Higher-Order Coverage Errors of Batching Methods via Edgeworth Expansions on \( t \)-Statistics

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Abstract

While batching methods have been widely used in simulation and statistics, it is open regarding their higher-order coverage behaviors and whether one variant is better than the others in this regard. We develop techniques to obtain higher-order coverage errors for batching methods by building Edgeworth-type expansions on \( t \)-statistics. The coefficients in these expansions are intricate analytically, but we provide algorithms to estimate the coefficients of the \( n^{-1} \) error term via Monte Carlo simulation. We provide insights on the effect of the number of batches on the coverage error where we demonstrate generally non-monotonic relations. We also compare different batching methods both theoretically and numerically, and argue that none of the methods is uniformly better than the others in terms of coverage. However, when the number of batches is large, sectioned jackknife has the best coverage among all.

Keywords — Batching methods, Edgeworth expansion, coverage errors, simulation analysis

1 Introduction

Batching methods are widely used in simulation analysis. The basic idea of these methods is to divide the data into batches and quantify the variability of point estimates by suitably combining the batch estimates. They are especially useful tools to construct confidence intervals (CIs) when the variance of the output is hard to compute, such as quantile [Nakayama, 2014] whose variance estimation involves density estimation, and in serially dependent problems and steady-state estimation [Asmussen and Glynn, 2007, Nakayama, 2007].

While widely used, the detailed coverage behaviors of batching methods, beyond the well-known asymptotic limits, are quite open. To understand and to better compare the statistical performances of these methods, however, this question seems imminent. To put things in perspective, note that a good CI should have a small coverage error, which refers to the difference between the empirical coverage and the prescribed target coverage. It is known that under regularity conditions, all batching methods are asymptotically exact, in the sense that they achieve the prescribed coverage level as the sample size increases. In other words, each method only have “higher-order” coverage errors that would converge to zero as the sample size increases. However, when the sample size is finite, this higher-order coverage error could be significant and also affected by the number of batches and method used, which is what we investigate mainly in this paper.

There are very few studies on the higher-order coverage errors of batching methods. The challenge is that the statistics used in these methods have an asymptotic \( t \)-distribution rather than a normal distribution, so conventional Edgeworth expansion cannot be directly applied. The most relevant result is the heuristic argument given in [Nakayama, 2014], which argue that since the estimator based on the entire empirical distribution has a smaller bias, the so-called sectioning appears to lead to a better coverage compared to batching. [Nakayama, 2014] supports this claim with numerical results.

In this paper, we develop tools to study higher-order expansions for the coverage probabilities of batching methods. Let \( K \) be the number of batches and suppose that each batch has \( n \) i.i.d. samples. When \( K \geq r + 3 \)
for some positive integer \( r \), under regularity conditions, we show that the coverage errors of batching methods can be expanded as a series of \( n^{-1/2} \) with residual \( O(n^{-r+1/2}) \). For symmetric CIs, we show that batching methods have coverage errors of order \( O(n^{-1}) \). To support the necessity of the assumption \( K \geq r + 3 \), we provide examples where such expansion does not exist when \( K = 2, r = 1 \). The coefficients in the expansion involve some integration that cannot be explicitly calculated in general, but for symmetric CIs, we design a simulation scheme to generate unbiased estimates for the coefficient of the \( n^{-1} \) error term, which is the leading term of the coverage error.

Our argument for coverage error expansions can be extended to more general cases without the i.i.d. assumption as long as there is an Edgeworth expansion for the joint distribution of the batch averages. We provide extensions to the scenario where the sample is a dependent data sequence with proper recurrence and mixing conditions, for which batching methods are commonly used. To ensure an Edgeworth expansion, however, we need to run variants of the batching methods that are slightly different from standard practice, one by leaving a gap between successive batches, and one using regenerative cycles. These variants allow us to explicitly analyze the coverage errors under data dependence.

In terms of methodology, our analysis utilizes Edgeworth expansion and Taylor’s expansion techniques combined with oddness and evenness arguments for functions. More precisely, we approximate the event that the target value is covered by the CI using a Taylor expansion argument where the coefficients are given by the implicit function theorem. Then, we study the probability of the approximated event by integrating with the Edgeworth expansion that leverages embedded normality. For a symmetric CI, we use an oddness and evenness argument to show that the coefficient of the \( n^{-1/2} \) term is 0. To our best knowledge, our line of techniques in deriving \( t \)-statistic expansions and applying it to the open question on higher-order coverage errors of batching methods appear the first in the literature.

By numerically comparing the theoretical coverages using our expansion (where the coefficients are estimated via simulation) and the actual coverages (estimated from repeated experiments), we show that our expansions give close approximations to the actual coverages. This allows us to compare the coverage errors of different batching methods and draw insights on the effect of the number of batches based on our expansion. From our analyses, we conclude that which method has smaller higher-order coverage error depends on problem parameters and none of them is uniformly better. However, for a fixed problem, we show that when \( K \) is large and \( n \) is fixed, batching suffers from a significant bias and has asymptotically 0 coverage, sectioning has an asymptotically incorrect coverage, while sectioned jackknife has asymptotically correct coverage. When the total number of data is fixed, coverage errors tend to increase as \( K \) increases. However, there is no monotonicity, meaning that for any batching method that we consider, when \( K \) is small, the coefficient could either increase or decrease as \( K \) increases depending on the problem parameters.

We summarize the main results and contributions of this paper:

1. **Building expansion techniques for \( t \)-statistics:** We develop techniques to study higher-order expansions for the distribution of statistics whose limiting distribution is \( t \). Our techniques utilize the implicit function theorem combining with embedded normality in the considered statistic that allows us to leverage established Edgeworth expansions as a building block.

2. **Higher-order expansions for coverage errors of batching methods:** With the \( t \)-statistic expansions, we obtain expansions for the coverage errors of batching methods, both in the case of i.i.d. data and when data comes from a dependent sequence with proper recurrence and mixing conditions. In the latter case, we provide two approaches to run the batching methods that allow explicit analyses on the coverage errors.

3. **Sufficient conditions on the number of batches \( K \):** To obtain our expansions with residuals of order \( O(n^{-(r+1)/2}) \), our theorem requires \( K \geq r + 3 \). We provide an example where an expansion with residual \( O(n^{-1}) \) does not exist when \( K = 2 \), which implies that the condition \( K \geq 3 \) is necessary when \( r = 1 \).

4. **Simulation-based algorithms to estimate coefficients in the expansions:** The coefficients in the expansions of coverage errors are intricate analytically, but amenable to simulation. We provide algorithms to estimate the coefficients of the \( n^{-1} \) term. We prove that the algorithms give unbiased estimates for the coefficients.
5. Insights on methods used and the effect of the number of batches: We show that none of the batching methods are uniformly better than the others, but when the number of data in each batch is fixed and $K \to \infty$, the coverage probability of batching goes to 0, the coverage probability of sectioning goes to a limit that is different from the nominal level, while the coverage probability of sectioned jackknife converges to the nominal level. When the total number of data is fixed, the coverage error tends to empirically increase as $K$ increases, but the error coefficient in our expansion is not monotone in $K$ and thus no theoretical monotonicity is achieved in general.

The rest of this paper is as follows. Section 2 reviews related literature. Section 3 introduces all considered batching methods. Section 4 presents our higher-order coverage error expansions. Section 5 extends these expansions to models with dependent data. Section 6 provides an algorithm to generate unbiased estimates for the $n^{-1}$ error terms for symmetric CIs. Section 7 discusses the asymptotic coverages as the number of batches grows. Section 8 validates our theoretical results via numerical experiments and uses our results to compare different methods and batch number choices. Technical proofs, some computation details, an alternative algorithm for batching, and additional numerical experiments are provided in the Appendix.

2 Literature review

We briefly review the literature on batching methods. Pope [1995] analyzes the coverage error of sectioning using Edgeworth expansion, but it focuses on the case when the number of batches goes to infinity so that the problem statistic can be approximated by normal. This is different from our analysis for the $t$ distribution approximation, which is our key novelty and faced challenge in this problem. For the CI half width, Schmeiser [1982] shows that if we assume the data size is large enough so that the non-normality of the batch estimators is negligible, then the expected half width would decrease as the number of batches increases, but the rate of decrease would become much slower when the number of batches is large. Similar observations are also made in Glynn and Lam [2018]. Jackknife can be used to reduce small-sample bias within sections, but at the cost of greater computation time and uncertainty about the variance inflation [Lewis and Orav, 1989].

Batching methods are commonly used in simulation output analysis, especially for steady state estimation where the data come from a dependent process. Alexopoulos and Seila [1996] use batching to study steady-state means and numerically test different strategies for choosing the number of batches. They also study overlapping batch means where different batches can overlap with each other. Steiger and Wilson [2002] also study steady-state means and proposes an algorithm called ASP to progressively increase the batch size until the batch means pass the independence test or multivariate normality test. Some refinements (ASP2, ASP3) are provided in Steiger et al. [2002], [2005]. Tafazzoli et al. [2008], [2011] propose SKART and N-SKART which are adjusted batching methods based on skewness and autoregression. Other algorithms concerning the CIs for steady-state means include Lada and Wilson [2006] (WASSP) and Lada and Wilson [2006] (SBATCH). Alexopoulos et al. [2014] use the idea of sectioning and batching to develop algorithms to build CIs for steady-state quantiles. Muñoz and Glynn [1997] uses batching methods for the estimation of non-linear functions of steady-state means. Dong and Glynn [2019a, b] use batching methods to decide the stopping time in sequential procedures and characterize the limiting distributions of the estimators at stopping times. Batching methods can also be used to estimate the variances of Markov chain Monte Carlo Geyer [1992] and the consistency of these variance estimators is established in Flegal and Jones [2010]. Jones et al. [2006]. Finally, Song and Schmeiser [1995], Flegal and Jones [2010] analyze optimal batch sizes that minimize the mean squared errors of batching variance estimators.

Batching can also be seen as a special type of the more general umbrella technique of standardized time series (STS), as shown in Example 3.1 of Glynn and Iglehart [1990]. Similar to batching methods, the idea of STS is to cancel out the variance term by taking the ratio between a point estimator and a variance estimator, but in a more general way where the variance estimator is viewed as a finite-sample approximation of a general functional of Brownian motions that is asymptotically independent of the point estimator. Schruben [1983] proposes STS as a method to construct CIs for the steady-state mean of a stationary process. Generalizations and properties of STS-type methods are studied extensively in the literature, including Glynn and Iglehart [1990], Goldsman and Schruben [1990], Calvin and Nakayama [2006], Antonini et al. [2009], Alexopoulos et al.
STS can also be used for constructing CIs for steady-state quantiles. Calvin and Nakayama [2013] and Alexopoulos et al. [2019, 2020] use STS to study steady-state quantiles and establish the asymptotic validity of the STS CI under different conditions.

Lastly, we mention a preliminary conference version of this work He and Lam [2021]. All contents in this paper are new except the argument on evenness and oddness that we utilize and the computation of expansions on some simple examples that we include in Appendix A.

3 Batching methods

Consider the problem of constructing a CI for $\psi(P)$ where $P$ is an unknown distribution, $\psi$ is a known statistical functional and we have data $X_1, \ldots, X_N$ drawn i.i.d. from $P$. Suppose the data size is $N = nK$. Divide the data into $K$ batches each with size $n$ and denote $\hat{P}_i$ as the empirical distribution for the $i$-th batch where $i = 1, 2, \ldots, K$. Denote $\hat{P}$ as the entire empirical distribution using all of the $N = nK$ data. By batching methods, in this paper we mean the following four variants:

- **Batching:** The batching CI is given by
  
  $$CI_B := \left( \frac{1}{K} \sum_i \psi(\hat{P}_i) \pm t_{K-1,\alpha/2} \frac{S_{\text{batch}}}{\sqrt{K}} \right)$$

  where $S_{\text{batch}}^2 = \frac{1}{K-1} \sum_{i=1}^{K} \left( \psi(\hat{P}_i) - \frac{1}{K} \sum_j \psi(\hat{P}_j) \right)^2$ and $t_{K-1,\alpha/2}$ is the upper $\alpha/2$-quantile of the $t_{K-1}$, the $t$-distribution with degree of freedom $K - 1$. That is, batching uses the batch estimates $\psi(\hat{P}_i)$ as primitives and the sample mean and sample variance of these batch estimates to construct a CI.

- **Sectioning:** The sectioning CI is given by
  
  $$CI_S := \left( \psi(\hat{P}) \pm t_{K-1,\alpha/2} \frac{S_{\text{sec}}}{\sqrt{K}} \right)$$

  where $S_{\text{sec}}^2 = \frac{1}{K-1} \sum_{i=1}^{K} \left( \psi(\hat{P}_i) - \psi(\hat{P}) \right)^2$. Compared with batching, sectioning uses the point estimate $\psi(\hat{P})$ constructed from the entire empirical distribution in both the center of the interval and the center in the variance estimator $S_{\text{sec}}^2$.

- **Sectioning-batching (SB):** The SB CI is
  
  $$CI_{SB} := \left( \psi(\hat{P}) \pm t_{K-1,\alpha/2} \frac{S_{\text{batch}}}{\sqrt{K}} \right)$$

  SB is a modified sectioning [Nakayama, 2014] that is viewed as a middle ground between batching and sectioning. It uses the same variance estimator $S_{\text{batch}}^2$ as batching, but the same interval center $\psi(\hat{P})$ as sectioning.

- **Sectioned jackknife (SJ):** Let $\hat{P}_{(i)}$ be the empirical distribution of all samples except for those from the $i$-th section. Let $J_i = K\psi(\hat{P}) - (K - 1)\psi(\hat{P}_{(i)})$. The SJ CI is given by
  
  $$CI_{SJ} := \left( \bar{J} \pm t_{K-1,\alpha/2} \frac{S_{\text{SJ}}}{\sqrt{K}} \right)$$

  where $S_{\text{SJ}}^2 = \frac{1}{K-1} \sum_{i=1}^{K} (J_i - \bar{J})^2$. SJ works in a similar way as conventional jackknife, but instead of considering the leave-one-out data, we leave one section or batch out. Like the conventional jackknife,
SJ is also known to be bias-corrected, but requires less computational cost (Section III.5b, Asmussen and Glynn [2007]).

Under regularity conditions, all four methods above are asymptotically exact, i.e., \( P(\psi(P) \in CI) \to 1 - \alpha \) as \( n \to \infty \) where \( \cdot \) can be \( B \), \( S \), \( SB \) or \( SJ \). For batching, this can be seen by the fact that the corresponding statistic has a limiting \( t_{K-1} \) distribution:

\[
W_B := \frac{\sqrt{nK} \left( \frac{1}{K} \sum_{i=1}^{K} \psi(\hat{P}_i) - \psi \right)}{\sqrt{\frac{1}{K-1} \sum_{i=1}^{K} \left( \sqrt{\frac{n}{K}} \psi(\hat{P}_i) - \sqrt{\frac{n}{K}} \psi(\bar{P}) \right)^2}} \Rightarrow t_{K-1}.
\]

Here \( \psi := \psi(P) \) is the target value and the limit is as \( n \to \infty \) with \( K \) fixed. Sectioning is also asymptotically exact since

\[
W_S := \frac{\sqrt{nK} \left( \psi(\bar{P}) - \psi \right)}{\sqrt{\frac{1}{K-1} \sum_{i=1}^{K} \left( \sqrt{\frac{n}{K}} \psi(\hat{P}_i) - \sqrt{\frac{n}{K}} \psi(\bar{P}) \right)^2}} = W_B + o_p(1) \Rightarrow t_{K-1}.
\]

Similar to sectioning and batching, \( SB \) is also asymptotically exact since

\[
W_{SB} := \frac{\sqrt{nK} \left( \psi(\bar{P}) - \psi \right)}{\sqrt{\frac{1}{K-1} \sum_{i=1}^{K} \left( \sqrt{\frac{n}{K}} \psi(\hat{P}_i) - \sqrt{\frac{n}{K}} \psi(\bar{P}) \right)^2}} = W_B + o_p(1) \Rightarrow t_{K-1}.
\]

Finally, the asymptotic exactness of \( SJ \) can be seen from

\[
W_{SJ} := \frac{\sqrt{nK} (J - \psi_0)}{\sqrt{\frac{1}{K-1} \sum_{i=1}^{K} \left( \sqrt{\frac{n}{K}} J_i - \sqrt{\frac{n}{K}} J \right)^2}} \Rightarrow t_{K-1}.
\]

To check that the last convergence indeed holds, consider the case \( \psi(P) = E_P X \) first where \( E_P \) denotes the expectation under \( P \). In this case, \( J_i = X_i \) so \( SJ \) is equivalent to batching and sectioning whose statistic has limit \( t_{K-1} \). More generally, with proper differentiability of \( \psi \), we can approximate \( \psi(\bar{P}) \) and \( \psi(\hat{P}_i) \) with \( E_{\bar{P}} IF(X) \) and \( E_{\hat{P}_i} IF(X) \) where \( IF(\cdot) \) is the influence function of \( \psi \) at \( P \). From this, we can get the same asymptotic distribution.

The four CIs we have introduced above are two-sided and symmetric in the sense that each of the CI has a midpoint at the respective point estimate. With the limiting distributions of the statistics given above, it is not hard to see that the following lower one-sided CIs are also valid: 

\[
\tilde{CI}_B := (-\infty, \frac{1}{K} \sum_i \psi(\hat{P}_i) + t_{K-1,\alpha} \frac{\hat{S}_{batch}}{\sqrt{K}}),
\]

\[
\tilde{CI}_S := (-\infty, \psi(\bar{P}) + t_{K-1,\alpha} \frac{\hat{S}_{batch}}{\sqrt{K}}), \tilde{CI}_{SB} := (-\infty, \psi(\bar{P}) + t_{K-1,\alpha} \frac{\hat{S}_{batch}}{\sqrt{K}}), \tilde{CI}_{SJ} := (-\infty, \bar{J} + t_{K-1,\alpha} \frac{\hat{S}_{SJ}}{\sqrt{K}}).
\]

Similarly, one can consider upper one-sided CIs with shape \( \psi(0, \infty) \) for some \( \psi \) or two-sided CIs that are not symmetric.

Although each of the four batching methods introduced above has asymptotically correct coverage, the coverage might be poor when we only have a finite sample. Note that \(-t_{K-1,\alpha/2} \leq W_B \leq t_{K-1,\alpha/2} \Rightarrow \psi \in CI_B \) and similar arguments hold for sectioning, \( SJ \) and \( SB \) and for one-sided CIs. Therefore, to study the higher-order coverage errors, it suffices to study the distributions of \( W_B, W_S, W_{SB} \) and \( W_{SJ} \), and how much they deviate from \( t_{K-1} \).

### 4 Expansions on batching methods with \( t \)-limits

For batching, by integrating over the Edgeworth expansion for batched estimates, we obtain the following.
Theorem 1 (Coverage error expansion for batching). Suppose that \( \psi(P_\lambda) \) has a valid Edgeworth expansion, in the sense that for some \( 0 < \sigma < \infty \),

\[
P \left( \frac{\sqrt{n} \left( \psi(P_\lambda) - \psi \right)}{\sigma} \leq q \right) = \Phi(q) + \sum_{j=1}^{r} n^{-j/2} p_j(q) \phi(q) + O \left( n^{-(r+1)/2} \right)
\]

holds uniformly over \( q \in \mathbb{R} \), and \( p_j \) is an even polynomial when \( j \) is odd and an odd polynomial when \( j \) is even. Here \( \Phi \) and \( \phi \) are the distribution function and density function of standard normal. Then:

- For any \( q \in \mathbb{R} \), there exists \( c_j^{(B,K)} \in \mathbb{R}, j = 1, 2, \ldots, r \), such that

\[
P(W_B \leq q) = \Phi(q) + \sum_{j=1}^{r} n^{-j/2} c_j^{(B,K)} + O(n^{-(r+1)/2})
\]

Here the coefficients \( c_j^{(B,K)} \) depends on \( K \), the distribution \( P \), the objective function \( \psi \) and the value of \( q \), but do not depend on \( n \).

- \( P(-q \leq W_B \leq q) = P(-q \leq t_{K-1} \leq q) + O(n^{-1}) \).

**Proof.** As long as we have a valid Edgeworth expansion for \( \sqrt{n} \left( \psi(P_\lambda) - \psi \right) \), noting that \( W_B \) is a function of \( \left( \sqrt{n} \left( \psi(P_\lambda) - \psi \right) \right)^{K}_{i=1} \), we can evaluate the probability \( P(W_B \leq q) \) based on integration. Let \( f(z) = \frac{1}{\sqrt{K^{r-1} \sum_{i=1}^{r} (z_i - \hat{z})^2}} \). Then one can check that

\[
W_B = f \left( \left( \sqrt{n} \left( \psi(P_\lambda) - \psi \right) / \sigma \right)^{K}_{i=1} \right)
\]

Therefore, from \([1]\), by integration we can get (here, the remainder term below has the claimed order because the testing region \( f(z) \leq q \) has a nice form: given \( z_1, \ldots, z_{i-1}, z_{i+1}, \ldots, z_K \), the values of \( z_i \) that makes \( f(z) \leq q \) can be described by at most two intervals, whose measures are uniformly controlled by \([1]\). See Appendix \([2]\) for a detailed proof on this.)

\[
P(W_B \leq q) = \int_{f(z) \leq q} \prod_{j=1}^{K} d \left( \Phi(z_j) + \sum_{j=1}^{r} n^{-j/2} p_j(z_j) \phi(z_j) \right) + O \left( n^{-(r+1)/2} \right).
\]

For a symmetric CI, by a similar integration, we have that

\[
P(-q \leq W_B \leq q)
\]

\[
= \int_{-q \leq f(z) \leq q} \prod_{j=1}^{K} d \left( \Phi(z_j) + n^{-1/2} p_1(z_j) \phi(z_j) \right) + O \left( n^{-1} \right)
\]

\[
=P(-q \leq t_{K-1} \leq q) + K n^{-1/2} \int_{-q \leq f(z) \leq q} \phi(z_1) \phi(z_2) \cdots \phi(z_K) (\phi(z_1) p_1(z_1) + p'_1(z_1)) dz 
\]

\[
+ O(n^{-1}).
\]

Here \( p'_1 \) is the derivative of \( p_1 \). Since \( p_1 \) is an even polynomial, \( -z_1 p_1(z_1) + p'_1(z_1) \) is an odd polynomial. In addition, note that the area \( \{-q \leq f(z) \leq q\} \) is symmetric around 0 since \( f(z) = -f(-z) \). Thus, the integration in the RHS above is 0. As a result, we have that \( P(-q \leq W_s \leq q) \) can be expanded as a power of \( n^{-1/2} \) and its leading term is of order \( n^{-1} \).

Theorem \([1]\) implies that the distribution of the batching statistic can be expanded as a series of \( n^{-1/2} \), and that the coverage error for the symmetric CI (i.e., a CI centered at the point estimate as introduced
in Section 3, given by batching is of order $O(n^{-1})$. The reasonableness of the condition (1) can be checked from Theorem 2.2 of Hall [1992]. Relation (2) is important for the proof, which says that $W_R$ can be written as a function of $\left(\sqrt{n} \left(\psi\left(\hat{P}_i\right) - \psi\right)\right)_{i=1}^K$ whose distribution is well understood by Edgeworth expansion. Moreover, this function does not depend on $n$, so in (3), when we integrate with respect to the Edgeworth expansion, the area of integration remains fixed when $n$ changes.

However, for other batching methods, the area is no longer the case. Consider sectioning for example. $W_S$ cannot be expressed as merely a function of $\left(\sqrt{n} \left(\psi\left(\hat{P}_i\right) - \psi\right)\right)_{i=1}^K$, but is also dependent on $\psi(\hat{P})$. Moreover, it is difficult to study the joint distribution of

$$\Lambda := \left(\sqrt{nK} \left(\psi\left(\hat{P}\right) - \psi\right), \left(\sqrt{n} \left(\psi\left(\hat{P}_i\right) - \psi\right)\right)_{i=1}^K\right)$$

via Edgeworth expansion, since its asymptotic joint distribution is degenerate. By the latter we mean that, under regularity conditions, $\sqrt{nK} \left(\psi\left(\hat{P}\right) - \psi\right) - \sqrt{K} \frac{1}{K} \sum_{i=1}^K \sqrt{n} \left(\psi\left(\hat{P}_i\right) - \psi\right) = o_p(1)$, which implies that the limiting distribution of $\Lambda \in \mathbb{R}^{K+1}$ has only $K$ degrees of freedom, hence is degenerate. Similarly for SJ, we note that SJ depends on $\psi(P), \psi(\hat{P}_{(1)}), \ldots, \psi(\hat{P}_{(K)})$, but again it appears difficult to study its joint distribution because of the asymptotic degeneracy.

To handle this issue, we focus on the smooth function model where $\psi(P) = f(E_P X)$. For this model, it is not difficult to see that each of $W_S, W_{SB}$ and $W_{SJ}$ can be written as a function of $\hat{\Lambda} := \left(\sqrt{n} \left(\hat{X}_j - E_P X\right)\right)_{i=1}^K$ whose distribution can be approximated by Edgeworth expansion. However, we still face some difficulties. To illustrate this, let’s take sectioning as an example and denote this function as $f$, which gives $W_S = f(\hat{\Lambda})$. As one can check, the function $f_{ij}(\cdot)$ would depend on $n$ (as long as $f$ is nonlinear), so the set of $\hat{\Lambda}$ that makes $f_{ij}(\cdot) \leq q$ depends on $n$. Therefore, a direct integration as in the proof of Theorem 1 will not give an expansion whose coefficients are free of $n$. To address this, we approximate the event $W_S \leq q$ by using a conditioning argument and studying the Taylor expansion for the critical value. More precisely, letting $A_i = \sqrt{n}(\hat{X}_i - E_P X)$, we consider the vector $A := (\hat{A}, A_1 - \hat{A}, \ldots, A_K - \hat{A}) \in \mathbb{R}^{dK}$ which can be seen as a linear transformation of $\hat{\Lambda}$ (so its Edgeworth expansion is also known). Let $A_{0,1} \in \mathbb{R}$ denote the first coordinate of $A$ and let $A' \in \mathbb{R}^{dK-1}$ denote the rest of the coordinates of $A$. We reformulate the event $W_S \leq q$ (whose probability we are interested in) as $A_{0,1} \leq F_{n}^{A'}$ where $F_{n}^{A'}$ is a function of $A'$ (and depend on $n$). The expansion for $F_{n}^{A'}$ w.r.t. $n^{-1/2}$ can be studied by the implicit function theorem. Moreover, the smoothness of (the Edgeworth approximation for) the distribution of $A_{0,1}$ can be used to argue that the contribution of the higher-order terms in the expansion for $F_{n}^{A'}$ to the final expectation is also of higher order. Therefore, with the expansion for $F_{n}^{A'}$, by integrating with the Edgeworth expansion for $A$ in a proper way, we get an expansion for the probability of $A_{0,1} \leq F_{n}^{A'}$ which is what we want. The detailed argument is given in Appendix D. We can show the following theorem regarding the validity and order of expansion for other batching methods.

**Theorem 2** (Coverage error expansions for all methods). Suppose that $\psi(\cdot)$ is a statistical functional mapping from distributions in $\mathbb{R}^d$ to $\mathbb{R}$ defined by $\psi(\hat{P}) = f(E_P X)$ for a vector $X \sim \hat{P}, X \in \mathbb{R}^d$. Assume the following Cramer’s condition holds for the distribution of $X_1 \in \mathbb{R}^d$ (recall that $X_1, \ldots, X_{nK}$ are drawn i.i.d. from $P$):

$$\limsup_{|t| \to \infty} |E_P \{\exp\{i \langle t, X \rangle\}\}| < 1,$$

(4)

Suppose that for some positive integer $r$, $X$ has finite moments up to order $r+2$ with nonsingular covariance, and $f$ is $r+1$ times differentiable in a neighborhood of $E_P X$ with $\nabla f(E_P X) \neq 0$. Then:

- If $K \geq r + 3$, then for any $q \in \mathbb{R}$, there exists $c_j^{(S,J,K)} \in \mathbb{R}, j = 1, 2, \ldots, r$, such that

$$P(W_{S,J} \leq q) = P(t_{K-1} \leq q) + \sum_{j=1}^{r} n^{-j/2} c_j^{(S,J,K)} + O(n^{-(r+1)/2})$$

Here the coefficients $c_j^{(S,J,K)}$ depends on $K$, the distribution $P$ that generates each $X_i$, the objective function $f$ and the value of $q$, but does not depend on $n$. 

• Suppose that \( K \geq 4 \). Then we have \( P(-q \leq W_{S,1} \leq q) = P(-q \leq t_{K-1} \leq q) + O(n^{-1}) \).

The same result holds if \( W_{S,1} \) is replaced by \( W_S \), \( W_{SB} \) or \( W_B \) and the coefficients \( c_j^{(S,J,K)} \), \( j = 1, 2, \ldots, r \) are replaced with a different set of coefficients corresponding to each method.

Theorem 2 gives results similar to Theorem 1 but has different assumptions and works for all batching methods. The assumptions on the Cramer’s condition, finiteness of moments, and the differentiability of \( f \) are common in the literature of Edgeworth expansion. The assumption that seems nontrivial is the requirement \( K \geq r + 3 \). In our proof, this condition is used to guarantee the finiteness of some terms that involve the moment of an inverse chi-squared distribution with \( K - 1 \) degrees of freedom. This condition may not be necessary in some cases, e.g., the simple examples in Appendix A. However, we also find examples where the claim of Theorem 2 does not hold when \( K \) is too small. The following proposition reveals that when \( K = 2 \), the magnitude of error for sectioning in the symmetric case is indeed larger than \( n^{-1} \). This implies that for Theorem 2 with \( r = 1 \) to hold, \( K \) should be at least 3 (unless there are other additional assumptions).

**Proposition 1** (Magnitude of error when \( K = 2 \)). Let \( \psi(\tilde{P}) = f(E_p[X], E_p[Y]) \), \( f(x, y) = x + y^2 \) and \((X, Y) \sim N(0, 2I_2) \) under \( P \) where \( I_2 \) is the 2-dimensional identity matrix,

\[
\Pr(-q \leq W_S \leq q) = \Pr(-q \leq t_1 \leq q) = \omega(n^{-1})
\]

but

\[
\Pr(-q \leq W_S \leq q) - \Pr(-q \leq t_1 \leq q) = o(n^{-1/2}).
\]

We also remark that in Theorem 2 the condition \( K \geq r + 3 \) could be potentially relaxed to \( K \geq r + 2 \) if we only need a residual \( o(n^{-r/2}) \) instead of \( O(n^{-(r+1)/2}) \). This could be done by conducting all the expansions in our proofs with reminder terms of the Peano type. A detailed argument of this would require some delicate but similar analysis as this paper.

## 5 Extensions to dependent data

Following from the discussion before Theorem 2 for the smooth function model, as long as the (scaled) batch averages have a valid joint Edgeworth expansion and other regularity conditions in Theorem 2 hold, we can show the validity of Edgeworth expansion for the resulting statistic. In what follows, we extend Theorem 2 to the setting where the data is a dependent sequence.

Consider a stationary dependent sequence (e.g., a Markov chain) \( X_1, X_2, \ldots \) and suppose we are interested in estimating \( f(Eg(X_1)) \) where the expectation is taken under the stationary measure and \( g \) maps from the state space of the data sequence to \( \mathbb{R} \). Here we introduce \( g \) because the Edgeworth expansion literature only works for the average of \( g(X_i) \)'s (which is one-dimensional) but not for the average of \( X_i \)'s (which can be multidimensional). Suppose we divide the data into batches each having \( n \) samples. Let \( \bar{g}_k \) denote the average of \( g(X_i) \) among the \( X_i \)'s in the \( k \)-th batch. For this model, under some conditions, Edgeworth expansion for the distribution of \( \sqrt{n}(\bar{g}_1 - Eg(X_1)) \) is known [Jensen 1989, Malinovskii 1987]. However, this is not sufficient to inform the joint distribution of \( (\sqrt{n}(\bar{g}_1 - Eg(X_1)), \ldots, \sqrt{n}(\bar{g}_K - Eg(X_1))) \) since we do not know the dependence among batches. Indeed, noting that \( Cor(g(X_n), g(X_{n+1})) \) (here \( Cor \) means correlation) would contribute \( \Phi(n^{-1}) \) to \( Cor(\sqrt{n}(\bar{g}_1 - Eg(X_1)), \sqrt{n}(\bar{g}_2 - Eg(X_1))) \), we expect that \( Cor(\sqrt{n}(\bar{g}_1 - Eg(X_1)), \sqrt{n}(\bar{g}_2 - Eg(X_1))) \) is of order \( n^{-1} \). Therefore, the dependence among batches would contribute \( n^{-1} \) to the Edgeworth expansion for the joint distribution which is not negligible for the higher-order coverage error. Without further information, it seems challenging to explicitly analyze the effect of dependence among batches. For this reason, we consider some modified schemes where different batch averages are independent or nearly independent.

### 5.1 Approach 1: Leave a gap between successive batches

Suppose that, between each two adjacent batches, we discard \( n^\delta \) data for some \( 0 < \delta < 1 \) (for convenience, suppose that after this operation, each batch has \( n \) data). Intuitively, with this gap, there is more independence between adjacent batches. After this operation, we construct the CIs in the same way as introduced in
Section 3. More precisely, following the convention therein, let \( \hat{\mathcal{P}}_i, i = 1, 2, \ldots, K \) denote the empirical distribution of \( X_i \)'s in the \( i \)-th batch (after leaving the gap). Let \( \hat{\mathcal{P}} = \frac{1}{K} \sum_{i=1}^{K} \hat{\mathcal{P}}_i \) and \( \hat{\mathcal{P}}(i) = \frac{1}{K-1} \sum_{1 \leq k \leq K, k \neq i} \hat{\mathcal{P}}_k \). Let \( \psi(\cdot) \) be defined as \( \psi(\hat{\mathcal{P}}) = f(E_{X \sim \hat{\mathcal{P}}} g(X)) \). With these, we construct the CIs \( CI_B, CI_S, CI_{SB}, CI_{SJ} \) and consider the associated statistics \( W_{SJ}, W_S, W_B, W_{SB} \) in terms of \( \psi(\cdot), \hat{\mathcal{P}}, \hat{\mathcal{P}}(i), i = 1, 2, \ldots, K \) using the same formulas as given in Section 3.

To proceed, we introduce the notion of mixing coefficient and Harris recurrence.

**Definition 1** (Mixing coefficient). For any two Borel \( \sigma \)-fields \( A \) and \( B \), define the mixing coefficient \( \alpha(A, B) := \sup_{A \in A, B \in B} |P(A \cap B) - P(A)P(B)|. \) For a stationary sequence \( X \) with \( \mathcal{F}_n := \sigma(X_1, \ldots, X_n) \), define \( \alpha(n) := \sigma(\mathcal{F}_0^\infty, \mathcal{F}_n^\infty) \).

**Definition 2** (Harris recurrence). A Markov chain \( X \) defined on state space \( \mathcal{X} \) is said to be Harris recurrent if there exists a measure \( \mu \) such that for any measurable set \( B \subset \mathcal{X} \) satisfying \( \mu(B) > 0 \), we have \( \mathcal{P}_\mu(X_n \in B, \text{i.o.}) = 1, \forall x \in \mathcal{X} \).

With the Edgeworth expansion proposed in Theorem 1 of Jensen [1989], we can show the following validity of the coverage error expansion:

**Theorem 3** (Coverage error expansions for batching methods on dependent data bearing recurrent atoms with gaps between successive batches). Suppose that \( X_i, i = 1, 2, \ldots \) is a Harris-recurrent and strictly stationary Markov chain with a recurrent atom \( A_0 \) and stationary distribution \( \mathcal{P} \). Moreover, suppose that \( n^{-3r} \alpha(n) \to 0 \) as \( n \to 0 \) for some positive integer \( r \). Let

\[
\tau = \min\{n > 0 : X_n \in A_0\}, G = \sum_{i=1}^{\tau} \{|g(X_i)| \}
\]

Suppose the uniform Cramer condition holds: there exists \( \delta' < 1 \) such that \( |E_{\mathcal{P}} \exp(iuX_1 + iv\tau)| < \delta' \) for all \( v \in \mathbb{R} \) and all \( u \in \mathbb{R}^d \) with \( ||u|| > c \). Suppose further that \( E_{\mathcal{P}} \tau^{r+3} < \infty \), \( E_{\mathcal{P}} \tau^{r+3} < \infty \). Suppose that \( f \) is \( r \) times differentiable in a neighborhood of \( E_{\mathcal{P}} g(X_1) \) and \( \nabla f(E_{\mathcal{P}} g(X_1)) \neq 0 \). Moreover, suppose that \( K \geq r + 3 \). Then for any \( q \in \mathbb{R} \), there exists \( c_{ij}^{(SJ,K)} \in \mathbb{R}, j = 1, 2, \ldots, r \), such that

\[
P(W_{SJ} \leq q) = P(t_{K-1} \leq q) + \sum_{j=1}^{r} n^{-j/2}c_{ij}^{(SJ,K)} + O(n^{-(r+1)/2})
\]

Here the coefficients \( c_{ij}^{(SJ,K)} \) depend on \( K \), the stationary distribution \( \mathcal{P} \), the objective function \( g \) and the value of \( q \), but does not depend on \( n \). The same result holds if \( W_{SJ} \) is replaced by \( W_S, W_{SB} \) or \( W_B \) and the coefficients \( c_{ij}^{(SJ,K)} \), \( j = 1, 2, \ldots, r \) are be replaced with a different set of coefficients corresponding to each method.

Theorem 3 stipulates that for a dependent data sequence satisfying proper conditions, the coverage error also has a valid expansion similar to Theorems 1 and 2. In Theorem 3, we didn’t make a claim that the coverage error of a symmetric CI is of order \( O(n^{-1}) \) since the expansion in Jensen [1989] doesn’t discuss the oddness and evenness of the polynomials in the Edgeworth expansion. But as long as we have this oddness and evenness, we can show that the coverage error for a symmetric CI is order \( O(n^{-1}) \) (see the second claim of Theorem 1 next).

We discuss the conditions introduced in Theorem 3. The Harris recurrence condition can be seen as a generalization of positive recurrent Markov chains with countable states while preserving some good properties for a rich theory. This condition can be easily verified in some settings beyond countable state space: for example, for the waiting time process in a queue, we can let \( \mu \) in Definition 2 (and also the recurrent atom as required in Theorem 3) be concentrated on the state “0”, then we can verify the Harris recurrence as long as “0” is a recurrent state. Similar setups using positive recurrent Harris chains also appear in IV.6b of Asmussen and Glynn [2007]. More generally, the Doeblin chains can be seen as special cases of recurrent Harris chains Malinovskii [1987]. Practical examples include M/G/1 waiting time processes, AR(1) processes, and
more general queueing systems as considered in the numerical examples of Chien [1994], Alexopoulos and Seila [1996], Steiger and Wilson [2002], Alexopoulos et al. [2013]. Conditions that can guarantee the mixing condition $n \to \infty \alpha(n) \to 0$ in the setting of Harris recurrent Markov chains can be found in Section 3.2 of Duchi et al. [2021]. Under those conditions, we actually have $\alpha(n) = c^n$ for some $c \in (0,1)$, so $n^{-r+1} \alpha(n) \to 0$ holds for arbitrary $\delta > 0$. Other assumptions on the finiteness of moments and Cramer condition are common in the study of Edgeworth expansion.

The following theorem does not require the existence of atom as in Theorem 3 but involves more complex notations in the statement. Moreover, we are able to conclude that the coverage error for a symmetric CI is of order $O(n^{-1})$ thanks to the knowledge of the oddness and evenness of the polynomials in the Edgeworth expansion in Malinovskii [1987].

**Theorem 4** (Coverage error expansions for batching methods on dependent data with gaps between successive batches). Suppose that $X_i, i = 1, 2, \ldots$ is a Harris-recurrent Markov chain and is strictly stationary. Moreover, suppose that $n^{r+1} \alpha(n) \to 0$ for some positive integer $r$. Let $P$ be the stationary distribution. Suppose that there exists a set $C$, a positive $\lambda$ and a probability measure $\varphi_C$ concentrated on $C$ such that

$$P_x (\cup_{i=1}^{\infty} \{X_i \in C\}) = 1$$

for any $x$ and

$$P_x (X_2 \in A) \geq \lambda \varphi_C(A)$$

for any $x \in C, A \subset C$. For any distribution $\alpha$, define $P_{\alpha,\lambda}$ as the measure of the process $\{(X_i, b_i), i = 1, 2, \ldots\}$ with initial distribution $P_{\alpha,\lambda}(X_1 \in dx, b_1 = \delta) = \alpha(dx)(\lambda \delta + (1 - \lambda)(1 - \delta))$

and transition probability

$$P_{\alpha,\lambda} ((x, 1), A \times \{\delta\}) = \begin{cases} (\lambda \delta + (1 - \lambda)(1 - \delta))P(x, A) & x \notin C \\ (\lambda \delta + (1 - \lambda)(1 - \delta))\varphi_C(A) & x \in C \end{cases}$$

and

$$P_{\alpha,\lambda} ((x, 0), A \times \{\delta\}) = \begin{cases} (\lambda \delta + (1 - \lambda)(1 - \delta))P(x, A) & x \notin C \\ (\lambda \delta + (1 - \lambda)(1 - \delta))Q(x, A) & x \in C \end{cases}$$

where $P(x, \cdot)$ is the transition probability of $X_i, i = 1, 2, \ldots$ and $Q(x, \cdot) = (1 - \lambda)^{-1}(P(x, \cdot) - \lambda \varphi_C(\cdot))$. Let

$$\tau = \min\{n > 0 : X_n \in C, b_n = 1\}, \tilde{g}(x) = g(x) - Eg(X_1), \Sigma_n = n^{-1/2} \sum_{i=1}^{n} \tilde{g}(X_i), G = \sum_{i=1}^{\tau} g(X_i).$$

Suppose that

1. $\limsup_{|t| \to \infty} |E_{\varphi_C,\lambda} \exp(itG)| < 1$.
2. $\sigma_G := E_{\varphi_C,\lambda} G^2 > 0$
3. $E_{\varphi_C,\lambda} r^{r+3} < \infty, E_{P,\lambda} r^{r+1} < \infty$
4. $E_{\varphi_C,\lambda} (\sum_{i=1}^{\tau} |g(X_i)|)^{r+3} < \infty, E_{P,\lambda} (\sum_{i=1}^{\tau} |g(X_i)|)^{r+1} < \infty$

Then,

- If $K \geq r + 3$, then for any $q \in \mathbb{R}$, there exists $\tilde{c}_{j}^{(S,J,K)} \in \mathbb{R}, j = 1, 2, \ldots, r$, such that

$$P(W_{S,J} \leq q) = P(t_{K-1} \leq q) + \sum_{j=1}^{r} n^{-j/2} \tilde{c}_{j}^{(S,J,K)} + O(n^{-(r+1)/2})$$

Here the coefficients $\tilde{c}_{j}^{(S,J,K)}$ depends on $K$, the stationary distribution $P$, the objective function $g$ and the value of $q$, but does not depend on $n$.

- Suppose that $K \geq 4$. Then $P(-q \leq W_{S,J} \leq q) = P(-q \leq t_{K-1} \leq q) + O(n^{-1})$. 
The same result holds if \( W_{SJ} \) is replaced by \( W_S, W_{SB} \) or \( W_B \) and the coefficients \( \tilde{c}_j^{(SJK)} \), \( j = 1, 2, \ldots, r \) are be replaced with a different set of coefficients corresponding to each method.

While the choices of \( C \) and \( \lambda \) in the statement of Theorem \( \text{[4]} \) seem to have some freedom, it is shown in Malinovskii \( \text{[1987]} \) that any choice would lead to the same Edgeworth expansion.

### 5.2 Approach 2: Decompose into regenerative cycles

Suppose that \( X_1, X_2, \ldots \) has a recurrent state \( a_0 \). Let \( T_1 = \inf \{ k > 0 : X_k = a_0 \} \) and for \( i \geq 2 \), let \( T_i = \inf \{ k > T_{i-1} : X_k = a_0 \} \). Let \( Y_i = \sum_{k=T_{i-1}}^{T_i} g(X_k) \). We may regard \( (Y_i, T_{i+1} - T_i) \) as the new data and perform batching for these data. For example, suppose that we are interested in \( \mathbb{E} \gamma g(X_1) \), where \( \pi \) is the stationary distribution. Note that

\[
T_i = \inf \{ k > T_i : X_k = a_0 \}.
\]

More concretely, we construct the CIs for \( \psi := \mathbb{E} \gamma g(X_1) \) in the following way. Let \( Q_i := (Y_i, T_{i+1} - T_i), i = 1, 2, \ldots, nK \). Let \( \hat{P} \) denote the entire, batched and leave-one-batch-out empirical distributions of \( \{Q_i\}_{i=1}^{nK} \) as introduced in Section \( \text{[3]} \). For any two-dimensional distribution \( \tilde{P} \), we define \( \psi(\tilde{P}) = \frac{\mathbb{E}_{\tilde{P}}[Q^{(1)}]}{\mathbb{E}_{\tilde{P}}[Q^{(2)}]} \), where \( Q \sim \tilde{P} \) and for \( j = 1, 2 \), \( Q^{(j)} \) stands for the \( j \)-th coordinate of \( Q \). Note that the target value can be written as \( \psi = \frac{\mathbb{E}_{\tilde{Q}}[Q^{(1)}]}{\mathbb{E}_{\tilde{Q}}[Q^{(2)}]} \) (where the expectation is taken under the true distribution of \( Q_1 \)). Construct \( CI_B, CI_S, CI_{SB}, CI_{SJ} \) and define the corresponding statistics \( \psi(\cdot), \hat{P}, \tilde{P}, \hat{P}(i) \) using the same formulas as in Section \( \text{[3]} \).

We have the following theorem regarding the validity of expansion:

**Theorem 5** (Coverage error expansions for batching methods on dependent data using regenerative cycles). Suppose that the following Cramer’s condition holds for the distribution of \( Q_i \):

\[
\limsup_{|t| \to \infty} |\mathbb{E}[\exp(i \langle t, Q_1 \rangle)]| < 1,
\]

Suppose that for some positive integer \( q, \) \( Q_1 \) has finite moments up to order \( r+2 \) with nonsingular covariance. Suppose that \( \mathbb{E}[T_2 - T_1] > 0 \). Then:

- If \( K \geq r + 3 \), then for any \( q \in \mathbb{R} \), there exists \( \tilde{c}_j^{(SJK)} \in \mathbb{R}, j = 1, 2, \ldots, r \), such that

\[
P(W_{SJ} \leq q) = P(t_{K-1} \leq q) + \sum_{j=1}^{r} n^{-j/2} \tilde{c}_j^{(SJK)} + O(n^{-(r+1)/2}).
\]

Here the coefficients \( \tilde{c}_j^{(SJK)} \) depends on \( K \), the true distribution of \( Q_1 \), and the value of \( q \), but does not depend on \( n \).

- Suppose that \( K \geq 4 \). Then we have \( P(-q \leq W_{SJ} \leq q) = P(-q \leq t_{K-1} \leq q) + O(n^{-1}) \).

The same result holds if \( W_{SJ} \) is replaced by \( W_S, W_{SB} \) or \( W_B \) and the coefficients \( \tilde{c}_j^{(SJK)} \), \( j = 1, 2, \ldots, r \) are be replaced with a different set of coefficients corresponding to each method.

### 6 An algorithm to estimate coefficients of the \( n^{-1} \) error via simulation

For this section, we mainly focus on the symmetric CIs whose errors are of order \( n^{-1} \) by Theorem \( \text{[2]} \). Consider the smooth function model where we want to construct a CI for \( f(EX) \). Recall that Theorem \( \text{[2]} \) implies that

\[
P(-q \leq W \leq q) = P(-q \leq t_{K-1} \leq q) + c_n^{-1} + O(n^{-3/2})
\]
where \( W \) can be either one of \( W_S, W_B, W_{SB} \) and \( W_{SJ} \) and \( c \) is a constant that depends on the method used, the number of batches \( K \), the underlying distribution \( P \), the function \( f \), and the critical point \( q \), but does not depend on \( n \). For some very simple examples, we can calculate \( c \) explicitly (see Section A). However, in general, \( c \) involves some integration that cannot be calculated explicitly. In this section, we give a simulation scheme to generate an unbiased estimator for \( c \) for each batching method. Our proposed algorithm is Algorithm 1 whose construction follows closely from the proof of Theorem 2. The polynomials \( p_1 \) and \( p_2 \) in Algorithm 1 are defined as follows, which are due to Skovgaard [1986]:

\[
\begin{align*}
p_1(x) &= \phi_\Sigma(x) \left[ 1 + \frac{1}{n} \chi_{ijk} \sigma^{ia} \sigma^{jb} \sigma^{kc} x_i x_j x_k - \frac{1}{2} \sigma^{ij} \chi_{ijkl} \right] \\
p_2(x) &= \phi_\Sigma(x) \left[ \frac{1}{n} \chi_{ijkl} \left( \sigma^{ia} \sigma^{jb} \sigma^{kc} \sigma^{ld} x_i x_j x_k x_l - 6 \sigma^{ia} \sigma^{ib} \sigma^{jc} \sigma^{kd} x_i x_j x_k x_l + 3 \sigma^{ij} \sigma^{kl} \right) \\
&+ \frac{1}{2} \chi_{ijkl} \left\{ \sigma^{ia} \sigma^{ib} \sigma^{jc} \sigma^{kd} \sigma^{lm} \sigma^{mn} \sigma^{op} x_i x_j x_k x_l x_m x_n x_o \right\} \right]
\end{align*}
\]

Here \( \phi_\Sigma(\cdot) \) is the density of \( N(0, \Sigma) \), \( \sigma^{ij} \) are the coordinates of matrix \( \Sigma^{-1} \), and \( \chi_{ijk} \) and \( \chi_{ijkl} \) stand for the joint cumulants of the coordinates of \( X \). The Einstein summation convention is used here, which means we sum over repeated indices. For example, we omit the summation symbol \( \sum \) when we write \( \chi_{ijk} \sigma^{ia} \sigma^{jb} \sigma^{kc} x_i x_j x_k \).

The following proposition asserts the correctness of the algorithm. The proof uses similar techniques as the proof of Theorem 2 but with more explicit algebra.

**Theorem 6** (Unbiasedness of simulation algorithm to estimate coefficients of \( n^{-1} \)). *Suppose that the conditions of Theorem 2 hold with \( r = 2 \), and the expansion is given as (7) where \( W \) can be any of \( W_S, W_B, W_{SB} \) and \( W_{SJ} \). Then, Algorithm 1 returns an unbiased estimator for \( c \).*

In what follows, we illustrate how to compute the polynomials \( a, b_1, b_2, d, e, E_2, b'_1, d' \) as required by Steps 2 and 3 of Algorithm 1 using sectioning as an example. The computation for other schemes can be found in Section B.

Let \( u = \nabla f, v = \nabla^2 f/2, w = \nabla^3 f/6 \). Recall the definition of \( A_0, B_i, i = 1, 2, \ldots, K \) in Algorithm 1. Then

\[
W_S = \frac{\sqrt{K} \left( f(m + n^{-1/2} A_0) - f_0 \right)}{\sqrt{K(K-1) \sum_{i=1}^K \left( \sqrt{n} f(m + n^{-1/2} X_i) - \sqrt{n} f(m + n^{-1/2} A_0) \right)^2}}
\]

\[
= \frac{\sqrt{K(K-1)}}{\sqrt{\sum_{i=1}^K \left( \left[ u, A_0 \right] + n^{-1/2} [v, A_0, A_0] + n^{-1} [w, A_0, A_0, A_0] \right)}} \sqrt{\sum_{i=1}^K \left[ w, A_0, A_0, A_0 \right] + O_p(n^{-3/2})}
\]

Here, \( [u, A_0] \) = \( u_i A_0, i \), \( [v, A_0, A_0] \) := \( v_{ij} A_0 A_0 \), \( [w, A_0, A_0, A_0] \) := \( w_{ijk} A_0 A_0 A_0 \). The leading term of the denominator is \( \sum_i [u, A_i] - A_0^2 \). The coefficient for \( n^{-1/2} \) is

\[
\lambda = 2 \sum_i [u, B_i] ([v, B_i + A_0, B_i + A_0] - [v, A_0, A_0])
\]

The coefficient for \( n^{-1} \) is

\[
e = \sum_i \left[ +2 [u, B_i] ([w, B_i + A_0, B_i + A_0] - [w, A_0, A_0])^2 \right]
\]

We also have \( a = [u, A_0], b_1 = [v, A_0, A_0], b_2 = [w, A_0, A_0] \). The derivatives w.r.t. \( A_0, 1 \) can be computed as

\[
b_1 = 2v_{11} A_0, 1 + 2 \sum_{j=1}^2 v_{ij} A_0, j = 2 \sum_{j=1}^d \sum_{j=1}^d v_{ij} A_0, j
\]
Algorithm 1 An unbiased simulation scheme to compute the coefficient of the $n^{-1}$ error term

Initialization: Derivatives of $f$ at $EX_1$ up to order 3, cumulants of $X_1$ up to order 4, testing statistic $W$. ($W$ can be either of $W_S, W_B, WS_B$ and $W_{SB}$ and is regarded as a function of batch averages and $n$)

1: Let $\Sigma = Var(X_1)$. Simulate $X_1, X_2, \ldots, X_K \overset{i.i.d.}{\sim} N(0, \Sigma)$. Let $A_0 = \frac{X_1 + \cdots + X_K}{K}, B_i = X_i - A_0, i = 1, 2, \ldots, K$.

2: Perform Taylor’s expansion on $W$ regarding $X_1, \ldots, X_K$ as the batch averages, and write it as $W = \sqrt{K(K-1)} \frac{a + n^{-1/2}b_1 n^{-1/2}b_2}{\sqrt{E_2+n^{-1/2}b_2}} + O_K(n^{-3/2})$. Express each of $a, b_1, b_2, \lambda, c, E_2$ as a polynomial of $A_0, B_1, B_2, \ldots, B_K$ (the expressions depend on the batching scheme we use. The expressions for sectioning is included in Section $[B]$. The expressions for other schemes are given in Section $[C]$).

3: Compute the derivative of $b_1$ and $\lambda$ w.r.t. $A_0, 1$ and denote them by $b'_1$ and $\lambda'$ respectively. Then let (denote $u = \nabla f(\bar{X}_1)$)

$$F_x = \frac{b_1}{\sqrt{2}} - \frac{1}{2} \frac{\lambda a}{\sqrt{2}}, F_{xx} = \frac{1}{\sqrt{2}} \left( a - \frac{c}{4} + b_1 \lambda + 2b_2 \right),$$

$$F_y = \frac{a'}{\sqrt{2}}, F_{xy} = b'_1 - \frac{1}{2} \frac{(\lambda a)'}{\sqrt{2}},$$

$$F_+ = \frac{q\sqrt{E_2}}{\sqrt{K(K-1)}} - \sum_{i=2}^d u_i A_0, i, F_- = \frac{-q\sqrt{E_2}}{\sqrt{K(K-1)}} - \sum_{i=2}^d u_i A_0, i.$$

4: Compute

$$y_x = \frac{-F_x/F_y|_{A_0=1=F_+}}{y_{xx} = -\left( F_{xx} + 2F_{xy} y_x \right) / F_y |_{A_0=1=F_+}},$$

$$y_x(-) = \frac{-F_x/F_y|_{A_0=1=F_-}}{y_{xx}(-) = -\left( F_{xx} + 2F_{xy} y_x \right) / F_y |_{A_0=1=F_-}}.$$

5: Derive the error term estimator:

$$ER = IC(A) \left[ \sum_{1 \leq i < j \leq K} p_1(x_i(A))p_1(x_j(A)) + \sum_{1 \leq i \leq K} p_2(x_i(A)) \right]$$

$$+ \phi_{\tilde{\sigma}_0}(F_+ - \mu) (p_1(x(A))) |_{A_0 = 1=F_+} (y_x(-)) + \phi_{\tilde{\sigma}_0}(F_+ - \mu) (\frac{1}{2} y_{xx})$$

$$- \phi_{\tilde{\sigma}_0}(F_- - \mu) (p_1(x(A))) |_{A_0 = 1=F_-} (y_x(-)) + \phi_{\tilde{\sigma}_0}(F_- - \mu) (\frac{1}{2} y_{xx})$$

$$+ \frac{1}{2} \left( \phi_{\tilde{\sigma}_0}(F_+ - \mu) \left( \frac{\left( F_+ - \mu \right)}{\tilde{\sigma}_0} \right) y_x^2 \right)$$

$$- \phi_{\tilde{\sigma}_0}(F_- - \mu) \left( \frac{\left( F_- - \mu \right)}{\tilde{\sigma}_0} \right) y_x^2.$$

Here, $(x_1(A), \ldots, x_K(A))^\top = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & \ldots & 1 & 1 \\ \vdots & \ddots & \vdots & \vdots \\ 1 & -1 & \cdots & -1 \end{pmatrix}$ and $C$ represents $-q \leq y$. The polynomials $p_1$ and $p_2$ are given in $[7]. \ \tilde{\sigma}_0 = (\sigma_0 - \sigma_{01} \sigma_{11} \sigma_{10})/K$, $\sigma_0$ is the variance of the first coordinate of $X_1$, $\sigma_{11}$ is the variance of the last $d-1$ coordinates of $X_1$, and $\sigma_{01}$ is their covariance. $\mu = \sigma_{01} \sigma_{11} A_0'$ where $A_0'$ is the vector of the last $d-1$ coordinates of $A_0$. $\phi_{\tilde{\sigma}}(\cdot)$ is the density of $N(0, \sigma)$.

Output: An unbiased estimator of $c$ in $[6]$ given by $ER$.
\[
\lambda' = 2 \sum_i \left[ u_i \beta_i \right] \left( \sum_{j=1}^{d} v_{ij} (B_{i,j} + A_{0,j}) - \sum_{j=1}^{d} v_{1j} A_{0,j} \right) = 4 \sum_i \left[ u_i \beta_i \right] \sum_{j=1}^{d} v_{1j} B_{i,j}.
\]

This gives all polynomials required by Steps 2 and 3 of Algorithm 1.

We also point out that when \( K = 2 \), the proposed algorithm may not work for batching, although in this case the error of batching has a valid expansion by Theorem 1. This is described in the next proposition.

**Proposition 2.** Consider the same setting as in Proposition 1. In this case, Algorithm 1 does not give the correct coefficient of the \( n^{-1} \) coverage error term of batching.

For batching (only), we can use an alternative algorithm that leverages Theorem 1. This algorithm, which is detailed in Appendix C, works regardless of the value of \( K \). When \( K \geq 5 \), both this algorithm and Algorithm 1 would give unbiased estimators for the coefficient of \( n^{-1} \) error term, but Algorithm 1 would have a smaller variance due to the conditioning argument in its construction.

### 7 Asymptotic coverages as number of batches grows

We close our theoretical developments with a discussion on the behaviors of batching methods when the number of batches \( K \) grows. For a general \( \psi(\cdot) \) and distribution \( P \), we have the following theorem regarding the asymptotic as \( K \to \infty \) when the number of samples in each batch is fixed:

**Theorem 7** (Asymptotic coverages as number of batches grows). Suppose that we are under the setting introduced in Section 3. In particular, we have i.i.d. data \( X_1, \ldots, X_{nK} \) drawn from \( P \). Suppose that \( \psi(\cdot) \) is continuously Gateaux differentiable at \( P \) with influence function \( IF \). Suppose that \( E\psi(\hat{P}_1) - \psi \neq 0 \) (i.e., \( \psi(\hat{P}_1) \) is a biased estimator of \( \psi \)), \( \text{Var}(\psi(\hat{P}_1)) < \infty \), and \( \text{Var}_P IF = \sigma^2, 0 < \sigma < \infty \). Fix \( n \) and let \( K \to \infty \). Then for any \( q > 0 \),

\[
P(-q \leq W_B \leq q) \to 0,
\]

\[
P(-q \leq W_S \leq q) \to \Phi \left( q \sqrt{nE(\psi(\hat{P}_1) - \psi)^2/\sigma} \right) - \Phi \left( -q \sqrt{nE(\psi(\hat{P}_1) - \psi)^2/\sigma} \right),
\]

while

\[
P(-q \leq W_{SJ} \leq q) \to \Phi(q) - \Phi(-q).
\]

Theorem 7 implies that when \( K \) is large, batching has a significant bias which could lead to an extremely small coverage. The sectioning statistic converges in distribution to a limit that is not standard normal, so its asymptotic coverage is different from the nominal level. In contrast, the SJ statistic converges to the standard normal, so SJ is the only method among all considered ones that is consistent in this regime. This observation is also consistent with the numerical findings in Nakayama [2014], who considers \( K = 10 \) and \( K = 20 \) and observes severe under-coverage for batching when \( K = 20 \) in some examples.

Finally, suppose we fix the total number of data and let \( K \) increases. In this case, for sectioning and batching, the performance could be bad because the number of data in each batch could be extremely small. On the other hand, SJ it reduces to a usual jackknife. So SJ is evidently superior in this case.

### 8 Numerical results

In this section, we run experiments to validate our expansions. Moreover, based on the coefficients of the \( n^{-1} \) error term and the derived theoretical coverage probabilities, we investigate the coverage performances of our considered batching methods and in terms of the number of batches in two regimes: when the number of data in each batch is fixed, and when the total data size is fixed.
8.1 Validation of expansions and simulation algorithm

In this subsection, we validate the correctness of our expansions and Algorithm 1 by comparing the theoretical with the actual coverage probabilities. Moreover, we investigate the effect of the number of batches on coverage error and compare different batching methods. We consider smooth function models where we want to construct a CI for $f(EX)$. In what follows, we present the numerical findings for different choices of $f$ and the distribution of $X$.

8.1.1 Normal

Consider the model $f(EX)$ where $X \sim N(0, 1)$ and $f(x) = x + x^2$. We estimate both the coverage errors given by our theoretical expansion and empirical experiments. Recall that $c$ is the coefficient for the $n^{-1}$ error term defined in (6). For the theoretical coverage probabilities, we first estimate $c$ via $10^4$ replications of Algorithm 1. Then an estimate of the theoretical coverage is given by the nominal level plus $cn^{-1}$. On the other hand, the actual coverage probabilities are estimated via $10^6$ experimental repetitions, where in each repetition we generate a new data set and compute the CI, and at the end we estimate the empirical coverages by taking the proportions of times where the CI covers the truth.

Figure 1 shows the result with a fixed number of samples per batch $n = 30$, and the number of batches $K$ ranging from 2 to 30 (note that although Theorem 6 requires $K \geq 5$ in general, for this example we also have the validity of expansion for $K = 2, 3, 4$). We see that for each batching method, the estimated theoretical coverage probabilities are close to the estimated actual coverage probabilities. This validates the correctness of our estimation for the error. When $K$ becomes large, the coverage probability of batching decreases quickly, while SJ has the smallest error among the four methods. For example, when the nominal level is 80% and $K = 30$, the estimated coverage probability of batching is only about 70%, which is 10% smaller than the nominal level, while SJ has the smallest error. On the other hand, when $K$ is small, this observation does not hold. In fact, when $K \leq 5$, batching has the smallest error while SJ has the largest error, which is exactly the opposite of the observation when $K$ is large. In addition, we observe that the critical value of $K$ where the comparison among methods changes depends on the nominal level: When the nominal level is 80%, batching has the largest coverage error when $K = 10$; however, when the nominal level is 95%, batching still has the smallest coverage error when $K = 10$. Moreover, we can see that for each method, the theoretical coverage (and thus the coefficient $c$) is not monotone in $K$. For example, when the nominal level is 95%, none of the curves is monotonically increasing or decreasing.

![Figure 1](image_url)

**Figure 1:** Theoretical and actual coverage probabilities for the model in Section 8.1.1. BT, ST, SBT, and SJT represents the estimated theoretical coverage probabilities of batching, sectioning, SB, and SJ, respectively. BA, SA, SBA, and SJA represents the estimated actual coverage probabilities of batching, sectioning, SB, and SJ, respectively.

8.1.2 Exponential and chi-square

Consider the model $\psi(P) = f(EBX, EBY)$. Let $X \sim exp(1)$, $Y \sim \chi^2_1$ and they are independent under the true distribution $P$. Let $f(x, y) = x + 2y + y^2 + x^3$. This is an example where the samples
are multidimensional with non-normal distribution. The cumulants are given by (note that there are no cross-cumulants by independence)

\[\kappa_2(X) = 1, \kappa_3(X) = 2, \kappa_4(X) = 6, \kappa_2(Y) = 1, \kappa_3(Y) = 2\sqrt{2}, \kappa_4(Y) = 12\]

We use \(4 \times 10^4\) replications of Algorithm 1 to estimate the theoretical coverage probabilities, and \(10^6\) experimental repetitions to estimate the actual coverage probabilities. We set \(n = 30\) and let \(K\) range from 4 to 30. The results are shown in Figure 2. The estimated theoretical coverage probabilities are again close to the actual coverage probabilities, although the differences appear slightly larger than the first example where the data is exactly normal. The increased differences are probably due to the need to estimate the error term induced by the non-normality of the underlying distribution. When \(K\) is large, we observe that SJ has the smallest coverage error. In comparison, batching has more significant under-coverage, while sectioning and SB have significant over-coverage issues. For example, when the nominal level is 80\%, the estimated coverage probability of batching is around 77\%, the estimated coverage probabilities of sectioning and SB are above 82\%, while the estimated coverage probability of SJ is close to the nominal level. But as in the previous example, this observation may not hold when \(K\) is small. For example, when the nominal level is 95\% and \(K = 5\), the estimated coverage probability of batching, sectioning and SB are between 94.75\% and 95\%, while the estimated coverage probability of SJ is smaller than 94.75\%, indicating that SJ has the largest error in this case.

**Figure 2:** Theoretical and actual coverage probabilities for the model in Section 8.1.2. The definitions of BT, ST, etc are the same as in Figure 1.

### 8.1.3 Normal and its square

Again consider the model \(\psi(\bar{P}) = f(E_P X, E_P Y)\). Let \(X \sim N(0, 1)\), \(Y = \frac{X^2 - 1}{\sqrt{2}}\) under the true distribution \(P\), and let \(f(x, y) = \sin(x + y^2)\). This is an example where the coordinates of the samples are dependent and \(f\) is not a polynomial. The joint cumulants can be computed as follows:

\[\kappa(X, X) = \kappa(Y, Y) = 1, \kappa(X, Y) = 0\]

\[\kappa(X, X, X) = \kappa(X, Y, Y) = 0, \kappa(X, X, Y) = \sqrt{2}, \kappa(Y, Y, Y) = 2\sqrt{2}\]

\[\kappa(X, X, X, Y) = \kappa(X, Y, Y, Y) = 0, \kappa(X, X, Y, Y) = 4, \kappa(Y, Y, Y, Y) = 12\]

Other setups are the same as the previous example. The results are shown in Figure 3. Again, the actual coverage probabilities are close to the estimated theoretical coverage probabilities. In this example, when \(K\) is large, we also observe that SJ has the smallest error and batching has significant under-coverage issues, which is consistent with the findings in the previous two examples. A difference with the previous examples is that, for sectioning, SB, and SJ, the coverage probabilities do not change much when \(K\) changes, which can be seen since the curves for these methods are close to horizontal.
8.2 Coverage error comparisons when fixing total data size

We investigate the coverage error when the total data size $N$ is fixed and $K$ changes. In this case, the number of data in each section is $N/K$ which will become smaller when $K$ is larger. We consider $N = 1000$ and $K$ ranges from 4 to 30. Since $N/K > 30$ which is large, we expect our asymptotic approximation to be accurate and estimate the coverage probability by the nominal level plus $c(N/K)^{-1}$. We consider the models in Section 8.1. The results are plotted in Figure 4. When $K$ is large, we observe a similar trend as in Section 8.1: SJ has the smallest coverage error, sectioning and SB have over-coverage issues, while batching has under-coverage issues. When $K$ is smaller, the coverage probabilities of all methods are close to the nominal level. This can be attributed to that when $K$ is small, there are sufficient samples in each section which makes the coverage error small.

8.3 Non-monotonicity of coverage errors in number of batches

Lastly, we also investigate the trend of the coefficient when fixing total data size (i.e., $Kc$). In general, the coefficient does not exhibit monotonicity behavior as $K$ increases. This can be seen from the estimated error coefficients reported in Table 1 which contains two experiments with different setups. In particular, from Experiment 1, we can see that the error coefficient of batching increases when $K$ goes from 5 to 7, and then decreases as $K$ increases from 7. The error coefficient of sectioning decreases when $K$ goes from 5 to 7, and then increases as $K$ increases from 7. The error coefficient of SB decreases when $K$ increases from 5 to 9, and then increases as $K$ increases from 9. So we conclude that the error coefficients of batching, sectioning and SB are not monotone. In Experiment 1, the error coefficient of SJ keeps decreasing as $K$ increases from 5 to 7, but in Experiment 2, we see that the coefficient of SJ increases as $K$ increases from 5 to 7. Therefore, the error coefficient of SJ is also not monotone in a particular direction.

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Figure 4: Theoretical coverage probabilities when \( N \) is fixed. (a)-(c), (d)-(f), and (g)-(i) correspond to the models in Sections 8.1.1, 8.1.2, and 8.1.3 respectively. The definitions of BT, ST, etc are the same as in Figure 1.
Table 1: Estimated error coefficients. Here $c_B$ represents the coefficient of the $n^{-1}$ coverage error term for batching as defined in [6] where we added subscript “B” to highlight its dependence on the method used. $c_S, c_{SJ}, c_{SB}$ are defined similarly. “CI” represents the half width of a 95% CI for the target quantity.

Experiment 1: $f(x) = x + x^2, X \sim N(0, 1)$, nominal level = 95%

|   | $K_{c_B}$ | CI-B | $K_{c_S}$ | CI-S | $K_{c_{SJ}}$ | CI-SJ | $K_{c_{SB}}$ | CI-SB |
|---|---------|-----|-----------|-----|------------|-------|-------------|-------|
| 5 | -0.383  | 0.008 | -1.088    | 0.014 | -1.368     | 0.016 | -1.207      | 0.015 |
| 6 | -0.266  | 0.011 | -1.209    | 0.016 | -1.613     | 0.014 | -1.423      | 0.017 |
| 7 | -0.246  | 0.015 | -1.251    | 0.019 | -1.795     | 0.013 | -1.532      | 0.019 |
| 8 | -0.335  | 0.019 | -1.233    | 0.022 | -1.917     | 0.012 | -1.611      | 0.022 |
| 9 | -0.592  | 0.023 | -1.157    | 0.025 | -2.014     | 0.012 | -1.673      | 0.026 |
|10 | -1.051  | 0.028 | -1.076    | 0.029 | -2.085     | 0.011 | -1.651      | 0.028 |
|11 | -1.628  | 0.030 | -0.911    | 0.033 | -2.143     | 0.011 | -1.639      | 0.032 |
|12 | -2.523  | 0.037 | -0.792    | 0.036 | -2.197     | 0.010 | -1.580      | 0.035 |
|13 | -3.559  | 0.041 | -0.626    | 0.039 | -2.244     | 0.010 | -1.520      | 0.038 |
|14 | -4.805  | 0.045 | -0.409    | 0.041 | -2.277     | 0.009 | -1.407      | 0.039 |
|15 | -6.273  | 0.050 | -0.207    | 0.044 | -2.305     | 0.009 | -1.299      | 0.040 |
|16 | -7.974  | 0.059 | 0.007     | 0.045 | -2.339     | 0.009 | -1.221      | 0.045 |
|17 | -9.854  | 0.062 | 0.308     | 0.045 | -2.355     | 0.009 | -1.055      | 0.046 |
|18 | -11.956 | 0.068 | 0.514     | 0.049 | -2.376     | 0.008 | -0.951      | 0.046 |
|19 | -14.347 | 0.074 | 0.774     | 0.051 | -2.398     | 0.008 | -0.798      | 0.047 |
|20 | -16.858 | 0.082 | 1.052     | 0.051 | -2.415     | 0.008 | -0.634      | 0.049 |
|21 | -19.538 | 0.090 | 1.352     | 0.052 | -2.427     | 0.008 | -0.495      | 0.055 |
|22 | -22.580 | 0.098 | 1.580     | 0.053 | -2.438     | 0.008 | -0.317      | 0.052 |
|23 | -25.873 | 0.105 | 1.812     | 0.058 | -2.447     | 0.008 | -0.143      | 0.053 |
|24 | -29.338 | 0.115 | 2.099     | 0.059 | -2.461     | 0.007 | 0.017       | 0.056 |
|25 | -33.002 | 0.123 | 2.463     | 0.057 | -2.473     | 0.007 | 0.159       | 0.055 |
|26 | -36.867 | 0.133 | 2.781     | 0.059 | -2.477     | 0.007 | 0.358       | 0.060 |
|27 | -41.014 | 0.144 | 3.040     | 0.059 | -2.485     | 0.007 | 0.574       | 0.057 |
|28 | -45.427 | 0.151 | 3.350     | 0.059 | -2.488     | 0.007 | 0.770       | 0.058 |
|29 | -49.949 | 0.166 | 3.611     | 0.063 | -2.500     | 0.007 | 0.926       | 0.059 |
|30 | -54.900 | 0.174 | 3.862     | 0.062 | -2.504     | 0.007 | 1.132       | 0.058 |

Experiment 2:

$f(x) = x_1 + x_2 + x_3 - 0.4x_1^2 - 0.06x_1x_2 - 2.13x_2^2 + 1.6x_3^2 - 1.79x_1^3 - 0.84x_1^2x_2 + 0.5x_1x_2^2 - 1.25x_3^3, X \sim N(0, I_3)$, nominal level = 80%.

|   | $K_{c_{SJ}}$ | CI-SJ |
|---|-------------|-------|
| 5 | -0.87       | 0.015 |
| 6 | -0.786      | 0.013 |
| 7 | -0.74       | 0.012 |
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A  Explicit Coverage Error Expansions for Simple Examples

Suppose that $K = 2$, $\psi(P) = f(E_P X) := E_P X + \lambda \left( E_P X \right)^2$ and $P_0$ is standard normal. In this case, the batched estimates are $\psi(P_i) = f(\hat{E}_{P_i} X) \overset{d}{=} f(\frac{1}{n}U_i)$ where $U_i \sim N(0, 1)$). For this model, the higher-order coverage errors can be computed explicitly via the following lemma.

Lemma 8. With the model introduced above, the higher-order coverage errors for batching, sectioning, SB and SJ can be expressed as

\begin{align*}
    &P(-q \leq W_B \leq q) - P(-q \leq t_1 \leq q) = \frac{\lambda^2}{n} \left( -q \left( q^2 - 1 \right)^2 \left( \frac{1}{q^2 + 1} \right)^4 \pi \right) + O(n^{-3/2}), \\
    &P(-q \leq W_S \leq q) - P(-q \leq t_1 \leq q) = \frac{\lambda^2}{n} \left( -q^5 \left( \frac{1}{q^2 + 1} \right)^3 \frac{4}{\pi} + q \left( \frac{1}{q^2 + 1} \right)^2 \frac{1}{\pi} \right) + O(n^{-3/2}), \\
    &P(-q \leq W_{SB} \leq q) - P(-q \leq t_1 \leq q) = \frac{\lambda^2}{n} \left( -q^5 \left( \frac{1}{q^2 + 1} \right)^3 \frac{4}{\pi} \right) + O(n^{-3/2}), \\
    &P(-q \leq W_{SJ} \leq q) - P(-q \leq t_1 \leq q) = \frac{\lambda^2}{n} \left( -q(q^2 + 1)^{-1} \frac{4}{\pi} \right) + O(n^{-3/2}).
\end{align*}

Proof. The test statistic for batching can be expressed as

\begin{align*}
    W_B = \sqrt{nK} \left( \frac{f\left( \frac{1}{\sqrt{n}} U_1 \right) + f\left( \frac{1}{\sqrt{n}} U_2 \right)}{2} \right) = \sqrt{\frac{2}{\pi}} \frac{\lambda}{\sqrt{n}} \left( \frac{U_1 + U_2}{2} \right),
\end{align*}

Denote $A_0 = \sqrt{\frac{U_1 + U_2}{2}}$ and $A_1 = \sqrt{\frac{U_1 - U_2}{2}}$ (note that they are independent). Then from the above,

\begin{align*}
    W_B = \frac{A_0 + \frac{\lambda}{\sqrt{2\sqrt{n}}} \left( A_0^2 + A_1^2 \right)}{|A_1| \sqrt{\left( 1 + \frac{\lambda}{\sqrt{n}} A_0 \right)^2}} = \frac{A_0 + \frac{\lambda}{\sqrt{2\sqrt{n}}} \left( A_0^2 + A_1^2 \right)}{|A_1| \left( 1 + \frac{\lambda}{\sqrt{n}} A_0 \right)}
\end{align*}

Here the second equality holds as long as $1 + \frac{\lambda}{\sqrt{n}} A_0 > 0$ which happens with probability $1 - O(e^{-n})$. Based on this expression for $W_S$, we study the event $W_B \leq q$:

\begin{align*}
    W_B \leq q \iff A_0 + \frac{\lambda}{\sqrt{2\sqrt{n}}} \left( A_0^2 + A_1^2 \right) \leq q \left| A_1 \right| \left( 1 + \frac{\lambda}{\sqrt{n}} A_0 \right)
\end{align*}

which is a quadratic function in $A_0$. It can be equivalently written as

\begin{align*}
    A_0 + \frac{\lambda}{\sqrt{2\sqrt{n}}} \left( A_0^2 - 2q |A_1| A_0 \right) \leq q |A_1| - \frac{\lambda}{\sqrt{2\sqrt{n}}} A_1^2
\end{align*}
We want to write the above as \( A_0 < V + O(n^{-3/2}) \) for some critical value \( V \) that is independent of \( A_0 \). From the above inequality, \( V \) satisfy

\[
V = q |A_1| + O_p(n^{-1/2}) =: q |A_1| + V_1
\]

for some \( V_1 = O_p(n^{-1/2}) \). Plugging this in (12) and solving for \( V \), we get

\[
V_1 = (q^2 - 1) \frac{A_1^2}{\sqrt{2\sqrt{n}}} + O(n^{-1}) =: (q^2 - 1) \frac{A_1^2}{\sqrt{2\sqrt{n}}} + V_2.
\]

Again, by plugging this in (12) and solving for \( V \), we have that \( V_2 \) satisfy

\[
V_2 = 0 + O_p(n^{-3/2}).
\]

So as a conclusion, with exponentially small error, \( W_B \leq t \iff A_0 \leq q |A_q| + (q^2 - 1) \frac{A_1^2}{\sqrt{2\sqrt{n}}} + O_p(n^{-3/2}) \). Similarly, \( W_B \geq -q \iff A_0 \geq -q |A_1| + (q^2 - 1) \frac{A_1^2}{\sqrt{2\sqrt{n}}} + O_p(n^{-3/2}) \). Based on this, for the coverage error we have

\[
P(-q \leq W_B \leq q) = P(-q \leq A_0 \leq q |A_q| + (q^2 - 1) \frac{A_1^2}{\sqrt{2\sqrt{n}}} + O_p(n^{-3/2}) \]

\[
- P(-q \leq A_0 \leq q |A_q|) + O(n^{-3/2})
\]

\[
= E_{A_1} \left[ \Phi \left[ q |A_1| + (q^2 - 1) \frac{A_1^2}{\sqrt{2\sqrt{n}}} \right] - \Phi \left[ -q |A_1| + (q^2 - 1) \frac{A_1^2}{\sqrt{2\sqrt{n}}} \right] \right] + O(n^{-3/2})
\]

\[
= E_{A_1} \left[ -\phi(q |A_1|) \frac{q^2 (q^2 - 1)^2}{2n} A_1^5 \right] + O(n^{-3/2})
\]

\[
= \frac{\lambda^2}{\sqrt{2\pi}} n \left[ -\frac{q (q^2 - 1)^2}{2} \left( \frac{1}{q^2 + 1} \right)^{3/4} \mu_5 \right] + O(n^{-3/2})
\]

\[
= \frac{\lambda^2}{n} \left[ -q (q^2 - 1)^2 \left( \frac{1}{q^2 + 1} \right)^{3/4} \pi \right] + O(n^{-3/2}).
\]

Here in the second equality, we condition on \( A_2 \) first and use that \( A_0 \) and \( A_1 \) are independent standard normals. Also \( \mu_i \) is the \( i \)-th absolute moment of the standard normal. So we have shown (8).

For sectioning, we can do a similar computation

\[
W_S = \frac{A_0 + \frac{\lambda}{\sqrt{2\sqrt{n}}} A_0^2}{|A_1| \sqrt{\left( 1 + \frac{\lambda A_1^2}{\sqrt{2\sqrt{n}}} A_0 \right) + \frac{\lambda^2 A_1^2}{2n} + |A_1| \left( 1 + \frac{\lambda A_1^2}{\sqrt{2\sqrt{n}}} \right) \left( 1 + \frac{\lambda^2 A_1^2}{4n} \right)}} + O_p(n^{-3/2}).
\]

and

\[
W_S \leq q \iff A_0 + \frac{\lambda}{\sqrt{2n}} (A_0^2 - 2q |A_1| A_0) \leq q |A_1| + q |A_1| \frac{\lambda^2 A_1^2}{4n}.
\]

After some algebra, we get

\[
W_S \leq q \iff A_0 \leq q |A_1| + \frac{\lambda}{\sqrt{2n}} q^2 A_1^2 + q |A_1| \frac{\lambda^2 A_1^2}{4n} + O_p(n^{-3/2})
\]

and

\[
W_S \geq -q \iff A_0 \geq -q |A_1| + \frac{\lambda}{\sqrt{2n}} q^2 A_1^2 - q |A_1| \frac{\lambda^2 A_1^2}{4n} + O_p(n^{-3/2}).
\]
Then we have that
\[
P(-q \leq W_S \leq q) = P\left(-q |A_1| + q^2 \frac{\sqrt{2 \sqrt{n} A_i^2}}{2n} \leq A_0 \leq q |A_1| + q^2 \frac{\sqrt{2 \sqrt{n} A_i^2}}{2n}\right) + O(n^{-3/2})
\]
\[
= E_{A_1} \left[ \Phi \left(q |A_1| + q^2 \frac{\sqrt{2 \sqrt{n} A_i^2}}{2n}\right) - \Phi \left(-q |A_1| + q^2 \frac{\sqrt{2 \sqrt{n} A_i^2}}{2n}\right) \right] + O(n^{-3/2})
\]
\[
= E_{A_1} \left[ \Phi (q |A_1|) - \Phi (-q |A_1|) + \frac{\lambda^2}{n} \phi (q |A_1|) \left(-q^5 |A_1|^5 \frac{1}{2} + \frac{1}{2} q |A_1|^3\right) \right] + O(n^{-3/2})
\]
Here the second equality follows by conditioning on $A_1$. Thus, the coverage error of sectioning is given by
\[
P(-q \leq W_S \leq q) - P(-q \leq t_1 \leq q) = E_{A_1} \left[ \frac{\lambda^2}{n} \phi (q |A_1|) \left(-q^5 |A_1|^5 \frac{1}{2} + \frac{1}{2} q |A_1|^3\right) \right] + O(n^{-3/2})
\]
\[
= \frac{\lambda^2}{n} \left(-q^5 \frac{1}{n} + \frac{1}{\pi} + q \frac{1}{n} \right) + O(n^{-3/2})
\]
so (9) is proved. The algebra for SB is quite similar to sectioning. Starting from the following expression for the sectioning statistic:
\[
W_{SB} = \frac{A_0 + \frac{\lambda}{\sqrt{2 \sqrt{n} A_0}} A_i^2}{|A_1| \sqrt{1 + \frac{\sqrt{2 \sqrt{n} A_0}}{|A_1|}^2}}
\]
We can do similar computations as above and get (10). For SJ, we have
\[
W_{SJ} = \frac{A_0 + \frac{\lambda}{\sqrt{2 \sqrt{n} A_0}} (A_i^2 - A_i^2)}{|A_1| \sqrt{1 + \frac{\sqrt{2 \sqrt{n} A_0}}{|A_1|}^2}}
\]
It follows that
\[
P(-q \leq W_{SJ} \leq q) = P(-q |A_1| + (q^2 + 1) \frac{\lambda}{\sqrt{2n} A_i^2} \leq A_0 \leq q |A_1| + (q^2 + 1) \frac{\lambda}{\sqrt{2n} A_i^2})
\]
which leads to (11).}

Lemma 8 indicates that these three methods have different higher-order coverage errors. More specifically, their leading term ($n^{-1}$ order term) in the error expansion is different. When $q \geq 1$ (which is usually the case; since 1 is the 75-percentile of the $t_1$ distribution), the RHS of each of (8)-(11) is negative, which implies that the actual coverage probability is smaller than the nominal coverage probability. With a little algebra, we can show that the RHS of (11) < RHS of (10) < RHS of (9) < RHS of (8) < 0. Thus, batching has the smallest higher-order coverage error and SJ has the largest higher-order coverage error.

However, if the underlying distribution is not normal, then we also need to consider the error induced by that. The joint density of $(\sqrt{n}X_1, \sqrt{n}X_2)$ admits an Edgeworth expansion where the coefficients are determined by the cumulants of $X$. For simplicity, consider the case when $EX^3 = EX = 0$ and $VarX = 1$. Let $\kappa_4 = EX^4 - 3$ be the 4-th cumulant. Then the density of $\sqrt{n}X_1$ has Edgeworth expansion $p_{X_1}(x) = \phi(x)(1 + \frac{1}{2\pi} \kappa_4 H_{e_4}(x)) + O(n^{-3/2})$. Here $H_{e_4}$ is the 4-th Hermite polynomial given by $H_{e_4}(x) = x^4 - 6x^2 + 3$.

Noting that all of $W_B, W_S, W_{SB}$ and $W_{SJ}$ can be expressed as $\frac{X_1 + X_2}{|X_1 - X_2|} + O_p(n^{-1/2})$, we have that the contribution of the error term in the Edgeworth expansion to the coverage error is given by (for both
where \( f(z_1, z_2) = \frac{z_1 + z_2}{|z_1 - z_2|} \). Therefore, the coverage errors become the RHS of (8) + (11) plus the above term. Noting that \( \kappa_4 \) can be positive or negative, we have that after adding the above term, it could be the case that 0 < RHS of (11) + (13) < (10) + (13) < RHS of (8) + (13) < RHS of (8) + (13). If this is the case, then the coverage error of SJ is the smallest.

### B Expansions for Other Schemes

In this section, we do Steps 2 and 3 of Algorithm 1 for SJ, batching, and SB. We will continue to use the notations introduced in Section 6.

#### B.1 Sectioned jackknife

We know that

\[
W_{SJ} = \frac{\sqrt{nK} (\bar{J} - \psi_0)}{\sqrt{\frac{1}{K-1} \sum_i (\sqrt{n} J_i - \sqrt{n} \bar{J})^2}}
\]

where

\[
J_i = K f(\bar{X}) - (K - 1) f \left( \frac{K \bar{X} - \bar{X}_i}{K - 1} \right)
\]

\[
= K f(m + n^{-1/2} A_0) - (K - 1) f \left( \frac{K (m + n^{-1/2} A_0) - (m + n^{-1/2} (A_0 + B_i))}{K - 1} \right)
\]

\[
= K f(m + n^{-1/2} A_0) - (K - 1) f \left( m + n^{-1/2} \left( A_0 - \frac{B_i}{K - 1} \right) \right)
\]

\[
= f_0 + K \left( n^{-1/2} [u, A_0] + n^{-1} [v, A_0, A_0] + n^{-3/2} [w, A_0, A_0, A_0] \right)
\]

\[
- (K - 1) \left( n^{-1/2} [u, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}] + n^{-3/2} [w, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}] \right)
\]

\[
= f_0 + n^{-1/2} [u, A_0 + B_i] + n^{-1} \left( K[v, A_0, A_0] - (K - 1)[v, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}] \right)
\]

\[
+ n^{-3/2} \left( K[w, A_0, A_0] - (K - 1)[w, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}] \right)
\]

and

\[
\bar{J} = \frac{1}{K} \sum_i J_i
\]

\[
= f_0 + n^{-1/2} [u, A_0] + n^{-1} \left( K[v, A_0, A_0] - \frac{K - 1}{K} \sum_i [v, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}] \right)
\]

\[
+ n^{-3/2} \left( K[w, A_0, A_0] - \frac{K - 1}{K} \sum_i [w, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}] \right)
\]
Therefore,
\[
\sum_{i=1}^{K} (\sqrt{n}J_i - \sqrt{n}J)^2
\]
\[
= \sum_{i=1}^{K} \left( [u, B_i] - n^{-1/2} \left[ (K - 1)[v, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}] - \frac{K - 1}{K} \sum_i [v, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}] \right] \right)^2
\]

The coefficient for \( n^{-1/2} \) is
\[
\lambda = -2 \sum_i [u, B_i] \left[ (K - 1)[v, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}] \right]
\]

The coefficient for \( n^{-1} \) is
\[
e = -2 \sum_i [u, B_i] (K - 1)[w, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}]
+ \sum_i \left( (K - 1)[v, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}] - \frac{K - 1}{K} \sum_i [v, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}] \right)^2
\]

We also have that \( a = [u, A_0], b_1 = K[v, A_0, A_0] - \frac{K - 1}{K} \sum_i [v, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}] = [v, A_0, A_0] - \frac{1}{K(K - 1)} \sum_i [v, B_i, B_i], \)

\[
b_2 = K[w, A_0, A_0] - \frac{K - 1}{K} \sum_i [w, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}, A_0 - \frac{B_i}{K - 1}]
\]

\[
b_1' = 2v_{11}A_{0,1} + 2 \sum_{j=2}^{d} v_{1j}A_{0,j} = 2 \sum_{j=1}^{d} v_{1j}A_{0,j}
\]

\[
\lambda' = -4(K - 1) \sum_i [u, B_i] \left( \sum_{j=1}^{d} v_{1j}(A_{0,j} - \frac{B_{i,j}}{K - 1}) - \sum_{j=1}^{d} v_{1j}A_{0,j} \right) = 4 \sum_i [u, B_i] \sum_{j=1}^{d} v_{1j}B_{i,j}
\]

We observe that the formulas for \( b_1' \) and \( \lambda' \) are the same as the corresponding formulas for sectioning.

### B.2 Batching

We have that
\[
W_B = \frac{\sqrt{nK} \left( \frac{1}{K} \sum_i f (m + n^{-1/2}X_i) - f_0 \right)}{\sqrt{\frac{1}{K - 1} \sum_{i=1}^{K} \left( \sqrt{n}f (m + n^{-1/2}X_i) - \sqrt{n}f (m + n^{-1/2}X_i) \right)^2}}
\]

Since
\[
f (m + n^{-1/2}X_i) = f_0 + n^{-1/2}[u, A_0 + B_i] + n^{-1}[v, A_0 + B_i, A_0 + B_i]
+ n^{-3/2}[w, A_0 + B_i, A_0 + B_i, A_0 + B_i]
\]

and
\[
\frac{1}{K} \sum_i f (m + n^{-1/2}X_i) = f_0 + n^{-1/2}[u, A_0] + n^{-1} \frac{1}{K} \sum_i [v, A_0 + B_i, A_0 + B_i]
+ n^{-3/2} \frac{1}{K} \sum_i [w, A_0 + B_i, A_0 + B_i, A_0 + B_i],
\]
we have $a = [u, A_0]$,

$$b_1 = \frac{1}{K} \sum_i [v, A_0 + B_i, A_0 + B_i],$$

$$b_2 = \frac{1}{K} \sum_i [w, A_0 + B_i, A_0 + B_i, A_0 + B_i]$$

and the denominator is

$$\sum_i \left( [u, B_i] + n^{-1/2} \left( [v, A_0 + B_i, A_0 + B_i] - \frac{1}{K} \sum_i [v, A_0 + B_i, A_0 + B_i] \right) \right)^2$$

Therefore,

$$\lambda = 2 \sum_i [u, B_i][v, A_0 + B_i, A_0 + B_i]$$

$$e = 2 \sum_i \left[ [u, B_i][w, A_0 + B_i, A_0 + B_i] + ( [v, A_0 + B_i, A_0 + B_i] - \frac{1}{K} \sum_i [v, A_0 + B_i, A_0 + B_i])^2 \right]$$

The expressions for $\lambda'$ and $b_1'$ are the same as for sectioning.

### B.3 Sectioning-batching

Just replace $\lambda$ and $e$ for sectioning with the $\lambda$ and $e$ for batching. Other steps are the same as before.

### C An Alternative Algorithm to Estimate Coefficient of the $n^{-1}$ Error for Batching

For batching (only), we propose an alternative algorithm given in Algorithm 2. It is not hard to see that Theorem 1 along with the Edgeworth expansion given in Section 2.3 of Hall [1992] imply the correctness of Algorithm 2. To illustrate how to use Algorithm 2 and compare with Algorithm 1, we consider the example in Proposition 1. More precisely, consider $f(x, y) = x + \lambda y^2$ where $X, Y \sim N(0, 1)$. Then $A_1 \overset{d}{=} (X, Y)$. The cumulants of $X + \lambda n^{-1/2}Y^2$ are given by

$$\kappa_{1,n} = \lambda n^{-1/2}, \kappa_{2,n} = 1 + 2\lambda^2 n^{-1}, \kappa_{3,n} = O(n^{-3/2}), \kappa_{4,n} = O(n^{-3/2}),$$

so we have $k_{1,2} = \lambda, k_{2,2} = 2\lambda^2$. Therefore,

$$h_1(x) = -\lambda \phi(x), h_2(x) = -x \frac{3}{2} \lambda^2 \phi(x).$$

Then, following Step 3 of Algorithm 2

$$p_1(x) = \lambda x \phi(x), p_2(x) = -\frac{3}{2} \lambda^2 \left(1 - x^2\right) \phi(x).$$

We run both Algorithms 1 and 2 $10^4$ times to estimate the theoretical coverage probabilities. The results are shown in Table 2. When $K = 2$, the estimated coverage probability of Algorithm 1 is 0.495 which is much lower than the estimated coverage probability (0.788), while Algorithm 2 gives a close approximation (0.774). The failure of Algorithm 1 in this case verifies Proposition 2. When $K \geq 3$, Algorithms 1 and 2 have close coverages. Indeed, the differences between the estimated coverage probabilities of the two algorithms are smaller than the corresponding CI half widths. We also observe that when $K \geq 4$, Algorithm 1 has a shorter CI. Note that the CI half width is computed as $1.96 \text{ empirical standard deviation} \sqrt{n_{\text{rep}}}$, where $n_{\text{rep}}$ is the number of replications which is $10^4$ for this example. Therefore, the shorter CI implies that Algorithm 1 has a smaller variance. This can be attributed to that the construction of Algorithm 1 employs a conditioning argument which helps reduce the variance. Another observation is that when $K$ is larger, the differences between the actual coverage probabilities and the estimated coverage probabilities become larger. This is because when $K$ is large, the coverage error of batching is quite large so that the approximation of coverage error via expansion is not accurate in this regime.
Table 2: Estimated coverage probabilities for batching. “Actual” stands for the actual coverage estimated from experimental repetitions. “ Alg 1” and “ Alg 2” stand for the estimated coverage probabilities given by Algorithms 1 and 2 respectively. CI half widths 1 and 2 are the corresponding CI half widths.

| K | Actual | Alg 1 | CI half width 1 | Alg 2 | CI half width 2 |
|---|--------|-------|-----------------|-------|-----------------|
| 2 | 0.788  | 0.495 | 0.024           | 0.774 | 0.007           |
| 3 | 0.765  | 0.742 | 0.013           | 0.730 | 0.008           |
| 4 | 0.742  | 0.710 | 0.006           | 0.715 | 0.009           |
| 5 | 0.717  | 0.685 | 0.006           | 0.684 | 0.010           |
| 6 | 0.695  | 0.649 | 0.005           | 0.644 | 0.011           |
| 7 | 0.673  | 0.617 | 0.005           | 0.619 | 0.012           |
| 8 | 0.652  | 0.585 | 0.005           | 0.590 | 0.013           |
| 9 | 0.632  | 0.555 | 0.005           | 0.561 | 0.014           |
| 10| 0.612  | 0.524 | 0.005           | 0.523 | 0.015           |
| 11| 0.592  | 0.493 | 0.005           | 0.481 | 0.015           |
| 12| 0.573  | 0.468 | 0.006           | 0.450 | 0.016           |
| 13| 0.555  | 0.437 | 0.006           | 0.431 | 0.017           |
| 14| 0.537  | 0.406 | 0.006           | 0.404 | 0.018           |
| 15| 0.520  | 0.376 | 0.006           | 0.378 | 0.019           |
| 16| 0.503  | 0.348 | 0.007           | 0.333 | 0.019           |
| 17| 0.486  | 0.313 | 0.007           | 0.308 | 0.020           |
| 18| 0.471  | 0.289 | 0.007           | 0.281 | 0.021           |
| 19| 0.455  | 0.258 | 0.007           | 0.240 | 0.021           |
| 20| 0.439  | 0.227 | 0.008           | 0.233 | 0.022           |
Algorithm 2 An unbiased simulation scheme to compute coefficient of the $n^{-1}$ error for batching

**Initialization:** derivatives of $f$ at $EX_1$ up to order 3, cumulants of $X_1$ up to order 4, testing statistic $W_B$.

1. Let $A_1 = \sqrt{n}(X_1 - EX_1)/Var([\nabla f, X_1 - EX_1])$. Algebraically compute the cumulants of $[\nabla f, A_1] + n^{-1}[\nabla f, A_1, A_1] + n^{-1}[\nabla f, A_1, A_1, A_1]$ up to order 4 (with residual $O(n^{-3/2})$), in terms of $n$ and the cumulants of $X_1$. Moreover, write the cumulants $\kappa_{i,n}, i=1,2,3,4$ (defined as the cumulants of order 1,2,3,4 respectively) as a series of $n^{-1/2}$: $\kappa_{1,n} = n^{-1/2}k_{1,2}, \kappa_{2,n} = 1 + n^{-1}k_{2,2} + O(n^{-3/2}), \kappa_{3,n} = n^{-1}k_{3,1} + O(n^{-3/2}), \kappa_{4,n} = n^{-1}k_{4,1} + O(n^{-3/2})$.

2. Let $h_1(x) = -\{k_{1,2} + \frac 16 k_{3,1}(x^2 - 1)\} \phi(x)$,

$$h_2(x) = -x\left(\frac 12(k_{2,2} + k_{1,2}^2) + \frac 1{24}(k_{4,1} + 4k_{1,2}k_{3,1})(x^2 - 3) + \frac 1{72}k_{3,1}^2(x^4 - 10x^2 + 15)\right) \phi(x).$$

Here $\phi(\cdot)$ is the pdf of standard normal

3. Let $p_1(x) = h_1'(x)/\phi(x)$ and $p_2(x) = h_2'(x)/\phi(x)$.

4. Generate $Z_1, Z_2, \ldots, Z_K$ i.i.d. from standard normal. Derive the error term estimator:

$$ER_B = IC(Z) \left[ \sum_{1 \leq i < j \leq K} p_1(Z_i)p_1(Z_j) + \sum_{1 \leq i \leq K} p_2(Z_i) \right].$$

Here, $C$ represents the set of $Z = (Z_1, \ldots, Z_K)$ such that $-q \leq \sqrt{K(K-1)} \frac{Z}{\sqrt{\sum_{i=1}^K (Z_i - \bar Z)^2}} \leq q$.

**Output:** An unbiased estimator of $c$ in $[\hat c]$ given by $ER_B$

---

**D Proof of Theorem 2**

*Proof.* We consider sectioned jackknife for example. The analysis for other methods is similar (indeed, easier). Moreover, in this proof we focus on the expansion for coverage of the symmetric CI, i.e., $P(-q \leq W_{SJ} \leq q)$. It will be clear that the proof could be easily adapted to the one-sided setting. We introduce some notations first. Denote $m := E_{\hat A_0} X$ and $A_i := \sqrt{n}(X_i - m)$ where $X_i$ is the $i$-th batch average. Let $A_0 = \frac{A_1 + \cdots + A_K}{K}$. For $1 \leq i \leq K$, let $B_i = A_i - A_0$. Denote $A_{0,j}, 1 \leq j \leq d$ to be the $j$-th coordinate of $A_0$. Define $B_{i,j}, 1 \leq i \leq K, 1 \leq j \leq d$ similarly. Denote $A$ as the $dK$-dimensional vector $(A_0, B_1, B_2, \ldots, B_{K-1})$. Denote $A'$ as the $(dK-1)$-dimensional vector $(A_{0,2}, \ldots, A_{0,d}, B_1, \ldots, B_{K-1})$. Let $\nabla f$ denote the gradient of $f$ at point $EX$.

First, we apply the Edgeworth expansion result in Theorem 20.1 of [Bhattacharya and Rao 2010] to approximate the distribution of batch averages (for the ease of reading, we included the statement of this theorem in Theorem 11, we have that there exist polynomials $p_j(a), 1 \leq j \leq r$, such that (we include more details on this step in Section D.3)

$$P(-q \leq W_{SJ} \leq q) = \hat P(-q \leq W_{SJ} \leq q) + O(n^{-(r+1)/2})$$

(14)

where under $\hat P$, $A_i, 1 \leq i \leq K$ has density $p(x) = \phi_\Sigma(x)(1 + \sum_{i=1}^r n^{-1/2} p_i(x))$ (Note that $p(x)$ can be negative when $n$ is small. In this case, we interpret $\hat P$ as a signed measure.). Here $\phi_\Sigma(x)$ is the limiting normal distribution of $A_i$. In the sequel, unless otherwise mentioned, each statement is under the approximated measure $\hat P$.

Although we have the expansion for the distribution of $A_i$ under $\hat P$, this does not easily imply an expansion for the distribution of $W_{SJ}$. This is because $W_{SJ}$ can not be expressed as a fixed function of $(A_1, A_2, \ldots, A_K)$. Indeed, $\psi(\hat P) = f\left(m + n^{-1/2} \left(\frac{K_0 - A}{K-1}\right)\right)$, which is dependent on $n$ even when each $A_i$ is given. Our way to handle this is to reformulate $-q \leq W_{SJ} \leq q$ as $E_{-}^{(n)} \leq A_{0,1} \leq E_{+}^{(n)}$. In other words,
we regard $W_{S,J}$ as a function of $(n^{-1/2}, A_{0,1}, A')$, and then solve for the possible values of $A_{0,1}$ (given $A'$ and $n^{-1/2}$) that makes $-q \leq W_{S,J} \leq q$. Essentially, this is done by applying the implicit function theorem. Heuristically, this is not difficult. But we will see that to get a valid expansion for $P(-q \leq W_{S,J} \leq q)$, more care must be taken to bound the moments of each term and the residual in the expansion. Let

$$E_2 = \sum_{i=1}^{K} \left( (\nabla f)^	op B_i \right)^2, F_+ = \frac{q\sqrt{E_2}}{\sqrt{K(K-1)}} - \sum_{i=2}^{d} \nabla f_i A_{0,i}, F_- = \frac{-q\sqrt{E_2}}{\sqrt{K(K-1)}} - \sum_{i=2}^{d} \nabla f_i A_{0,i}.$$

As one can check, when $n = \infty$, the expressions of $F_+^n$ and $F_-^n$ would be given by $F_+$ and $F_-$ respectively. The following lemma states that $F_+^n$ and $F_-^n$ have expansion around $F_+$ and $F_-$ and the terms in the expansion have bounded moments.

**Lemma 9.** Suppose that the conditions of Theorem 1 hold. There exist $F_+^n$ and $F_-^n$ (functions of $A'$ and depend on $n$), such that

$$\hat{P} \left( \{-q \leq W_{S,J} \leq q\} \Delta \left\{ F_-^n \leq A_{0,1} \leq F_+^n \right\} \right) = O(n^{-(r+1)/2}).$$

Moreover, the powers $(F_+^n - F_+)^l$ and $(F_-^n - F_-)^l$, $l = 1, 2, \ldots, r + 1$ have expansion

$$\left( F_+^n - F_+ \right)^l = \sum_{m=1}^{r} n^{-m/2} \sqrt{E_2} \frac{p_{l,m}(A')}{E_2} + n^{-(r+1)/2} R_{F,l}$$

where each $p_{l,m}(A')$ is a polynomial of $A'$ and there exist $c > 0$ such that $E \left[ \left| \sqrt{E_2} \frac{p_{l,m}(A')}{E_2} \right|^{1+c} \right] < \infty$, $E \left[ |R_{F,l}|^{1+c} \right] < \infty$. Here, the expectation is taken under the limiting normal distribution of $A'$.

Based on this, we can write $-q \leq W_{S,J} \leq q$ as

$$F_-^n(A_{0,2}, \ldots, A_{0,d}, B_1, \ldots, B_{K-1}) \leq A_{0,1} \leq F_+^n(A_{0,2}, \ldots, A_{0,d}, B_1, \ldots, B_{K-1}).$$

Corresponding to $A = (A_0, B_1, B_2, \ldots, B_{K-1})$, let $a = (a_0, b_1, b_2, \ldots, b_{K-1})$ where each of $a_0, b_1, \ldots, b_{K-1}$ has $d$ coordinates. Corresponding to $A'$, let $a'$ be a with its first coordinate removed, i.e., $a' = (a_0, \ldots, a_{d}, b_1, \ldots, b_{K-1})$. Then, following (14) and a linear transformation argument, we have that there exist $p_{j,A}(a), 1 \leq j \leq r$, such that

$$\hat{P}(-q \leq W_{S,J} \leq q) = \int \phi_{\Sigma}(a) \left( 1 + \sum_{j=1}^{r} n^{-j/2} p_{j,A}(a) \right) da = \int \phi_{\Sigma'}(a') \left[ \int_{F_-^n}^{F_+^n} \phi_{\tilde{a}_0,a_{0,1} - \hat{\mu}_0} \left( 1 + \sum_{j=1}^{r} n^{-j/2} p_{j,A}(a) \right) da_0,1 \right] da'$$

(15)

Here, $\Sigma$ is the variance of $A$, $\Sigma'$ is the variance of $A'$, $\tilde{a}_0$ and $\hat{\mu}_0$ are the conditional variance and expectation of $A_{0,1}$ given $A'$, when $A' = a'$ (under their joint limiting normal distribution), so that we have $\phi_{\Sigma'}(a')\phi_{\tilde{a}_0,a_{0,1} - \hat{\mu}_0} = \phi_{\Sigma}(a)$where $\Sigma$ is covariance of $A = (A_0, B_1, \ldots, B_{K-1})$. For the inner integration, we have the following...
D.1 The error of a symmetric CI is of order $n^{-1}$

Consider sectioning first. Since we have shown the validity of the expansion as a series of $n^{-1/2}$ in the first part, to show that the error is of order $O(n^{-1})$ it suffices to show that the order is of order $o(n^{-1/2})$. With some Taylor expansion arguments as in Section D.2, we can see that $W_S$ is given by

$$W_S = \frac{\nabla f^T \cdot A_0 + \frac{1}{2\sqrt{nK}} A_0^T \left[ \nabla^2 f \right] A_0}{\sqrt{\frac{1}{K-1} \sum_{k=1}^{K} \left( \frac{\nabla f^T \cdot A_k}{\sqrt{K}} \right)^2 \left( 1 + \frac{1}{\sqrt{nK}} (A_k^T c_b + c_a) \right)}} + O_p \left( n^{-1} \right)$$

$$= \frac{\nabla f^T \cdot A_0 + \frac{1}{2\sqrt{nK}} A_0^T \left[ \nabla^2 f \right] A_0}{\sqrt{\frac{1}{K-1} \sum_{k=1}^{K} \left( \frac{\nabla f^T \cdot A_k}{\sqrt{K}} \right)^2 \left( 1 - \frac{1}{2\sqrt{nK}} (A_k^T c_b + c_a) \right)}} + O_p \left( n^{-1} \right).$$ (17)

where $c_a = \frac{\sum_{k=1}^{K} \frac{\nabla f^T B_k}{\sqrt{nK}} B_k}{\sum_{k=1}^{K} \left( \frac{\nabla f^T B_k}{\sqrt{nK}} \right)^2}, c_b = \frac{2 \sum_{k=1}^{K} \frac{\nabla f^T B_k}{\sqrt{nK}} B_k}{\sum_{k=1}^{K} \left( \frac{\nabla f^T B_k}{\sqrt{nK}} \right)^2}$ (both of them are functions of $B_1, \ldots, B_K$)

Denote the above function as $g_n(A_0, B_1, \ldots, B_{K-1})$ (note that $B_K = -(B_1 + \cdots + B_{K-1})$ so we do not need to include $B_K$ as an argument of $g_n$). Since $(A_0, B_1, \ldots, B_{K-1})$ is a linear transformation of the batch averages, and the batch averages have valid Edgeworth expansions, we have that the joint distribution of $A_0, B_1, \ldots, B_{K-1}$ admits a valid multivariate Edgeworth expansion:

$$P((A_0, B_1, \ldots, B_{K-1}) \in B) = \int_B \phi_C(z)(1 + \frac{n^{-1/2} p(z)}{2})d\mathbf{z} + o(n^{-1/2})$$
for all Borel sets $B$. Here $\tilde{\Sigma}$ denotes the covariance of $(A_0, B_1, \ldots, B_{K-1})$, and $p(z)$ is an odd polynomial. For the probability that $-q \leq W_S \leq q$, we have that
\[
P(-q \leq W_S \leq q) = P(-q \leq \frac{g_n}{n} (B_0, B_1, \ldots, B_{K-1}) \leq q) + o(n^{-1/2})
\]
\[
= \int_{-q \leq g_n(z) \leq q} \phi_{\tilde{\Sigma}}(z) + n^{-1/2} \phi_{\tilde{\Sigma}}(z) p(z) \, dz + o(n^{-1/2})
\]
\[
= \int_{-q \leq g_n(z) \leq q} \phi_{\tilde{\Sigma}}(z) \, dz + n^{-1/2} \int_{-q \leq g_n(z) \leq q} \phi_{\tilde{\Sigma}}(z) p(z) + o(n^{-1/2}).
\]

Here $g_\infty(z) = \lim_{n \to \infty} g_n(z) = \sqrt{\frac{f^T \cdot z_0}{\sum_{k=1}^{K} \left( \frac{\sum_{l=1}^{K} f_l Z_l}{\sqrt{K}} \right)^2}}$ and in the last equality above, we used that $g_\infty(z) - g(z) = O(n^{-1/2})$. Also note that $g_\infty$ satisfies $g_\infty(z) = g_\infty(-z)$ so $\int_{-q \leq g_\infty(z) \leq q} \phi_{\tilde{\Sigma}}(z)p(z) = 0$. Hence from the above displayed equality,
\[
P(-q \leq W_S \leq q) = \int_{-q \leq g_n(z) \leq q} \phi_{\tilde{\Sigma}}(z) \, dz + O(n^{-1})
\]
\[
= P(-q \leq t_{K-1} \leq q) + \int_{-q \leq g_n(z) \leq q} \phi_{\tilde{\Sigma}}(z) \, dz - \int_{-q \leq g_\infty(z) \leq q} \phi_{\tilde{\Sigma}}(z) \, dz + O(n^{-1}).
\]  

Here we used $P(-q \leq t_{K-1} \leq q) = \int_{-q \leq g_\infty(z) \leq q} \phi_{\tilde{\Sigma}}(z) \, dz$ since the limiting distribution of $W_S$ is $t_{K-1}$. Now it suffices to study the difference between $P(-q \leq g_n(Z_0, Z_1, \ldots, Z_{K-1}) \leq q)$ and its counterpart as $n \to \infty$ and show that the difference is $o(1/n)$, where $Z_0, Z_1, \ldots, Z_{K-1}$ follows from the limiting normal distribution of $(A_0, B_1, \ldots, B_{K-1})$. In particular, we note that $Z_0$ is independent of $Z_1, \ldots, Z_{K-1}$ since $\text{Cov}(A_0, B_i) = 0$ for each $i = 1, 2, \ldots, K$. For this probability, we can compute it as follows:
\[
P(-q \leq g_n(Z_0, Z_1, \ldots, Z_{K-1}) \leq q) = \int_{-q \leq g_n(z) \leq q} \phi_{\tilde{\Sigma}}(z) \, dz + o(1)
\]
\[
= \int_{-q \leq Z_0 + \frac{1}{2\sqrt{nK}} Z_0^T \left[ \nabla^2 f \right] Z_0 \leq q} \phi_{\tilde{\Sigma}}(z) \, dz + o(1)
\]
\[
= \int_{-q \leq Z_0 + \frac{1}{2\sqrt{nK}} Z_0^T \left[ \nabla^2 f - c_0(Z) \nabla f^T \right] Z_0 \leq q} \phi_{\tilde{\Sigma}}(z) \, dz + o(1)
\]
\[
= \int_{-q \leq Z_0 + \frac{1}{2\sqrt{nK}} \left[ \nabla f \right]^T Z_0 \leq q} \phi_{\tilde{\Sigma}}(z) \, dz + o(1)
\]
Here corresponding to $c_a$ and $c_b$, we let $c_a(Z) = \frac{\sum_{k=1}^{K} \frac{\nabla f^T Z_k}{\sqrt{K}} \left[ \nabla^2 f \right] Z_k}{\sum_{k=1}^{K} \frac{\nabla f^T Z_k}{\sqrt{K}}}$. Conditional on $Z_1, \ldots, Z_{K-1}$ (note that the value of $c_a, c_b$ is determined by $Z_1, \ldots, Z_{K-1}$), by normality of the distribution of $Z_0$ and Edgeworth expansion, we know that the conditional distribution function for $\nabla f^T \cdot Z_0 + \frac{1}{2\sqrt{nK}} Z_0^T \left[ \nabla^2 f - b \nabla f^T \right] Z_0$ can be expanded as $\Phi(q) + n^{-1/2} \tilde{p}_1(q) \phi(q) + O(n^{-1})$ where $\tilde{p}_1$ is even (this evenness claim follows since $\nabla f^T \cdot Z_0 + \frac{1}{2\sqrt{nK}} Z_0^T \left[ \nabla^2 f - b \nabla f^T \right] Z_0$ is a polynomial with the same form...
as Theorem 2.1 of [Hall 1992]. Thus, conditional on $Z_1, \ldots, Z_{K-1}$, the above probability is given as (denote $q' = q \sqrt{ \frac{1}{K-1} \sum_{k=1}^{K} \left( \frac{\nabla f^T \cdot Z_k}{\sqrt K} \right)^2 }$)

$$
\Phi \left( q' \left( 1 + \frac{c_a(Z)}{2\sqrt{nK}} \right) \right) + n^{-1/2} \tilde{p}_1(q') \phi(q') - \Phi \left( -q' \left( 1 + \frac{c_a(Z)}{2\sqrt{nK}} \right) \right) - n^{-1/2} \tilde{p}_1(q') \phi(q') + O(n^{-1})
$$

which is (by the evenness of $\tilde{p}_1$)

$$
\Phi (q') - \Phi (-q') + \phi(q') \frac{c_a(Z)}{\sqrt{nK}} + O(n^{-1}).
$$

Taking expectation w.r.t. $(Z_1, \ldots, Z_{K-1})$ and note that $E[\Phi (q') - \Phi (-q')] = P(-q \leq g_\infty (Z_0, Z_1, \ldots, Z_{K-1}) \leq q)$, we conclude that

$$
P(-q \leq g_n (Z_0, Z_1, \ldots, Z_{K-1}) \leq q) - P(-q \leq g_\infty (Z_0, Z_1, \ldots, Z_{K-1}) \leq q)
$$

$$
= E_{Z_1, \ldots, Z_{K-1}} \left[ \phi(q') \left( 1 + \frac{a}{\sqrt{nK}} \right) \right] + O(n^{-1})
$$

Noting that $a$ is odd (and $q'$ is even) in $Z_1, \ldots, Z_{K-1}$, we have that the expectation is 0, so the above difference is indeed $O(n^{-1})$.

To see that $W_{SB}$ has the same property, notice that

$$
n S_{sec}^2 = n S_{batch}^2 + \frac{K}{K-1} \left( \sqrt{n} \psi (\hat{P}) - \frac{1}{K} \sum_{i=1}^{K} \sqrt{n} \psi (\hat{P}_i) \right)^2 = n S_{batch}^2 + O_p(1)
$$

Here the second equality holds since $\sqrt{n} \psi (\hat{P}) - \frac{1}{K} \sum_{i=1}^{K} \sqrt{n} \psi (\hat{P}_i) = O(n^{-1/2})$, which can be seen by plugging in expansions

$$
\sqrt{n} \left( \psi (\hat{P}_k) - \psi (P_0) \right) = \nabla f^T \cdot A_0 + \frac{1}{2\sqrt{nK}} A_0^T \left[ \nabla^2 f \right] A_0 + O_p \left( n^{-1} \right)
$$

$$
\sqrt{n} (\hat{P}_k - P_0) = \frac{1}{\sqrt K} \nabla f^T (A_0 + B_k) + \frac{n^{-1/2}}{2\sqrt K} (A_0 + B_k)^T \left[ \nabla^2 f \right] (A_0 + B_k) + O_p \left( n^{-1} \right), k = 1, 2, \ldots, K
$$

and using the equation $\sum_{i=1}^{K} B_i = 0$. This implies $W_{SB} = W_S + O_p(n^{-1})$. Since we have shown $P(-q \leq W_S \leq q) = O(n^{-1})$, the same holds for $W_{SB}$.

Next, we consider sectioned jackknife. By examining the expansion for $W_{SJ}$ in Section 13, we have that similar to (17),

$$
W_{SJ} = \frac{\nabla f^T \cdot A_0 + \frac{1}{\sqrt{2nK}} A_0^T \left[ \nabla^2 f \right] A_0 + n^{-1/2} \tilde{c}_d}{\sqrt{\frac{1}{K-1} \sum_{k=1}^{K} \left( \frac{\nabla f^T \cdot A_k}{\sqrt K} \right)^2}} \left( 1 - \frac{1}{2\sqrt{nK}} (A_0^T \tilde{c}_b + \tilde{c}_a) \right) + O_p \left( n^{-1/2} \right),
$$

(19)

where $\tilde{c}_a$ is odd in $(B_1, \ldots, B_K)$ and $\tilde{c}_b, \tilde{c}_d$ are even in $(B_1, \ldots, B_K)$. Compared to sectioning, the difference is that we have a new term $\tilde{c}_d$. Following the argument for sectioning, it suffices to show that the difference between

$$
P \left( \frac{q' - \frac{c_a(Z)}{2\sqrt{nK}}}{1 - \frac{c_a(Z)}{2\sqrt{nK}}} - n^{-1/2} \tilde{c}_d(Z) \leq \nabla f^T \cdot Z_0 + \frac{1}{2\sqrt{nK}} Z_0^T \left[ \nabla^2 f - \tilde{c}_b(Z) \nabla f^T \right] Z_0 \leq \frac{q'}{1 - \frac{c_a(Z)}{2\sqrt{nK}}} - n^{-1/2} \tilde{c}_d(Z) \right)
$$

and $P(-q \leq g_\infty (Z_0, Z_1, \ldots, Z_{K-1}) \leq q)$ is $o(n^{-1/2})$. But note that the above probability is

$$
\Phi \left( q' \left( 1 + \frac{\tilde{c}_b(Z)}{2\sqrt{nK}} \right) - n^{-1/2} \tilde{p}_1(Z) \phi(q') \right)
$$

$$
- \Phi \left( -q' \left( 1 + \frac{\tilde{c}_a(Z)}{2\sqrt{nK}} \right) - n^{-1/2} \tilde{p}_1(Z) \phi(q') \right) - n^{-1/2} \tilde{p}_1(q') \phi(q') + O(n^{-1})
$$

From this, we can see that the contribution of $\tilde{c}_d$ to the $n^{-1/2}$ error is cancelled. Therefore, proceeding as in the proof for sectioning to handle $\tilde{c}_a$, we get the desired result.
D.2 Proof of Lemma 9

First, we give a lemma that helps bound the moments for the inverse of \( E_2 \). The proof is deferred to Section D.2.1

**Lemma 10.** Under our assumptions in Theorem 2, we have that for any \( \epsilon < 1 \), there exists \( c > 0 \) such that
\[
\tilde{E} \left[ E_2^{-(r+1+\epsilon)/2} \right]^{1+c} < \infty.
\]

Then, we give the proof of Lemma 9

**Proof.** Consider \( F^{(n)}_{i} \) for example. Note that when \( W_{S,J} = q \), we have that \( \sqrt{nK} (\hat{J} - \psi_0) = q \sqrt{K^{-1} \sum_{i=1}^{K} (\sqrt{nJ_i} - \sqrt{n}\bar{J})^2} \).

We can do a Taylor expansion for each \( \psi(\hat{P}_{(i)}) = f \left( m + n^{-1/2} \left( \frac{K A_0 - A_i}{K-1} \right) \right) \) and \( \psi(\hat{P}) = f \left( m + n^{-1/2} \left( \frac{K A_0 - A_i}{K-1} \right) \right) \):

\[
\psi(\hat{P}_{(i)}) = \psi_0 + \sum_{m=1}^{r} n^{-m/2} \sum_{1 \leq i_1 \ldots i_m \leq d} \nabla f_{i_1 \ldots i_m}(m) \left( \frac{K A_0 - A_i}{K-1} \right)_{i_1} \ldots \left( \frac{K A_0 - A_i}{K-1} \right)_{i_m} + n^{-(r+1)/2} \sum_{1 \leq i_1 \ldots i_m \leq d} \nabla f_{i_1 \ldots i_m}(\xi) \cdot \left( \frac{K A_0 - A_i}{K-1} \right)_{i_1} \ldots \left( \frac{K A_0 - A_i}{K-1} \right)_{i_{r+1}}
\]

for some \( \xi \) on the line segment between \( m \) and \( m + n^{-1/2} \left( \frac{K A_0 - A_i}{K-1} \right) \). Moreover, the residual \( R \) can be bounded by \( C \sum_{i=0}^{K} \| A_i \| r+1 \) where \( C \) and \( C_i \) in the sequel are constants independent of \( n \). By the continuity of the \( (r+1) \)-th derivative of \( f \), we may pick some \( \delta > 0 \) such that \( \sup_{\|x-m\| \leq \delta} \| \nabla^{r+1} f \| \) is bounded. Note that when \( \left\| n^{-1/2} \left( \frac{K A_0 - A_i}{K-1} \right) - m \right\| \leq \delta \), the last term in the preceding displayed equation can be bounded by \( C n^{-(r+1)/2} \sup_{\|x-m\| \leq \delta} \| \nabla^{r+1} f \| \sum_{i=0}^{K} \| A_i \| r+1 \). Since we assumed that \( X \) has finite \( r+2 \) moments, (by Markov’s inequality) we can show that the probability that this \( \left\| n^{-1/2} \left( \frac{K A_0 - A_i}{K-1} \right) - m \right\| > \delta \) is of order \( O(n^{-(r+1)/2}) \). Therefore, we conclude that with probability \( 1 - O(n^{-(r+1)/2}) \), the residual of the Taylor expansion is bounded by \( C n^{-(r+1)/2} \sum_{i=0}^{K} \| A_i \| r+1 \) for some \( C \) independent of \( n \). Similar expansion holds for \( \psi(\hat{P}) \). With these expansions, notice that each of \( J_i \) and \( \bar{J} \) can be written as linear combinations of \( \psi(\hat{P}_{(i)}) \) and \( \psi(\hat{P}) \), we also have an expansion for them:

\[
J_i = \psi_0 + n^{-1/2} (\nabla f)^T A_i + \sum_{j=2}^{r} n^{-j/2} p_{i,j}(A) + n^{-(r+1)/2} R_i
\]

\[
\bar{J} = \psi_0 + n^{-1/2} (\nabla f)^T A_0 + \sum_{j=2}^{r} n^{-j/2} \bar{p}_{j}(A) + n^{-(r+1)/2} \bar{R}
\]

where each \( p_{i,j}(A) \) is a polynomial in \( A \) of order \( j \), \( R_i \) can be bounded by \( C_1 \sum_{i=0}^{K} \| A_i \| r+1 \) (with probability \( 1 - O(n^{-(r+1)/2}) \)), \( \bar{p}_j \) and \( \bar{R} \) are the average of \( p_{i,j}, R_i, 1 \leq i \leq K \) respectively. Therefore, when \( W_{S,J} = q \) or equivalently \( \sqrt{nK} (\bar{J} - \psi_0) = q \sqrt{\bar{1}/K \sum_{i=1}^{K} (\sqrt{nJ_i} - \sqrt{n}\bar{J})^2} \), we have (using the expansion for \( J_i \) and \( \bar{J} \) above)

\[
\left| \sqrt{K} \left( \nabla f \cdot A_0 + \sum_{j=1}^{r} n^{-\frac{j}{2}} \bar{p}_{j+1}(A) \right) - q \sqrt{\frac{E_2 + \sum_{j=1}^{r} n^{-\frac{j}{2}} p_{j+1}(A) + n^{-\frac{r+1}{2}} R}} \right| \leq n^{-\frac{r+1}{2}} R_3 \tag{20}
\]

where \( E_2 = \sum_{i=1}^{K} \left( (\nabla f)^T (A_i - A_0) \right)^2, p_{j+1}(A) = \sum_{i=1}^{K} (\nabla f)^T (A_i - A_0) q_i(A), q_i(A) \) is a polynomial of \( A \). For each \( j = 3, 4, \ldots, r+1 \), \( p_{j+1}(A) \) is a polynomial of \( A \), and \( |R_2|, |R_3| \) can be bounded by \( C_2 \sum_{i=0}^{K} \| A_i \| r+1 \) (with probability \( 1 - O(n^{-(r+1)/2}) \)).
Observe that
\[ \sqrt{E_2 + \sum_{j=1}^{r} n^{-\frac{j}{2}} p_{j+1}^{(1)}(A) + n^{-\frac{r+1}{2}} R_2} = \sqrt{E_2} \left( 1 + \frac{\sum_{j=1}^{r} n^{-\frac{j}{2}} p_{j+1}^{(1)}(A)}{E_2} + \frac{n^{-\frac{r+1}{2}} R_2}{E_2} \right) \]

By a Taylor expansion for the composition of \( \sqrt{1+x} \) with \( 1 + \frac{\sum_{j=1}^{r} n^{-\frac{j}{2}} p_{j+1}^{(1)}(A)}{E_2} + \frac{n^{-\frac{r+1}{2}} R_2}{E_2} \), we have that the above can be expanded as follows
\[ \sqrt{E_2} \left( 1 + \frac{\sum_{j=1}^{r} n^{-\frac{j}{2}} p_{j+1}^{(1)}(A)}{E_2} + \frac{n^{-\frac{r+1}{2}} R_2}{E_2} \right)^{\frac{n}{2}} \]

Here, \( p_{j+1}^{(2)}(A) \) can be bounded by \( E_2^{\frac{r}{2}} \) times a polynomial of \( A \) and \( R_4 \) can be bounded by \( E_2^{\frac{r+1}{2}} \) times a polynomial of \( A \). (The proof is given in Section D.2.1). Therefore, by Lemma 10, each of \( \frac{\sqrt{E_2}}{E_2^{\frac{r}{2}}} \), \( 1 \leq j \leq r \) and \( \frac{R_4}{E_2^{\frac{r+1}{2}}} \) has finite \( 1 + c \) moment for some \( c > 0 \). Putting (21) into (20), we get that
\[ \sqrt{E_2} \left( \nabla f \cdot A_0 + \sum_{j=1}^{r} n^{-\frac{j}{2}} p_{j+1}(A) \right) - q \sqrt{E_2} \left( 1 + \frac{\sum_{j=1}^{r} n^{-\frac{j}{2}} p_{j+1}^{(2)}(A)}{E_2} \right) \leq n^{-\frac{r+1}{2}} R_3. \]

Therefore, with an error of \( (\frac{1}{\sqrt{R \nabla f}} + o(1)) (n^{-\frac{r+1}{2}} R_3 \) (note that \( E_2 \) does not depend on \( A_{0,1} \) so the leading term for the derivative of \( A_{0,1} \) is \( \sqrt{K \nabla f} \)), we can find the critical value for \( A_{0,1} \) that makes \( W_{s,j} = q \) (i.e., \( F_{+}^{(n)} \)) by solving
\[ \sqrt{K} \left( \nabla f \cdot A_0 + \sum_{j=1}^{r} n^{-\frac{j}{2}} p_{j+1}(A) \right) - q \sqrt{E_2} \left( 1 + \frac{\sum_{j=1}^{r} n^{-\frac{j}{2}} p_{j+1}^{(2)}(A)}{E_2} \right) = 0 \]

Denote the LHS above as \( F(A_{0,1}, n^{-1/2}) \). Observe that \( F(A_{0,1}, n^{-1/2}) \) is a polynomial whose coefficients are determined by \( A' \). We are interested in solving \( A_{0,1} \) as a function of \( n^{-1/2} \) (denote by \( y(x) \)) and get the derivatives of \( y(\cdot) \) via implicit function theorem. We have that
\[ F_x + F_y y_x = 0 \Rightarrow y_x = -F_x / F_y, \]
\[ F_{xx} + 2F_x y_x + F_y y_{xx} = 0 \Rightarrow y_{xx} = -(F_{xx} + F_x y_x) / F_y. \]

Here \( F_x, F_y \) stands for the derivative of \( F \) with its first and second argument, respectively. From (22), we have that \( \frac{\partial^{m+1}}{\partial x^m \partial y} F \big|_{x=0} \) has form \( \sqrt{E_2} E_2^{\frac{m}{2}} (A') \) where \( \left| p_m^{(3)}(A') \right| \) can be bounded by \( E_2^{\frac{m}{2}} \) times a polynomial of \( A' \) (which follows from (21)). Also note that \( F_y = \sqrt{K} (\nabla f)_1 \neq 0 \). With this observation, by induction similar to the above displayed derivations, we can show that \( \frac{\partial^m}{\partial x^m} y(x) \big|_{x=0}, 1 \leq m \leq r+1 \) has form \( \sqrt{E_2} E_2^{\frac{m}{2}} (A') \) where \( \left| p_m^{(4)}(A') \right| \) can also be bounded by \( E_2^{\frac{m}{2}} \) times a polynomial of \( A' \). Therefore, by Taylor expansion on \( y(\cdot) \) around 0, we have
\[ F_{+}^{(n)} = y(n^{-1/2}) = F_{+} + \sum_{m=1}^{r} \frac{n^{-m/2}}{m!} \sqrt{E_2} \frac{p_m^{(3)}(A')}{E_2^{m/2}} + n^{-(r+1)/2} R_5 \]

Moreover, the residual \( R_5 \) has form \( \sqrt{E_2} E_2^{\frac{r+1}{2}} (A') \) where \( \left| p_{r+1}(A') \right| \) can be bounded by \( E_2^{\frac{r+1}{2}} \) times a polynomial of \( A' \) (similar to the argument for the form of the residual term in the proof of (21)), which has finite \( 1 + c \) moment by Lemma 10.
More generally, for \((F_+^{(n)} - F_+)^l\), since it can be written as \((y(n^{-1/2}) - y(0))^l\), with the derivatives for \(y\), we also have its expansion of form (heuristically, we can see the following expansion by taking the \(l\)-th power in the preceding expansion, but that would induce a power of \(R_1\) which may not have finite expectation)

\[
(F_+^{(n)} - F_+)^l = \sum_{m=1}^{r} n^{-m/2} \sqrt{E_2^m} \frac{p_{l,m}(A')}{E_2^m} + n^{-(r+1)/2} R_{F,l},
\]

where \(|p_{l,m}(A')|\) can be bounded by \(E_2^{m/2}\) times a polynomial of \(A'\) and the residual \(R_{F,l}\) has form \(\sqrt{E_2^{p_{l,r+1}(A')}}\) where \(|p_{l,r+1}(A')|\) can be bounded by \(E_2^{(r+1)/2}\) times a polynomial of \(A'\). This gives the form of expansion as claimed. The finiteness of \(1 + c\) moment follows from Lemma \([10]\) (note that the existence of \(1 + c\) moment preserves when we multiply a polynomial of \(A'\)).

\[\square\]

### D.2.1 Proof of Lemma \([10]\)

**Proof.** It suffices to show that \(E \left[ E_2^{-(r+1+\epsilon)/2} \right] < \infty\) for any \(\epsilon < 1\) (once we can show this, the claim holds for any \(c\) such that \((r + 1 + \epsilon)(1 + c)/2 < r + 2\)). Note that the limiting distribution of \(E_2^{-1}\) follows a inverse-chi-squared distribution with \(K - 1\) degrees of freedom, whose density is proportional to \(x^{-K/2-1}e^{-1/2x}\). When \(K \geq r + 3\),

\[
\int_1^\infty x^{-K/2-1} e^{-1/2x} x^{(r+1+\epsilon)/2} dx \leq \int_1^\infty x^{-(3-\epsilon)/2} e^{-1/2x} dx < \infty
\]

also, because of the \(e^{-1/2x}\) term in the expression of the density, it is clear that \(\int_0^1 x^{-K/2-1} e^{-1/2x} x^{(r+1+\epsilon)/2} dx < \infty\). Therefore, \(\int_0^\infty x^{-K/2-1} e^{-1/2x} x^{(r+1)/2} dx < \infty\), which means that under the limiting distribution, \(E_2^{-(r+1+\epsilon)/2}\) has finite expectation. This means

\[
\int E_2 (a)^{-(r+1+\epsilon)/2} \phi_{\Sigma}(a_1) \ldots \phi_{\Sigma}(a_K) da_1 \ldots da_K < \infty.
\]

Here \(E_2(a_1, \ldots, a_K) := \sum_{i=1}^{K} (\nabla f(EX)^T (a_i - \bar{a}))^2\) is the function such that \(E_2(A_1, \ldots, A_K) = E_2\). Moreover, for any \(c\) such that \((r + 1 + \epsilon)(1 + c)/2 < r + 2\) we still have

\[
\int \left[ E_2 (a)^{-(r+1+\epsilon)/2} \right]^{1+c} \phi_{\Sigma}(a_1) \ldots \phi_{\Sigma}(a_K) da_1 \ldots da_K < \infty.
\]

Therefore, for any \(p(a)\) that is polynomial in \(a\), by Holder’s inequality and the fact that \(p(A)\) has an arbitrary order of moments under the limiting distribution, we have

\[
\int E_2 (a)^{-(r+1+\epsilon)/2} p(a) \phi_{\Sigma}(a_1) \ldots \phi_{\Sigma}(a_K) da_1 \ldots da_K < \infty. \tag{23}
\]

Observing that \(E \left[ E_2^{-(r+1+\epsilon)/2} \right]\) can be written as

\[
\int E_2 (a)^{-(r+1+\epsilon)/2} \left( 1 + \sum_i n^{-i/2} p_i^{(5)}(a) \right) \phi_{\Sigma}(a_1) \ldots \phi_{\Sigma}(a_K) da_1 \ldots da_K,
\]

from (23) we conclude the desired result. \(\square\)

**Proof of (24).** Let \(z(h) := 1 + \sum_{i=1}^{r} \frac{h^{i+1}p_i^{(1)}(A)}{E_2} + h^{r+1}R_2\) and \(r(x) := \sqrt{1 + x}\). By Taylor expansion, we have that

\[
r(z(n^{-1/2})) = r(z(0)) + \sum_{k=1}^{r} \frac{d^k}{dh^k} (r \circ z)(h)\big|_{h=0} n^{-k/2} + \frac{d^{r+1}}{dh^{r+1}} (r \circ z)(h)\big|_{h=0} n^{-(r+1)/2} \tag{24}
\]
for some $0 < h' < n^{-1/2}$. Therefore, to get (21), it suffices to argue that the derivatives of $r \circ z$ have the claimed forms.

By the chain rule, we have

$$\frac{d}{dh} (r \circ z)(h) = r'(z(h))z'(h)$$

$$\frac{d^2}{dh^2} (r \circ z)(h) = r''(z(h)) (z'(h))^2 + r'(z(h))z''(h)$$

In general, by induction, it is not hard to show that $\frac{d^k}{dh^k} (r \circ q)(h)$ can be written as

$$\frac{d^k}{dh^k} (r \circ q)(h) = \sum_{i=1}^{k} \left( \frac{d^i}{dh^i} (r \circ q)(h) \right)$$

Here $r^{[i]}$ denote the $i$-th derivative of $r$ and $z^{[i]}$, $\ldots$, $z^{[i]}$ are similarly defined. Note that $\left| p_2^{(1)}(A) \right| = \left| \sum_{t=1}^{K} (\nabla f)^T (A_t - A_0) q_t(A) \right| \leq \sqrt{E_2} \sum_{t=1}^{K} \| \nabla f \|_2 q_t(A)$ (see the expression for $p_2^{(1)}(A)$ after (20)), we have

$$z'(0) = \frac{p_2^{(1)}(A)}{E_2} \quad \text{where } p_2^{(1)}(A) \text{ can be bounded by } \sqrt{E_2} \text{ times a polynomial of } A.$$ 

For any $k \geq 2$, the expression of $z(h)$ we also have that $z^{[k]}(0) = \frac{p_2^{(k)}(A)}{E_2}$ where $p_2^{(k)}(A)$ can be bounded by $E_2^{k-1}$ times a polynomial of $A$. Note that when $k \geq 2$ we have $k - 1 \geq k/2$ and $E_2$ itself is bounded by a polynomial of $A$, we also have that $p_2^{(k)}(A)$ can be bounded by $E_2^{k/2}$ times a polynomial of $A$. Therefore, for any $i_1 \ldots i_k$ such that $i_1 + \cdots + i_k = k$, $z^{[i_1]}(0) \ldots z^{[i_k]}(0) = \frac{p_k^{[i_1]}(A)}{E_2}$ where $p_k^{[i_1]}(A)$ can be bounded by $E_2^{k/2}$ times a polynomial of $A$. Also note that $r^{(i_0)}(z(0))$ is a constant that does not depend on $A$. So by (21) we have that $\frac{d^k}{dh^k} (r \circ q)(h) = \frac{p_k^{[i_1]}(A)}{E_2}$ where $p_k^{[i_1]}(A)$ can be bounded by $E_2^{k/2}$ times a polynomial of $A$. From this, by (24), we get (21) except for the residual.

The additional difficulty for handling the residual is that the derivatives are evaluated at a point that is not 0. But as we will show, the knowledge that $0 < h' < n^{-1/2}$ suffices to control the residual. When $k \geq 2$, we note that

$$z^{[k]}(h) = \sum_{j=k}^{r} \left( \binom{k}{j} h^{j-k} p_{j+1}^{(1)}(A) \right) E_2 = \left( \frac{k}{r + 1} \right) h^{r+1-k} R_2$$

When $h < 1/2$, we have that

$$|z^{[k]}(h)| \leq \sum_{j=k}^{r} \left( \binom{k}{j} \right) \left( \frac{k}{r + 1} \right) \frac{R_2}{E_2}$$

The RHS can be bounded by $\frac{p_k^{[i_1]}(A)}{E_2}$ where $p_k^{[i_1]}(A)$ can be bounded by $E_2^{k/2}$ times a polynomial of $A$, as in the $h = 0$ case discussed above. When $k = 1$, we have that

$$z'(h) = z'(0) + h \left[ \sum_{j=2}^{r} j h^{j-2} p_{j+1}^{(1)}(A) \right] + \left( r + 1 \right) \frac{R_2}{E_2}$$

It follows from Lemma 10 that $P(E_2^{-1/2} > n^{1/2}) = O(n^{-(r+1)/2})$. Therefore, with probability $1 - O(n^{-(r+1)/2})$ we can assume that $n^{-1/2} < \sqrt{E_2}$. Therefore, for any $h < n^{-1/2}$,

$$|z'(h)| \leq |z'(0)| + \sum_{j=k}^{r} \left( \binom{k}{j} \right) \left( \frac{k}{r + 1} \right) \frac{R_2}{E_2^{1/2}}.$$
Since we have shown that \( z'(0) = \frac{p_2(0)(A)}{E_2} \) where \( p_2(0)(A) \) can be bounded by \( \sqrt{E_2} \) times a polynomial of \( A \), from the above we have that \( |z'(h)| \leq \frac{p_2(0)(A)}{E_2} \) where \( p_2(0)(A) \) can be bounded by \( \sqrt{E_2} \) times a polynomial of \( A \). Moreover, note that for any \( h < n^{-1/2} \),

\[
|z(h) - 1| = \left| \sum_{j=1}^{r} h_j p_j(A) \right| + h_r \frac{R_2}{E_2}
\leq h \left[ \sum_{i=1}^{K} \|\nabla f\|_{2} q_i(A) \right] + h_r \left| \frac{p_j(A)}{E_2} \right| + h_r \frac{R_2}{E_2}
\leq n^{-(1 - \frac{r+1}{2})/2} \left[ \sum_{i=1}^{K} \|\nabla f\|_{2} q_i(A) \right] + n^{-r}\left( \sum_{j=2}^{r} \frac{p_j(A)}{E_2} \right) + n^{-r+1}\frac{R_2}{E_2}
\]

when \( n^{-1/2} < E_2^{-(r+1)/2} \)

By Lemma 10 we have that \( n^{-1/2} < E_2^{-(r+1)/2} \) = 1 - \( O(n^{-r+1/2}) \) when \( \epsilon > 0 \) is sufficiently small. Note that the RHS above is smaller than 1/2 with high probability (i.e., with probability 1 - \( O(e^{-n^\alpha}) \) for some \( \alpha > 0 \) since it has the form \( n^{-\alpha} \) times polynomials of \( A \), which has moments of arbitrary order under \( \hat{P} \)). Therefore, with probability 1 - \( O(n^{-r+1/2}) \), we have that \( |z(h) - 1| < 1/2 \). This gives an absolute bound for \( z^{(0)}(z(h)) \). With this and the bounds for \( z'(h) \) and \( z^{(k)}(h) \), \( k \geq 2 \) that we derived, by (25) we have that the residual of (24) gives the claimed form of residual in (21).

D.3 Proof of (14)

Consider the i.i.d. sequence

\[ X_i := (X_i, X_{n+i}, \ldots, X_{(K-1)n+i}), i = 1, 2, \ldots, n \]

Then, the vector of all batch averages can be seen as the average of \( X_i, i = 1, 2, \ldots, n \). With the imposed conditions on \( X_i \), it is not hard to verify that the distribution of \( X_i \) satisfies the conditions in Theorem 11. We regard the indicator \( I_{-d}^{-d}(X_1, \tilde{X}_2, \ldots, \tilde{X}_K) := I(\tilde{q} \leq W_{SJ} \leq q) \) as a function of all the batch averages, which is in turn a function of \( X \). Therefore, we may let \( f \) in Theorem 11 be this function. Now we are in the setting of Theorem 11 so it suffices to show that the residual guaranteed by Theorem 11 is of order \( O(n^{-r+1/2}) \). We choose \( s = r + 3 \) in Theorem 11. Then, since \( f \) is bounded by 1, we have that \( M_{\epsilon}(f) \leq 1 \) which implies that \( M_{\epsilon}(f) \delta_{1}(n) = o(n^{-r+1/2}) \). Next, we show that the other residual term given in Theorem 11 i.e., \( \omega_f(2e^{-dn} : \Phi_{0,V}) = O(n^{-r+1/2}) \), is bounded by \( O(n^{-r+1/2}) \). Here, \( V \) is the product distribution of \( K \) r.v. with covariance equal to the covariance of \( X_1 \). This is heuristically correct since this term represents the oscillation of \( f \) in an exponentially small neighborhood.

Consider the function of batch averages induced by the SJ statistic

\[
W_{SJ}(x) := \frac{\sqrt{K} \left( J(x) - f(EX) \right)}{\sqrt{1 - r} \sum_{i=1}^{K} (J_i(x) - J(x))^2}
\]

where \( J_i(x) = K f(x) - (K-1) f(x_{(i)}) \). For its gradient, we have that

\[
\nabla W_{SJ}(x) = \frac{\sqrt{K(K-1)} \nabla J}{\sqrt{\sum_{i=1}^{K} (J_i(x) - J(x))^2}} - \frac{\sqrt{K(K-1)} \left( J(x) - f(EX) \right) \sum_{i=1}^{K} (J_i(x) - J(x)) (\nabla J_i - \nabla J)}{\sum_{i=1}^{K} (J_i(x) - J(x))^2 \sqrt{\sum_{i=1}^{K} (J_i(x) - J(x))^2}}
\]

(28)

Since our target is to bound \( \omega_{I_{-d}}(2e^{-dn} : \Phi_{0,V}) \) which is the oscillation under the limiting normal distribution, in what follows, we suppose all \( X_i \) are normal with variance \( \Sigma \). By Gaussian concentration, with probability \( 1 - O(n^{-r+1/2}) \) we have that \( \| \tilde{X}_i - EX \| \leq \delta \) for each \( i = 1, 2, \ldots, K \) where \( \delta \) is a value.
such that \( \sup_{\|x-Ex\| \leq \delta} \nabla f(x) \leq C \). Moreover, from the assumption that \( \text{Var}_P X \) is nonsingular and \( \nabla f \neq 0 \), it is not hard to show that there exists \( \lambda > 0 \) such that \( P \left( \sup_{\|x-X\| \leq \gamma} \sum_{i=1}^{K} (J_i(x) - \bar{J}(x))^2 < n^{-\lambda} \right) = O(n^{-(r+1)/2}) \). Therefore, from the preceding displayed equation, we conclude that there exist \( \lambda > 0 \) such that

\[
P \left( \sup_{\|x-X\| \leq \gamma} \|W_{SJ}(x)\| \leq n^{\lambda} C \right) = 1 - O(n^{-(r+1)/2}).
\]

Therefore, by Lagrange mean value theorem, we have that

\[
P \left( \sup_{\|x-X\| \leq \gamma} \|W_{SJ}(x) - W_{SJ}(X)\| \leq n^{\lambda-\epsilon} C \right) = 1 - O(n^{-(r+1)/2}). \tag{29}
\]

Pick any \( 0 < \gamma' < \gamma \). Note that \( P \left( q - e^{-\gamma'n} \leq W_{SJ}(X) \leq q + e^{-\gamma'n} \right) = O(n^{-(r+1)/2}) \) since otherwise \( W_{SJ} \) would have unbounded density around \( q \). Similarly \( P \left( -q - e^{-\gamma'n} \leq W_{SJ}(X) \leq -q + e^{-\gamma'n} \right) = O(n^{-(r+1)/2}) \).

Note also that \( n^\lambda e^{-\gamma'n} C \) can be bounded by \( Ce^{-\gamma'n} \). Therefore, from (29) we get

\[
P \left( \sup_{\|x-X\| \leq \gamma} \|I(-q \leq W_{SJ}(x) \leq q) - I(-q \leq W_{SJ}(X) \leq q)\| = 1 \right) = O(n^{-(r+1)/2})
\]

which implies that \( \bar{\omega}_{I_{SJ}} (e^{-\gamma'n}, \Phi_{0,V}) = O(n^{-(r+1)/2}) \).

## E Proofs of Other Theorems

### Proof of [3].

Denote \( Z_i = \sqrt{n} \left( \psi(\hat{P}_i) - \psi \right) / \sigma, i = 1, 2, \ldots, K \). Let \( \hat{P} \) be the measure (possibly signed when \( n \) is small) such that

\[
\hat{P} \left( (-\infty, q) \right) = \Phi(q) + \sum_{j=1}^{r} n^{-j/2} p_j(q) \phi(q)
\]

Let \( P_0 \) be the measure induced by the distribution of \( Z_i \), i.e., \( P_0 \left( (-\infty, q) \right) = P(Z_i \leq q) \). It suffices to show that

\[
\left| P_0^{\otimes n} \left( \{z_1, \ldots, z_K : f(z) \leq q\} \right) - \hat{P}^{\otimes n} \left( \{z_1, \ldots, z_K : f(z) \leq q\} \right) \right| = O(n^{-(r+1)/2}) \tag{30}
\]

Here \( P_0^{\otimes n} \) stands for the product measure of \( n \) copies of \( P \). Then, note that \( f(z_1, \ldots, z_K) \leq q \iff (K-1)/K (z_1 + \cdots + z_K)^2 \leq q \sum_{i=1}^{K} (z_i - \frac{1}{K} \sum_j z_j)^2 \), which can be formulated as

\[
z_1 \in \left[ z^-(z_2, \ldots, z_K), z^+(z_2, \ldots, z_K) \right]
\]

or

\[
z_1 \in (-\infty, z^- (z_2, \ldots, z_K)) \cup [z^+(z_2, \ldots, z_K), \infty)
\]

where \( z^+, z^- \) are the two roots of \( z_1 \) that solve \( (K-1)/K (z_1 + \cdots + z_K)^2 = q \sum_{i=1}^{K} (z_i - \frac{1}{K} \sum_j z_j)^2 \). Therefore, applying [1] at \( z^+ \) and \( z^- \), by the uniformity assumption we have that there exists a deterministic \( C \) such that

\[
\left| P_0 \left( \{z_1 : f(z_1, z_2, \ldots, z_K) \leq q\} \right) - \hat{P} \left( \{z_1 : f(z_1, z_2, \ldots, z_K) \leq q\} \right) \right| \leq C n^{-(r+1)/2}, \forall z_2, \ldots, z_K.
\]

Therefore, by Fubini’s theorem,

\[
\left| P_0^{\otimes n} \left( \{z_1, \ldots, z_K : f(z) \leq q\} \right) - \hat{P} \times P_0^{\otimes (n-1)} \left( \{z_1, \ldots, z_K : f(z) \leq q\} \right) \right|
\]

\[
= \left| P_0^{\otimes (n-1)} \left( P_0 \left( \{z_1 : f(z_1, z_2, \ldots, z_K) \leq q\} \right) - \hat{P} \left( \{z_1 : f(z_1, z_2, \ldots, z_K) \leq q\} \right) \right) \right|
\]

\[
\leq P_0^{\otimes (n-1)} C n^{-(r+1)/2}
\]

\[
= C n^{-(r+1)/2}
\]
Similarly, for any \( i = 0, 1, \ldots, K - 1 \), we can show that

\[
\begin{align*}
|\tilde{P}^\otimes i \times P_0^\otimes(n-i) (\{z_1, \ldots, z_K : f(z) \leq q\}) - \tilde{P}^\otimes(i+1) \times P_0^\otimes(n-i-1) (\{z_1, \ldots, z_K : f(z) \leq q\})| \\
\leq C_n^{-r+1/2} \left| \tilde{P}^\otimes i \times P_0^\otimes(n-i) \left( P_0(\{z_{i+1} : f(z_1, z_2, \ldots, z_K) \leq q\}) - \tilde{P}(\{z_{i+1} : f(z_1, z_2, \ldots, z_K) \leq q\}) \right) \right|
\end{align*}
\]

Here for a signed measure \( P \), \( |P| \) stands for \( P^+ + P^- \) where \( P^+ \), \( P^- \) are the positive and negative parts of \( P \). By the definition of \( \tilde{P} \), we have \( |\tilde{P}|(\mathbb{R}) = \int_{-\infty}^{\infty} \frac{d}{dq} \left( \Phi(q) + \sum_{j=1}^r n^{-j/2} p_j(q) \phi(q) \right) dq \) which can be uniformly bounded over all \( n \). Hence \( |\tilde{P}|(\mathbb{R}) \leq C_1 < \infty \) where \( C_1 \) does not depend on \( n \). Therefore, from the above we have

\[
|\tilde{P}^\otimes i \times P_0^\otimes(n-i) (\{z_1, \ldots, z_K : f(z) \leq q\}) - \tilde{P}^\otimes(i+1) \times P_0^\otimes(n-i-1) (\{z_1, \ldots, z_K : f(z) \leq q\})| \leq C C_1 n^{-(r+1)/2}
\]

Summing the above over \( i = 0, 1, \ldots, K - 1 \) and applying the triangle inequality, we get that

\[
|P_0^\otimes n (\{z_1, \ldots, z_K : f(z) \leq q\}) - \tilde{P}^\otimes n (\{z_1, \ldots, z_K : f(z) \leq q\})| \leq C \sum_{i=0}^{K-1} C_1 n^{-(r+1)/2}
\]

which gives (30).

\[ \square \]

**Proof of Proposition 7** The notations essentially follows from the notations in the proof of Theorem 2. But to make things concrete we will introduce them again for this example. Suppose that the batch averages multiplied by \( \sqrt{n} \) are given by \((X_1, Y_1)\) and \((X_2, Y_2)\) (both of them are 2-d standard normal) Let \( A_{0,1} = \frac{X_1+X_2}{2}, A_{0,2} = \frac{Y_1+Y_2}{2}, B_{1,1} = -B_{2,1} = \frac{X_1-X_2}{2}, B_{1,2} = -B_{2,2} = \frac{Y_1-Y_2}{2} \) (note that \( A_{0,1}, A_{0,2}, B_{1,1}, B_{1,2} \) are standard normal and independent). We have that

\[
W_S = \sqrt{2} \frac{A_{0,1} + n^{-1/2} (A_{0,2})^2}{\sqrt{\left( (B_{1,1} + n^{-1/2} Y_1^2 - n^{-1/2} A_{0,2}^2)^2 + (B_{2,1} + n^{-1/2} Y_2^2 - n^{-1/2} A_{0,2}^2)^2 \right)}}
\]

\[
= \sqrt{2} \frac{\left[ A_{0,1} + n^{-1/2} (A_{0,2})^2 \right]}{\sqrt{2B_{2,1}^2 + n^{-1/2} A_{0,2} B_{1,1} B_{1,2} + n^{-1} \left( (B_{2,2} + A_{0,2})^2 - A_{0,2}^2 \right)^2 + (B_{2,2} + A_{0,2})^2 - A_{0,2}^2}}
\]

Therefore, \( W_S \leq q \) can be written as

\[
A_{0,1} \leq F_+^{(n)} := \frac{q}{\sqrt{2}} \sqrt{2B_{2,1}^2 + n^{-1/2} A_{0,2} B_{1,1} B_{1,2} + n^{-1} \left( B_{1,2}^4 + 8B_{1,2}^2 A_{0,2}^2 \right)} - n^{-1/2} A_{0,2}^2.
\]

Similarly, \( W_S \geq -q \) is equivalent to

\[
A_{0,1} \geq F_-^{(n)} := -\frac{q}{\sqrt{2}} \sqrt{2B_{2,1}^2 + n^{-1/2} A_{0,2} B_{1,1} B_{1,2} + n^{-1} \left( B_{1,2}^4 + 8B_{1,2}^2 A_{0,2}^2 \right)} - n^{-1/2} A_{0,2}^2.
\]

So we have \( P(-q \leq W_S \leq q) = P(F_-^{(n)} \leq A_{0,1} \leq F_+^{(n)}) = E \left[ \Phi(F_+^{(n)}) - \Phi(F_-^{(n)}) \right] \) where \( \Phi \) is the c.d.f. of standard normal. Let \( F_+ = \frac{q}{\sqrt{2}} \sqrt{2B_{2,1}^2} \) and \( F_- = -\frac{q}{\sqrt{2}} \sqrt{2B_{2,1}^2} \). By the definition of \( t_1 \) distribution, we have
that \( P(-q \leq t_1 \leq q) = E[\Phi(F_+) - \Phi(F_-)] \). Therefore, the coverage error, i.e., \( |P(-q \leq W_S \leq q) - P(-q \leq t_1 \leq q)| \), can be expressed as
\[
E \left[ \left( \Phi(F_2^n) - \Phi(F_1^n) \right) - \left( \Phi(F_2^n) - \Phi(F_1^n) \right) \right]
\]
which by Taylor expansion can be expressed as
\[
\left| E \left[ \phi(F_+)(F_2^n - F_1^n) + \phi'(\xi_+)(F_2^n - F_1^n)^2 - \phi(F_-)(F_2^n - F_1^n) - \phi'(\xi_-)(F_2^n - F_1^n)^2 \right] \right|
\]
for some \( \xi_+, \xi_- \in \mathbb{R} \). Note that \( F_+ = -F_- \) and \( \phi(F_+) = \phi(F_-) \). So from the preceding we get that the coverage error is
\[
\left| E \left[ \phi(F_+)(F_2^n - F_1^n) - 2F_1^n + \phi'(\xi_+)(F_2^n - F_1^n)^2 - \phi'(\xi_-)(F_2^n - F_1^n)^2 \right] \right|.
\] (31)

We study \( F_2^n - F_1^n \). We observe that
\[
\sqrt{2B_{1,1}^2 + n^{-1/2}A_{0,2}B_{1,1}B_{1,2} + n^{-1} \left( B_{1,1}^4 + 8B_{1,2}^2A_{0,2}^2 \right)} - \sqrt{2B_{1,1}^2} \]
\[
= n^{-1/2}A_{0,2}B_{1,1}B_{1,2} + n^{-1} \left( B_{1,1}^4 + 8B_{1,2}^2A_{0,2}^2 \right)
\]
is dominated by (note that \( 2B_{1,1}^2 + n^{-1/2}A_{0,2}B_{1,1}B_{1,2} + n^{-1} \left( B_{1,1}^4 + 8B_{1,2}^2A_{0,2}^2 \right) \geq n^{-1} \left( B_{1,1}^4 + 8B_{1,2}^2A_{0,2}^2 \right) - n^{-1}A_{0,2}^2B_{1,2}^2 \geq \frac{1}{2}n^{-1} \left( B_{1,1}^4 + 8B_{1,2}^2A_{0,2}^2 \right) )
\]
\[
\frac{n^{-1/2} \left| A_{0,2}B_{1,1}B_{1,2} \right|}{\sqrt{2B_{1,1}^2}} + n^{-1/2} \frac{B_{1,1}^4 + 8B_{1,2}^2A_{0,2}^2}{\sqrt{2}} = n^{-1/2} \left| A_{0,2}B_{1,1}B_{1,2} \right| + 2n^{-1/2} \sqrt{B_{1,1}^4 + 8B_{1,2}^2A_{0,2}^2}
\]
Therefore
\[
\left| F_2^n - F_1^n \right| \leq n^{-1/2} \left( \frac{\left| A_{0,2}B_{1,1}B_{1,2} \right|}{\sqrt{2}} + 2 \sqrt{B_{1,1}^4 + 8B_{1,2}^2A_{0,2}^2} \right).
\] (32)

We note that the RHS is bounded by \( n^{-1/2} \) times a polynomial of normal which have arbitrary order of moments. Also note that the derivative of normal density is uniformly bounded, we have that
\[
E \left[ \phi'(\xi_+)(F_2^n - F_1^n)^2 \right] = O(n^{-1}).
\]
Similarly we have \( E \left[ \phi'(\xi_-)(F_2^n - F_1^n)^2 \right] = O(n^{-1}) \). Therefore, by (31) we have that the coverage error is
\[
\left| E \left[ \phi(F_+)(F_2^n - F_1^n - 2F_1^n) \right] + O(n^{-1}) \right|.
\] (33)

Note that conditional on \( B_{1,1} \), the expectation \( E \left[ \phi(F_+)(F_2^n - F_1^n - 2F_1^n) \big| B_{1,1} \right] \) is always positive (which is implied by the positiveness of the second order derivative in (35)). Also note that \( \phi(F_+) \) is uniformly bounded away from 0 when \( B_{1,1} \) belongs to a bounded set. Therefore, to show that the above is \( \omega(n^{-1}) \), it suffices to show that
\[
E \left[ F_2^n - F_1^n - 2F_1^n \big| B_{1,1} \leq M \right] = \omega(n^{-1}).
\]

Plugging in the expressions for \( F_1^n, F_2^n, F_+ \), the above can be restated as: for independent \( X, Y, Z \sim N(0,1) \), we want to show that
\[
\lim_{n \to \infty} nE \left[ \sqrt{2X^2 + n^{-1/2}XY Z + n^{-1} \left( Y^4 + 8Y^2Z^2 \right)} - \sqrt{2X^2}; |X| \leq M \right] = \infty.
\] (34)

To show this, we let \( f(h) = \sqrt{2X^2 + hXY Z + h^2 (Y^4 + 8Y^2Z^2)} \). Then we have that \( Ef'(0) = E \frac{X Y Z}{2\sqrt{2X^2}} = 0 \), and for any \( \theta \in [0, h] \) we have that
\[
f''(\theta) = \frac{8X^2Y^4 + 63X^2Y^2Z^2}{4(2X^2 + \theta XY Z + \theta^2 (Y^4 + 8Y^2Z^2))^{3/2}} \geq \frac{8X^2Y^4 + 63X^2Y^2Z^2}{4(2X^2 + h |XY Z| + h^2 (Y^4 + 8Y^2Z^2))^{3/2}}.
\] (35)
By Taylor expansion, we have that \( f(h) = f(0) + f'(0)h + \frac{1}{2}f''(\theta_h)h^2 \). Therefore,

\[
E \left[ \frac{f(h) - f(0)}{h^2}; |X| \leq M \right] = \frac{1}{2} E \left[ f''(\theta_h); |X| \leq M \right] \\
\geq E \left[ \frac{8X^2Y^4 + 63X^2Y^2Z^2}{4(2X^2 + h|XYZ| + h^2(Y^4 + 8Y^2Z^2))^{3/2}}; |X| \leq M \right]
\]

By monotone convergence, the RHS goes to \( \infty \) as \( h \to 0 \) (note that \( E \left[ |X|^{-1}; |X| \leq M \right] = \infty \)). Let \( h = n^{-1/2} \), we get (34).

To show that the coverage error of sectioning is \( o(n^{-1/2}) \), from (33) it suffices to show that

\[
E \left[ \phi(F_+)(F_+^{(n)} - F_-^{(n)} - 2F_+) \right] = o(n^{-1/2}).
\]

From the boundness of \( \phi(F_+) \) and the positivity of the conditional distribution on \( B_{1,1} \), it suffices to show that \( E \left[ F_+^{(n)} - F_-^{(n)} - 2F_+ \right] = o(n^{-1/2}) \), which can be restated as: for independent \( X, Y, Z \sim N(0, 1) \), we want to show that

\[
\lim_{n \to \infty} \sqrt{n}E \left[ \sqrt{2X^2 + n^{-1/2}XYZ + n^{-1}(Y^4 + 8Y^2Z^2)} - \sqrt{2X^2} \right] = 0
\]

Or equivalently

\[
\lim_{n \to \infty} E \left[ \frac{XYZ + n^{-1/2}(Y^4 + 8Y^2Z^2)}{\sqrt{2X^2 + n^{-1/2}XYZ + n^{-1}(Y^4 + 8Y^2Z^2) + 2X^2}} \right] = 0
\]

This can be shown by dominated convergence with dominating function given by \( \frac{YZ}{\sqrt{2}} + 2\sqrt{Y^4 + 8Y^2Z^2} \) (see the derivation of (32)).

**Proof of Theorem 2.** Let \( \bar{g}_k \) denote the average of \( g(X_i) \) for all \( X_i \) in the \( k \)-th section. From the mixing condition, since the gap between sections is of order \( n^\epsilon \), we have that for each \( k_1 \neq k_2 \) and measurable sets \( A_{k_1}, A_{k_2} \), \( |P(\bar{g}_{k_1} \in A_{k_1}, g_{k_2} \in A_{k_2}) - P(\bar{g}_{k_1} \in A_{k_1})P(g_{k_2} \in A_{k_2})| \leq \alpha(n^\delta) = o(n^{-r/2}) \). It is not hard to see that by applying this for \( K - 1 \) times, we will get that for any \( A_1, A_2, \ldots, A_K \), we have that

\[
|P(\bar{g}_1 \in A_1, \bar{g}_2 \in A_2, \ldots, \bar{g}_K \in A_K) - P(\bar{g}_1 \in A_1) \ldots P(\bar{g}_K \in A_K)| \leq K\alpha(n^\delta) = o(n^{-(r+1)/2}). \tag{36}
\]

Therefore, to study the joint distribution of \( \bar{g}_1, \ldots, \bar{g}_K \), it suffices to look at the marginal distributions.

For these marginal distributions, by Theorem 1 of [Jensen 1989], we have that

\[
P(\sqrt{n}(\bar{g}_1 - Eg(X_1)) \in B) = \int_B \phi_{\Sigma}(x) \sum_{j=1}^r n^{j/2}q_j(x)dx + O(n^{-(r+1)/2}) \tag{37}
\]

uniformly over \( B \) satisfying \( \phi_{\Sigma}((\delta B)^c) < \epsilon \) where \( (\delta B)^c := \{ x : d(x, B) < \epsilon, x \notin B \} \) (heuristically, this means the area of the boundary of \( B \) is bounded) and \( q_j, j = 1, 2, \ldots, r \) are polynomials. Combining this with (36), and doing integration, we again get (14) with \( A_i \) replaced by \( \sqrt{n}(\bar{g}_1 - Eg(X_1)) \). Therefore, following the proof of Theorem 2 we get the desired result.

**Proof of Theorem 3.** The proof for the first part is almost identical to the proof of Theorem 3. The only difference is that we use the Edgeworth expansion result in [Malinovskii 1987] to conclude that (here all probabilities are taken under the stationary measure)

\[
\sup_{x \in R} \left| P \left( \frac{\sqrt{a}}{\sigma_F \Sigma f_{\cdot,n}} \leq x \right) - \Phi(x) - \sum_{j=1}^r n^{-j/2} \tilde{q}_j(x)\phi(x) \right| = O(n^{-(r+1)/2}).
\]
Using the above expansion to take the place of \[37\], and proceed as in the proof of Theorem \[3\] we get the desired result.

For the second part, we note that the coefficient for the \(n^{-1/2}\) term in the Edgeworth expansion given in Malinowski [1987] (more precisely, the polynomial \(q_1(x)\) in its Theorem 1) is an even polynomial. Therefore, with the same oddness and evenness argument as in the proof of Theorem \[2\] we get the claimed result. 

**Proof of Theorem \[2\]** Based on the approximation \(W = \sqrt{K(K-1)} [u, A_0] + n^{-1/2} b_1 + n^{-1/2} b_2 + O_p(n^{-3/2})\), we may further do Taylor expansion and get that

\[
W = \sqrt{K(K-1)} \frac{[u, A_0] + n^{-1/2} b_1 + n^{-1/2} b_2}{\sqrt{E_2 + n^{-1/2} \lambda + n^{-1} e}}
\]

\[
= \sqrt{K(K-1)} \left[ u, A_0 \right] + n^{-1/2} b_1 + n^{-1/2} b_2 \left( 1 + \frac{n^{-1/2}}{E_2} \left( \frac{\lambda}{E_2} + \frac{e}{E_2} \right) \right)^{-1/2}
\]

\[
= \sqrt{K(K-1)} \left[ u, A_0 \right] + n^{-1/2} b_1 + n^{-1/2} b_2 \left( 1 - \frac{1}{2} n^{-1/2} \frac{\lambda}{E_2} - \frac{n^{-1}}{2} \frac{e}{E_2} + \frac{3}{8} n^{-1} \frac{\lambda^2}{E_2^2} \right)
\]

\[
= \frac{K(K-1)}{\sqrt{E_2}} \left[ u, A_0 \right] + n^{-1/2} b_1 + n^{-1/2} b_2 \left( 1 - \frac{1}{2} n^{-1/2} \frac{\lambda}{E_2} - \frac{n^{-1}}{2} \frac{e}{E_2} + \frac{3}{8} n^{-1} \frac{\lambda^2}{E_2^2} \right)
\]

Let \(F = \frac{W}{\sqrt{K(K-1)}}\). Let \(F_+\) and \(F_-\) denote the value of \(A_0\), such that the value of \(W\) is equal to \(q\) and \(-q\) when \(n = \infty\), respectively. Then indeed we have that \(F_+ = \frac{q \sqrt{E_2}}{\sqrt{K(K-1)}} - \sum_{i=2}^d u_i A_0, i\) and \(F_- = -\frac{-q \sqrt{E_2}}{\sqrt{K(K-1)}} - \sum_{i=2}^d u_i A_0, i\). Denote \(F_x, F_y\) as the derivative of \(F\) w.r.t. \(n^{-1/2}\) and \(A_0, i\) respectively when \(n^{-1/2} = 0, A_0, i = F_+\). Let \(F_{xx}, F_{xy}, F_{yy}\) be the corresponding second-order derivatives (note that we actually have \(F_{yy} = 0\) since when \(n^{-1/2} = 0\), the only term is \(\sqrt{K(K-1)} [u, A_0] / \sqrt{E_2}\) which is linear in \(A_0, i\)). Then

\[
F_x = \frac{b_1}{\sqrt{E_2}} - \frac{1}{2} n^{-1/2} \lambda \frac{\lambda}{E_2} \frac{a'}{\sqrt{E_2}} - \frac{1}{\sqrt{E_2}} \frac{u_1}{\sqrt{E_2}}
\]

\[
F_y = \frac{a'}{\sqrt{E_2}} - \frac{1}{2} n^{-1/2} \lambda \frac{\lambda'}{E_2} - \frac{1}{2} n^{-1} \frac{\lambda^2}{E_2^2}
\]

Therefore,

\[
F_x + F_y y_x = 0 \Rightarrow y_x = -F_x / F_y
\]

\[
F_{xx} + 2 F_{xy} y_x + F_{yy} y_x^2 + F_{xy} y_{xx} = 0 \Rightarrow y_{xx} = -(F_{xx} + 2 F_{xy} y_x) / F_y
\]

By a second-order Taylor expansion, we have that when \(W = q\),

\[
A_{0,1} = F_+^{(n)} = F_+ + n^{-1/2} y_x + \frac{1}{2} n^{-1} y_{xx} + O_p(n^{-3/2})
\]

and similarly when \(W = -q\),

\[
A_{0,1} = F_-^{(n)} = F_- + n^{-1/2} y_x + \frac{1}{2} n^{-1} y_{xx} + O_p(n^{-3/2})
\]
where \( y_x^- \) and \( y_{xx}^- \) are the counterpart of the derivatives at \( (n^{-1/2}, A_{0,1}) = (0, F_0) \). Then, we have that

\[
P(-q \leq W \leq q) = \int_{F_0}^{F_+} \phi_\Sigma(a) \left( 1 + \sum_{j=1}^{2} n^{-j/2} p_{j,A}(a) \right) da_{0,1} da' + O(n^{-3/2})
\]

\[
= \int_{F_0}^{F_+} \phi_\Sigma(a) \left( 1 + \sum_{j=1}^{2} n^{-j/2} p_{j,A}(a) \right) da_{0,1} da'
+ \int \left( \left[ \phi_\Sigma(a) \left( 1 + n^{-1/2} p_{1,A}(a) \right) \right]_{a_{0,1}=F_+} \left( n^{-1/2} y_x + \frac{1}{2} n^{-1} y_{xx} \right) \right) da' \\
+ \int \left( \left[ \phi_\Sigma(a) \left( 1 + n^{-1/2} p_{1,A}(a) \right) \right]_{a_{0,1}=F_-} \left( n^{-1/2} y_x^- + \frac{1}{2} n^{-1} y_{xx}^- \right) \right) da' \\
+ \frac{1}{2} \int \left( \left. \frac{\partial}{\partial a_{0,1}} \left[ \phi_\Sigma(a) \right] \right|_{a_{0,1}=F} y_x^2 \right) da' + O(n^{-3/2}).
\]

Hence, the \( n^{-1} \) error term is given by

\[
\int_{F_0}^{F_+} \phi_\Sigma(a) \left( p_{2,A}(a) \right) da_{0,1} da' + \int \left( \left[ \phi_\Sigma(a) \left( p_{1,A}(a) \right) \right]_{a_{0,1}=F_+} \left( y_x \right) \right) da' \\
+ \int \left( \left[ \phi_\Sigma(a) \left( 1 + n^{-1/2} p_{2,A}(a) \right) \right] \right) da' + \frac{1}{2} \int \left( \left. \frac{\partial}{\partial a_{0,1}} \left[ \phi_\Sigma(a) \right] \right|_{a_{0,1}=F} y_x^2 \right) da' \tag{38}
\]

Note that the joint density of \((\sqrt{n} (X_1 - m), \ldots, \sqrt{n} (X_K - m)) = (A_0 + B_1, A_0 + B_2, \ldots, A_0 + B_{K-1}, A_0 - B_1 - B_2 - \cdots - B_{K-1})\) is given by

\[
p(x) = \phi_\sigma(x_1) \cdots \phi_\sigma(x_K) \prod_i \left( 1 + n^{-1/2} p_1(x_i) + n^{-1} p_2(x_i) \right)
\]

The formulas for \( p_1(x) \) and \( p_2(x) \), given in [7], can be found in Skovgaard [1986], p172. Therefore, after a linear transformation, we get that the density of \( A = (A_0, B_1, \ldots, B_{K-1}) \) is

\[
p_A(a) = p(x) \left| \det \left( \frac{Dx}{Da} \right) \right| = K p(x) = \phi_\Sigma(a) \prod_i \left( 1 + n^{-1/2} p_1(x_i) + n^{-1} p_2(x_i) \right) + O(n^{-3/2}).
\]

(Note that, since \( \frac{Dx}{Da} = \begin{pmatrix} 1 & 1 & \cdots & 1 \\
1 & 1 & \cdots & 1 \\
\vdots & \vdots & \ddots & \vdots \\
1 & -1 & \cdots & -1 \end{pmatrix} \), we have that its determinant is \( K \).) This gives \( p_1(a) = p_1(x_1(a)) + \cdots + p_1(x_K(a)) \), and \( p_2(a) = \sum_{1 \leq i < j \leq K} p_1(x_i(a)) p_1(x_j(a)) + \sum_{1 \leq i \leq K} p_2(x_i(a)) \). Therefore, the first term in (38) is

\[
E_C p_2(x) = E_C \left[ \sum_{1 \leq i < j \leq K} p_1(x_i(A)) p_1(x_j(A)) + \sum_{1 \leq i \leq K} p_2(x_i(A)) \right]
\]

where \( C \) represents the area where

\[
-q \leq \sqrt{K(K-1)} \frac{[u, A_0]}{\sqrt{\sum_{i=1}^{K} \left( [u, A_i - A_0] \right)^2}} \leq q.
\]

For the second term of (38), we have that
\[ \int \left( \begin{array}{c}
\phi_S(a) (p_1(a)) |_{a_0,1=F_+} (y_z)
- \phi_S(a) (p_1(a)) |_{a_0,1=F_-} (y_z^-) 
\end{array} \right) da' = E \left( \begin{array}{c}
\phi_{\sigma_0}(F_+ - \mu) (p_1(a)) |_{a_0,1=F_+} (y_z)
- \phi_{\sigma_0}(F_- - \mu) (p_1(a)) |_{a_0,1=F_-} (y_z^-) 
\end{array} \right) \]

Here \( \sigma_0 = (\sigma_0 - \sigma_0 \sigma_1^{-1} \sigma_{10}) / K, \sigma_0 \) is the variance of the first dimension of \( X \), \( \mu = \sigma_0 \sigma_1^{-1} \mu_0 \). The expectation is taken under the limiting normal distribution of \( a' \). We explain why the above is true. Observe that \( \phi_{\sigma_0} (- \mu) \) is the conditional density of \( A_{0,1} \) given \( A' \) (under their joint limiting distribution), which implies \( \phi_S(a) = \phi_{\sigma_0}(F_+ - \mu) \phi_S(a') \). Moreover, it follows from the definition of expectation that \( \int [\phi_S(a')g(a')] da' = Eg(A') \) where \( A' \) follows from its limiting normal distribution. Therefore, we have the preceding displayed equality. Similar argument holds for the third and last terms of (38). Therefore, the summation of the last three terms of (38) is

\[
E \left( \begin{array}{c}
\phi_{\sigma_0}(F_+ - \mu) (p_1(a)) |_{a_0,1=F_+} (y_z)
- \phi_{\sigma_0}(F_- - \mu) (p_1(a)) |_{a_0,1=F_-} (y_z^-) 
\end{array} \right) + E \left( \begin{array}{c}
\phi_{\sigma_0}(F_+ - \mu) \left( \frac{1}{2} y_{x^2} \right)
- \phi_{\sigma_0}(F_- - \mu) \left( \frac{1}{2} y_{z^2} \right) 
\end{array} \right)
\]

Here, the expectation is taken under the asymptotic normal distribution of \( A' \).

Proof of Proposition 2: For batching, the event \( P(-q \leq W_B \leq q) \) could be written as (recall that \( X_i, Y_i, i = 1, 2 \) corresponds to the scaled batch averages and has standard normal distribution, and are independent)

\[
- \frac{q}{\sqrt{2}} \leq \frac{X_1 + X_2}{2} + \frac{1}{n-1/2} \frac{Y_1^2 + Y_2^2}{X_1 - X_2} \leq \frac{q}{\sqrt{2}}
\]

the critical points for \( (X_1 + X_2)/2 \) (which corresponds to \( F'_1 \) and \( F'_0 \) in the proof of Theorem 2) are given by

\[
\frac{q}{\sqrt{2}} \left| \frac{X_1 - X_2}{2} \right| \left| 1 + \frac{1}{n-1/2} \frac{Y_1^2 - Y_2^2}{X_1 - X_2} \right| \leq \frac{q}{\sqrt{2}}
\]

and

\[
- \frac{q}{\sqrt{2}} \left| \frac{X_1 - X_2}{2} \right| \left| 1 + \frac{1}{n-1/2} \frac{Y_1^2 - Y_2^2}{X_1 - X_2} \right| \leq \frac{q}{\sqrt{2}}
\]

However, when \( K = 2 \), since the probability that \( 1 + \frac{1}{n-1/2} \frac{Y_1^2 - Y_2^2}{X_1 - X_2} > 0 \) is not \( o(n^{-1}) \), the above can not be approximated by (with error \( o_p(n^{-1}) \)) dropping the absolute value whose resulting value is

\[
\frac{q}{\sqrt{2}} \left| \frac{X_1 - X_2}{2} \right| \left( 1 + \frac{1}{n-1/2} \frac{Y_1^2 - Y_2^2}{X_1 - X_2} \right) \leq \frac{q}{\sqrt{2}}
\]

and

\[
- \frac{q}{\sqrt{2}} \left| \frac{X_1 - X_2}{2} \right| \left( 1 + \frac{1}{n-1/2} \frac{Y_1^2 - Y_2^2}{X_1 - X_2} \right) \leq \frac{q}{\sqrt{2}}
\]

On the other hand, dropping the absolute value operation exactly corresponds to what is done using the current expansion scheme:

\[
\left| 1 + n^{-1/2} \frac{Y_1^2 - Y_2^2}{X_1 - X_2} \right| = \sqrt{1 + 2n^{-1/2} \frac{Y_1^2 - Y_2^2}{X_1 - X_2} + n^{-1} \left( \frac{Y_1^2 - Y_2^2}{X_1 - X_2} \right)^2}
\]

\[
= 1 + n^{-1/2} \frac{Y_1^2 - Y_2^2}{X_1 - X_2} + \frac{n^{-3/2}}{(X_1 - X_2)^3}
\]

Though the residual has a coefficient \( n^{-3/2} \), its contribution is actually larger since \( \frac{1}{(X_1 - X_2)^3} \) does not have finite expectation.
Proof of Theorem 11. As \( K \to \infty \), \( S_{\text{batch}} \to \sqrt{n \text{Var}(\hat{P}_1)} \). But \( \sqrt{nK} \left( \frac{1}{K} \sum_{i=1}^{K} \psi(\hat{P}_i) - \psi \right) \to \text{sign}(E(\psi(\hat{P}_1) - \psi)) \cdot \infty \). Thus \( W_B \) either converges to \( \infty \) or \( -\infty \) which implies \( P(-q \leq W_B \leq q) \to 0 \). Similarly, since

\[
\left| S_{\text{sec}}^2 - \frac{1}{K-1} \sum_{i=1}^{K} (\psi(\hat{P}_i) - \psi)^2 \right| \leq \frac{K}{K-1} (\psi(\hat{P}) - \psi)^2 = o_P(1),
\]

by the strong law of large numbers and Slutsky’s theorem we have \( S_{\text{sec}} \to \sqrt{E(\psi(\hat{P}_1) - \psi)^2 } \) (as \( K \to \infty \)).

Also note that by the differentiability of \( \psi \) implies the asymptotic result \( \sqrt{nK} (\psi(\hat{P}) - \psi) \Rightarrow N(0, \sigma^2) \).

Therefore, we get the claim for \( P(-q \leq W_S \leq q) \). The claim that \( P(-q \leq W_{SJ} \leq q) \Rightarrow \Phi(q) - \Phi(-q) \) can be seen by regarding each batch as a multidimensional data and applying the consistency of the usual jackknife (e.g. Theorem 2.3 of Shao and Tu 1995).

\( \square \)

F Edgeworth Expansion for Smooth Function Models

For completeness, we introduce the Edgeworth expansion result in Bhattacharya and Rao 2010. Let

\[
M_s(f) := \left\{ \sup_{x \in R^k} \frac{1}{(1 + \|x\|^s)^{-1}} |f(x)| \right\}^{s > 0}
\]

\[
\omega_f(R^k) = \sup_{x,y \in R^k} |f(x) - f(y)| \quad \text{for } s = 0.
\]

Let \( \omega_f(\epsilon, x) := \sup_{d(x', x) \leq \epsilon} f(x') - \inf_{d(x', x) \leq \epsilon} f(x') \),

\( \omega_f(\epsilon, \mu) := \int \omega_f(\epsilon, x) d\mu(x) \). Heuristically, \( \omega_f(\epsilon, x) \) measures the oscillation of \( f(x) \) in an \( \epsilon \)-neighborhood of \( x \), which is then averaged over \( x \) w.r.t. measure \( \mu \) to give \( \omega_f(\epsilon, \mu) \).

Theorem 11. Let \( \{X_n : n > 1\} \) be an i.i.d. sequence of random vectors with values in \( R^k \) whose common distribution \( Q_1 \) satisfies Cramer’s condition. Assume that \( Q_1 \) has mean zero and a finite \( s \)-th absolute moment for some integer \( s > 3 \). Let \( V \) denote the covariance matrix of \( Q_1 \) and \( \chi_\nu \) its \( \nu \)-th cumulant (\( 3 < |\nu| < s \)). Then for every real-valued, Borel-measurable function \( f \) on \( R^k \) satisfying

\[
M_s'(f) < \infty
\]

for some \( s', 0 < s' \leq s \), one has

\[
\left| \int f d \left( Q_n - \sum_{\nu=0}^{s-2} n^{-j/2} p_j (-\Phi_{0,V} : (\chi_\nu)) \right) \right| < M_{s'}(f) \delta_1(n) + c(s, k) \omega_f(2n^{-\gamma n : \Phi_{0,V}})
\]

where \( Q_n \) is the distribution of \( n^{-1/2} (X_1 + \cdots + X_n) \), \( \gamma \) is a suitable positive constant, and

\[
\delta_1(n) = o\left(n^{-(s'-2)/2}\right), \quad (n \to \infty)
\]

Moreover, \( c(s, k) \) depends only on \( s \) and \( k \), and the quantities \( \gamma, \delta_1(n) \) do not depend on \( f \).