            | log(MSE_a) log(MSE_b) MSE_b/MSE_a | Time_a | Time_b | Time_b/Time_a |
| BR($\times 10^3$) | B | R | log(MSE_a) | log(MSE_b) | MSE_b/MSE_a | Time_a | Time_b | Time_b/Time_a |
| 1          | 100 | 10 | 1515 | 2 | -33.484 | -33.685 | 0.818 | 8.362 | 4.786 | 0.572 |
|            | 50  | 20 | 1515 | 2 | -33.659 | -34.651 | 0.371 | 12.317 | 10.981 | 0.891 |
|            | 20  | 50 | 1515 | 12 | -33.592 | -35.576 | 0.138 | 26.709 | 27.013 | 1.011 |
|            | 10  | 100 | 1515 | 23 | -33.496 | -35.829 | 0.097 | 49.304 | 51.323 | 1.041 |
| 2          | 100 | 20 | 1515 | 5 | -34.332 | -34.732 | 0.670 | 17.112 | 11.409 | 0.667 |
|            | 50  | 40 | 1515 | 10 | -34.158 | -35.354 | 0.302 | 26.255 | 22.125 | 0.843 |
|            | 25  | 80 | 1515 | 19 | -34.105 | -35.845 | 0.175 | 44.727 | 41.897 | 0.937 |
|            | 10  | 200 | 1515 | 47 | -34.158 | -36.166 | 0.134 | 99.914 | 102.899 | 1.030 |
| 3          | 100 | 30 | 1515 | 8 | -34.505 | -35.184 | 0.507 | 26.483 | 18.336 | 0.692 |
|            | 75  | 40 | 1515 | 10 | -34.692 | -35.441 | 0.473 | 31.459 | 22.653 | 0.720 |
|            | 50  | 60 | 1515 | 15 | -34.671 | -35.592 | 0.398 | 40.848 | 33.448 | 0.819 |
|            | 25  | 120 | 1515 | 29 | -34.568 | -35.828 | 0.284 | 68.062 | 64.730 | 0.951 |
| 4          | 100 | 40 | 1515 | 11 | -34.864 | -35.271 | 0.666 | 35.481 | 25.258 | 0.712 |
|            | 50  | 80 | 1515 | 20 | -34.971 | -35.862 | 0.410 | 54.585 | 44.874 | 0.822 |
|            | 40  | 100 | 1515 | 25 | -35.126 | -35.847 | 0.487 | 63.572 | 55.229 | 0.869 |
|            | 20  | 200 | 1515 | 48 | -34.854 | -36.236 | 0.251 | 108.775 | 105.261 | 0.968 |
Table 4: Detailed results are reported for the Airline Data with $N = 1.01 \times 10^6$ and $n = 5000$.

| Setting I | Setting II | MedSE | SD/$SD_a$ | CPU Time | Time/$Time_a$ |
|-----------|------------|-------|------------|-----------|---------------|
| $BR(\times 10^3)$ | $B$ | $R$ | $BR^*$ | $R^*$ | $BR^*_{b}/BR^*_{a}$ | $SD_b/SD_{a}$ | $Time_a$ | $Time_b$ | $Time_b/Time_a$ |
| 1  | 100 | 10 | 1895 | 3 | 0.999 | 0.717 | 11.680 | 8.936 | 0.765 |
|  | 50 | 20 | 1895 | 5 | 1.007 | 0.507 | 19.740 | 14.533 | 0.736 |
|  | 20 | 50 | 1895 | 14 | 0.995 | 0.361 | 42.512 | 39.622 | 0.932 |
|  | 10 | 100 | 1895 | 27 | 1.003 | 0.199 | 80.443 | 75.841 | 0.943 |
| 2  | 100 | 20 | 1895 | 6 | 0.996 | 0.658 | 23.897 | 17.300 | 0.724 |
|  | 50 | 40 | 1895 | 11 | 1.005 | 0.459 | 40.162 | 31.282 | 0.779 |
|  | 25 | 80 | 1895 | 22 | 1.001 | 0.322 | 70.489 | 61.872 | 0.878 |
|  | 10 | 200 | 1895 | 55 | 1.004 | 0.233 | 160.895 | 153.872 | 0.956 |
| 3  | 100 | 30 | 1895 | 9 | 1.001 | 0.697 | 36.061 | 25.634 | 0.711 |
|  | 75 | 40 | 1895 | 12 | 0.999 | 0.591 | 45.321 | 34.053 | 0.751 |
|  | 50 | 60 | 1895 | 17 | 0.998 | 0.567 | 60.520 | 47.971 | 0.793 |
|  | 25 | 120 | 1895 | 34 | 1.001 | 0.354 | 106.135 | 95.358 | 0.898 |
| 4  | 100 | 40 | 1895 | 12 | 1.001 | 0.736 | 48.309 | 33.988 | 0.704 |
|  | 50 | 80 | 1895 | 23 | 1.004 | 0.505 | 80.832 | 64.703 | 0.800 |
|  | 40 | 100 | 1895 | 29 | 0.999 | 0.455 | 95.977 | 81.399 | 0.848 |
|  | 20 | 200 | 1895 | 56 | 0.999 | 0.331 | 172.232 | 156.615 | 0.909 |