On Variance Estimation of Random Forests

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Abstract

Ensemble methods, such as random forests, are popular in applications due to their high predictive accuracy. Existing literature views a random forest prediction as an infinite-order incomplete U-statistic to quantify its uncertainty. However, these methods focus on a small subsampling size of each tree, which is theoretically valid but practically limited. This paper develops an unbiased variance estimator based on incomplete U-statistics, which allows the tree size to be comparable with the overall sample size, making statistical inference possible in a broader range of real applications. Simulation results demonstrate that our estimators enjoy lower bias and more accurate coverage rate without additional computational costs. We also propose a local smoothing procedure to reduce the variation of our estimator, which shows improved numerical performance when the number of trees is relatively small. Further, we investigate the ratio consistency of our proposed variance estimator under specific scenarios. In particular, we develop a new “double U-statistic” formulation to analyze the Hoeffding decomposition of the estimator’s variance.

Keywords: U-statistic, Hoeffding decomposition, statistical inference, subbagging

1 Introduction

Random forest is a tree-based ensemble model, first introduced by Breiman (2001). It consists of a collection of random tree models while each tree is built on a random subsample from the training data. Additional randomization, such as random feature space (Breiman, 2001) and random cutoff points (Geurts et al., 2006), are injected into the recursively partitioning process of a tree construction for improved performances.

In recent years, there is an increasing interest in statistical inference for bagging models, including random forests. To estimate the variance of random forest predictions, Sexton and Laake (2009) utilize the jackknife and bootstrap mechanism. Wager et al. (2014) further propose to use jackknife and infinitesimal jackknife (IJ, Efron (2014)). Wager and Athey (2018) further apply the IJ estimation on random forests built under honesty property and perform inference of heterogeneous treatment effects. On the other hand, Mentch and Hooker (2016) consider the variance estimation based on trees using subsamples (sampled

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without replacement) of the training data. They view a random forest estimator as a random kernel Infinite
Order U-statistic (Frees, 1989), $U_n$ and use Monte Carlo variance estimators to approximate the asymptotic
variance of $U_n$. Recent developments under this topic also include Zhou et al. (2021) and Peng et al. (2021).
Zhou et al. (2021) propose a “balanced method” estimator, which significantly reduces the computational
cost from Mentch and Hooker (2016). Peng et al. (2021) further study the bias and consistency of the IJ
estimator and propose alternative variance estimators with classical jackknife and regression approaches.

An important line of research that underlies statistical inference for random forests is the asymptotic
normality of the forests estimator. For forests based on subsamples, (Mentch and Hooker, 2016) first show
the asymptotic normality of its estimator under a U-statistic framework with growing tree (kernel) size
$k = o(\sqrt{n})$, where $k$ is the subsampling size and $n$ is the training sample size. Unfortunately, the conditions
in Mentch and Hooker (2016) for asymptotic normality cannot hold simultaneously. Further conditions and
proofs are given in DiCiccio and Romano (2022), Zhou et al. (2021) and Peng et al. (2019). Zhou et al.
(2021) set the connection between U-statistics and V-statistics and develop similar asymptotic results for
V-statistic, where subsamples are taken with replacement. Wager and Athey (2018) show the asymptotic
unbiasedness and normality of random forests built with honest trees. Their work allow a larger tree size
($o(n^{\beta})$ with $0.5 < \beta < 1$) than that in Mentch and Hooker (2016). In particular, their analysis shows that the
inference is useless for small tree size $k$ with growing samples size $n$, by showing that the random forests
can be asymptotically biased. Peng et al. (2019) develop the notation of generalized U-statistic and show its
asymptotic normality with $k = o(n)$ and a linear growth rate assumption of $\xi_{d,k}^2$ (see Equation (3)).

Many questions still remain unanswered for variance estimation of random forests. In particular, the
theoretical guarantee for the estimators in the above literature is provided when the variance of the U-
statistic is approximated well by the variance of its Hajek projection. However, such approximation are
usually not compatible with large $k$. Practitioners tend to use a large subsample size for higher accuracy.
For example, it is typical to use a fixed proportion of the total sample size, i.e., $k = \beta n$ for some $0 < \beta \leq 1$
(Breiman, 2001; Geurts et al., 2006).

To address this, we propose a new class of estimation approach for unbiased variance estimator, called
**Matched Sample Variance Estimator**, which is suitable under large tree size $k \leq n/2$. Our approach is
motivated by estimating all terms in the Hoeffding decomposition of $\text{Var}(U_n)$, instead of barely estimating
its leading term or the Hajek projection. Moreover, our estimator is computationally efficient and can be
directly calculated from a fitted random forest. In addition, we propose a local smoothing strategy to reduce
the variance of our estimator and thus improve the coverage of the corresponding confidence interval. We
also propose a computational strategy to extend the method to $k > n/2$.

Current literature usually focuses on the asymptotic property of $U_n$ while there is very limited analysis on
the properties of the variance estimator of $\text{Var}(U_n)$. To the best of our knowledge, the asymptotic property
of an unbiased variance estimator of U-statistics has not been well studied even for fixed $k$. Our theoretical
contribution is two-fold. First, we show that when $k \leq n/2$, our estimator coincides with approaches in the
previous literature (Wang and Lindsay, 2014; Folsom, 1984), although they are proposed from a completely
different perspective (see Section 3.5 for a detail discussion). Secondly, we prove the ratio consistency for
our variance estimator under $k = o(\sqrt{n})$, which has never been established previously. Our result serves as a first attempt in this direction. Technically, the proposed estimator can be expressed as a U-statistic, however, existing tools and assumptions used in Mentch and Hooker (2016) and DiCiccio and Romano (2022) cannot be directly applied. Hence, we employ a new concept called Double U-statistic (see Section 4.4) to analyze the ratio consistency. Interestingly, we illustrate that there is no general theory for the normality of $U_n$ when $k$ is comparable to $n$. Hence further explorations along this line of topic is much needed.

2 Background

2.1 Random Forests as U-statistics

Given a set of $n$ i.i.d. observations $X_n = (X_1, ..., X_n)$ and an unbiased estimator, $h(X_1, ..., X_k)$, of the parameter of interest $\theta$ with $k \leq n$, the U-statistic (Hoeffding, 1948) defined in the following is a minimum-variance unbiased estimator of $\theta$:

$$
U_n = \left(\frac{n}{k}\right)^{-1} \sum_{1 \leq j_1 < \cdots < j_k \leq n} h(X_{j_1}, \ldots, X_{j_k}) = \left(\frac{n}{k}\right)^{-1} \sum_{S_i \subseteq X_n} h(S_i),
$$

where each $S_i$ is a subset of $k$ samples from the original $X_n$. Note that without the risk of ambiguity, we drop $k$ in the notation of U-statistics. Random forests with subbagging samples can be viewed as such estimators (Mentch and Hooker, 2016). In particular, if we let each $X_j = (x_j, y_j)$ be the vector of observed covariates $x_j \in \mathbb{R}^d$ and outcome $y_j \in \mathbb{R}^1$, and view $h(S_i)$ as a tree estimator that predicts the outcome at a specific target point $x_0$, then in a broad view, a random forest is an average of such tree estimators. The goal of this paper is to provide new strategies for estimating the variance of a random forest under scenarios that existing methods are not suitable for. However, a few subtle differences should be clarified before we proceed.

First, the original random forest (Breiman, 2001) uses bootstrap samples, i.e. sampling with replacement, to build each tree. This can be view as a V-statistic and the connection has been discussed in Zhou et al. (2021). Later developments of random forests such as Geurts et al. (2006) show that sampling without replacement, i.e. subbagging, can perform equally well. Hence, we will restrict our discussion to this subbagging setting. Secondly, unlike traditional examples of U-statistics, the subsample size $k$ usually grows with $n$, as implemented in a random forest. This is referred to as the Infinite-Order U-statistic (IOUS). As a consequence, $\binom{n}{k}$ is too large and it is computationally infeasible to exhaust all such subsamples. In practice, a random forest model usually fits a pre-specified, say $B$ number of trees, where $B$ is a reasonably large number. The incomplete U-statistic is defined as

$$
U_{n,B} = \frac{1}{B} \sum_{i=1}^{B} h(S_i)
$$

Hence, this belongs to the class of incomplete U-statistics (Lee, 1990). Such differences will be addressed.
in the methodology section.

Lastly, we note that most random forest models use a random kernel function \( h(\cdot) \) instead of a deterministic one. This is mainly due to the mechanics of random feature selection (Breiman, 2001) and random splitting point (Geurts et al., 2006) when fitting each tree. Such randomness reduces correlations among individual trees and thus improves the performance of random forests over single trees and other ensemble approaches (Breiman, 1996). To be specific, we may label such randomness as \( w_i \)'s, which are generated from a certain distribution \( F_w \). Hence a random forest is represented as a random kernel, incomplete and infinite order U-statistic, given as

\[
U_{w,n,B} = \frac{1}{B} \sum_{i=1}^{B} h^{(w)}(S_i).
\]

Mentch and Hooker (2016) show that \( U_{w,n,B} \) converges in probability to \( U_{w,n,B}^* = E_w(U_{w,n,B}) \) under suitable conditions and when \( B \) diverges to infinity at a fast rate of \( n \). It should be noted that the exact mechanism of \( w \) on the kernel \( h \) is still unclear and is an open question. For the sake of estimating the variance of U-statistics, given \( B \) large enough, the theoretical analysis of random U-statistic can be reasonably reduced to analyzing the non-random U-statistic \( U_{w,n,B}^* \).

With the above clarifications, the focus of this paper is on estimating the variance of a non-random and incomplete U-statistic, i.e. \( U_{n,B} \), for large \( k \). Our analysis starts with a classical result of the variance of U-statistics. In particular, the variance of an order-\( k \) complete U-statistics is given by Hoeffding (1948):

\[
\text{Var}(U_n) = \left( \begin{array}{c} n \\ k \end{array} \right)^{-1} \sum_{d=1}^{k} \left( \begin{array}{c} k \\ d \end{array} \right) \left( \begin{array}{c} n-k \\ k-d \end{array} \right) \xi_{d,k}^2,
\]

where \( \xi_{d,k}^2 \) is the covariance between two kernels \( h(S_1) \) and \( h(S_2) \) with \( S_1 \) and \( S_2 \) sharing \( d \) overlapping samples, i.e., \( \xi_{d,k}^2 = \text{Cov}(h(S_1), h(S_2)) \), with \( |S_1 \cap S_2| = d \). Here both \( S_1 \) and \( S_2 \) are size-\( k \) subsamples. Alternatively, we can represent \( \xi_{d,k}^2 \) as (Lee, 1990),

\[
\xi_{d,k}^2 = \text{Var}[E(h(S)|X_1, ..., X_d)].
\]

Such a form will be utilized in the following discussion. Finally, we note that the gap between variances of an incomplete U-statistic and its complete counterpart can be understood as

\[
\text{Var}(U_{n,B}) = \text{Var}[E(U_{n,B}|X_n)] + E[\text{Var}(U_{n,B}|X_n)] = \text{Var}(U_n) + E[\text{Var}(U_{n,B}|X_n)].
\]

where the additional term \( E[\text{Var}(U_{n,B}|X_n)] \) depends on the subsampling scheme. In particular, when all subsamples are sampled with replacement from \( X_n \), we have (Lee, 1990)

\[
\text{Var}(U_{n,B}) = (1 - \frac{1}{B})\text{Var}(U_n) + \frac{1}{B}\xi_{k,k}^2.
\]

This suggests that the gap between the two can be closed by using a large \( B \). Hence, we shall first restrict
our discussion under the complete U-statistics setting and then extend it to an incomplete U-statistic based one.

3 Methodology

The main technical challenge for estimating the variance is when \( k \) grows in the same order as \( n \), i.e., \( k = \beta n \) for some \( \beta \in (0, 1) \). This is rather common in practice and many existing implementations since \( k \) essentially controls the depth of a tree, which is the major factor that determines the bias of the model. However, existing methods mainly focus on a small \( k \) scheme, with various assumptions with the growth rate of \( k \). We shall demonstrate that existing methods will encounter significant bias in such a scenario.

After investigating existing methods, and establishing new connections, our proposed estimator *Matched Sample Variance Estimator* will be given in Sections 3.3 and 3.4, these methods are suitable when \( k \leq \frac{n}{2} \). Its extensions when \( \frac{n}{2} < k < n \) will be discussed in Section 3.7. Furthermore, we introduce a local smoothing approach to reduce variations of the proposed estimator in Section 3.8.

3.1 Existing Methods and Limitations

Continuing from the decomposition of \( \text{Var}(U_n) \) (3), by further defining the coefficient \( \gamma_{d,k,n} = \left( \begin{array}{c} n \\ k \end{array} \right)^{-1} \left( \begin{array}{c} k \\ d \end{array} \right) \left( \begin{array}{c} n-k \\ k-d \end{array} \right) \), we have \( \text{Var}(U_n) = \sum_{d=1}^{k} \gamma_{d,k,n} \xi_{d,k}^2 \). It is easy to see that \( \gamma_{d,k,n} \) corresponds to the probability mass function (PMF) of a hypergeometric (HG) distribution with parameters \( n, k \) and \( d \). A graphical demonstration of such coefficients under different \( k \) and \( d \) settings, with \( n = 100 \), is provided in Figure 1. Many existing methods (Mentch and Hooker, 2016; DiCiccio and Romano, 2022) rely on the asymptotic approximation of \( \text{Var}(U_n) \) when \( k \) is small, e.g., \( k = o(n^{1/2}) \). Under such settings, the first coefficient \( \gamma_{1,k,n} = \left[ 1 + o(1) \right] \frac{k^2}{n} \) dominates all remaining ones, as we can see in Figure 1 when \( k = 10 \). In this case, to estimate \( \text{Var}(U_n) \), it suffices to estimate the leading covariance term \( \xi_{1,k}^2 \) if the \( \xi_{k,k}/(k\xi_{1,k}^2) \) is bounded.

![Hypergeometric Prob. Mass (n = 100)](image)

Figure 1: Probability mass function of hypergeometric distribution with \( n = 100 \) and different \( k \).

However, when \( k \) is of the same order as \( n \), i.e., \( k = \beta n \), the density of HG distribution concentrates
around $d = \beta^2 n$ instead of $d = 1$ (see e.g., Figure 1, with $k = 20$ or 50). In particular, given $k, n \to \infty$, $k/n \to \beta \in (0, 1)$ with certain conditions, the probability mass function of HG distribution can be approximated by the normal density function (Nicholson, 1956). Hence, the variance will be mainly determined by terms with large $d$ in the decomposition, and only estimating $\xi_{1,k}^2$ will introduce significant bias.

Alternatively, another theoretical strategy proposed by Wager and Athey (2018); Peng et al. (2019) may be used under $k = o(n)$ setting, if the $U$ statistic can be understood through the Hajek projection with additional regularity conditions. In this case, the variance of a U-statistic can be well approximated by the variance of a linearised version, while its estimates can be realized using the infinitesimal jackknife procedure Efron and Stein (1981). However, this is usually at the cost of requiring specific mechanics, such as “honesty” when fitting the tree model (Wager and Athey, 2018; Athey et al., 2019), and it is not clear what would be the consequences if these conditions are violated.

Existing variance estimator methods are mainly divided into two categories, depending on whether or not to explicitly estimate $\xi_{d,k}^2$. With the Hajek projection guarantee, Wager and Athey (2018) avoids the estimation of any individual $\xi_{d,k}^2$ and directly estimates the variance of $U_n$. Our empirical evaluation using such estimators shows that they usually overestimate the variance when $k$ is large. On the other hand, Mentch and Hooker (2016) and Zhou et al. (2021) explicitly estimate $\xi_{1,k}^2$ and $\xi_{k,k}^2$, where $\xi_{1,k}^2$ leads to the leading variance of $\text{Var}(U_n)$ and $\xi_{k,k}^2$ compensates the additional variance of incomplete U-statistics. However, based on our previous analysis, merely estimating these two terms is no longer sufficient when $k = \beta n$. Moreover, it becomes empirically difficult to provide an accurate estimate for either $\xi_{1,k}^2$ or $\xi_{k,k}^2$, since one has to numerically approximate the $\text{Var}$ and $\text{E}$ operations in Equation (4) (Mentch and Hooker, 2016; Zhou et al., 2021). To estimate $\xi_{1,k}^2$, their strategy starts withholding one shared sample, e.g., $X_pq$, and varying the remaining samples in $S$ among existing observations $X_n$. After approximating the $\text{E}$ operator, one alters the held sample $X_{(1)}$ randomly and approximates the $\text{Var}$ operator. However, as one can expect, when $k = \beta n$, these subsamples highly overlap with each other, leading to correlation among different estimations of the $\text{E}$ operator, and large bias in the $\text{Var}$ approximation. In Section 5, we provide numerical evidence to show their bias and the advantage of our strategy.

To conclude, it appears to be computationally and theoretically inevitable to estimate all or at least a large amount of $\xi_{d,k}^2$ terms for an unbiased variance estimator. At the first glance, this seems to be impossible. However, the following analysis shows that we may achieve this through an alternative view of the variance decomposition, which then motivates a convenient incomplete and computationally feasible version. Our method uncovers a connection with the literature on the variance calculation of complex sample designs (Folsom, 1984) and shares interesting identical complete and incomplete forms with Wang and Lindsay (2014) while Wang and Lindsay (2014)’s estimators are motivated from the moments of $U_n$. These connections will be discussed in Section 3.5.
3.2 An Alternative View of the Variance Decomposition

Instead of directly estimating each $\xi^2_{d,k}$ (4) for $d = 1, 2, \ldots, k$, we decompose it into two parts by the law of total variance,

$$
\xi^2_{d,k} = \text{Var}[E(h(S)|X_1, \ldots, X_d)] = \text{Var}(h(S)) - E[\text{Var}(h(S)|X_1, \ldots, X_d)] := V(h) - \xi^2_{d,k},
$$

(7)

where $V(h) := \text{Var}(h(S))$ and $\xi^2_{d,k} := E[\text{Var}(h(S)|X_1, \ldots, X_d)]$. In this representation, $V(h)$ is the variance of a tree estimator while the conditional variance part of $\xi^2_{d,k}$ concerns the variance of a tree with $d$ samples fixed. We can then combine this decomposition with Equation (3) to obtain

$$
\text{Var}(U_n) = V(h) - \sum_{d=0}^{k} \gamma_{d,k,n} \xi^2_{d,k} := V(h) - V(S),
$$

(8)

where $\xi^2_{0,k} := V(h)$ and $V(S) := \sum_{d=0}^{k} \gamma_{d,k,n} \xi^2_{d,k}$. Note that we add and subtract $\gamma_{0,k,n} \xi^2_{0,k}$ from (3) to make the coefficient of $V(h)$ to be 1. The above formulation is valid not only when $k \leq n/2$ but whenever $k$ is less than $n$. In particular, when $k > n/2$, the first $2k - n$ terms in $V(S)$ would vanish since $\gamma_{d,k,n} = 0$ for $d < 2k - n$, given that the overlaps between two size-$k$ subsamples would be at least $2k - n$. The advantage of such formulation over the variance decomposition (3) is that when $k \leq n/2$, there exist computationally convenient unbiased sample estimators of both quantities on the right-hand side. However, when $k > n/2$, the main difficulty is on estimating $\text{Var}(h(S))$, which may require bootstrapping, and cannot be directly obtained without fitting additional trees outside the ones used in calculating the forest. Hence, for our discussion, we would mainly restrict to the $k \leq n/2$ case, while the $k > n/2$ case will be discussed in Section 3.7. In the following, we will first present the estimation of $V(S)$, which involves an infinite sum when $k$ grows with $n$, then $V(h)$, is relatively straightforward provided that $k \leq n/2$.

3.3 Variance Estimation for Complete U-statistics

Ideally, estimators of $V(S)$ and $V(h)$ with $k \leq n/2$ can both be computed directly from a fitted random forest without posing much additional computational cost. This seems to be a tall task given that we are estimating an infinite sum $V(S)$. However, we shall see that the sample variance of all fitted trees $h(S_i)$ can produce an unbiased estimator. Again, we start with the complete case to facilitate the argument. The incomplete case shall become natural.

3.3.1 Joint Estimation of the Infinite Sum: $V(S)$

Suppose we pair subsamples $S_i$ and $S_j$ among $\binom{n}{k}$ subsamples and let $d = |S_i \cap S_j| = 0, 1, \ldots, k$. Then for each $d$, there exist $N_{d,k,n} = \binom{n}{d}^2 \gamma_{d,k,n}$ pairs of subsamples $S_i, S_j$ such that $|S_i \cap S_j| = d$. Note that for any such pair, $[h(S_i) - h(S_j)]^2/2$ is an unbiased estimator of $\xi^2_{d,k} = \text{Var}(h(S)|X_1, \ldots, X_d)$. We may then
construct an unbiased estimator of $\hat{\xi}^2_{d,k}$ that utilizes all such pairs:

$$\hat{\xi}^2_{d,k} = N^{-1}_{d,k,n} \sum_{|S_i \cap S_j| = d} [h(S_i) - h(S_j)]^2 / 2.$$  (9)

This motivates us to combine all such terms in the infinite sum, which surprisingly leads to the sample variance of all trees (kernels). This is demonstrated in the following proposition, suggesting that we may jointly estimate them without explicitly analyzing every single term. The proof is collected in Appendix F.

**Proposition 3.1.** Given a complete U-statistic $U_n$, and the estimator $\hat{\xi}^2_{d,k}$ defined in Equation (9), when $k \leq n/2$, we have the following unbiased estimator of $V^p_\mathcal{S}$:

$$\hat{\S} := \binom{n}{k}^{-1} \sum_{i} [h(S_i) - U_n]^2,$$  (10)

satisfying that $\hat{\S} = \sum_{d=0}^{k} \gamma_{d,k,n,n^2_{d,k}}$. and $E(\hat{\S}) = V^S$.

Furthermore, when $k > n/2$, the first $2k - n$ terms in the summation $\sum_{d=0}^{k}$ is removed since corresponding $\gamma_{d,k,n} = 0$.

This proposition suggests that $\hat{\S}$, the sample variance of all $h(S_i)$, is an unbiased estimator of the infinite sum $V^S = \sum_{d=0}^{k} \gamma_{d,k,n,n^2_{d,k}}$. Its incomplete U-statistic based version should be straightforward to calculate since we can simply obtain samples from all possible trees to estimate this quantity. This can be computed without any hassle since they are exactly the trees used to obtain a random forest. However, additional considerations may facilitate the estimation of the other term $V^h$ so that both can be done simultaneously without fitting additional trees.

**3.3.2 Estimation of Tree Variance: $V^h$**

The idea of estimating $V^h$ follows from the fact that $[h(S_i) - h(S_j)]^2 / 2$ is an unbiased estimator of the tree variance if the pair $S_i$ and $S_j$ do not contain any overlapping samples. Actually, $\hat{\xi}^2_{0,k}$ introduced in the last section is such an estimator. Hence, given that $k \leq n/2$, by Equation (9) we have the following unbiased estimator of $V^h$:

$$\hat{\S} = \hat{\xi}^2_{0,k} = \binom{n}{k}^{-1} \binom{n-k}{d}^{-1} \sum_{|S_i \cap S_j| = 0} [h(S_i) - h(S_j)]^2 / 2.$$  (11)

Therefore, we combine estimators $\hat{\S}$ (10) and $\hat{\S}$ (11) to get an unbiased estimator of $\text{Var}(U_n)$:

$$\hat{\text{Var}}(U_n) = \hat{\S} - \hat{\S}.$$  (12)
3.4 Variance Estimation for Incomplete U-statistics

Based on the previous demonstration, we can also construct an incomplete estimator of \( \text{Var}(U_n) \) by drawing random subsamples instead of exhausting all \( \binom{n}{k} \) subsamples. However, if we obtain these subsamples through completely random draws, very few of them would be mutually exclusive \((d = 0)\), especially when \( k \) is large. This causes difficulty for estimating the tree-variance \( V^{(h)} \) since only the mutually exclusive pairs should be used. Hence, a new subsampling strategy is needed to allow sufficient pairs of subsamples to estimate both \( V^{(h)} \) and \( V^{(S)} \). In addition, due to this new sampling strategy, the variance of new incomplete U-statistic has a different incomplete correction term than the one in (6). This should be done by estimating the inflation term \( \text{E}[\text{Var}(U_{n,B}|X_n)] \) in Equation (5). Note that this sampling strategy is only applied to \( k \leq n/2 \) settings. The case for \( k \geq n/2 \) will be presented in Section 3.7.

The following “matched group” sampling scheme is proposed by a simple idea, intended sampling \((S_i, S_j)\)'s that \( |S_i \cap S_j| = 0 \), so we can estimate \( V^{(h)} \). First, we can sample \( M \) mutually exclusive subsamples, \((S_1, ..., S_M)\) namely “a matched group”, from \((X_1, ..., X_n)\), where \( 2 \leq M \leq \lfloor n/k \rfloor \). This enable us to estimate \( V^{(h)} \) by its sample variance. In particular, when \( M = 2 \), the unbiased estimator is \( [h(S_1) - h(S_2)]^2/2 \) for \( |S_1 \cap S_2| = 0 \). Then, we repeat this \( B \) times to obtain \( B \) such matched groups. Denote the subsamples in the \( b \)-th matched group as \( S^{(b)}_1, S^{(b)}_2, ..., S^{(b)}_M \), such that \( S^{(b)}_i \cap S^{(b)}_{i'} = \emptyset \) for \( i \neq i' \).

We use a new notation \( U_{n,B,M} \) to denote the resulting \( U \) statistics

\[
U_{n,B,M} = \frac{1}{MB} \sum_{i=1}^{M} \sum_{b=1}^{B} h(S^{(b)}_i). \tag{13}
\]

This is different from the conventional incomplete U-statistic \( U_{n,B} \) with random subsamples. Though \( M = 2 \) is enough for estimating \( V^{(h)} \), we recommend to choose \( M = \lfloor n/k \rfloor \). Because fixing the number of subsamples, i.e. \( B^* := M \cdot B \), a larger \( M \) leads to a smaller \( \text{Var}(U_{n,B,M}) \), which is a direct consequence of the following proposition.

**Proposition 3.2.** For a general incomplete U-statistic with \( M \cdot B \) samples sampled by the matching sampling scheme in last section,

\[
\text{Var}(U_{n,B,M}) = \left( 1 - \frac{1}{B} \right) \text{Var}(U_n) + \frac{1}{MB} V^{(h)}. \tag{14}
\]

The proof is deferred to Appendix E.1. It is interesting to note that when fixing the total number of trees \( M \cdot B \) and let \( M \geq 2 \), the variance of \( U_{n,B,M} \) is always smaller than the variance of \( U_{n,B} \) given in (6). However, these two are identical when \( M = 1 \).

Based on this new sampling scheme, we can propose estimators \( \hat{V}^{(h)}_{B,M} \) and \( \hat{V}^{(S)}_{B,M} \) as analogues to \( \hat{V}^{(h)} \) and \( \hat{V}^{(S)} \) respectively. Denote the collection of tree predictions as \( \{h(S^{(b)}_i)\}_{i,b} \) for \( i = 1, 2, ..., M, \; b = 1, 2, ..., B \). A sample variance within each group \( b \), \( \frac{1}{M-1} \sum_{i=1}^{M} [h(S^{(b)}_i) - \bar{h}^{(b)}]^2 \), is an unbiased estimator of \( V^{(h)} \). Here \( \bar{h}^{(b)} = \frac{1}{M} \sum_{i=1}^{M} h(S^{(b)}_i) \) is the group mean. Thus the average of the above estimators over all groups becomes our following \( \hat{V}^{(h)}_{B,M} \) (15). \( \hat{V}^{(S)}_{B,M} \) (16) is again the sample variance of all kernels but we use
Instead of MB as the denominator.

\[
\hat{V}_{B,M}^{(b)} = \frac{1}{B} \sum_{b=1}^{B} \frac{1}{M - 1} \sum_{i=1}^{M} \left[ h(S_i^{(b)}) - \bar{h}^{(b)} \right]^2, \quad (15)
\]

\[
\hat{V}_{B,M}^{(S)} = \frac{1}{MB - 1} \sum_{b=1}^{B} \sum_{i=1}^{M} \left( h(S_i^{(b)}) - U_{n,B,M} \right)^2. \quad (16)
\]

Note that \( \hat{V}_{B,M}^{(h)} \) is still an unbiased of \( V^{(h)} \) while \( \hat{V}_{B,M}^{(S)} \) introduces a small bias when estimating \( V^{(S)} \). We use the following proposition to quantify the bias. We note that we can correct this bias by using a linear combination of \( \hat{V}_{B,M}^{(h)} \) and \( \hat{V}_{B,M}^{(S)} \).

**Proposition 3.3.** For the sample variance estimator \( \hat{V}_{B,M}^{(S)} \) defined on the matched groups subsamples with \( M \cdot B \geq 2 \), we denote \( \delta_{B,M} := \frac{M-1}{MB - 1} \). Then,

\[
E \left( \hat{V}_{B,M}^{(S)} \right) = (1 - \delta_{M,B})V^{(S)} + \delta_{M,B}V^{(h)}. \quad (17)
\]

This leads to the following unbiased estimator of \( \text{Var}(U_{n,B,M}) \). The proof of both Propositions 3.3 and 3.4 is collected in Appendix F.

**Proposition 3.4.** Given \( M \cdot B \) subsamples from the matched group sampling scheme, \( B \geq 1 \), and \( M \geq 2 \), the following is an unbiased estimator of \( \text{Var}(U_{n,B,M}) \), namely “Matched Sample Variance Estimator”.

\[
\widehat{\text{Var}}(U_{n,B,M}) = \hat{V}_{B,M}^{(h)} - MB - 1 \hat{V}_{B,M}^{(S)}. \quad (18)
\]

When considering random kernels, both estimators \( \hat{V}_{B,M}^{(h)} \) and \( \hat{V}_{B,M}^{(S)} \) will be inflated due to the additional randomness of \( w \). However, the inflation is offset to a large extent after taking the difference between these two quantities. Our simulation results show that using random kernels does not introduce noticeable bias.

### 3.5 Connection with Existing Methods

To the best of our knowledge, there are two existing methods (Wang and Lindsay, 2014; Folsom, 1984) that share close connections with our proposed one. It is interesting to discuss the relationships and differences between our view of the variance decomposition versus these existing approaches. Wang and Lindsay (2014) proposed partition-based, unbiased variance estimators of both complete and incomplete U-statistics. Their estimation of \( \text{Var}(U_n) \) is motivated by \( E(U_n^2) - E^2(U_n) \). This second-moment view of the estimator leads to an ANOVA type of estimator that uses the within and between-variances of the groups (see Wang and Lindsay, 2014, page 1122). Although with different motivations, we can show that their complete and sample version estimators are equivalent to ours after some careful calculation. This is shown in Appendix F.

On the other hand, Folsom (1984) is a method proposed for sampling design problems. It follows a sequence of works such as the Horvitz-Thompson estimator (Horvitz and Thompson, 1952) and the Sen-
Yates-Grundy estimators (Yates and Grundy, 1953; Sen, 1953) in the sample survey literature. However, the authors only derived a variance estimator of complete U-statistic through a purely algebraic approach without considering the incomplete case. Interestingly, their complete variance estimator is also the same as our proposed one, and hence equivalent to Wang and Lindsay (2014).

The unique feature of our estimator is its conditional variance view. This motivates sample estimators in both \( k \leq n/2 \) and \( k > n/2 \) settings (see more details in Section 3.7 for the latter setting). Given \( k \leq n/2 \) and choosing \( M = \lfloor n/k \rfloor \), our estimators coincide with those in both Wang and Lindsay (2014) and Folsom (1984). However, when \( k > n/2 \), their estimators do not naturally exist. While Folsom (1984) sees “no practical utility in the general case” (page 68) of these estimators back in 1984, and Wang and Lindsay (2014) does not realize the connection and equivalence between the two U-statistic’s variance estimators (see Remark 1 therein), our formulation bridges these works in the literature, and extends its potential under \( k > n/2 \).

### 3.6 The Algorithm

**Algorithm 1:** Matched Sample Variance Estimator \((k \leq n/2)\)

**Input:** \( n, k, M, B, \) training set \( \mathcal{X}_n \), and testing sample \( x^* \)

**Output:** \( \hat{\text{Var}}(U_{n,B,M}) \)

1. **Construct matched samples:**
   
   for \( b = 1, 2, \ldots, B \) do
   
   Sample the \( b \)-th matched group \( \{S_1^{(b)}, S_2^{(b)}, \ldots, S_M^{(b)}\} \) such that \( S_i^{(b)} \)s are mutually exclusive, i.e.,
   
   \[ S_i^{(b)} \cap S_i^{(b')} = \emptyset \text{ for } i \neq i'. \]

2. **Fit trees and obtain predictions:**
   
   Fit random trees for each subsample \( S_i^{(b)} \) and obtain prediction \( \hat{h}(S_i^{(b)}) \) on the target point \( x^* \).

3. **Calculate the variance estimator components:**
   
   8. Forest average: \( U_{n,B,M} = \frac{1}{MB} \sum_{i=1}^{M} \sum_{b=1}^{B} h(S_i^{(b)}) \)
   
   9. Within-group average: \( \bar{h}^{(b)} = \frac{1}{M} \sum_{i=1}^{M} h(S_i^{(b)}) \)
   
   10. Tree variance in (15): \( \hat{V}_{B,M}^{(b)} = \frac{1}{MB} \sum_{b=1}^{B} \frac{1}{M-1} \sum_{i=1}^{M} (h(S_i^{(b)}) - \bar{h}^{(b)})^2 \)
   
   11. Tree sample variance in (16): \( \hat{V}_{B,M}^{(S)} = \frac{1}{MB-1} \sum_{i=1}^{M} \sum_{b=1}^{B} (h(S_i^{(b)}) - U_{n,B,M})^2 \)
   
   12. **The final variance estimator** (18)
   
   \[ \hat{\text{Var}}(U_{n,B,M}) = \hat{V}_{B,M}^{(b)} - (1 - \frac{1}{MB})\hat{V}_{B,M}^{(S)} \]

Based on the previous illustration, we summarize the proposed method in Algorithm 1. We call \( \hat{\text{Var}}(U_{n,B,M}) \) the Matched Sample Variance Estimator. The algorithm is adaptive to any \( k \leq n/2 \), where \( n \) is not necessarily a multiplier of \( k \).
3.7 Extension to $k > n/2$

The previous estimator $\overline{\text{Var}}(U_{n,B,M})$ (18) is restricted to $k \leq n/2$ due to the sampling scheme. However, this does not prevent the application of formulation (8), $\text{Var}(U_n) = V^{(h)} - V^{(S)}$. Neither Folsom (1984) or Wang and Lindsay (2014) provide further discussions under $k > n/2$. In this section, we discuss a simple generalization.

Note that this $U_{n,B,M=1}$ degenerates to a $U_{n,B}$ in (6). Re-applying Propositions (3.2) and (8) with $M = 1$, we can obtain the variance of an incomplete $U$ statistic sampled randomly with replacement:

$$\text{Var}(U_{n,B,M=1}) = V^{(h)} - \frac{B-1}{B}V^{(S)}.$$  

By Proposition 3.3, $\hat{V}^{(S)}_{B,M=1} = \frac{1}{B-1} \sum_{b=1}^{B} (h(S_b) - U_{n,B,M=1})^2$ is still an unbiased estimator of $V^{(S)}$. However, $V^{(h)}$ has to be estimated with a different approach since any pair of trees would share at least some overlapping samples. A simple strategy is to use bootstrapping. This means that we need to generate another set of trees, each sampled with replacement, and calculate their variance as the estimator of $V^{(h)}$.

We remark that these additional trees through bootstrapping will introduce an additional computational burden since they are not used in forest averaging. In our simulation study, we simply fit the same number of $B$ trees for the bootstrap estimator. The goal of this generalization is to explore the potential. Limitations and future work are discussed in the discussion section.

3.8 Locally Smoothed Estimator

Using the proposed variance estimator, we could construct confidence intervals for $U_{n,B,M}$ accordingly, provided that the corresponding random forest estimator is asymptotically normal. The asymptotic normality of random forests has been partially studied recently, e.g., Athey et al. (2019), and is still an open question. Our focus is not on the properties of random forests themselves. Instead, we are only interested in the behavior of various variance estimators, which can further lead to constructing confidence intervals. However, even though the proposed estimator is unbiased, large variance of this estimator may still result in an under-coverage of the corresponding confidence interval. To alleviate this issue, one natural idea is to use local smoothing. Hence, we propose a Matched Sample Smoothing Variance Estimator (MS-s). The improvement of variance reduction will be demonstrated in the simulation study, e.g., Table 1 and Figure 2.

Denote a variance estimator on a future test sample $x^*$ as $\hat{\sigma}^2_{RF}(x^*)$. We randomly generate $N$ neighbor points $x_1^*, \ldots, x_N^*$ and obtain their variance estimators $\hat{\sigma}^2_{RF}(x_1^*), \ldots, \hat{\sigma}^2_{RF}(x_N^*)$. Then, the locally smoothed estimator is defined as the average:

$$\bar{\hat{\sigma}}^2_{RF}(x^*) = \frac{1}{N+1} \left[ \hat{\sigma}^2_{RF}(x^*) + \sum_{i=1}^{N} \hat{\sigma}^2_{RF}(x_i^*) \right].$$  

(19)

Due to the averaging with local target samples, there is naturally a bias-variance trade-off. This is a rather classical topic, and there can be various ways to improve such an estimator based on the literature. Our
goal here is to provide a simple illustration. In the simulation section, we consider generating 10 neighbors on an $\ell_2$ ball centered at $x^*$. The radius of the ball is set to be the Euclidean distance from $x^*$ to the closest training sample. More details are provided by Algorithm 2 in Appendix K. This smoothing approach effectively improves the coverage rate, especially when the number of trees is small. Also, we found that the performance is not very sensitive to the choice of neighbor distance.

4 Theoretical Results

4.1 Limitation of Normality Theories

Many existing works in the literature have developed the asymptotic normality of $U_n$ given $k = o(\sqrt{n})$ to $o(n)$ under various regularity conditions (Mentch and Hooker, 2016; Wager and Athey, 2018; DiCiccio and Romano, 2022; Zhou et al., 2021). Although our estimator is proposed for the case $k = \beta n$, we need to acknowledge that there is no universal normality of $U_n$ for such a large $k$ setting. As we will see in the following, there are both examples and counter-examples for the asymptotic normality of $U_n$ with large $k$, depending on the specific form of the kernel.

Essentially, when a kernel is very adaptive to local observations without much randomness, i.e., 1-nearest neighbors, and the kernel size is at the same order of $n$, there are too many dependencies across different $h(S_i)$’s. This prevents the normality of $U_n$. On the other hand, when the kernel size is relatively small, there is enough variation across different kernel functions to establish normality. This is the main strategy used in the literature. In practice, it is difficult to know a priori what type of data dependence structure these $h(S_i)$’s may satisfy. Thus, the normality of a random forest with large subsample sizes is still an open question and requires further understanding of its kernel. In the simulation study, we observe that the confidence intervals constructed with the normal quantiles work well, given that data are generated with Gaussian noise (see Section 5.1).

Example 4.1. Given covariate-response pairs: $Z_1 = (x_1, Y_1), \ldots, Z_n = (x_n, Y_n)$ as training samples, where $x_i$’s are unique and deterministic numbers and $Y_i$’s i.i.d. $F$ such that $E(Y_i) = \mu > 0$, $\text{Var}(Y_i) = \sigma^2$), for $i = 1, 2, \ldots, n$. We want to predict the response for a given testing sample $x^*$.

Suppose we have two size-$k$ ($k = \beta n$) kernels: 1) a simple (linear) average kernel: $h(S) = \frac{1}{k} \sum_{j=1}^{k} Y_j$; 2) a 1-nearest neighbor (1-NN) kernel, which predicts using the closest training sample of $x^*$ based on the distance of $x$. Without loss of generality, we assume that $x_i$’s are ordered such that $x_i$ is the $i$-th nearest sample to $x^*$. We denote corresponding sub-bagging estimator as $U_{\text{mean}}$ and $U_{1-\text{NN}}$ respectively. It is trivial to show that

$$U_{\text{mean}} = \frac{1}{n} \sum_{i=1}^{n} Y_n, \quad U_{1-\text{NN}} = \sum_{i=1}^{n-k+1} a_i Y_i,$$

where $a_i = \binom{n-i}{k-1} / \binom{n}{k}$ and $\sum_{i=1}^{n-k+1} a_i = 1$. Accordingly, we have $\text{Var}(U_{\text{mean}}) = \frac{1}{n^2} \sigma^2$ and $\text{Var}(U_{1-\text{NN}}) \geq a_i^2 \text{Var}(Y_i) = \frac{k^2}{n^2} \sigma^2 = \beta^2 \sigma^2$. Since $U_{\text{mean}}$ is a sample average, we still obtain asymptotic normality after
scaling by \( \sqrt{n} \). However, \( \beta = k/n > 0 \), \( a_1 \) makes a significant proportion in the sum of all \( a_i \)'s and \( \text{Var}(U_{1-NN}) \) does not decay to 0 as \( n \) grows. Hence, asymptotic normality is not satisfied for \( U_{1-NN} \).

### 4.2 Ratio Consistency of Variance Estimator

Denote our unbiased variance estimator of complete U-statistic (12) as \( \hat{V}_u \). The theoretical focus of this paper is to show its ratio consistency, i.e., \( \hat{V}_u/E(\hat{V}_u) \xrightarrow{P} 1 \), where \( \xrightarrow{P} \) denotes convergence in probability. However, based on the previous observation, this becomes a tall task under the \( k = \beta n \) setting, since explicit assumptions have to be made for random forests. Instead, as the first attempt to investigate such estimators, we focus on the \( k = o(\sqrt{n}) \) setting, which is prevalent in the current literature. This is in fact already a challenging task. To the best of our knowledge, there is no existing work analyzing the asymptotic behavior of \( \hat{V}_u \) (as also noted by Wang and Lindsay (2014) which shares the same empirical versions), even under fixed \( k \). The difficulty lies in the complexity of both the structure of its kernel (see \( \psi \) in (20)) and the 4-way overlapping between size 2k subsamples, to be illustrated later. When \( k = \beta n \), the ratio consistency may not hold even for \( U_n \), let alone for \( \hat{V}_u \). In this case, the existence of ratio consistency highly depends on the form of the kernel, which we would like to leave for future studies.

The theoretical analysis focuses on the variance estimator for complete U-statistic, since the connection with the incomplete version is apparent when \( B \) is large enough. The section is organized as follows. In Section 4.3, we present preliminaries. In Section 4.5, we discuss the difficulties in this analysis and introduce certain new strategies. In Section 4.4, we introduce the concept of “double U-statistic” as a tool to represent the variance estimator. The main results are presented in Section 4.6. Details of assumptions and notations are deferred to Appendix B.

### 4.3 Preliminaries of the Variance of U-statistics

Recall the equivalence with Wang and Lindsay (2014) as the complete U-statistic based variance estimator, we can rewrite \( \hat{V}_u = \hat{V}^{(h)} - \hat{V}^{(S)} \) (12) as an order-2k U-statistic:

\[
\hat{V}_u = \left( \frac{n}{2k} \right)^{-1} \sum_{S^{(2k)} \subseteq \mathcal{X}_n} \psi \left( S^{(2k)} \right),
\]

where \( S^{(2k)} \) is a size-2k subsample set and \( \psi \left( S^{(2k)} \right) \) is the corresponding size-2k kernel. The size-2k kernel \( \psi \left( S^{(2k)} \right) \) in Equation (20) is defined as follows. First, it can be decomposed as the difference between two size-2k kernels: \( \psi \left( S^{(2k)} \right) := \psi_k \left( S^{(2k)} \right) - \psi_0 \left( S^{(2k)} \right) \) (See Wang and Lindsay, 2014, page 1138). Here \( \psi_{k'} \left( S^{(2k)} \right) \) for \( k' = 0, 1, 2, \ldots, k \) satisfies

\[
\psi_{k'} \left( S^{(2k)} \right) = \left( \frac{n}{2k} \right) \left( \frac{n}{k} \right)^{-1} \left( n - k + k' \right)^{-1} \sum_{d=0}^{k'} \frac{1}{N_d} \sum_{s_1, s_2 \subseteq S^{(2k)}, |s_1 \cap s_2| = d} h \left( S_1 \right) h \left( S_2 \right),
\]

where

\[
N_d = \frac{\binom{n}{k} \binom{n-k}{k'} \binom{n-k}{k'} \binom{n-k'-k'}{k'}}{\binom{n}{2k}}.
\]
where \( N_d = \binom{n-2k+d}{d} \) is some normalization constant and \( S_1, S_2 \) are size-\( k \) subsample sets. To be more specific, fixing any \( S_1 \) and \( S_2 \) s.t. \(|S_1 \cap S_2| = d\), \( N_d \) is the number of different size-2\( k \) sets \( S^{(2k)} \) which are supersets of \( S_1 \) and \( S_2 \).

Similar to a regular U-statistic, for an order-2\( k \) U-statistic \( \hat{V}_u \), given two subsample sets \( S_1^{(2k)} \) and \( S_2^{(2k)} \), the variance of \( \hat{V}_u \) can be decomposed as

\[
\text{Var} \left( \hat{V}_u \right) = \left( \frac{n}{2k} \right)^{-1} \sum_{c=1}^{2k} \binom{2k}{c} \binom{n-2k}{2k-c} \sigma^2_{c,2k},
\]

where \( \sigma^2_{c,2k} \) is the covariance between \( \psi(S_1^{(2k)}) \) and \( \psi(S_2^{(2k)}) \), i.e.,

\[
\sigma^2_{c,2k} := \text{Cov} \left[ \psi(S_1^{(2k)}), \psi(S_2^{(2k)}) \right], \text{s.t. } |S_1^{(2k)} \cap S_2^{(2k)}| = c, \text{ for } c = 1, 2, ..., 2k.
\]

We remark that in this paper, \( S \) refers to a size-\( k \) set and \( S^{(2k)} \) refers to a size-2\( k \) set. Accordingly, notations \( d = |S_1 \cap S_2| \) and \( \xi_{d,k}^2 = \text{Cov}[h(S_1), h(S_2)] \) are associated with order-\( k \) U-statistic \( \bar{U}_n \) while notations \( c = |S_1^{(2k)} \cap S_2^{(2k)}| \) and \( \sigma^2_{c,2k} = \text{Cov}[\psi(S_1^{(2k)}), \psi(S_2^{(2k)})] \) are associated with order-2\( k \) U-statistic \( \hat{V}_u \).

### 4.4 Double U-statistic

In this section, we propose the Double U-statistic structure and show that \( \hat{V}_u \) is a Double U-statistic. The way to utilize this structure will be highlighted in Section 4.5. The advantage of this tool is to break down our variance estimator into lower order terms, which levitate the difficulty involved in analyzing \( \sigma^2_{c,2k} \).

**Definition 4.2** (Double U-statistic). *For an order-\( k \) U-statistic, we call it Double U-statistic if its kernel function \( h \) is a weighted average of U-statistics.*

Essentially, a Double U-statistic is an “U-statistic of U-statistic”. Recall by Equation (20), \( \hat{V}_u = \left( \frac{n}{2k} \right)^{-1} \sum_{S^{(2k)} \subseteq X_n} \psi \left( S^{(2k)} \right) \). \( \hat{V}_u \) involves a size-2\( k \) kernel \( \psi \). However, by Equation (21), the kernel \( \psi \) has a complicated form. The following proposition shows that we can further decompose \( \psi \) into linear combinations of \( \varphi_d \)'s, which are still U-statistics.

**Proposition 4.3** (\( \hat{V}_u \) is a Double U-statistic). *The order-2\( k \) U-statistic \( \hat{V}_u \) defined in Equation (20) is a Double U-statistic. Its kernel \( \psi \left( S^{(2k)} \right) \) can be represented as a weighted average of U-statistics, such that*

\[
\psi \left( S^{(2k)} \right) := \sum_{d=1}^{k} w_d \left[ \varphi_d \left( S^{(2k)} \right) - \varphi_0 \left( S^{(2k)} \right) \right].
\]

Here each \( \varphi_d \) is the U-statistic with size-(2\( k - d \)) asymmetric kernel as following

\[
\varphi_d \left( S^{(2k)} \right) = M^{-1}_{d,k} \sum_{S_1, S_2 \subseteq S^{(2k)}, |S_1 \cap S_2| = d} h(S_1)h(S_2), \text{ for } d = 0, 1, 2, ..., k;
\]

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Then, we can represent \( \sigma \) introduce the following decomposition of \( w \) a speed even faster than the geometric series. In our later analysis, we can show that the first term, \( \hat{\eta} \) existing tools such as those proposed by Mentch and Hooker (2016) and DiCiccio and Romano (2022).

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subsamples and hence a covariance between kernels involves 4-way overlaps (see discussions in Appendix

Proposition 4.4 (Decomposition of \( \sigma^2 \)). For any size-2k subsample sets \( S_{1}^{(2k)} , S_{2}^{(2k)} \), s.t. \( |S_{1}^{(2k)} \cap S_{2}^{(2k)} | = c \) and \( 1 \leq c \leq 2k, 1 \leq d_1, d_2 \leq k \), we define

\[
\eta_{c,2k}^{2}(d_1 , d_2 ) := \text{Cov} \left[ \varphi_{d_1} \left( S_{1}^{(2k)} \right) \varphi_{d_2} \left( S_{2}^{(2k)} \right) \right].
\]

Then, we can represent \( \sigma^2 \) as weighted sum of \( \eta_{c,2k}^{2}(d_1 , d_2 ) \)'s.

\[
\sigma^2_{c,2k} = \sum_{d_1 = 1}^{k} \sum_{d_2 = 1}^{k} w_{d_1} w_{d_2} \eta_{c,2k}^{2}(d_1 , d_2 ).
\]

This Proposition 4.4 can be directly concluded by combining the alternative form of \( U_n \)'s kernel \( \psi \) in Equation (24) and the definition of \( \eta_{c,2k}^{2}(d_1 , d_2 ) \). With the help of Double U-statistic structure, upper bounding \( \sigma^2 \) can be boiled down to the analysis of \( \eta_{c,2k}^{2}(d_1 , d_2 ) \). Detailed analysis of this connection is provided in the proof road-map (Appendix D.1) and the technical lemmas section (Appendix G). Note that we can further decompose \( \eta_{c,2k}^{2}(d_1 , d_2 ) \) (see Appendix H.5), so \( \sigma^2_{c,2k} \) can be viewed as a weighted sum of \( \text{Cov} \left[ h(S_2)h(S_2), h(S_3)h(S_3) \right] \)'s.

4.5 Technical Highlight

To show the ratio consistency of \( \hat{V}_u \), we need to upper bound \( \text{Var}(\hat{V}_u) \). However, our \( \hat{V}_u \) is not a regular fixed order or Infinite Order U-statistic. Though its order is 2k, there are further overlaps within size-2k subsamples and hence a covariance between kernels involves 4-way overlaps (see discussions in Appendix B). This unique structure renders many results for Infinite Order U-statistics inapplicable. In particular, existing tools such as those proposed by Mentch and Hooker (2016) and DiCiccio and Romano (2022) cannot be applied to our problem. Hence, we need to develop new strategies to analyze \( \text{Var}(\hat{V}_u) \) (22). First, we will introduce the Double U-statistic structure of \( \hat{V}_u \), which helps discover a cancellation effect inside \( \hat{V}_u \) (See Proposition 4.3) and reduce the analysis of \( \sigma^2_{c,2k} \) terms in Equation (22) into a lower level covariance problem. Based on the Double U-statistic structure, we break down \( \text{Var}(\hat{V}_u) \) into a 3-step analysis.

In step 1, utilizing the Double U-statistic structure, we are able to represent \( \hat{V}_u \)'s kernel, \( \psi \), as a weighted
average of new U-statistics $\varphi$’s, i.e., $\psi(S(2k)) = \sum_{d=0}^{k} w_d \varphi_d(S(2k))$, where the coefficient $w_d$ exhibits a cancellation pattern (see Proposition 4.3). In step 2, we upper bound the covariance $\eta_{c,2k}(d_1, d_2)$ (27) (see the discussion in the Double U-statistics section) by performing further cancellation analysis through pairing $\varphi_d(S(2k))$ with $\varphi_0(S(2k))$. Note that $\sigma_{c,2k}^2$ can be decomposed as a weighted sum of $\eta_{c,2k}^2(d_1, d_2)$. In step 3, we show that an upper bound of $\sigma_{c,2k}^2$ is the dominant term in upper bounding $\text{Var}(\hat{V}_u)$. This is achieved by upper bounding $\sigma_{c,2k}^2$ in $\text{Var}(\hat{V}_u)$ for all $c$. A proof road map is presented in Appendix D.1.

In the existing literature (Mentch and Hooker, 2016; DiCiccio and Romano, 2022; Zhou et al., 2021), assumptions are made to bound the ratio of last term, $\xi_{d,k}^2$, over first term, $\xi_{d,k}^2$, for $\text{Var}(U_n)$. Such assumptions of $\xi_{d,k}^2$ is reasonable for $U_n$ derived from random forests, however, since the variance estimator $\hat{V}_u$ has a complicated structure, similar assumptions of $\sigma_{c,2k}^2$ are difficult to verify and possibly violated, which is demonstrated in Appendix C.4. In this paper, we first make a weaker assumption (Assumption 2) on $\xi_{d,k}^2$. Moreover, instead of direct assumptions on $\sigma_{c,2k}^2$, we further decompose $\sigma_{c,2k}^2$ (see Section 4.4) and make primitive assumptions on its component $\text{Cov}[h(S_1)h(S_2), h(S_3)h(S_1)]$. These assumptions are easy to validate and interpret. Then, we quantify all $\sigma_{c,2k}^2$ by a tighter bound for finite $c$ and a looser bound for general $c = 1, 2, ..., 2k$. We introduce Assumption 3 to describe the overlapping structure between two size-$2k$ subsamples. Further relaxation is presented in Appendix I. We also introduce Assumption 4 and 5 to control the growth rate of “fourth-moment terms” in the covariance calculation.

We remark that it is easier to understand the effect of these cancellation patterns in steps 1 and 2 through a simplified example, linear average kernel (see Appendix J), where we also discuss difficulties arising from the nature of Double U-statistic and the implicit cancellation pattern for a general kernel.

### 4.6 Main Results

We now present the main results. As a direct consequence of this theorem, the ratio consistency property is provided in Corollary 4.7.

**Theorem 4.5** (Asymptotic variance of $U_n$ and $\hat{V}_u$). Under Assumptions 1 - 5, we can bound $\text{Var}(U_n)$ (3) and $\text{Var}(\hat{V}_u)$ (22) as

$$\text{Var}(U_n) = (1 + o(1)) \frac{k^2}{n} \xi_{d,k}^4,$$

$$\text{Var}(\hat{V}_u) = O \left( \frac{k^2}{n} \sigma_{c,2k}^2 \right),$$

where $\sigma_{c,2k}^2 := \Theta(\frac{k^2}{n} \xi_{d,k}^4)$ is the upper bound of $\sigma_{c,2k}^2$ given by Proposition G.2 in Appendix G.

The proof is collected in Appendix D.3. The quantification of $\text{Var}(U_n)$ (29) and $\text{Var}(\hat{V}_u)$ (30) requires controlling the growth pattern of $\xi_{d,k}^4$ and $\sigma_{c,2k}^2$. We impose direct assumption on $\xi_{d,k}^4$ (Assumption 2) but not on $\sigma_{c,2k}^2$, which makes our analysis different from previous works. In particular, (29) can be inferred from a more general Proposition 4.6 given below, however, the proof of (30) is much more involved. For (30), we first investigate the $\eta_{c,2k}^2(d_1, d_2)$ (27) as components of $\sigma_{c,2k}^2$ and then bound $\sigma_{c,2k}^2$ for small $c$ (Proposition...
G.2) and for every $c$ (Proposition G.3). The proof also involves a “truncation trick”. Details are collected in Appendix D.1 and Appendix G.

**Proposition 4.6** (Asymptotic variance of infinite order U-statistics). For a complete U-statistic $U_n$ with size-$k$ kernel and $k = o(\sqrt{n})$, assume that $\xi^2_{1,k} > 0$ and there exists a non-negative constant $C$ such that

$$\limsup_{k \to \infty} 2 \xi^2_{1,k} / (d \xi^2_{1,k}) = C.$$ 

Then,

$$\lim_{n \to \infty} \frac{\text{Var}(U_n)}{(k^2 \xi^2_{1,k}/n)} = 1.$$ 

This proposition relaxes the conditions in Theorem 3.1 in DiCiccio and Romano (2022) and also motivates our strategy to bound $\text{Var}(\hat{V}_u)$. The proof is collected in Appendix D.4. Our condition allows $\xi^2_{d,k}/\xi^2_{1,k}$ to grow at a factorial rate of $d$. This is a much weaker condition than the one used in the existing literature (Mentch and Hooker, 2016; Zhou et al., 2021; DiCiccio and Romano, 2022) which assumes $\xi^2_{d,k}/(k^2 \xi^2_{1,k}) = O(1)$. In particular, since the relation $k \xi^2_{d,k} \leq d \xi^2_{k,k}$ always holds (Lee, 1990), their condition is equivalent to $\xi^2_{d,k}/(d \xi^2_{1,k}) \leq C$ for $d = 2, 3, \ldots, k$ and certain positive $C$, which only allows $\xi^2_{d,k}/\xi^2_{1,k}$ to grow at a linear rate with $d$.

**Corollary 4.7** (Ratio consistency of $\hat{V}_u$). Under Assumptions 1 - 5,

$$\frac{\text{Var}(\hat{V}_u)}{(E(\hat{V}_u))^2} = O\left(\frac{1}{n}\right),$$

which implies that $\hat{V}_u/E(\hat{V}_u) \xrightarrow{P} 1$.

This shows the ratio consistency of the variance estimator $\hat{V}_u$, as a corollary of Theorem 4.5. The proof is collected in Appendix D.2. Note that this is the consistency of $\hat{V}_u/E(\hat{V}_u)$ rather than only $\hat{V}_u$. Because the latter, $\hat{V}_u \xrightarrow{P} 0$, is trivial when $E(\hat{V}_u) = \text{Var}(U_n) \to 0$ as $n$ grows to infinity. To the best of our knowledge, this is the first time that the ratio consistency of an unbiased variance estimator for a U-statistic with growing order is proved.

## 5 Simulation Study

We present simulation studies to compare our variance estimator with existing methods (Zhou et al., 2021; Wager and Athey, 2018). We consider both the smoothed and non-smoothed versions, denoted as “MS-s” and “MS”, respectively. The balance estimator and its bias-corrected version in Zhou et al. (2021) are denoted as “BM” and “BM-cor”. The infinitesimal jackknife in Wager and Athey (2018) is denoted as “IJ”. Our simulation does not include the Internal Estimator and the External Estimator in Mentch and Hooker (2016), since BM method has been shown to be superior to these estimators (Zhou et al., 2021).

### 5.1 Simulation Settings

We consider two different underlying regression settings:
1. MARS: \( g(x) = 10\sin(\pi x_1x_2) + 20(x_3 - 0.05)^2 + 10x_4 + 5x_5; \quad \mathcal{X} = [0, 1]^6. \)

2. MLR: \( g(x) = 2x_1 + 3x_2 - 5x_3 - x_4 + 1; \quad \mathcal{X} = [0, 1]^6. \)

The MARS model is proposed by Friedman (1991) for the multivariate adaptive regression splines. It has been used previously by Biau (2012); Mentch and Hooker (2016). The second model is a simple multivariate linear regression. In both setting, features are generated uniformly from the feature space and responses are generated by \( g(x) + \epsilon, \) where \( \epsilon \overset{iid}{\sim} \mathcal{N}(0, 1). \)

We use \( n = 200 \) as total training sample size and pick different tree subsample sizes: \( k = 100, 50, 25 \) for \( k \leq n/2 \) setting and \( k = 160 \) for \( k > n/2 \) setting. The numbers of trees are \( n_{\text{trees}} = B \cdot M = 2000, 10000, 20000. \) For tuning parameters, we set \( \text{mtry} \) (number of variables randomly sampled as candidates at each split) as 3, which is half of the dimension, and set \( \text{nodesize} \) parameter to \( 2\lfloor \log(n) \rfloor = 8. \) We repeat the simulation \( N_{mc} = 1000 \) times to evaluate the performance of different estimators. Our proposed methods, BM and BM-cor estimators are implemented using the \texttt{RLT} package available on GitHub. The IJ estimators are implemented using \texttt{grf} and \texttt{ranger}. Each estimation method and its corresponding ground truth (see details in the following) is generated by the same package. Note that we do not use the honest tree setting by Wager and Athey (2018) since it is not essential for estimating the variance.

To evaluate the performance, we consider both the bias of the variance estimator and the corresponding confidence interval’s coverage rate. The coverage is in terms of the mean of the random forest estimator, i.e., \( \mathbb{E}(\hat{f}(x^*)) \) (see the following description for “ground truth”). We choose to evaluate the coverage based on this quantity instead of the true model value, i.e. \( f(x^*), \) because our focus is the variance estimation of \( \hat{f}(x^*) \) instead of the model prediction. Furthermore, the random forest itself can be a biased model. In our numerical study, we want to rule out the influence of such bias in the coverage evaluation. To obtain the ground truth of the variance of a random forest, we consider a numerical approach: First, we generate the training dataset 10000 times and fit a random forest to each training data. Then, we use the mean and variance of 10000 forest predictions as the approximation of \( \mathbb{E}(\hat{f}(x^*)) \) and \( \text{Var}(\hat{f}(x^*)), \) where \( \hat{f}(x^*) \) denotes a forest prediction at a testing sample \( x^*. \) We use the relative bias and the confidence interval (CI) converge as the evaluation criteria. The relative bias is defined as the ratio between the bias and the ground truth of the variance estimation. The \( 1 - \alpha \) confidence interval is constructed using \( \hat{f} \pm Z_{\alpha/2} \sqrt{\hat{V}_u} \) with standard normal quantile \( Z_{\alpha/2}. \) We notice that the ground truth generated under different packages has small difference (see Appendix K), which is mainly due to the subtle difference in packages’ implementation.

The variance estimation is performed and evaluated on two types of testing samples for both MARS and MLR data. The first type is a “central sample” with \( x^* = (0.5, \ldots, 0.5). \) The second type includes 50 random samples whose every coordinate is independently sampled from a uniform distribution between \([0, 1].\) And these testing samples are fixed for all the experiments. We use the central sample to show the distribution of variance estimators over 1000 simulations (see Figure 2, first row). We use the 50 random samples to evaluate the average bias and the CI coverage rate (see the second and third row of Figure 2 and Tables 1 and 2).
5.2 Results for $k \leq n/2$

Figure 2: A comparison of different methods on MARS data. Each column figure panel represents tree size: $k = n/2, n/4, n/8$ respectively. The first row: boxplots of relative variance estimators on the central test sample over 1000 simulations. The red diamond symbol in the boxplot indicates the mean. The second row: boxplots of 90% CI coverage for 50 testing samples. The third row: coverage rate averaged over 50 testing samples with $nTrees = 20000$, where the black reference line $y = x$ indicates the desired coverage rate.

Figure 2 focuses on the evaluation on MARS data. The subfigures present the distribution of variance estimators on the central sample and corresponding CI coverage on 50 testing samples. As mentioned before, we use relative estimators to compare the bias objectively, avoiding the influence caused by different packages. The figure for MLR data is provided in Appendix K, which shows similar patterns. For both MARS and MLR, Table 1 shows the 90% CI coverage rate, and Table 2 shows the relative bias of variance estimation. The presented coverage of each method is averaged over 50 testing samples, and the standard deviation (followed in the bracket) reflects the variation over these. In addition, we observe that the CI constructed by the true variance achieves desired confidence level (see Appendix K). This shows that based on our simulation setting, the random forest estimators are approximately normally distributed. As a sum-
Table 1: 90% CI Coverage Rate averaged on 50 testing samples. The number in the bracket is the standard deviation of coverage over 50 testing samples.

|       | nTrees |       |       |       |       |       |
|-------|--------|-------|-------|-------|-------|-------|
|       |        | k = n/2 |       | k = n/4 |       | k = n/8 |
|       | 2000   | 20000  | 2000  | 20000  | 2000  | 20000  |
| MARS  |        |        |       |       |       |       |
| MS    | 81.2% (2.0%) | 85.8% (1.6%) | 82.3% (2.6%) | 87.7% (1.2%) | 81.8% (2.6%) | 88.1% (1.1%) |
| MS-s  | 87.7% (2.7%) | 88.7% (2.7%) | 87.7% (2.6%) | 89.1% (2.5%) | 86.9% (2.0%) | 88.9% (1.7%) |
| BM    | 81.3% (3.2%) | 65.4% (2.0%) | 91.4% (1.9%) | 81.2% (1.5%) | 93.8% (1.1%) | 86.3% (1.1%) |
| BM-cor| 16.7% (9.0%) | 59.8% (1.6%) | 71.7% (2.3%) | 78.8% (1.4%) | 83.0% (1.1%) | 84.7% (1.1%) |
| IJ    | 95.4% (1.0%) | 96.6% (1.0%) | 89.9% (1.5%) | 90.7% (1.0%) | 91.7% (1.6%) | 87.8% (0.9%) |
|       |        |        |       |       |       |       |
| MARS  |        |        |       |       |       |       |
| MS    | 83.3% (1.4%) | 86.4% (1.2%) | 84.5% (1.5%) | 88.2% (1.0%) | 84.1% (1.6%) | 88.9% (1.0%) |
| MS-s  | 88.8% (1.6%) | 89.6% (1.5%) | 89.1% (1.6%) | 90.3% (1.5%) | 88.6% (1.6%) | 90.3% (1.2%) |
| BM    | 79.4% (2.0%) | 64.7% (1.4%) | 90.7% (1.3%) | 80.9% (1.3%) | 93.8% (0.9%) | 86.6% (1.2%) |
| BM-cor| 23.1% (5.6%) | 59.9% (1.6%) | 73.0% (1.9%) | 78.7% (1.4%) | 83.6% (1.4%) | 85.2% (1.2%) |
| IJ    | 95.6% (0.8%) | 96.5% (0.6%) | 89.5% (1.1%) | 91.1% (1.1%) | 91.4% (1.1%) | 88.1% (1.2%) |

Table 2: Relative bias (standard deviation) over 50 testing samples. For each method and testing sample, the relative bias is evaluated over 1000 simulations.

|       | nTrees |       |       |       |       |       |
|-------|--------|-------|-------|-------|-------|-------|
|       |        | k = n/2 |       | k = n/4 |       | k = n/8 |
|       | 2000   | 20000  | 2000  | 20000  | 2000  | 20000  |
| MARS  |        |        |       |       |       |       |
| MS    | -0.3% (1.7%) | -0.2% (1.4%) | -0.2% (2.0%) | 0.1% (1.3%) | 0.3% (1.8%) | 0.5% (1.3%) |
| MS-s  | 2.0% (13.0%) | 2.3% (13.5%) | 1.8% (12.2%) | 1.9% (12.5%) | 0.8% (8.5%) | 1.2% (8.7%) |
| BM    | -28.8% (8.6%) | -64.1% (1.1%) | 20.6% (12.2%) | -30.9% (1.6%) | 40.5% (9.1%) | -12.0% (1.5%) |
| BM-cor| -101.1% (8.1%) | -71.4% (1.0%) | -52.4% (3.9%) | -38.3% (0.9%) | -24.4% (1.7%) | -18.6% (1.1%) |
| IJ    | 102.3% (21.5%) | 103.5% (21.8%) | 36.6% (10.1%) | 20.8% (9.2%) | 67.4% (15.4%) | 11.5% (6.7%) |
| MARS  |        |        |       |       |       |       |
| MS    | 0.3% (2.7%) | 0.1% (2.1%) | -0.1% (2.0%) | 0.0% (1.8%) | 0.0% (2.1%) | -0.2% (1.6%) |
| MS-s  | 6.0% (7.4%) | 6.2% (7.4%) | 5.8% (7.1%) | 6.1% (7.0%) | 4.8% (4.9%) | 4.6% (5.0%) |
| BM    | -36.2% (3.8%) | -65.4% (0.9%) | 11.4% (5.9%) | -32.4% (1.4%) | 32.1% (5.8%) | -13.7% (1.5%) |
| BM-cor| -95.0% (3.2%) | -71.3% (0.7%) | -50.1% (1.8%) | -38.6% (1.1%) | -24.7% (1.2%) | -19.6% (1.1%) |
| IJ    | 87.8% (15.0%) | 88.6% (14.7%) | 27.1% (5.7%) | 17.1% (5.8%) | 53.1% (11.4%) | 6.6% (5.1%) |
mary over different tree sizes, MS and MS-s demonstrate consistent better performance over other methods, especially when tree size $k$ is large, i.e., $k = n/2$. The advantages are demonstrated in two aspects: the accurate CI coverage and small bias.

First, the third row of Figure 2 shows that MS-s method achieves the best CI coverage under every $k$, i.e., the corresponding line is nearest to the reference line: $y = x$. MS performs the second best when $k = n/2$ and $n/8$. Moreover, the CI coverages of the proposed methods are stable over different testing samples with a small standard deviation (less than 3%), as demonstrated in Table 1. Secondly, considering the bias of the variance estimation, our methods show a much smaller bias compared to all other approaches (Figure 2, first row). More details of the relative bias are summarized in Table 2. The averaged bias of MS is smaller than 0.5% with a small standard deviation, which is mainly due to the Monte Carlo error. MS-s has a slightly positive average bias (0% to 6.2%), but it is still much smaller than the competing methods. The standard deviation of bias for MS-s is around 4.3% to 13.6%, which is comparable to IJ.

On the other hand, the performance of competing methods varies. When tree size $k = n/2$, BM, BM-cor and IJ methods show large bias. But the performance is improved for smaller tree sizes. Noticing that these methods are theoretically designed for small $k$, so this is expected. BM and BM-cor tend to underestimate the variance in most settings, while IJ tends to overestimate. In Table 2, on MARS data with 20000 $nTrees$, the bias of both BM and BM-cor is more than −50%, with severe under-coverage (65.4%, 59.8%), while IJ leads to over-coverage. When the tree size is small as $k = n/8$, these methods still display a mild but noticeable bias. The proposed methods still outperform them when more trees ($nTrees = 20000$) are used, as shown in Table 2, the last column.

The number of trees ($nTrees$) has a significant impact on performance. First, as the number of trees grows, all estimators’ variation decreases (Figure 2: first row). Since our estimators are mostly unbiased, our CI coverages benefit from large $nTrees$. For example, the 90% CI coverages of MS on MARS data are 81.2% ($k = n/2$) and 81.8% ($k = n/8$) with $nTrees = 2000$, which increase to 85.8% and 88.1% respectively with $nTrees = 20000$. On the other hand, the performance of competing methods do not necessarily benefit from increasing $nTrees$. For example, BM is over-coverage with $nTrees = 2000$ but under-coverage with $nTrees = 20000$ when $k = n/4$ or $n/8$. In fact related estimation inflation phenomenon has been discussed in Zhou et al. (2021), and the BM-cor is used to reduced the bias. When $k = n/8$, the gap between BM and BM-cor diminishes as $nTrees$ grows. However, this is no longer true when $k$ is large since the dominating term used in their theory cannot be applied anymore.

Finally, we would like to highlight the connection between the estimator’s bias and its CI coverage, which motivates our smoothing strategy. The normality of forest prediction and the unbiasedness of variance estimator do not necessarily result in a perfect CI coverage rate. Though the MS estimator is unbiased, it still displays significant variations, which leads to under-coverage. This issue also exists for IJ. On MARS with $k = n/8$ and $nTrees = 20000$, IJ has a positive bias (11.5%), but its CI is still under-coverage and even worse than the proposed methods since its variance is much larger. As we have discussed, one solution is to increase the number of trees. An alternative method, especially when $nTrees$ is relatively small, is to perform local averaging as implemented in MS-s. The heights of boxplots clearly demonstrate the variance
reduction effect. Consequently, MS-s method with only 2000 trees shows better coverage than MS method with 20000 trees when \( k = n/2 \) (see Table 1). However, MS-s method may suffer from a mild bias issue, and the choice of neighbor points may affect its variance. Hence we still recommend using larger trees when it is computationally feasible.

5.3 Results for \( k > n/2 \)

As discussed in Section 3.7, when \( n/2 < k < n \), we cannot jointly estimate \( V^h \) and \( V^S \) jointly so additional computational cost is introduced. In this simulation study, we attempt to fit additional \( nTrees \) with bootstrapping (sampling with replacement) subsamples to estimate \( V^h \) so we denote our proposed estimator and smoothing estimator as “MS(bs)” and “MS-s(bs)”. We note that grf package does not provide IJ estimator when \( k > n/2 \) so we generate the IJ estimator and corresponding ground truth by ranger package.

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Table 3: 90% CI coverage, relative bias, and standard deviation averaged on 50 testing samples. Tree size \( k = 0.8n \). The calculation follows previous tables.

| Model  | nTrees | 90% CI Coverage | Relative Bias |
|--------|--------|-----------------|---------------|
|        |        | 2000            | 20000         | 2000 | 20000 |
| MARS   | MS(bs) | 94.2% (2.8%)    | 95.4% (2.4%)  | 128.4% (64.8%) | 136.6% (67.2%) |
|        | MS-s(bs)| 97.7% (1.5%)   | 98.1% (1.3%)  | 132.2% (66.7%) | 140.6% (69.1%) |
|        | BM     | 51.4% (3.8%)    | 33.9% (1.7%)  | -80.4% (3.1%)  | -92.1% (0.5%)  |
|        | BM-cor | 0.0% (0.0%)     | 13.5% (4.5%)  | -143.0% (12.1%)| -98.3% (1.3%)  |
|        | IJ     | 88.0% (4.6%)    | 87.1% (3.7%)  | -0.8% (25.2%)  | -5.6% (16.3%)  |
| MLR    | MS(bs) | 94.3% (1.9%)    | 95.2% (1.7%)  | 98.4% (24.7%)  | 103.9% (25.4%) |
|        | MS-s(bs)| 96.6% (1.3%)   | 97.0% (1.2%)  | 104.8% (24.9%) | 110.3% (25.6%) |
|        | BM     | 47.9% (2.3%)    | 32.4% (1.5%)  | -83.4% (1.2%)  | -92.6% (0.3%)  |
|        | BM-cor | 0.0% (0.0%)     | 15.9% (2.4%)  | -132.7% (4.3%) | -97.5% (0.5%)  |
|        | IJ     | 99.4% (0.3%)    | 99.2% (0.3%)  | 182.8% (21.7%) | 175.8% (16.7%) |

As seen from Table 3, all methods suffer from severe bias, but our methods and IJ are comparable and better than BM and BM-cor methods. More specifically, our proposed method generally over-covers due to overestimating the variance. The IJ method shows good accuracy on MARS data but has more severe over-coverage than our methods on MLR. Overall, to obtain a reliable conclusion of statistical inference, we recommend avoiding using \( k > n/2 \). This can be a reasonable setting when \( n \) is relatively large, and \( k = n/2 \) can already provide an accurate model.

6 Real Data Illustration

We consider the Seattle Airbnb Listings \(^1\) dataset obtained from Kaggle. The goal is to predict the price of the target Airbnb unit in Seattle. We use a subset of data that consists of 7515 samples and nine covariates: latitude, longitude, room type, bedroom number, bathroom number, accommodates, review number, having

\(^1\)https://www.kaggle.com/shanelev/seattle-airbnb-listings
a rating, and the rating score. Detailed information of this dataset and missing value processing is described in Appendix L.

Given the large sample size, we fit 40000 trees in the random forest to reduce the variation of the variance estimator. The tree size is fixed as half of the sample size: $k = 3757$. We construct 12 testing samples at 3 locations: Seattle-Tacoma International Airport (SEA Airport), Seattle downtown, and Mercer Island. We further consider four bedroom/bathroom settings as (1/1), (2/1), (2/2), and (3/2). Details of the latitude and longitude of these locations and other covariates are described in Appendix L. The price predictions along with 95% confidence intervals are presented in Figure 3. Overall, the prediction results match our intuitions. In particular, we can observe that the confidence interval of the 1B1B-type unit at SEA Airport does not overlap with those corresponding to the same type of unit at the other two locations. This is possible because the accommodations around an airport usually have lower prices due to stronger competition. We also observe that 2-bathroom units at SEA Airport and downtown have higher prices than 1-bathroom units. However, the difference between 2B2B and 3B2B units at SEA Airport is insignificant.

7 Discussion

From the perspective of $U$-statistics, we propose a new variance estimator for random forest predictions. This is the first estimator designed for large tree size, i.e. $k = \beta n$. Moreover, new tools and strategies are developed to study the ratio consistency of the estimator. Below we describe several issues and extensions open for further investigation.

First, our current methods are initially developed for the case $k \leq n/2$. The difficulty of extending to the $k > n/2$ region is to estimate the tree variance, i.e. $V^{(h)}$. We proposed to use bootstrapped trees to extend the method to $k > n/2$. However, this could introduce additional bias and also leads to large variation. We
suspect that Bootstrapping may be sensitive to the randomness involved in fitting trees. Since we estimate \( V^{(k)} \) and \( V^{(S)} \) separately, the randomness of the tree kernel could introduce different added variance, which leads to non-negligible bias.

Secondly, we developed a new double-\( U \) statistics tool to prove ratio consistency. This is the first work that analyzes the ratio consistency of a minimum-variance unbiased estimator (UMVUE) of a \( U \)-statistic’s variance. The tool can be potentially applied to theoretical analyses of a general family of \( U \)-statistic problems. However, our ratio consistency result is still limited to \( k = o(n^{1/2-\epsilon}) \) rather than \( k = \beta n \), which is a gap between the theoretical guarantee and practical applications. The limitation comes from the procedure we used to drive the Hoeffding decomposition of the variance estimator’s variance. In particular, we want the leading term dominating the variance while allowing a super-linear growth rate of each \( \sigma^2_{c,2k} \) in terms of \( c \). Hence, the extension to the \( k = \beta n \) setting is still open and may require further assumptions on the overlapping structures of double-\( U \) statistics.

Thirdly, in our smoothed estimator, the choice of testing sample neighbors can be data-dependent and relies on the distance defined by the forests. It is worth considering more robust smoothing methods for future work.

Lastly, this paper focuses on the regression problem using random forest. This variance estimator can also be applied to the general family of subbagging estimators. Besides, we may further investigate the uncertainty quantification for variable importance, the confidence interval for classification probability, the confidence band of survival analysis, etc.

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# Supplementary Material of “On Variance Estimation of Random Forests”

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A  

Notations

| Notations | Description |
|-----------|-------------|
| \( \mathcal{O} \) | \( a = \mathcal{O}(b) \): exists \( C > 0 \), s.t. \( a \leq Cb \). |
| \( \Theta, \Omega \) | \( a = \Omega(b) \iff \exists b = \Theta(a) \). |\( a = \Theta(b) \iff a = \mathcal{O}(b) \) and \( a = \Theta(b) \). |
| \( U_n, h \) | \( U_n \) is the U-statistic with size-\( k \) kernel \( h \). |
| \( \hat{V}_u, \psi \) | \( \hat{V}_u \) denotes the estimator \( (20) \) of \( \text{Var}(U_n) \), which is a U-statistic with size-\( 2k \) kernel \( \psi \). |
| \( S \) | \( S \) denotes the size-\( k \) subsample set associated with kernel \( h \). |
| \( S^{(2k)} \) | \( S^{(2k)} \) denotes the size-\( 2k \) subsample set associated with kernel \( \psi \). |
| \( c, d_1, d_2 \) | Given \( S_1, S_2 \subset S_1^{(2k)}, S_3, S_4 \subset S_2^{(2k)} \), \( c = |S_1^{(2k)} \cap S_2^{(2k)}| \), \( d_1 = |S_1 \cap S_2| \), and \( d_2 = |S_3 \cap S_4| \). |
| \( \varphi_d, w_d \) | See \( \psi(S^{(2k)}) = \sum_{d=0}^{k} w_d \varphi_d (S^{(2k)}) \) \( (25) \). \( \varphi_d(S^{(2k)}) \) is still a U-statistic. |
| \( \bar{w}_d \) | \( \bar{w}_d = \mathcal{O}(k^{2d}/(d!n^d)) \) is the upper bound of \( w_d \) given by Equation \( (26) \). |
| \( \xi^2_{d,k} \) | \( \xi^2_{d,k} = \text{Cov}[h(S_1), h(S_2)] \) is first used in \( (3) \). |
| \( \sigma^2_{c,2k} \) | \( \sigma^2_{c,2k} = \text{Cov}[\psi(S_1^{(2k)}), \psi(S_2^{(2k)})] \) is first used in \( (22) \). |
| \( \eta^2_{c,2k}(d_1, d_2) \) | \( \eta^2_{c,2k}(d_1, d_2) \) is introduced by further decomposing \( \sigma^2_{c,2k} \) in \( (27) \). |
| \( \sigma^2_{c,2k} \) | \( \sigma^2_{c,2k} \) is an upper bound of \( \sigma^2_{c,2k} \) given by Propositions \( G.2 \) and \( G.3 \). |
| \( \rho \) | \( \rho := \text{Cov}[h(S_1)h(S_2), h(S_3)h(S_4)] \) \( (31) \). |
| \( \text{DoF} \) | The number of free parameters to determine \( \text{Cov}[h(S_1)h(S_2), h(S_3)h(S_4)] \). |
| \( \vec{r} \) | \( \vec{r} \) is a \( 9 \)-dimensional vector defined in \( (37) \), describing the 4-way overlapping among \( S_1, S_2, S_3, S_4 \). \( |\vec{r}| \) is the \( \ell_1 \) vector norm of \( \vec{r} \). |
| \( r_{i*}, r_{*j}, r^{*} \) | \( r_{i*} = \sum_{j=0}^{2} r_{ij}, r_{*j} = \sum_{i=0}^{2} r_{ij} \), and \( r^{*} = (r_{0*}, r_{1*}, r_{2*}, r_{*0}, r_{*1}, r_{*2}) \). |
| \( \rho(\vec{r}) \) | \( \rho(\vec{r}) \) is the \( 9 \) DoF representation of \( \rho \) (see Assumption \( 3 \)). |
| \( F_c^{(k)} \) | \( F_c^{(k)} \) \( (34) \) is the upper bound of \( \rho \), given that \( |S_1^{(2k)} \cap S_2^{(2k)}| = c \). |
| \( \rho(\vec{r}, d_1, d_2) \) | This is a notation emphasizing \( 11 \) DoF of \( \rho \) used in Appendix \( I \). |
| \( \hat{\rho}(\vec{r}) \) | \( \hat{\rho}(\vec{r}) \) is the \( 9 \) DoF benchmark of used in Assumption \( 6 \). |
| \( \text{Influential Overlaps} \) | The samples in \( S_1^{(2k)} \cap S_2^{(2k)} \). |

Table 4: Summary of Notations

B  

Assumptions

In this section, we present assumptions and notations necessary for the theoretical results. Assumption \( 1 \) controls the growth rate of kernel size \( k \) in terms of \( n \). Assumption \( 2 \) controls the growth rate of \( \xi^2_{d,k} \)
regarding $d$. We will show that this is a relaxation of $\xi^2_{k,k}/(k\xi^2_{1,k}) = \mathcal{O}(1)$ used by Mentch and Hooker (2016), Zhou et al. (2021), and DiCiccio and Romano (2022). In addition, we do not impose assumptions on $\sigma^2_{c,2k}$, which is difficult to validate due to $\hat{V}_u$’s complicated structure. Instead, we introduce Assumptions 3-5, which are imposed on a primitive term $\text{Cov}(h(S_1)h(S_2), h(S_3)h(S_4))$. More discussions and supporting examples of our assumptions are collected in Appendix C. Later, a relaxation of Assumption 3 and the proof under the new assumption is collected in Appendix I.

**Assumption 1.** There exist a constant $\epsilon \in (0, 1/2)$, so that the growth rate of kernel size $k$ regarding sample size $n$ is bounded as $k = \mathcal{O}(n^{1/2-\epsilon})$.

Previous works on Infinite-Order U-statistics usually bound the growth rate of $k$ by $k = o(\sqrt{n})$. This Assumption 1 is slightly stronger, which enables our variance truncation strategies (see Lemmas G.4 and G.8 in Appendix G).

**Assumption 2.** $\forall k \in \mathbb{N}^+, \xi^2_{1,k} > 0$ and $\xi^2_{k,k} < \infty$. There exist a universal constant $a_1 \geq 1$ independent of $k$, satisfying that

$$\sup_{d=2,3,\ldots,k} \frac{\xi^2_{d,k}}{d^a_1 \xi^2_{1,k}} = \mathcal{O}(1).$$

This assumption is weaker than those used in Mentch and Hooker (2016), Zhou et al. (2021), and DiCiccio and Romano (2022). To show that $\xi^2_{1,k}$ dominates $\text{Var}(U_n)$, these existing literature assumes that $\xi^2_{k,k}/k\xi^2_{1,k} = \mathcal{O}(1)$. Their assumption implies our Assumption 2 with $a_1 = 1$ (see the discussions below Proposition 4.6).

If we impose a direct assumption on the growth rate of $\sigma^2_{c,2k}$ like the one on $\xi^2_{1,k}$ (Assumption 2), the proof of Theorem 4.5 will be straightforward. However, such assumptions on $\sigma^2_{c,2k}$ are non-primitive and difficult to check in practice. Instead, since $\hat{V}_u$ is a Double U-statistic, $\sigma^2_{c,2k}$ can be decomposed into a weighted sum of $\eta^2_{2k}(d_1,d_2)$’s, which can be further decomposed into a weighted sum of $\text{Cov}[h(S_1)h(S_2), h(S_3)h(S_4)]$. In the following part of this section, we will first investigate this summand, $\text{Cov}[h(S_1)h(S_2), h(S_3)h(S_4)]$, and then proposed Assumptions 3-5 accordingly. To simplify the notation, we define

$$\rho := \text{Cov}[h(S_1)h(S_2), h(S_3)h(S_4)].$$

(31)

Given that $h(S)$ is a symmetric kernel, $\rho$ depends on the 4-way overlapping structure of $S_1, S_2, S_3,$ and $S_4$, which involves 11 different overlapping sets: 6 different 2-way overlapping, $S_1 \cap S_2, S_1 \cap S_3, S_1 \cap S_4, S_2 \cap S_3, S_2 \cap S_4, S_3 \cap S_4$; 4 different 3-way overlapping, $S_1 \cap S_2 \cap S_3, S_1 \cap S_2 \cap S_4, S_1 \cap S_3 \cap S_4, S_2 \cap S_3 \cap S_4$; and a 4-way overlapping $S_1 \cap S_2 \cap S_3 \cap S_4$. Hence, it natural to use an eleven-parameter quantity to describe $\rho$. We denote the number of these parameters as the “Degrees of Freedom” (DoF) of $\rho$. Moreover, since $S_1, S_2 \subset S_1^{(2k)}$ and $S_3, S_4 \subset S_2^{(2k)}$, there are two types of different overlapping: “within $S_1^{(2k)}$, $S_2^{(2k)}$”, and “between $S_1^{(2k)}$ and $S_2^{(2k)}$”. In particular, $d_1 = |S_1 \cap S_2|$ and $d_2 = |S_3 \cap S_4|$ describes the overlapping within $S_1^{(2k)}$ and $S_2^{(2k)}$ respectively. Apart from $S_1 \cap S_2$ and $S_3 \cap S_4$, the other 9
overlapping sets can describe the overlapping between $S_1^{(2k)}$ and $S_2^{(2k)}$, since any of these sets is a subset of $S_1^{(2k)} \cap S_2^{(2k)}$. So we denote the information from these 9 overlapping sets by a 9-dimensional vector $\underline{r}$, whose definition is collected in Appendix C.1.

However, it may not be necessary to know all $r_1, d_1, d_2$ values to calculate this covariance $\rho$. For example, in the linear average kernel (Example C.2 in Appendix C.2), $\rho$ only depends on $\underline{r}$. Hence, we impose the following assumption.

**Assumption 3.** We assume that $\rho$, i.e. $\text{Cov}[h(S_1)h(S_2), h(S_3)h(S_4)]$, only depends on 9 DoF denoted by $\underline{r}$. Hence, there exists a function $\rho(\underline{r})$, satisfying

$$\rho(\underline{r}) = \rho.$$  

(32)

By this assumption, we reduce the DoF of $\rho$ from 11 to 9, assuming that the “within $S_1^{(2k)}$, $S_2^{(2k)}$ overlapping” has no impact on $\rho$. This simplifies a cancellation pattern when analyzing $\eta_{c,2k}(d_1, d_2)$. In Appendix C, we provide a comprehensive discussion on this assumption. As mentioned previously, we will validate this assumption on the example of linear average kernel (see Example C.2). We also provide an example to show the difficulty of reducing DoF below 9 by only considering two-way overlaps. This shows that our assumption may not be further simplified without making further specific assumptions on the kernel functions themselves. Besides, in Appendix I, we impose a relaxation of this assumption, in which DoF of $\rho$ can still be 11 but, with some constraints. Proof using the relaxed assumption will also be collected in Appendix I.

**Assumption 4** (Ordinal Covariance). $\forall$ size-$k$ subset $S_1, S_2, S_3, S_4$ and $S_1', S_2', S_3', S_4'$, denote corresponding $\text{Cov}[h(S_1)h(S_2), h(S_3)h(S_4)]$ as $\rho$ with $\underline{r}$ and $\rho'$ with $\underline{r}'$ respectively. Then

$$\rho \geq \rho', \text{ if } r_{ij} \geq r'_{ij}, \forall i, j = 0, 1, 2.$$  

In addition, given size-$k$ sets $S'$, $S''$ and $\underline{r}$, satisfying $|S' \cap S''| = c$ and $|\underline{r}| = c$, then

$$\rho \leq \text{Cov}[h(S')^2, h(S'')^2].$$  

(33)

To simplify the notation, we denote the RHS of above inequality as $F_c^{(k)}$:

$$F_c^{(k)} := \text{Cov}[h(S')^2, h(S'')^2].$$  

(34)

Assumption 4 implies that more overlapping leads to larger $\rho$. This is a reasonable consequence to expect. For every $c = |S_1^{(2k)} \cap S_2^{(2k)}|$, it also provides an upper bound of $\rho$ in Equation (34), where $F_c^{(k)}$ refers to the case with “most overlapping”, where $S_1 = S_2, S_3 = S_4$. The overlapping associated with $F_c^{(k)}$ is visualized in Figure 5 in Appendix C. A corollary of Assumption 4 is that $\rho \geq 0$, because $\rho$ is 0 when $r_{ij} = 0, \forall i, j = 0, 1, 2$. Note that $\rho \geq 0$ can be viewed as a analogue to $\xi_{d,k}^2 \geq 0$ for $d = 1, 2, ..., k$ in a regular U-statistics setting (Lee, 1990).
Assumption 5. For $F_c^{(k)}$ defined in Assumption 4,

$$\frac{F_1^{(k)}}{\xi_{1,k}^4} = O(1).$$  \(35\)

There exist a universal constant $a_2 \geq 1$ independent of $k$, satisfying

$$\sup_{c=2,3,\ldots,2^k} \frac{F_c^{(k)}}{c^{a_2} F_1^{(k)}} = O(1).$$  \(36\)

Equation (35) implies that a fourth-moment term cannot be too large compared to a second moment term $\xi_{1,k}^4$. This can be verified on a linear average kernel with some basic moment assumption. The purpose of Equation (36) is to impose an assumption on the growth rate of $\rho$ similar to $\xi_{d,k}^2$ in Assumption 2. Hence, we first upper bound the 9-DoF $\rho^{(k)}$ by $F_c^{(k)}$, which has just 1 free parameter $c$. Then we assume a the polynomial growth rate of $F_c^{(k)}$ regarding $c$ by Assumption 5. We note that for some specific kernel, Assumption 5 can be implied by Assumption 2 (see Example C.4 in Appendix C).

C Discussion of Assumptions

In this section, we provide the definition of the 9-dimensional vector $r$ as well as the discussion and validation examples for Assumption 3-5.

C.1 $r$ Notation of “Between $S_1^{(2k)}$ and $S_2^{(2k)}$ Overlapping”

Definition C.1 (Between $S_1^{(2k)}$, $S_2^{(2k)}$ overlapping structure of $\rho$). First, we denote the samples in $S_1^{(2k)} \cap S_2^{(2k)}$ as Influential Overlaps of $\rho$ (31).

Given size-2k set of subsamples $S_1^{(2k)}$, $S_2^{(2k)}$, and size-k set of subsamples $S_1$, $S_2 \subset S_1^{(2k)}$, $S_3$, $S_4 \subset S_2^{(2k)}$, denote $c = |S_1^{(2k)} \cap S_2^{(2k)}|$, $d_1 = |S_1 \cap S_2|$, $d_2 = |S_3 \cap S_4|$. Then, we denote $T_0 = S_1 \cap S_2$, $T_1 = S_1 \setminus S_2$, $T_2 = S_2 \setminus S_1$, $T_0' = S_3 \cap S_4$, $T_1' = S_3 \setminus S_4$, and $T_2' = S_3 \setminus S_4$ (see Figure 4). Based on the above, we further denote $r_{ij} := |R_{ij}| := |T_i \cap T_j|$ for $i, j = 0, 1, 2$. With the above notations, a 9-dimensional vector $r$ is defined as follows:

$$r := (r_{00}, r_{01}, r_{02}, r_{10}, r_{11}, r_{12}, r_{20}, r_{21}, r_{22})^T.$$  \(37\)

We further define the norm of $r$: $|r| = \sum_{i=0}^2 \sum_{j=0}^2 r_{ij}$. Note that each sample in $(S_1 \cup S_2 \cup S_3 \cup S_4) \cap (S_1^{(2k)} \cap S_2^{(2k)})$ is counted exactly once in $r$ so $r \leq c$. 
Example C.2. It is easy to verify that $\rho$ can be represented as a weighted average of $a_{1,n}\text{cov}_{1} + a_{2,n}\text{cov}_{2} + a_{3,n}\text{cov}_{3}$, where $\text{cov}_{3}$ is 0. Moreover, by the definition of $\text{cov}_{1}$ and $\text{cov}_{2}$, it is easy to verify that $a_{1,n}$ only depends on $r_{ij}$ for $(i, j) \neq (0, 0)$ and $a_{2,n}$ only depends on $r_{0,0}$. This verifies
Assumption 3 on this linear average kernel. Besides, we can also show that $F^{(k)}$ in (34) (see Assumption 4) is a quadratic function of $c$ for this kernel.

In addition to the above example, the following discussion shows that we may not able to further reduce the $DoF$ from 9 to 4 by a stronger assumptions. When $E(h(S)) = 0$, it is natural to consider the following fourth cumulant of $\rho$:

$$
cum_4[h(S_1), h(S_2), h(S_3), h(S_4)] = \rho - \Cov[h(S_1), h(S_3)]\Cov[h(S_2), h(S_4)] - \Cov[h(S_1), h(S_4)]\Cov[h(S_2), h(S_3)].
$$

If $cum_4[h(S_1), h(S_2), h(S_3), h(S_4)]$ in (38) is a lower order term of $\rho$, the $DoF$ can be reduced to 4, i.e. $|S_1 \cap S_3|, |S_1 \cap S_4|, |S_2 \cap S_3|,$ and $|S_2 \cap S_4|$. However, Example C.3 shows that this does not hold even for a linear average kernel.

**Example C.3.** Given size-$k$ sets $S_1, S_2, S_3, S_4$ s.t. $S_t = (X_1, Y_1^{(l)}, \ldots, Y_{k-1}^{(l)})$, $X_1, Y_j^{(l)}$ are i.i.d. $E(X_1) = 0, \Var(X_1) > 0, \forall j = 1, 2, \ldots, k-1$ and $l = 1, 2, 3, 4$. By (38) and some direct calculations, we have $\rho = \frac{\Var(X_1)}{k^2}, \Cov[h(S_1), h(S_3)] = \frac{\Var(X_1)}{k^2}$. Plugging in the above equations, we have

$$
\frac{cum_4[h(X_1), h(X_2), h(X_3), h(X_4)]}{2\Cov[h(S_1), h(S_3)]^2} = \frac{\Var(X_1^2) - 2\Var^2(X_1)}{2\Var^2(X_1)}.
$$

As long as $\Var(X_1^2) - 2\Var^2(X_1) > 0$, which is common for non-Gaussian $X_1$, Equation (39) is larger than $o(1)$. This implies that the fourth cumulant is not always a lower order of $\rho$.

We can further verify that given the kernel function is simple quadratic average kernel $h(S_1) = h(X_1, \ldots, X_k) = \frac{1}{k^2} [\sum_{i=1}^k X_i]^2$, even if $X_i$’s are i.i.d. standard Gaussian, the fourth cumulant is still not a lower order term of $\rho$.

### C.3 Discussion of Assumption 4

In Equation (34), $F_c^{(k)}$ is defined as an upper bound for $\rho$ for a given $c$. As illustrated by Figure 5: the more samples shared by $S_1$ and $S_2$, $h(S_1)h(S_2)$ becomes closer to $h(S')^2$. Therefore, given that $|S_1^{(2k)} \cap S_2^{(2k)}| = c$, $F_c$ has the most overlapping among all $\rho$.

![Figure 5: An example of ordinal covariance assumption](image-url)
This assumption is trivial when considering the linear average kernel again: $h(S_l) = \frac{1}{k} \sum_{i=1}^{k} X^{(l)}_i$, for $l = 1, 2, 3, 4$. In particular, considering $(S_1, S_2, S_3, S_4)$ s.t.

$$|S_1 \cap S_2 \cap S_3 \cap S_4| = |(X^{(1)}, ..., X^{(1)})| = c$$

and $(S', S'')$ s.t. $|S' \cap S''| = c$, the equality in Equation (33) attains, i.e.,

$$\rho = k^{-4} \text{Var} \left[(X^{(1)}_1 + ... + X^{(1)}_c)^2 \right] = \text{Cov} \left[h(S')^2, h(S'')^2 \right]. \quad (40)$$

It is also straightforward to verify the assumption under simple quadratic average kernel function $h(S) = \frac{1}{k}[\sum_{i=1}^{k} X_i]^2$.

### C.4 Discussion of Assumption 5

Assumption 2 shows a polynomial growth rate of the second moment term $\xi_{d,k}^2$ while Assumption 5 shows a polynomial growth rate of the fourth moment term $F^{(k)}$. Assumption 5 also assumes $F^{(k)}$ is not a higher order term of $\xi_{1,k}^4$. To better illustrate the idea of Assumption 5, we consider the following example with an oversimplified setting: the cum$_4$ term is 0 in Equation (38). Note that linear average kernel with iid. standard Gaussian $X_i$’s satisfies this setting.

**Example C.4.** Suppose there is no fourth order cumulant term in Equation (38), by Equation (40), $F^{(k)}$ can be simplified as $\xi^2_{r22,k} \xi^2_{r22,k} + \xi^2_{r22,k} \xi^2_{r22,k} = 2\xi^4_{r22,k} = 2\xi^4_{c,k}$. This also implies (35): $F^{(k)} / \xi_{1,k}^4 = \mathcal{O}(1)$. We further remark that in this example, Assumption 5 can be implied by Assumption 2. To be more specific, as demonstrated in the following equation, $a_2$ in (36) is $2a_1$, where $a_1$ is provided in Assumption 2.

$$\frac{F^{(k)}_c}{F^{(k)}_1} = \frac{2\xi^4_{c,k}}{\xi^2_{1,k}} = 2 \left( \frac{\xi^2_{c,k}}{\xi^2_{l,k}} \right)^2 = \mathcal{O}(c^{2a_1}), \text{ for } c = 1, 2, ..., k. \quad (41)$$

By Lemma G.3 (see Appendix G), a natural upper bound for $\sigma_{c,2k}^2$ is $F^{(k)}_c$ (34). Hence, even if $\xi_{d,k}^2$ has a linear growth rate regarding $d$, $F^{(k)}$ still can growth at a quadratic rate of $c$ (see (41)). Therefore, we cannot assume $\sigma_{2k,2k}^2/(2k\sigma_{2,2k}^2) = \mathcal{O}(1)$., which is the common assumption on the counterpart $\xi^2_{1,2k}$ (Mentch and Hooker, 2016; Zhou et al., 2021; DiCiccio and Romano, 2022). That is one reason that Assumptions 3-5 are imposed on the primitive term $\rho$ instead of on $\sigma_{c,2k}^2$. 

35
where i.e. \( \text{Var} \) \( \hat{v} \)

The follow Equation (42) is a road map to upper bound \( \text{Var}(\hat{V}_u) \).

\[
\text{Var}(\hat{V}_u) = \sum_{c=1}^{2k} v_c \sigma^2_{c,2k} \leq \sum_{c=1}^{2k} v_c \sigma^2_{c,2k} \overset{(\ast)}{=} \sum_{c=1}^{T_1} v_c \sigma^2_{c,2k} \overset{(\ast\ast)}{=} v_1 \sigma^2_{1,2k} \overset{(\ast\ast\ast)}{=} \frac{k^4}{n^3} F_1^{(k)}.
\] (42)

Here \( v_c := \left( \frac{n}{2k} \right)^{-1} \left( \frac{2k}{c} \right)^{\frac{n-2k}{2k-c}} \) is the coefficients in the Heoffding decomposition of \( \text{Var}(\hat{V}_u) \) (22), \( \sigma^2_{c,2k} \) is the upper bound of \( \sigma^2_{c,2k} \) given by Propositions G.2 and G.3. “f \approx g” means that \( f = O(g) \) and \( g = O(f) \) (same as the “Big \( \Theta \)”), and \( F_1^{(k)} \) is defined in (34). We interpret the inequalities in (42) as follows.

- The first inequality \( \leq \) is derived through upper bounding \( \sigma^2_{c,2k} \)'s by Propositions G.2 (a tighter bound for \( c = 1, 2, ..., T_1 \)) and G.3 (a loose bound for \( c = T_1 + 1, .., 2k \)). These lemmas further depend on both tighter and loose upper bounds of \( \eta^2_{c,2k}(d_1, d_2) \) (Lemma G.5 and G.6), since each \( \sigma^2_{c,2k} \) can be decomposed weighted sum of \( \eta^2_{c,2k}(d_1, d_2) \)'s (28). Details of these arguments are presented in Appendix G.

- The first asymptotic notation \( \approx \) (denoted by *) is derived by Lemma G.4. Here \( T_1 = \left\lceil \frac{1}{\epsilon} \right\rceil + 1 \) does not grow with \( n \), where \( \epsilon \) controls the growth rate of \( k \) (see Assumption 1).

- The second and last asymptotic notation \( \approx \) (denoted by ** and ***) is derived by Theorem 4.5, showing that the leading term dominates \( \text{Var}(\hat{V}_u) \).

We remark that since \( E(\hat{V}_u) = \text{Var}(U_n) \) also goes to 0 when \( n \) grows to infinity, the ratio consistency of \( \hat{V}_u \) requires a very fast convergence rate of \( \text{Var}(\hat{V}_u) \). This rate can not be achieved if we use only the loose bound of \( \sigma^2_{c,2k} \) in Proposition G.3. Instead, we need a tighter bound in Proposition G.2, but only for the first \( T_1 \) terms.

D.2 Proof of Corollary 4.7

Proof of Corollary 4.7. To show \( \frac{\hat{V}_u}{E(\hat{V}_u)} \overset{P}{\to} 1 \) as \( n \to \infty \), it suffice to show the \( L_2 \) convergence of \( \hat{V}_u/E(\hat{V}_u) \), i.e. \( \text{Var}(\hat{V}_u)/(E(\hat{V}_u))^2 \to 0 \) as \( n \to \infty \).

By plugging Equation (29) and (30) from Theorem 4.5, we have

\[
\frac{\text{Var}(\hat{V}_u)}{(E(\hat{V}_u))^2} = \frac{O \left( \frac{k^2}{n} \sigma^2_{1,2k} \right)}{\left[ (1 + o(1)) \frac{k^2}{n} \xi_{1,k} \right]^2} = O \left( \frac{n}{k^2} \frac{\sigma^2_{1,2k}}{\xi_{1,k}} \right).
\] (43)

where \( \sigma^2_{1,2k} = \Theta(\frac{k^2}{n^2} F_1^{(k)}) \) is the upper bound of \( \sigma^2_{1,2k} \) given by Proposition G.2. By Assumption 5, \( F_1^{(k)} = \)
\( O(\xi_{1,k}^4) \). Plugging \( \sigma_{1,2k}^2 \) into Equation (43), we conclude that
\[
\frac{\text{Var}(\hat{V}_u)}{(E(\hat{V}_u))^2} = O\left( \frac{1}{n} \right).
\]

\[\square\]

### D.3 Proof of Theorem 4.5

We first present a technical proposition to be used soon.

**Proposition D.1.** For any integer \( c \), s.t. \( 1 \leq c \leq k \) and \( k = o(\sqrt{n}) \),
\[
\binom{n}{k}^{-1} \binom{k}{c} \binom{n-k}{k-c} \leq \frac{1}{c!} \left( \frac{k^2}{n-k-1} \right)^c.
\]

**Proof of Proposition D.1.** This proof is provided by DiCiccio and Romano (2022). We first write the combinatorial numbers as factorial numbers
\[
\binom{n}{k}^{-1} \binom{k}{c} \binom{n-k}{k-c} = \frac{(n-k)!k!}{n!} \frac{k!}{(k-c)!} \frac{(n-k)!}{(k-c)!(n-2k+c)!} = \frac{1}{c!} \left[ \frac{k!}{(k-c)!(k-c)!} \right] \left[ \frac{(n-k)!(n-k)!}{n!(n-2k+c)!} \right].
\]

It suffices to upper bound things inside two square brackets separately. We have
\[
\left[ \frac{k!}{(k-c)!(k-c)!} \right] \leq k^{2c}, \tag{45}
\]
\[
\frac{(n-k)!(n-k)!}{n!(n-2k+c)!} = \frac{(n-k)(n-k-1)\cdots(n-2k+c+1)}{n(n-1)\cdots(n-k+1)} \leq \left[ \frac{1}{n-k+1} \right]^c. \tag{46}
\]

Combining (45) and (46) into (44), we completes the proof. \(\square\)

**Proof of Theorem 4.5.** First, we show Equation (29). By Proposition 4.6 and Assumption 2, we can conclude that
\[
\lim_{n \to \infty} \frac{\text{Var}(U_n)}{\frac{k^2 \sigma_{1,k}^2}{n}} = 1.
\]
Secondly, we show Equation (30).

\[ \text{Var}(\hat{V}_n) \approx \text{Var}(T_1)(\hat{V}_n) = \sum_{c=1}^{T_1} \binom{n}{2k}^{-1} \binom{2k}{c} \binom{n-2k}{2k-c} \sigma_{c,2k}^2 \]

(47)

\[ = \sum_{c=1}^{T_1} \binom{n}{2k}^{-1} \binom{2k}{c} \binom{n-2k}{2k-c} O\left(\frac{k^2}{n^2} F_c^{(k)}\right) \]

(48)

\[ = \sum_{c=1}^{T_1} O\left(\frac{k^{2c+2}}{n^{c+2}} F_c^{(k)}\right) \]

(49)

\[ = O\left(\frac{k^4}{n^2} F_1^{(k)}\right). \]

(50)

Here, (47) is concluded by Lemma G.4. (48) is concluded by \( \sigma_{c,2k}^2 = O\left(\frac{k^2}{n^2} F_c^{(k)}\right) \) (Proposition G.2). (49) is concluded by \( \binom{n}{2k}^{-1} \binom{(n-2k)}{2k-c} = \left[1 + o(1)\right] \frac{k^{2c}}{n^c} \) for \( c = 1, 2, \ldots, T_1 \) (Proposition D.1). (50) is concluded by the bounded growth rate of \( F_c^{(k)} \) in Assumption 5 and finite \( T_1 \). If we denote \( \frac{k^2}{n} F_1^{(k)} \) as \( \tilde{\sigma}_{1,2k}^2 \), we conclude that \( \text{Var}(\hat{V}_n) = O\left(\frac{k^2}{n^2} \tilde{\sigma}_{1,2k}^2\right) \).

D.4 Proof of Proposition 4.6

Proof of Proposition 4.6. For \( k = o(\sqrt{n}) \), we want to show \( \lim_{n \to \infty} \frac{\text{Var}(U_n)}{k^2 \tilde{\sigma}_{1,k}^2} = 1 \). First notice that for the coefficient leading term \( \binom{n}{k}^{-1} \binom{k}{d} \binom{k-n-d}{k-1} \xi_{d,k}^2 \), we have

\[ \binom{n}{k}^{-1} \binom{k}{d} \binom{k-n-d}{k-1} = \frac{(n-k)!(n-k)!}{(n-1)!(n-2k+1)!} \to 0, \quad \text{as} \quad n \to \infty. \]

(51)

Therefore, it suffices to show that the rest part of \( \text{Var}(U_n) \) is dominated by the leading term:

\[ \lim_{n \to \infty} \frac{\binom{n}{k}^{-1} \sum_{d=2}^{k} \binom{k}{d} \binom{k-n-d}{k-1} \xi_{d,k}^2}{\frac{k^2}{n} \tilde{\sigma}_{1,k}^2} = 0. \]

By Proposition D.1, the numerator of the above can be bounded as

\[ \left(\frac{n}{k}\right)^{-1} \sum_{d=2}^{k} \binom{k}{d} \binom{k-n-d}{k-1} \xi_{d,k}^2 \leq \sum_{d=2}^{k} \frac{k^{2d}}{d!(n-k+1)d!} \xi_{d,k}^2 \sum_{d=2}^{k} b_n^{-1} \xi_{d,k}^2, \]

(52)

where \( b_n = \frac{k^2}{n-k-1} \). Notice that \( n < 2(n-k+1) \), so we have

\[ \frac{\binom{n}{k}^{-1} \sum_{d=2}^{k} \binom{k}{d} \binom{k-n-d}{k-1} \xi_{d,k}}{\frac{k^2}{n} \tilde{\sigma}_{1,k}^2} \leq \frac{n}{n-k+1} \sum_{d=2}^{k} b_n^{-1} \xi_{d,k}^2 \leq \frac{2}{d!} b_n^{-1} \xi_{d,k}^2. \]

(53)
By Assumption 2, the growth rate of $\xi_d^2$ is bounded, there exists a uniform constant $C$ s.t. $\frac{\xi_d^2}{\xi_1^2} \leq Cd!$ for $d = 2, 3, ..., k$. Therefore, the RHS of Equation (53) is bounded as

$$\sum_{d=2}^{k} \frac{1}{d!} b_{n}^{d-1} \xi_d^2 \xi_1^2 - k \leq \sum_{d=2}^{k} \frac{1}{d!} b_{n}^{d-1} \frac{C d! \xi_d^2}{\xi_1^2} \leq C \sum_{d=2}^{k} b_{n}^{d-1} = C b_{n}^{1} \frac{1 - b_{n}^{k-1}}{1 - b_{n}^{1}} \leq C \frac{b_{n}}{1 - b_{n}}. \tag{54}$$

The RHS of (54) goes to 0 when $n \to \infty$, since $b_{n} = \frac{k^2}{n-k-1} \to 0$. This completes the proof. □

### E Proof of Double U-Statistics

#### E.1 Proof of Proposition 4.3

**Proof of Proposition 4.3. Proof of Equation (24).**

We first show the following equation.

$$\psi \left( S^{(2k)} \right) = \sum_{d=0}^{k} u_d \psi_d \left( S^{(2k)} \right). \tag{55}$$

Wang and Lindsay (2014) have proved that $\hat{V}_u$ is an U-statistic with size-$2k$ kernel (Equation (20)):

$$\hat{V}_u = Q(k) - Q(0) = \binom{n}{2k}^{-1} \sum_{S^{(2k)} \subseteq X_n} \left[ \psi_k \left( S^{(2k)} \right) - \psi_0 \left( S^{(2k)} \right) \right];$$

$$\psi_k \left( S^{(2k)} \right) = \binom{n}{2k} \binom{n}{k}^{-1} \binom{n}{k}^{-1} \sum_{d=0}^{k} A_1 \frac{1}{N_d} \sum_{S_1, S_2 \subseteq S^{(2k)}} h(S_1) h(S_2),$$

$$\psi_0 \left( S^{(2k)} \right) = \binom{n}{2k} \binom{n}{k}^{-1} \binom{n-k}{k}^{-1} \frac{1}{N_0} \sum_{S_1, S_2 \subseteq S^{(2k)}} h(S_1) h(S_2),$$

where $N_d = \binom{n-2k+d}{d}$. Denote

$$A_1 := \binom{n}{2k} \binom{n}{k}^{-2}, \quad A_{1,0} := \binom{n}{2k} \binom{n}{k}^{-1} \binom{n-k}{k}^{-1}. \tag{56}$$

Rewrite $\psi_k \left( S^{(2k)} \right) - \psi_0 \left( S^{(2k)} \right)$ by the order of $d$. Notice that there is a $\sum_{d=0}^{k}$ in $\psi_k \left( S^{(2k)} \right)$ but $d$ can
only be 0 in \( \psi_0 \left( S^{(2k)} \right) \). Hence, there is a cancellation for \( h(S_1)h(S_2) \) s.t. \( d = |S_1 \cap S_2| = 0 \), thus we have

\[
\psi_k \left( S^{(2k)} \right) - \psi_0 \left( S^{(2k)} \right) = A_1 \sum_{d=1}^{k} \frac{1}{N_d} M_{d,k} \sum_{S_1, S_2 \subseteq S^{(2k)}} h(S_1) h(S_2) + (A_1 - A_{1,0}) \frac{1}{N_0} \sum_{S_1, S_2 \subseteq S^{(2k)}} h(S_1) h(S_2).
\]

For the RHS of above equation, multiply and divide \( M_{d,k} \) inside \( \sum_{d=1}^{k} \):

\[
\psi_k \left( S^{(2k)} \right) - \psi_0 \left( S^{(2k)} \right) = \sum_{d=1}^{k} \left[ A_1 \frac{1}{N_d} M_{d,k} \frac{1}{M_{d,k}} \sum_{S_1, S_2 \subseteq S^{(2k)}} h(S_1) h(S_2) \right] w_d + \left[ (A_1 - A_{1,0}) \frac{1}{N_0} M_{0,k} \frac{1}{M_{0,k}} \sum_{S_1, S_2 \subseteq S^{(2k)}} h(S_1) h(S_2) \right] w_0.
\]

We denote

\[
w_d := \frac{A_1}{N_d} M_{d,k}, \quad \text{for } d = 1, 2, \ldots, k;
\]
\[
w_0 := \frac{(A_1 - A_{1,0}) M_{0,k}}{N_0};
\]
\[
\varphi_d(S^{(2k)}) := \frac{1}{M_{d,k}} \sum_{S_1, S_2 \subseteq S^{(2k)}} h(S_1) h(S_2), \quad \text{for } d = 1, 2, \ldots, k;
\]
\[
\varphi_0(S^{(2k)}) := \frac{1}{M_{0,k}} \sum_{S_1, S_2 \subseteq S^{(2k)}} h(S_1) h(S_2).
\]

Thus we have

\[
\psi_k \left( S^{(2k)} \right) - \psi_0 \left( S^{(2k)} \right) = \sum_{d=1}^{k} \left[ w_d \varphi_d(S^{(2k)}) \right] + w_0 \varphi_0(S^{(2k)}) = \sum_{d=0}^{k} w_d \varphi_d(S^{(2k)}).
\]

Given that \( \sum_{d=0}^{k} w_d = 0 \) is true (to be proved soon), then \( w_0 = -\sum_{d=1}^{k} w_d \). Therefore,

\[
\psi \left( S^{(2k)} \right) = \sum_{d=0}^{k} w_d \varphi_d \left( S^{(2k)} \right) = \sum_{d=1}^{k} w_d \varphi_d \left( S^{(2k)} \right) - \left( \sum_{d=1}^{k} w_d \right) \varphi_0 \left( S^{(2k)} \right)
\]
\[
= \sum_{d=1}^{k} w_d \left[ \varphi_d \left( S^{(2k)} \right) - \varphi_0 \left( S^{(2k)} \right) \right].
\]

**Proof of Equation Equation (26)**

First, we show that \( \sum_{d=0}^{k} w_d = 0 \). As discussed above, \( w_d \) is a product of three normalization constants: \( A_1 = \binom{n}{2k} \binom{n}{k}^{-2} \) and \( A_{1,0} = \binom{n}{2k} \binom{n}{k}^{-1} \binom{n-k}{k}^{-1} \) are the normalization constant to rewrite \( Q(k) \) and \( Q(0) \).
as a U-statistic; \( M_{d,k} := \binom{2k}{d} (\binom{2k-d}{k-d})^2 \) is the number of pairs \( S_1, S_2 \subset S^{(2k)} \) s.t. \( |S_1 \cap S_2| = d; N_d = \binom{n-2k+d}{d} \) is defined in Equation (21).

\[
    w_0 = \frac{(A_1 - A_{1,0}) M_{0,k}}{N_0}; \quad w_d = \frac{A_1 M_{d,k}}{N_d}, \quad \text{for } d = 1, 2, \ldots, k.
\]

Since \( A_{1,0} > A_1 > 0, M_{d,k} > 0, N_d > 0 \), we have \( w_d > 0, \forall d \geq 1 \) and \( w_0 < 0 \). Then we show \( \sum_{d=0}^{k} w_d = 0 \). Though this can be justified by direct calculation, we present a more intuitive proof. Recall \( \hat{V}_u = Q(k) - Q(0) \). By the definition of \( Q(k), Q(k) \) can be represented as a weighted sum of \( h(S_1)h(S_2) \), i.e., \( \sum_{1 \leq i,j \leq n} a_{ij} h(S_i)h(S_j) \), where \( \sum_{1 \leq i < j \leq n} a_{ij} = 1 \). Thus, \( Q(k) - Q(0) \) can be represented in a similar way:

\[
    Q(k) - Q(0) = \sum_{1 \leq i < j \leq n} a'_{ij} h(S_i)h(S_j),
\]

where \( \sum_{1 \leq i,j \leq n} a'_{ij} = 0 \). Therefore \( \psi_k \left( S^{(2k)} \right) - \psi_0 \left( S^{(2k)} \right) \), as the kernel of U-statistic \( Q(k) - Q(0) \), can also be represented in the form of a weighted sum:

\[
    \psi_k \left( S^{(2k)} \right) - \psi_0 \left( S^{(2k)} \right) = \sum_{1 \leq i < j \leq n} b_{ij} h(S_i)h(S_j), \quad (57)
\]

where \( \sum_{1 \leq i,j \leq n} b_{ij} = 0 \) since \( \psi_k \left( S^{(2k)} \right) - \psi_0 \left( S^{(2k)} \right) \) is an unbiased estimator of \( Q(k) - Q(0) \). On the other hand, for \( d = 0, 1, 2, \ldots, k, \varphi_d \left( S^{(2k)} \right) \) is still a U-statistic, which can be represented in the form of a weighted sum:

\[
    \varphi_d \left( S^{(2k)} \right) = \sum_{1 \leq i,j \leq n} c_{ij}^{(d)} h(S_i)h(S_j), \quad (58)
\]

where \( \sum_{1 \leq i,j \leq n} c_{ij}^{(d)} = 1 \). Since \( \psi_k \left( S^{(2k)} \right) - \psi_0 \left( S^{(2k)} \right) = \sum_{d=0}^{k} w_d \varphi_d \left( S^{(2k)} \right) \), by comparing Equation (57) and (58), we have \( \sum_{d=1}^{k} w_d \sum_{1 \leq i,j \leq n} c_{ij}^{(d)} = \sum_{1 \leq i < j \leq n} b_{ij} \). Since \( \sum_{1 \leq i,j \leq n} c_{ij}^{(d)} = 1 \) and \( \sum_{1 \leq i,j \leq n} b_{ij} = 0 \), we can take \( h(S_i) = 1 \) for \( i = 1, 2, \ldots, n \) and conclude that

\[
    \sum_{d=0}^{k} w_d = 0.
\]

Secondly, we present the details to bound \( w_d = A_1 M_{d,k}/N_d \), for \( d = 1, 2, \ldots, k \). Plug in the expression of \( A_1, M_{d,k}, N_d \), we have

\[
    w_d = \left[ \binom{n}{2k} \binom{n}{k}^{-2} \right] \left[ \binom{2k}{d} \binom{2k-d}{k-d} \binom{2k-2d}{k-d} \right] / \binom{n-2k+d}{d} = \left[ \frac{n!}{(n-k)!k!} \right] \left[ \frac{(2k)!}{(2k-d)!} \right] \left[ \frac{(2k-d)!}{d!} \right] \left[ \frac{(n-2k)!}{(n-2k-d)!} \right].
\]

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After direct cancellation of the same factorials, we have

\[ w_d = \frac{(n - k)!}{n!(n - 2k + d)!} \left( \frac{k!}{(k - d)!} \right) \cdot \frac{1}{d!}. \]  

(59)

For Part I in (59),

\[ \frac{(n - k)!}{n!(n - 2k + d)!} = \frac{\prod_{i=0}^{k-d-1} (n - k - i)}{\prod_{i=0}^{k-1} (n - i)} = [1 + o(1)] \frac{1}{n^d}. \]

The last equality is because for any \( k = o(\sqrt{n}), d \leq k \), we have

\[ \frac{\prod_{i=0}^{k-d-1} (n - k - i)}{\prod_{i=0}^{k-1} (n - i)} \leq \frac{1}{\prod_{i=0}^{d-1} (n - k - d - i)} \leq \frac{1}{(n - k)^d} = [1 + o(1)] \frac{1}{n^d}. \]

On the other hand,

\[ \frac{\prod_{i=0}^{k-d-1} (n - k - i)}{\prod_{i=0}^{k-1} (n - i)} \geq \frac{1}{n^d}. \]

Combining \( \leq \) and \( \geq \), we have \([1 + o(1)] \frac{1}{n^d}\). For Part II (59),

\[ \frac{k!}{(k - d)!} = \frac{1}{\prod_{i=0}^{d-1} (k - d - i)} = k(k - 1)\ldots(k - d + 1) \leq k^{2d}. \]

Particularly, when \( d \) is fixed, we have \( k! = (k - d)! = k(k - 1)\ldots(k - d + 1) \leq [1 + o(1)] k^{2d} \). Combining Part I, II, III in (59), we have

\[ w_d = \begin{cases} 
[1 + o(1)] \left( \frac{1}{d!} \left( \frac{k^2}{n} \right)^d \right) & \forall \text{ finite } d; \\
O \left( \frac{1}{d!} \left( \frac{k^2}{n} \right)^d \right) & \forall d = 1, 2, \ldots, k. 
\end{cases} \]

\[ \square \]

F  Proof of Results in Methodology Section

F.1 Variance of Incomplete U-statistics \( U_{n,B,M} \)

Proof of Proposition 3.2. This is an extension of the results by Wang (2012, Section 4.1.1) and Wang and Lindsay (2014).

Comparing \( \text{Var}(U_{n,B,M}) = (1 - \frac{1}{B}) \text{Var}(U_n) + \frac{1}{MB} V^{(b)}(14) \) with \( \text{Var}(U_{n,B}) = \text{Var}(U_n) + E[\text{Var}(U_{n,B} | X_n)] \)
(5), it suffices to show that
\[
\mathbb{E} \left[ \text{Var}(U_{n,B} | \mathcal{X}_n) \right] = \frac{1}{MB} V^{(h)} - \frac{1}{B} \text{Var}(U_n).
\]

Here we adopt an alternative view of a complete U-statistic \( U_n \) with \( k \leq n/2 \) by Wang and Lindsay (2014). Follow our notation of “matched group”, we can always take \( M = \lfloor n/k \rfloor \) mutually disjoint subsamples \( S_1, \ldots, S_M \) from \( (X_1, \ldots, X_n) \), such that \( |S_i \cap S_j| = 0 \) for \( 1 \leq i < j \leq M \). Wang and Lindsay (2014) take integer \( M = n/k \) while we allow \( 2 \leq M \leq \lfloor n/k \rfloor \). Recall such \( (S_1^{(b)}, \ldots, S_M^{(b)}) \) as a “matched group”, where \( b \) is the index of group. Let \( G_{n,k,M} \) be the collection of all such matched groups constructed from \( n \) samples, i.e.,
\[
G_{n,k,M} = \left\{ (S_1^{(b)}, \ldots, S_M^{(b)}) : \cup_j S_j^{(b)} \subset \mathcal{X}_n, \text{ and } S_i^{(b)} \cap S_j^{(b)} = \emptyset, \forall 1 \leq i, j \leq M \right\}. \tag{60}
\]

Then, an alternative representation of \( U_n \) is
\[
U_n = \frac{1}{M |G_{n,k,M}|} \sum_{b=1}^{M} \sum_{i=1}^{M} S_i^{(b)}. \tag{61}
\]

This form seems redundant because there are some replicate subsample among all \( S_i^{(b)} \)’s. However, for incomplete U-statistic \( U_{n,B,M} \), each \( (S_1^{(b)}, \ldots, S_M^{(b)}) \) can be viewed as a sample from \( G_{n,k,M} \). Hence, Wang (2012) show that \( B \cdot \text{Var}(U_{n,B} | \mathcal{X}_n) = \frac{1}{|G_{n,k,M}|} \sum_{b=1}^{M} |G_{n,k,M}| (\bar{h}(b) - U_n)^2 \), where \( \bar{h}(b) = \frac{1}{M} \sum_{i=1}^{M} h(S_i^{(b)}) \), \( S_i^{(b)} \)’s are all subsamples associated with the complete U-statistic \( U_n \) on \( \mathcal{X} \). However, Wang (2012) and Wang and Lindsay (2014) do not provide a simple expression in the form of \( V^{(h)} \) and \( \text{Var}(U_n) \). We further simplify \( B \text{Var}(U_{n,B} | \mathcal{X}_n) \) as follows,
\[
B \cdot \mathbb{E} \left[ \text{Var}(U_{n,B} | \mathcal{X}_n) \right] = \mathbb{E} \left( \frac{1}{|G_{n,k,M}|} \sum_{b=1}^{M} (\bar{h}(b) - U_n)^2 \right) = \mathbb{E} \left[ \frac{1}{|G_{n,k,M}|} \sum_{b=1}^{M} \left( (\bar{h}(b) - E(U_n)) - (U_n - E(U_n)) \right)^2 \right]
\]
\[
= \frac{1}{|G_{n,k,M}|} \sum_{b=1}^{M} \mathbb{E} \left( (\bar{h}(b) - E(U_n))^2 \right) + \frac{1}{|G_{n,k,M}|} \sum_{b=1}^{M} \mathbb{E} \left( (U_n - E(U_n))^2 \right)
\]
\[
- 2 \mathbb{E} \left( \frac{1}{|G_{n,k,M}|} \sum_{b=1}^{M} (\bar{h}(b) - E(U_n))(U_n - E(U_n)) \right)
\]
\[
= \text{Var} \left( \bar{h}^{(1)} \right) - \text{Var}(U_n)
\]
\[
= \frac{1}{M} V^{(h)} - \text{Var}(U_n).
\]

In the above equations, the first equality is the conclusion by Wang (2012); the next-to-last equality holds
F.2 Unbiasedness of Variance Estimators

Proof of Proposition 3.1. First, we restrict the discussion given \( k \leq n/2 \). We first show that \( \hat{V}^{(S)} = \sum_{d=0}^{k} \gamma_{d,k,n} \hat{\xi}^2_{d,k} \). By the discussion in Section 3.3.1, we have \( N_{d,k,n} = \binom{n}{k}^2 \gamma_{d,k,n} \). For a complete U-statistic with \( k \leq n/2 \), \( N_{d,k,n} = \binom{n}{k} \binom{n-k}{k-d} \binom{k}{d} \) and we denote \( N = \binom{n}{k} > 0 \). Then,

\[
\sum_{d=0}^{k} \gamma_{d,k,n} \hat{\xi}^2_{d,k} = \sum_{d=0}^{k} N^{-2} N_{d,k,n} \hat{\xi}^2_{d,k} \\
= N^{-2} \sum_{1 \leq i \leq N} \sum_{1 \leq j \leq N} \sum_{d=0}^{k} 1 \{|S_i \cap S_j| = d\} [h(S_i) - h(S_j)]^2 / 2 \\
= N^{-2} \left[ 2 \sum_{1 \leq i < j \leq N} \sum_{d=0}^{k-1} 1 \{|S_i \cap S_j| = d\} [h(S_i) - h(S_j)]^2 / 2 \right] \\
= \frac{N(N-1)}{N^2} \left[ \binom{N}{2}^{-1} \sum_{1 \leq i < j \leq N} [h(S_i) - h(S_j)]^2 / 2 \right] \\
= \frac{N-1}{N} \left[ \frac{1}{N-1} \sum_{i=1}^{N} [h(S_i) - U_n]^2 \right] \\
= \frac{1}{N} \sum_{i=1}^{N} [h(S_i) - U_n]^2 = \hat{V}^{(S)}
\]

Here, the second equality holds by plugging in the definition of \( N_{d,k,n} \) and interchanging the finite summation \( \sum_{d \in \mathcal{D}} \) with \( \sum_{1 \leq i < j \leq B} \). The third equality omits the cases with \( i = j \), where \( h(S_i) - h(S_j) = 0 \). The second to last equality holds because the sample variance is essentially an order-2 U-statistic, with kernel \( (h(S_i) - h(S_j))^2 / 2 \).

Then, as we demonstrated in Section 3.3.1, \( \text{E}(\hat{\xi}^2_{d,k}) = \xi^2_{d,k} \) for \( d = 0, 1, ..., k \). Hence we conclude that

\[
\text{E} \left( \hat{V}^{(S)} \right) = \sum_{d=0}^{k} \gamma_{d,k,n} \text{E}(\hat{\xi}^2_{d,k}) = \sum_{d=0}^{k} \gamma_{d,k,n} \xi^2_{d,k} = V^{(S)}.
\]

Secondly, we extend the previous argument to the setting \( n/2 < k < n \). We denote \( \mathcal{D} = \{d \in \mathbb{N}^*|0 \leq d \leq k, \gamma_{d,k,n} > 0\} \). We can define \( \hat{V}^{(S)} = \sum_{d \in \mathcal{D}} \gamma_{d,k,n} \hat{\xi}^2_{d,k} \). We want to show that

\[
\hat{V}^{(S)} = \frac{1}{N} \sum_{i=1}^{N} [h(S_i) - U_n]^2, \\
\text{E}(\hat{V}^{(S)}) = V^{(S)}.
\]
Similar to previous proof

\[ \hat{V}'(S)' = \sum_{d \in \mathcal{D}} N^{-2} N_{d,k,n} \hat{\xi}^2_{d,k} \]

\[ = N^{-2} \left[ 2 \sum_{1 \leq i < j \leq N} \sum_{d \in \mathcal{D} \setminus \{k\}} 1 \{|S_i \cap S_j| = d\} \frac{[h(S_i) - h(S_j)]^2}{2} \right] \]

\[ = \frac{N(N-1)}{N^2} \left[ \binom{N}{2}^{-1} \sum_{1 \leq i < j \leq N} [h(S_i) - h(S_j)]^2 / 2 \right] \]

\[ = \frac{N - 1}{N} \left[ \frac{1}{N-1} \sum_{i=1}^{N} [h(S_i) - U_n]^2 \right] \]

\[ = \frac{1}{N} \sum_{i=1}^{N} [h(S_i) - U_n]^2 \]

Since each \( \hat{\xi}^2_{d,k} \) is still an unbiased estimator of \( \xi^2_{d,k} \), similarly, we have \( \mathbb{E}(\hat{V}'(S)') = V'(S) \). Remark that the summation in Equation (62) is over \( d \in \mathcal{D} \) instead of \( d = 0, 1, 2, \ldots, n \). This is because \( \gamma_{d,k,n} \) is 0 for small \( d \), given \( k > n/2 \). In other words, when \( k > n/2 \), several terms of \( \gamma_{d,k,n} \xi^2_{d,k} \) in the Hoeffding decomposition (3) is already 0.

\[ \square \]

**Proof of Proposition 3.3.** Since a sample variance is an order-2 U-statistic,

\[ \hat{V}'_{B,M} = [(BM - 1)BM]^{-1} \sum_{i=1}^{M} \sum_{j=1}^{B} \sum_{(i',j') \neq (i,j)} \left[ h(S^{(j)}_i) - h(S^{(j')}_{i'}) \right] \]

\[ = [(BM - 1)BM]^{-1} \sum_{i=1}^{M} \sum_{j=1}^{B} \left( \sum_{(i',j') \in A(i,j)} + \sum_{(i',j') \in B(i,j)} \right) \left[ h(S^{(j)}_i) - h(S^{(j')}_{i'}) \right] \]

\[ := [(BM - 1)BM]^{-1} \sum_{i=1}^{M} \sum_{j=1}^{B} \left( \sum_{(i',j') \in A(i,j)} + \sum_{(i',j') \in B(i,j)} \right) \hat{v}_{(i,j,i',j')} \]

where \( A(i,j) = \{(i',j')|i' \neq i, j' = j, 1 \leq i' \leq M, 1 \leq j' \leq B\} \); \( B(i,j) = \{(i',j')|j' \neq j, 1 \leq i' \leq M, 1 \leq j' \leq B\} \). We note that \( |A(i,j)| = M - 1 \) and \( |B(i,j)| = [(B - 1)(M - 1)] \) for any \( (i,j) \). To further simply our notation, we also denote \( \hat{v}_{(i,j,i',j')} = [h(S^{(j)}_i) - h(S^{(j')}_{i'})] / 2 \).

Fixing \( (i,j) \), for any \( (i',j') \in A(i,j), S^{(j')}_{i'} \) and \( S^{(j)}_i \) are the same but not identical. Hence, \( \hat{v}_{(i,j,i',j')} \) is an unbiased estimator of \( \hat{V}'(h) \). Furthermore, the sample variance within group \( j \) is also a U-statistic, which can be alternatively represented as an order-2 U-statistic: \( [M(M-1)]^{-1} \sum_{i=1}^{M} \sum_{i' \neq i} \hat{v}_{(i,j,i',j')} \). Thus, by
summation over all $j$ and the symmetry, we have
\[
[(BM - 1)BM]^{-1} \sum_{i=1}^{M} \sum_{j=1}^{B} \left( \sum_{(i', j') \in A(i, j)} E(\hat{\nu}_{(i, j', j')}) \right) \\
= [(BM - 1)BM]^{-1} \sum_{i=1}^{M} \sum_{j=1}^{B} |A(i, j)|V^{(h)} := \delta_{M,B}V^{(h)},
\]

(64)

where $\delta_{M,B} = \frac{M - 1}{MB - 1}$.

Fixing $(i, j)$, for any $(i', j') \in B(i, j)$, $S_{i}^{(j)}$ and $S_{i'}^{(j')} are in different matched group. Since each matched group are sampled independently, $S_{i}^{(j)}$ and $S_{i'}^{(j')} are independently sampled from $X_n$. By the theory of finite population sampling (Cochran, 2007), for $(i', j') \in B(i, j)$,
\[
E(\hat{\nu}_{(i, j, i', j')}) = E[E(\hat{\nu}_{(i, j, i', j')}|X_n)] = E\left[\left(\frac{n}{k}\right)^{-1} \sum_{S_i \in X_n} (h(S_i) - U_n)^2\right] = V^{(S)}
\]

Thus, the normalized summation over all such $\hat{\nu}_{(i, j, i', j')}$ satisfies that
\[
[(BM - 1)BM]^{-1} \sum_{i=1}^{M} \sum_{j=1}^{B} \sum_{(i', j') \in B(i, j)} E(\hat{\nu}_{(i, j, i', j')}) \\
= [(BM - 1)BM]^{-1} \sum_{i=1}^{M} \sum_{j=1}^{B} |B(i, j)|V^{(S)} := (1 - \delta_{M,B})V^{(S)}.
\]

(65)

Combining Equations (64) and (65), we conclude that
\[
E\left(\hat{V}^{(S)}_{B,M}\right) = (1 - \delta_{M,B})V^{(S)} + \delta_{M,B}V^{(h)}.
\]

Proof of Proposition 3.4. On one hand, by Proposition 3.3
\[
E\left(\hat{\text{Var}}(U_{n,B,M})\right) = E(\hat{V}^{(h)}_{B,M}) - \frac{MB - 1}{MB}E(\hat{V}^{(S)}_{B,M}) \\
= V^{(h)} - \frac{MB - 1}{MB} \left[ (1 - \frac{M - 1}{MB - 1})V^{(S)} + \frac{M - 1}{MB - 1}V^{(h)} \right] \\
= \frac{MB - M + 1}{MB}V^{(h)} - \frac{B - 1}{B}V^{(S)}.
\]

On the other hand, by $\text{Var}(U_n) = V^{(h)} - V^{(S)}$ (8) and Proposition and 3.2,
\[
\text{Var}(U_{n,B,M}) = \frac{B - 1}{B}\text{Var}(U_n) + \frac{1}{MB}V^{(h)} = \frac{MB - M + 1}{MB}V^{(h)} - \frac{B - 1}{B}V^{(S)}.
\]
Hence, we conclude the unbiasedness of our incomplete variance estimator:

$$E\left(\hat{\text{Var}}(U_{n,B,M})\right) = \text{Var}(U_{n,B,M}).$$

### F.3 Equivalence of Two complete Variance Estimators

We denote the proposed variance estimator (12) and the variance estimator of complete U-statistics as $\hat{V}'_u$ and $\hat{V}''_u$ respectively. Note that Wang and Lindsay (2014)’s estimator involves the notation of matching group (see $G_{n,k,M}$ in Appendix F.1) while ours does not. To simplify the notation, we denote $\mathcal{B} = |G_{n,k,M}|$ and $\tilde{h}(b) = \frac{1}{M_M} \sum_{i=1}^{M_M} h(S_i^{(b)})$, for $b = 1, 2, \ldots, \mathcal{B}$. Under this notation, the alternative form (with $G_{n,k,M}$) of $U_n$ (61) is $\frac{1}{MB_M} \sum_{b=1}^{\mathcal{B}} \sum_{i=1}^{M} h(S_i^{(b)})$. Then $\hat{V}'_u$ and $\hat{V}''_u$ can be represented as follows.

$$\hat{V}'_u = \hat{V}(h) - \hat{V}(S),$$

$$\hat{V}''_u = \frac{\sigma^2_{WP}}{M} - \sigma^2_{BP},$$

where $\hat{V}(S) = \binom{n}{k}^{-1} \sum_{i=1}^{\binom{n}{k}} (h(S_i) - U_n)^2$ (10); $\hat{V}(h) = \binom{n}{k} \binom{n-k}{d} \sum_{|S_i \cap S_j| = 0} [h(S_i) - h(S_j)]^2 / 2$ (11); $\sigma^2_{WP} = \frac{1}{\mathcal{B}} \sum_{b=1}^{\mathcal{B}} \frac{1}{M_M} \sum_{i=1}^{M} (h(S_i^{(b)}) - \tilde{h}(b))^2$; $\sigma^2_{BP} = \frac{1}{\mathcal{B}} (\tilde{h}(b) - U_n)^2$.

We note that our complete U-statistic variance estimator is identical to that by Folsom (1984).

**Proposition F.1.** Our complete variance estimator $\hat{V}'_u$ is equivalent to the estimator $\hat{V}''_u$ proposed by Wang and Lindsay (2014).

**Proof.** To simplify the notation, we denote

$$A_1 := \frac{1}{MB_M} \sum_{b=1}^{\mathcal{B}} \sum_{i=1}^{M} (h(S_i^{(b)}))^2, \quad A_2 := U_n^2, \quad A_3 := \frac{1}{\mathcal{B}} \sum_{b=1}^{\mathcal{B}} (\tilde{h}(b))^2.$$

To show the equivalence between $\hat{V}'_u$ and $\hat{V}''_u$, we will show that they are the same linear combination of $A_1, A_2, A_3$. First, it is trivial to verify that $\sigma^2_{WP}$ and $\sigma^2_{BP}$ are linear combinations of $A_1, A_2, A_3$:

$$\sigma^2_{WP} = \frac{M}{M-1} (A_1 - A_3), \quad \sigma^2_{BP} = A_3 - A_2. \quad (67)$$

Secondly, we show that $\hat{V}(h) = \sigma^2_{WP}$ by showing that $\hat{V}(h)$ also equals to $\frac{M}{M-1} (A_1 - A_3)$. Considering the summation $\frac{1}{M-1} \sum_{i=1}^{M} (h(S_i^{(b)}) - \tilde{h}(b))^2$ in $\sigma^2_{WP}$, it can be represented as

$$\binom{M}{2}^{-1} \sum_{i=1}^{M} \sum_{j \neq i} (h(S_i^{(b)}) - h(S_j^{(b)}))^2 / 2.$$
Since $G_{n,k,M}$ is a set of all permutation of disjoint $(S_1^{(b)}, \ldots, S_M^{(b)})$, we have

$$\sigma_{WP}^2 = \frac{1}{B} \sum_{b=1}^B \binom{M}{2}^{-1} \sum_{i=1}^M \sum_{j \neq i} \frac{(h(S_i^{(b)}) - h(S_j^{(b)}))^2}{2}$$

$$= \binom{n}{k}^{-1} \binom{n-k}{k}^{-1} \sum_{|S_i \cap S_j| = 0} [h(S_i) - h(S_j)]^2/2 = \hat{V}^{(h)}.$$

Similarly, we can show that our incomplete Variance estimator (18) is equivalent to the counterpart in Wang and Lindsay (2014, page 1124). Given $B$ matching groups and $M$ subsamples in each group, we have

$$\hat{V}^{(S)} = \frac{n}{k}^{-1} \sum_{i=1}^n h(S_i)^2 - U_n^2. $$

Due to the definition of $G_{n,k,M}$, the collection $\{S_i^{(b)}\}_{i,b}$ are basically replications of $\{S_i\}_{i=1}^n$. Hence, $(\binom{n}{k})^{-1} \sum_{i=1}^n h(S_i)^2 = A_1$, which implies that

$$\hat{V}^{(S)} = A_1 - A_2. $$

Therefore, we can represent both $\hat{V}_u'$ and $\hat{V}_u''$ with $A_1, A_2, A_3$ by (67) and (68) as follows:

$$\hat{V}_u' = \hat{V}^{(h)} - \hat{V}^{(S)} = \frac{M}{M-1} (A_1 - A_3) - (A_1 - A_2) = \frac{1}{M-1} A_1 + 2A_2 - \frac{1}{M-1} A_3,$$

$$\hat{V}_u'' = \sigma_{WP}^2/M - \sigma_{BP}^2 = \frac{1}{M-1} (A_1 - A_3) - (A_3 - A_2) = \frac{1}{M-1} A_1 + A_2 - \frac{M}{M-1} A_3.$$

This conclude that $\hat{V}_u' = \hat{V}_u''$. Note that $\hat{V}^{(h)} - \hat{V}^{(S)} = \sigma_{WP}^2/M - \sigma_{BP}^2$, however, $\hat{V}^{(h)} \neq \sigma_{WP}^2/M$ and $\hat{V}^{(S)} \neq \sigma_{BP}^2$. Our and Wang and Lindsay (2014)'s estimators are proposed under different perspectives.

### F.4 Equivalence of Two Incomplete Variance Estimators

Similarly, we can show that our incomplete Variance estimator (18) is equivalent to the counterpart in Wang and Lindsay (2014, page 1124). Given $B$ matching groups and $M$ subsamples in each group, we denote the above estimators as $\hat{V}_u^{(inc)}'$ and $\hat{V}_u^{(inc)}''$ respectively:

$$\hat{V}_u^{(inc)'} := \hat{V}^{(h)}_{B,M} - \frac{MB}{MB} \hat{V}^{(S)}_{B,M}, \quad \hat{V}_u^{(inc)''} := \sigma_{WP}^2/M - \sigma_{BP}^2,$$

where $\hat{\sigma}_{WP}^2 := \frac{1}{(M-1)B} \sum_{b=1}^B \sum_{i=1}^M (h(S_i^{(b)}) - \bar{h}(b))^2$, $\sigma_{BP}^2 := \frac{1}{B} \sum_{b=1}^B (\bar{h}(b) - U_n)^2$, and $\bar{h}(b) = \frac{1}{M} \sum_{i=1}^M h(S_i^{(b)})$. As analogues to $A_1, A_2, A_3$ (66) in Appendix F.3, we denote

$$\tilde{A}_1 := \frac{1}{MB} \sum_{b=1}^B \sum_{i=1}^M (h(S_i^{(b)}))^2, \quad \tilde{A}_2 := U_{n,B,M}^2, \quad \tilde{A}_3 := \frac{1}{B} \sum_{b=1}^B (\bar{h}(b))^2.$$ 

Similarly, it is trivial to verify that $\hat{V}^{(h)}_{B,M}$ (15), $\hat{V}^{(S)}_{B,M}$ (16), $\hat{\sigma}_{WP}^2$ and $\sigma_{BP}^2$ can be represented as linear
combinations of $\tilde{A}_1, \tilde{A}_2$ and $\tilde{A}_3$ as follows:

\[
\hat{V}^{(h)}_{B,M} = \hat{\sigma}^2_{WP} = \frac{MB}{M-1}(\tilde{A}_1 - \tilde{A}_3), \quad \hat{V}^{(S)}_{B,M} = \frac{MB}{M-1}(\tilde{A}_1 - \tilde{A}_2), \quad \sigma^2_{BP} = \tilde{A}_3 - \tilde{A}_2.
\]

By plugging the above into equation (69), we have

\[
\hat{V}^{(inc)'}_u = \hat{V}^{(h)}_{B,M} - \frac{MB-1}{MB} \hat{V}^{(S)}_{B,M} = \frac{1}{M-1}\tilde{A}_1 + \tilde{A}_2 - \frac{M}{M-1}\tilde{A}_3
\]

\[
\hat{V}^{(inc)''}_u = \hat{\sigma}^2_{WP}/M - \hat{\sigma}^2_{BP} = \frac{1}{M-1}\tilde{A}_1 + \tilde{A}_2 - \frac{M}{M-1}\tilde{A}_3.
\]

Hence, we conclude that $\hat{V}^{(inc)'}_u = \hat{V}^{(inc)''}_u$.

### G Technical Propositions and Lemmas

In this section, we present the technical propositions and lemmas. The proofs of these results are collected in Appendix H.

**Proposition G.1.** The value of $\psi(S^{(2k)})$ does not depend on $E[h(X_1, \ldots, X_k)]$. Therefore, WLOG, we can assume the kernel is zero-mean, i.e. $E[h(X_1, \ldots, X_k)] = 0$

The proof of this proposition is collected in Appendix H.1.

**G.1 Results of $\sigma^2_{c,2k}$**

First, we present Propositions G.2 and G.3. The former provides a precise bound of $\sigma^2_{c,2k}$ for some fixed $c$ while the latter provides rough bound for $1 \leq c \leq 2k$.

**Proposition G.2 (Bound $\sigma^2_{c,2k}$ for finite $c$).** Fix $T_1 = \left\lfloor \frac{1}{c} \right\rfloor + 1$. Under Assumptions 1 - 5, for any $c$ that $1 \leq c \leq T_1$,

\[
\sigma^2_{c,2k} = O\left(\frac{k^2}{n^2} F_{c}^{(k)}\right).
\]

Based on the upper bound, we define $\tilde{\sigma}^2_{c,2k} := C\frac{k^2}{n^2} F_{c}^{(k)}$, where $C$ is a generic positive constant.

**Proposition G.3 (Bound $\sigma^2_{c,2k}$ for any $c$).** Under Assumptions 1 - 5, for any $1 \leq c \leq 2k$, we have

\[
\sigma^2_{c,2k} = O(F_{c}^{(k)}).
\]

The proof of the above propositions is collected in Appendix H.2 and Appendix H.3 respectively. These results depend on the further decomposition of $\sigma^2_{c,2k}$ into weighted sum of $\eta^2_{c,2k}(d_1, d_2)$’s, which is later discussed in Appendix G.2. In particularly, we can show that $\eta^2_{c,2k}(1, 1)$ dominates $\sigma^2_{c,2k}$ for $c = 1, 2, \ldots, T_1$.

Note that the upper bound in Proposition G.2 actually works for any fixed and finite $c$. As a corollary of the above results, we can show the following lemma.
Lemma G.4 (Truncated Variance Lemma I). Under Assumptions 1-5, there exists a constant $T_1 = \left\lfloor \frac{1}{\epsilon} \right\rfloor + 1$, such that

$$\lim_{n \to \infty} \frac{\text{Var} \left( \hat{V}_n \right) - \text{Var}(T_1) \left( \hat{V}_n \right)}{\text{Var}(T_1) \left( \hat{V}_n \right)} = 0,$$  

(70)

where

$$\text{Var}^{(T_1)} \left( \hat{V}_n \right) := \left( \frac{n}{2k} \right)^{-1} \sum_{c=1}^{T_1} \left( \begin{array}{c} 2k \\ c \end{array} \right) \left( n - 2k \right) \left( 2k - c \right) \sigma_{c,2k}^2,$$  

(71)

$$\text{Var}^{(T_1)} \left( \hat{V}_n \right) := \left( \frac{n}{2k} \right)^{-1} \sum_{c=1}^{T_1} \left( \begin{array}{c} 2k \\ c \end{array} \right) \left( n - 2k \right) \left( 2k - c \right) \tilde{\sigma}_{c,2k}^2.$$  

(72)

Here, we denote $\tilde{\sigma}_{c,2k}^2$ as the upper bound of $\sigma_{c,2k}^2$ given by Proposition G.2.

The proof of Lemma G.4 is collected in Appendix H.4. This implies that to bound $\text{Var}(\hat{V}_n)$, it suffices to bound the weighted average of first $T_1$ terms of $\sigma_{c,2k}^2$, instead of all $2k$ terms. Note that we use $\tilde{\text{Var}}$ instead of $\text{Var}$ in the denominator of (70). Here $T_1 = \left\lfloor \frac{1}{\epsilon} \right\rfloor + 1$ does not grow with $n$. It only relies on $\epsilon$, which quantifies the growth rate of $k$ with respect to $n$ (see Assumption 1.). For example, if $k = n^{1/3}$, i.e., $\epsilon = 1/6$, then we can choose $T_1 = 7$. Hence, to show $\sigma_{1,2k}^2$ dominates in $\text{Var}(\hat{V}_n)$ when $n \to \infty$, it suffices to show that $\sigma_{1,2k}^2$ dominates in $T_1$-truncated $\text{Var}^{(T_1)}(\hat{V}_n)$ when $n \to \infty$.

G.2 Results of $\eta_{c,2k}^2(d_1, d_2)$

Given the decomposition $\sigma_{c,2k}^2 = \sum_{d_1=1}^{k} \sum_{d_2=1}^{k} w_{d_1} w_{d_2} \eta_{c,2k}^2(d_1, d_2)$ (see (28) in Proposition 4.4). To bound $\sigma_{c,2k}^2$, we should study $\eta_{c,2k}^2(d_1, d_2)$ (28). The results of $\eta_{c,2k}^2(d_1, d_2)$ are presented in this section.

Lemma G.5. Under Assumptions 1-5, for $1 \leq c \leq T_1$, $d_1, d_2 \leq T_2$,

$$\eta_{c,2k}^2(d_1, d_2) = O \left( \frac{1}{k^2} F_c^{(k)} \right).$$

Lemma G.6. Under Assumptions 1-5, for $c = 1, 2, \ldots, 2k$, $1 \leq d_1, d_2 = 1, 2, \ldots, k$,

$$\eta_{c,2k}^2(d_1, d_2) = O(F_c^{(k)}).$$

Similar to the “two-type” upper bounds of $\sigma_{c,2k}^2$, Lemma G.5 provides a precise bound of $\eta_{c,2k}^2(d_1, d_2)$ for bounded $c$ and $d_1, d_2$ while Lemma G.6 provides a rough bound of $\eta_{c,2k}^2(d_1, d_2)$ for all $c, d_1, d_2$. The proof of the above lemmas are collected in Appendix H.5 and Appendix H.6 respectively. The proof demonstrates the cancellation pattern by matching $\rho$ (31).

With the above bounds on $\eta_{c,2k}^2(d_1, d_2)$, we introduce the following truncated $\sigma_{c,2k}^2$ and show Lemma G.8, which implies that to bound $\sigma_{c,2k}^2$, it suffices to bound the first finite $\eta_{c,2k}^2(d_1, d_2)$ terms in its decomposition (28).
Definition G.7 (Truncated $\sigma^2_{c,2k}$). Let $T_2 = \lfloor \frac{1}{c} \rfloor + 1$. We define $\psi^{(T_2)}$, a $T_2$-truncated $\psi$ as

$$
\psi^{(T_2)}(S^{(2k)}):= \sum_{d=1}^{T_2} w_c \left( \varphi_d \left( S^{(2k)} \right) - \varphi_0 \left( S^{(2k)} \right) \right). \tag{73}
$$

Hence, given two size-2$k$ subsamples $S_1^{(2k)}$ and $S_2^{(2k)}$ that $|S_1^{(2k)} \cap S_2^{(2k)}| = c$, a $T_2$-truncated of $\sigma^2_{c,2k}$ are defined as:

$$
\sigma^2_{c,2k,(T_2)} := \text{Cov}(\psi^{(T_2)}(S_1^{(2k)}),\psi^{(T_2)}(S_2^{(2k)})) = \sum_{d_1=1}^{T_2} \sum_{d_2=1}^{T_2} w_{d_1}w_{d_2} \sigma^2_{c,2k}(d_1,d_2). \tag{74}
$$

Lemma G.8 (Truncated Variance Lemma II). Under Assumptions 1 - 5, there exists a constant $T_2 = \lfloor \frac{1}{c} \rfloor + 1$, such that for any $c \leq T_1$,

$$
\lim_{k \to \infty} \frac{\sigma^2_{c,2k} - \sigma^2_{c,2k,(T_2)}}{\tilde{\sigma}^2_{c,2k}} = 0,
$$

where $\tilde{\sigma}^2_{c,2k,(T_2)}$ is the upper bound of $\sigma^2_{c,2k,(T_2)}$ given in Proposition G.2.

The proof is collected in Appendix H.7. Similar to the idea of Lemma G.4, using Lemma G.8 the upper bound $\sigma^2_{c,2k}$ (28) only involves the sum of $T_2^2$ terms, i.e., $\sigma^2_{c,2k,(T_2)}$ rather than $k^2$ terms. Here $T_2$ is again finite and does not grow with $k$. Though $T_1$ and $T_2$ take the same value, we note that $T_1$ is the truncation constant for $\text{Var}(\hat{V}_u)$ in (71) while $T_2$ is the truncation constant for $\sigma^2_{c,2k}$ in (74).

H Proof of Technical Propositions and Lemmas

H.1 Proof of Proposition G.1

Proof of Proposition G.1. Suppose $E(h(S_1)) = \mu$ and we rewrite $h(S_1) = h_0(S_1) + \mu$, where $E(h_0(S_1)) = 0$. Then $\varphi_d(S^{(2k)})$ defined in (25) can be written as

$$
\varphi_d(S^{(2k)}) = \frac{1}{M_{d,k}} \sum_{S_1,S_2 \in S^{(2k)}, |S_1 \cap S_2| = d} h_0(S_1)h_0(S_2) + [h_0(S_1) + h_0(S_2)] \mu + \mu^2. \tag{75}
$$

Plug Equation (75) into Equations (20) and (24). By the fact that $\sum_{d=0}^{k} w_d = 0$ and the symmetry of U-statistic, the terms of $\mu$ and $\mu^2$ are cancelled. Consequently, $\hat{V}_u$ does not depend on $\mu$, so W.L.O G., we assume that $\mu = 0$. \qed
H.2 Proof of Proposition G.2

Proof of Proposition G.2. This proof relies on the technical lemmas in Appendix G.2. First, by Lemma G.8, to upper bound $\sigma_{c,2k}^2$, it suffices to upper bound the following $\sigma_{c,2k,(T_2)}^2$ (74)

$$\sigma_{c,2k,(T_2)}^2 = \sum_{d_1=1}^{T_2} \sum_{d_2=1}^{T_2} w_{d_1} w_{d_2} \eta_{c,2k}^2(d_1, d_2),$$

where $w_d = \lfloor 1 + o(1) \rfloor \left[ \frac{1}{d} \left( \frac{k^2}{n} \right)^d \right], \forall d \leq T_2$.

By Lemma G.5: fixing any $c$ s.t. $1 \leq c \leq T_2$, $\eta_{c,2k}^2(d_1, d_2) = \mathcal{O}\left( \frac{F_c(k)}{k^2} \right)$, $\forall d_1, d_2 \leq T_2$. Besides, since $d_1$ and $d_2$ are bounded by a constant $T_2$. $w_1^2$ dominates the summation $\sum_{d_1=1}^{T_2} \sum_{d_2=1}^{T_2} w_{d_1} w_{d_2}$. We have

$$\sigma_{c,2k,(T_2)}^2 = \sum_{d_1=1}^{T_2} \sum_{d_2=1}^{T_2} w_{d_1} w_{d_2} \eta_{c,2k}^2(d_1, d_2) = \mathcal{O}\left( \frac{F_c(k)}{k^2} \right) \sum_{d_1=1}^{T_2} \sum_{d_2=1}^{T_2} w_{d_1} w_{d_2}$$

$$= \mathcal{O}\left( \frac{F_c(k)}{k^2} \right) [1 + o(1)] w_1^2 = \mathcal{O}\left( \frac{k^2}{n^2} \right) F_c(k).$$

Here, the last equality is derived by plugging in $w_1 = \lfloor 1 + o(1) \rfloor \frac{k^2}{n}$.

\hfill \Box

H.3 Proof of Proposition G.3

Proof of Proposition G.3. This lemma again relies on the upper bound of $\eta_{c,2k}^2(d_1, d_2)$ in Appendix G.2. By Proposition 4.4, we can decompose $\sigma_{c,2k}^2$ as

$$\sigma_{c,2k}^2 = \sum_{d_1=1}^{k} \sum_{d_2=1}^{k} w_{d_1} w_{d_2} \eta_{c,2k}^2(d_1, d_2),$$

First, we investigate the coefficient of $\eta_{c,2k}^2(d_1, d_2)$. By Proposition 4.3, we have $\sum_{d_1=1}^{k} w_{d_1} < 1$. Thus, we attain

$$\sum_{d_1=1}^{k} \sum_{d_2=1}^{k} w_{d_1} w_{d_2} = (\sum_{d_1=1}^{k} w_{d_1})(\sum_{d_2=1}^{k} w_{d_2}) < 1.$$

By Lemma G.6, we have $\eta_{c,2k}^2(d_1, d_2) = \mathcal{O}(F_c)$ for $c = 1, 2, 3, \ldots, 2k$. Hence, combining the bounds on $w_d$ and $\eta_{c,2k}^2(d_1, d_2)$, we conclude that

$$\sigma_{c,2k}^2 = \mathcal{O}(F_c^{(k)})$$

We remark that the summation $\sum_{d_1=1}^{k} w_{d_1}$ can attain a lower order of 1, which may imply a tighter bound of $\sigma_{c,2k}^2$. 

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H.4 Proof of Lemma G.4

Proof. Let $T_1 = \lfloor \frac{1}{k} \rfloor + 1$. Recall Equation (22) $\text{Var} \left( \hat{V}_{\text{u}} \right) = \left( \frac{n}{2k} \right)^{-1} \sum_{c=1}^{2k} \left( \frac{c}{2k-1} \right) \sigma_{c,2k}^2$. We first present the intuition of this lemma. $\text{Var}(\hat{V}_u)$ is a weighted sum of $\sigma_{c,2k}^2$, where the coefficient of $\sigma_{c,2k}^2$ decays with $c$ at a rate even faster than a geometric rate. If the growth rate of $\sigma_{c,2k}^2$ is not too fast, then the tail terms can be negligible. This involves both the precise upper bound of $\sigma_{1,2k}^2$ (Proposition G.2) and the rough upper bound of $\sigma_{c,2k}^2$ for $c \geq T_1 + 1$ (Proposition G.3).

First, $\left( \frac{n}{2k} \right)^{-1} \left( \frac{n-2k}{1} \right) \sigma_{1,2k}^2 \leq \text{Var}(T_1) \left( \hat{V}_u \right)$ since the former is the first term in the latter and all the other terms are positive. Therefore, it suffices to show

$$\frac{\text{Var} \left( \hat{V}_u \right) - \text{Var}(T_1) \left( \hat{V}_u \right)} {\left( \frac{n}{2k} \right)^{-1} \left( \frac{n-2k}{1} \right) \sigma_{1,2k}^2} = \frac{\sum_{c=T_1+1}^{2k} \left( \frac{n}{2k} \right)^{-1} \left( \frac{n-2k}{c} \right) \sigma_{c,2k}^2} {\left( \frac{n}{2k} \right)^{-1} \left( \frac{n-2k}{1} \right) \sigma_{1,2k}^2} \to 0. \quad (76)$$

We bound the numerator and denominator in Equation (76) separately. For the denominator, by the analysis of Equation (51), we have

$$\left( \frac{n}{2k} \right)^{-1} \left( \frac{n-2k}{1} \right) \sigma_{1,2k}^2 = \left[ 1 + o(1) \right] \frac{4k^2 \sigma_{1,2k}^2}{n}. \quad (77)$$

For the numerator, by Proposition G.3 and assumption 5, $\sigma_{c,2k}^2 = O(F_{c}^{(k)}) = o(c^{a_2}F_{1}^{(k)})$. Therefore, it suffices to show that

$$\frac{\sum_{c=T_1+1}^{2k} \left( \frac{n}{2k} \right)^{-1} \left( \frac{n-2k}{c} \right) o(c^{a_2}F_{1}^{(k)})} {\left( \frac{n}{2k} \right)^{-1} \left( \frac{n-2k}{1} \right) \sigma_{1,2k}^2} = \frac{O \left( \left\{ \left( \frac{n}{2k} \right)^{-1} \left( \frac{n-2k}{c} \right) o(c^{a_2}F_{1}^{(k)}) \right\}_{c=T_1+1}^{2k} \right)} {n} \to 0. \quad (78)$$

The equality in (78) is given by Proposition H.1. The followed $\frac{n}{2k} \to \infty$ in (78) is given by Proposition H.2. This completes the proof. 

Proposition H.1. Under Assumptions 1 - 5,

$$\frac{\sum_{c=T_1+1}^{2k} \left( \frac{n}{2k} \right)^{-1} \left( \frac{n-2k}{c} \right) c^{a_2}F_{1}^{(k)}} {\left( \frac{n}{2k} \right)^{-1} \left( \frac{n-2k}{T_1+1} \right) (T_1 + 1)^{a_2}F_{1}^{(k)}} \to 0, \text{ as } n \to \infty \quad (79)$$

Proof. The proof of Proposition H.1 is similar to the proof of Proposition 4.6. The idea is that the sum of tail coefficients is a geometric sum and thus dominates the growth rate of moments.

First to consider the coefficient $\frac{\sum_{c=T_1+1}^{2k} \left( \frac{n}{2k} \right)^{-1} \left( \frac{n-2k}{c} \right) c^{a_2}F_{1}^{(k)}} {\left( \frac{n}{2k} \right)^{-1} \left( \frac{n-2k}{T_1+1} \right) (T_1 + 1)^{a_2}F_{1}^{(k)}}$. By Proposition D.1 and our analysis in Equ-
tion (52) and (53), let \( b_n = \frac{4k^2}{n-2k+1} \) which is the common ratio in the geometric sequence.

\[
\sum_{c=T_1+2}^{2k} \left( \frac{2k}{n} \right)^{-1} \left( \frac{2k}{T_1+1} \right) \left( \frac{n-2k}{2k-T_1-1} \right) \leq \sum_{c=T_1+2}^{2k} \left( 1 + o(1) \right) \frac{(T_1 + 1)!}{c!} b_n^{c-(T_1+1)}.
\] (80)

Second, combining \( c^{\alpha_1} \) with (80), it's again the problem of geometric series with common ratio \( b_n = o(1) \). We have

\[
\text{LHS of (79)} \leq \sum_{c=T_1+2}^{2k} \mathcal{O} \left( \frac{c^{\alpha_2}}{c!} \right) b_n^{c-(T_1+1)} \leq \sum_{c=T_1+2}^{2k} \mathcal{O}(1) b_n^{c-(T_1+1)} \leq \sum_{c=1}^{\infty} \mathcal{O}(1) b_n^c = \mathcal{O}(1)b_n \to 0,
\] (81)

where the last equality is concluded by the sum of geometric series.

**Proposition H.2.** Under Assumptions 1 - 5,

\[
\frac{\left( \frac{n}{2k} \right)^{-1} \left( \frac{2k}{T_1+1} \right) \left( \frac{n-2k}{2k-T_1-1} \right) C'(T_1 + 1)^{\alpha_2} F_1^{(k)}}{\sigma^2_{1,2k}} = o\left( \frac{1}{k^2} \right) \to 0.
\] (82)

In Equation (82), the upper bound of \( c = T_1 + 1 \) term of the numerator is a lower order term compared to the denominator.

**Proof.** It suffices bound two separate parts in Equation (82),

\[
\frac{\left( \frac{n}{2k} \right)^{-1} \left( \frac{2k}{T_1+1} \right) \left( \frac{n-2k}{2k-T_1-1} \right)}{k^2 n} = o\left( \frac{1}{n^2} \right),
\] (83)

\[
\frac{C'(T_1 + 1)^{\alpha_2} F_1^{(k)}}{\sigma^2_{1,2k}} = \mathcal{O}\left( \frac{n^2}{k^2} \right).
\] (84)

Then, combining Equation (83) and (84), we have

\[
\text{LHS of (82)} \leq o\left( \frac{1}{n^2} \right) \mathcal{O}\left( \frac{n^2}{k^2} \right) = o\left( \frac{1}{k^2} \right) \to 0.
\]

We first show Equation (83), i.e., bound the ratio of coefficient. Similar to the analysis for Equation (53), by Proposition D.1, we have

\[
\left( \frac{n}{2k} \right)^{-1} \left( \frac{2k}{T_1+1} \right) \left( \frac{n-2k}{2k-T_1-1} \right) \leq \left( \frac{2k}{T_1+1} \right)^{2(T_1+1)} \frac{1}{(T_1 + 1)!} \left( \frac{1}{(T_1 + 1)!} \right)^{b_n^{T_1+1}},
\]

where \( b_n = \frac{4k^2}{n-2k+1} \). Therefore the ratio of coefficient,

\[
\frac{\left( \frac{n}{2k} \right)^{-1} \left( \frac{2k}{T_1+1} \right) \left( \frac{n-2k}{2k-T_1-1} \right)}{4k^2 n} \leq [1 + o(1)] \frac{1}{(T_1 + 1)!} b_n^{T_1}.
\]
It remains to show \( b_{nT}^{\gamma_1} = o(\frac{1}{n^2}) \). By \( T_1 = \left\lceil \frac{1}{\epsilon} \right\rceil + 1 \) and \( k = \mathcal{O}(n^{1/2-\epsilon}) \), we have

\[
\eta_{nT}^{\gamma_1} \leq \left( \frac{4k^2}{n} \right)^{1/\epsilon + 1} = \mathcal{O}(n^{-2\epsilon} \epsilon^{1/\epsilon + 1}) = o\left( \frac{1}{n^2} \right).
\] (85)

Second, we show (84), i.e., bound the ratio of moments. By Lemma G.8 and G.2, \( \sigma_{1,2k}^2 = \mathcal{O}(k^2/n^2 F_{1,k}^{(k)}) \) and \( \tilde{\sigma}_{1,2k}^2 = \Theta(k^2/n^2 F_{1,k}^{(k)}) \). We have

\[
\frac{\text{Cov}(T_1 + 1)^{a_2} F_{1,k}^{(k)}}{\tilde{\sigma}_{1,2k}^2} = \mathcal{O}(n^2/k^2(T_1 + 1)^{a_2}) = \mathcal{O}(\frac{n^2}{k^2}).
\] (86)

\[\square\]

H.5 Proof of Lemma G.5

Proof of Lemma G.5. First, we present a sketch of this proof. Given \( S_{1}^{(2k)} \) and \( S_{2}^{(2k)} \), our strategy tracks the distribution of Influential Overlaps, i.e., the samples in \( S_{1}^{(2k)} \cap S_{2}^{(2k)} \). We will decompose \( \eta_{i,2k}^{2}(d_1, d_2) \) as a finite weighted sum:

\[
\eta_{i,2k}^{2}(d_1, d_2) = \sum_{i} a_i b_i,
\] (87)

where \( i \) is the summation index to be specified later. Based on this form, we will show \( a_i = \mathcal{O}(\frac{1}{c}) \) and \( b_i = \mathcal{O}(F_{c}^{(k)}) \) for each \( i \). Since (87) is a finite sum, we can conclude \( \eta_{i,2k}^{2}(d_1, d_2) = \mathcal{O} \left( \frac{1}{c} F_{c}^{(k)} \right) \). Details of (87) will be presented later. We remark that it is straightforward to upper bound \( \eta_{i,2k}^{2}(d_1, d_2) \) by enumerating all the possible 4-way overlapping cases of \( S_1, S_2, S_3, S_4 \) given \( c, d_1, d_2 \) for small \( c \). However, the growth of \( c \) from 1 to 2, 3, 4, ..., \( T_2 \) makes “enumerating” impossible.

We start the proof by reviewing the definition of \( \eta_{i,2k}^{2}(d_1, d_2) \) (27):

\[
\eta_{i,2k}^{2}(d_1, d_2) = \text{Cov} \left[ \varphi_{d_1} (S_{1}^{(2k)}) - \varphi_{0} (S_{1}^{(2k)}) , \varphi_{d_2} (S_{2}^{(2k)}) - \varphi_{0} (S_{2}^{(2k)}) \right],
\]

where \( \varphi_d (S_{2}^{(2k)}) = \left( \begin{smallmatrix} \binom{2k}{d} \binom{2k-d}{d} \binom{2k-2d}{k-d} \end{smallmatrix} \right)^{-1} \sum_{S_1, S_2 \subseteq S_{2}^{(2k)}, |S_1 \cap S_2| = d} h(S_1) h(S_2) \) (25). The following proof is collected as two parts. First, we propose an alternative representation of the covariance \( \text{Cov} \left[ \varphi_{d_1} (S_{1}^{(2k)}), \varphi_{d_2} (S_{2}^{(2k)}) \right] \), which helps discover the cancellation pattern of \( \eta_{i,2k}^{2}(d_1, d_2) \) (27). Secondly, we derive Equation (87) and specify \( a_i \)’s and \( b_i \)’s.

First, we notice that \( \varphi_d (S_{2}^{(2k)}) \) (25) is a weighted average of the product of two kernels \( h(S_1) h(S_2) \):

\[
\varphi_d (S_{2}^{(2k)}) = \left[ \binom{2k}{d} \binom{2k-d}{d} \binom{2k-2d}{k-d} \right]^{-1} \sum_{S_1, S_2 \subseteq S_{2}^{(2k)}, |S_1 \cap S_2| = d} h(S_1) h(S_2).
\]

Denote \( \sum_{F_{1,2}} \) as summation over all pairs of \( S_1, S_2 \), s.t. \( S_1, S_2 \subseteq S_{2}^{(2k)}, |S_1 \cap S_2| = d \). Similarly, we can
also denote $\sum_{P_{34}}$. Then, we can represent the covariance $\text{Cov}[\varphi_{d_1}(S^{(2k)}_1), \varphi_{d_2}(S^{(2k)}_2)]$ as

$$\text{Cov} \left[ \varphi_{d_1}(S^{(2k)}_1), \varphi_{d_2}(S^{(2k)}_2) \right] = \text{Cov} \left[ M_{d_1}^{-1} \sum_{P_{12}} h(S_1)h(S_2), M_{d_2}^{-1} \sum_{P_{34}} h(S_3)h(S_4) \right] \tag{88}$$

$$= M_{d_1}^{-1} M_{d_2}^{-1} \sum_{P_{12}} \sum_{P_{34}} \rho \tag{89}$$

$$= \sum_{\text{feasible } \varpi} p(\varpi,d_1,d_2,c)\rho. \tag{90}$$

In the above equations,

$$p(\varpi,d_1,d_2,c) := M_{d_1}^{-1} M_{d_2}^{-1} \sum_{(S_1,S_2,S_3,S_4)} 1 \{\text{overlapping structure of } S_1, S_2, S_3, S_4 \text{ satisfies } (\varpi,d_1,d_2)\};$$

$$M_{d} = \binom{2k-2d}{d} \binom{2k-d}{k-d}$$

is the number of pairs of sets in the summation. The equality in (90) holds by combining the $\rho$ terms with the same $\varpi$ (see definition of $\varpi$ in Appendix C.1). Since it is difficult to figure out the exact value of $p(\varpi,d_1,d_2,c)$, we further propose the following proposition to show an alternative representation of $\text{Cov}[\varphi_{d_1}(S^{(2k)}_1), \varphi_{d_2}(S^{(2k)}_2)]$.

**Lemma H.3.** Denote $r_{i*} = \sum_{j=0}^{2^d} r_{ij}$ and $r_{*j} = \sum_{i=0}^{2^d} r_{ij}$, for $i,j = 0, 1, 2$ and vector $\varpi^* := (r_{00}, r_{10}, r_{20}, r_{01}, r_{11}, r_{21})$, we have

$$\text{Cov} \left[ \varphi_{d_1}(S^{(2k)}_1), \varphi_{d_2}(S^{(2k)}_2) \right] = \sum_{\text{feasible } \varpi^*} p(\varpi*,r_{00},r_{10},r_{20},d_1,c)p(\varpi*,r_{01},r_{11},r_{21},d_2,c)g(\varpi^*,d_1,d_2). \tag{91}$$

Here $p(\varpi*,r_{00},r_{10},r_{20},d_1,c)$ and $p(\varpi*,r_{01},r_{11},r_{21},d_2,c)$ are non-negative and satisfy the following. For non-negative integers $x_0, x_1, x_2$ that $x_0 + x_1 + x_2 \leq c$,

$$p(x_0,x_1,x_2,d,c) := \binom{d}{x_0} \binom{k-d}{x_1} \binom{k-d}{x_2} \binom{d}{c-x_0-x_1-x_2} \binom{2k}{c}^{-1} = O(k^{x_1+x_2-c}). \tag{92}$$

g(\varpi^*,d_1,d_2) is the following weighted average of $\rho$, where the weight is some constant $p(\varpi^*)$ satisfying that $\sum_{\varpi^*} p(\varpi^*) = 1$.

$$g(\varpi^*,d_1,d_2) := \sum_{\varpi} p(\varpi,\varpi^*)\rho. \tag{93}$$

The proof of Lemma H.3 is deferred to the end of Appendix H.5. Under Assumption 3, $\rho$ does not depend on $d_1, d_2$. Hence, $g(\varpi^*,d_1,d_2)$ also does not depend on $d_1, d_2$. We further denote $G(\varpi^*) = g(\varpi^*,d_1,d_2)$. Then,

$$\text{Cov} \left[ \varphi_{d_1}(S^{(2k)}_1), \varphi_{d_2}(S^{(2k)}_2) \right] = \sum_{\text{feasible } \varpi^*} p(\varpi*,r_{00},r_{10},r_{20},d_1,c)p(\varpi*,r_{01},r_{11},r_{21},d_2,c)G(\varpi^*). \tag{94}$$

We remark that $p(\varpi*,r_{00},r_{10},r_{20},d_1,c)$ and $p(\varpi*,r_{01},r_{11},r_{21},d_2,c)$ can be viewed as some probability mass function with parameters $c, d_1, d_2$ (see the proof of Lemma H.3). As a corollary of (92), when $c - x_1 - x_2 > d$, 

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Notice that since $S_1^{(2k)}$ is independent of $S_2^{(2k)}$, $\sum_{\text{feasible } \xi^*} c$ can be written as two sequential sums: $\sum_{(r_0, r_1, r_2, r_3)} \sum_{(r_0, r_1, r_2, r_3)}$. Therefore, by plugging the expression of $\text{Cov}[\varphi_{d_1}(S_1^{(2k)}), \varphi_{d_2}(S_2^{(2k)})]$ into $\eta_{c,2k}(d_1, d_2)$ (27), we have

$$\eta_{c,2k}^2(d_1, d_2) = \text{Cov} \left[ \varphi_{d_1} \left( S_1^{(2k)} \right) - \varphi_0 \left( S_1^{(2k)} \right), \varphi_{d_2} \left( S_2^{(2k)} \right) - \varphi_0 \left( S_2^{(2k)} \right) \right]$$

$$= \sum_{\text{feasible } \xi^*} \left[ p(r_0, r_1, r_2, d_1, c) - p(r_0, r_1, r_2, 0, c) \right] \left[ p(r_0, r_1, r_2, d_2, c) - p(r_0, r_1, r_2, 0, c) \right] G(r^*)_{b_i}$$

We have two observations on the above Equation (95). First, this $\eta_{c,2k}^2(d_1, d_2) = \sum_i a_i b_i$ is a finite summation because $c \leq T_1$. Hence, to show $\eta_{c,2k}^2 = O(F_\xi^{(k)}/k^2)$, it suffices to bound every term $a_i b_i$. Secondly, by Lemma H.3, $b_i = G(r^*)$ is a weighted average of $\rho$ where the non-negative weights $\sum_{\xi^*} p_{(\xi, \xi^*)} = 1$. Hence, each $b_i$ is naturally bounded by the upper bound of $\rho$. We conclude that $b_i = O(F_\xi^{(k)})$. Therefore, it remains to show that $a_i = O(k^{-2})$ for every $i$. This is provided by the following lemma.

**Lemma H.4.** Fixing integer $d, c \geq 0$, for any tuple of non-negative integers $(x_0, x_1, x_2)$ s.t. $\sum_{i=0}^2 x_i \leq c$,

$$p(x_0, x_1, x_2, d, c) - p(x_0, x_1, x_2, 0, c) = O\left( \frac{1}{k} \right).$$

The proof is collected later in Appendix H.5. This completes the proof of Lemma G.5. We remark that though there exists $p(x_0, x_1, x_2, d, c) \simeq 1$ for some $(x_0, x_1, x_2)$, $p(x_0, x_1, x_2, d, c) - p(x_0, x_1, x_2, 0, c)$ is always at the order of $O\left( \frac{1}{k} \right)$. \(\square\)

**Remark H.5.** This proof has proceeded under Assumption 3. It can be adapted to a weaker assumption: Assumption 6. The according proof using this new assumption will be present in Appendix I, where we cannot exactly cancel two $\rho$ with the same $\xi$ but different $d$.

We present the proof of two important technical facts in the above proof: Lemma H.3 and Lemma H.4.

**Proof of Lemma H.3.** First, we derive Equation (91) from Equation (90):

$$\text{Cov} \left[ \varphi_{d_1} \left( S_1^{(2k)} \right), \varphi_{d_2} \left( S_2^{(2k)} \right) \right] = \sum_{\text{feasible } \xi} p_{(\xi, d_1, d_2, c)} \rho_i.$$

Given that $c = |S_1^{(2k)}, S_2^{(2k)}|$, $d_1 = |S_1 \cap S_2|$ and $d_2 = |S_3 \cap S_4|$, suppose we randomly sample a feasible $S_1, S_2, S_3, S_4$ from all possible cases, we can use a 9-dimension random variable $\mathbf{R}$ to denote the 4-way overlapping structure of $S_1, S_2, S_3, S_4$. Hence, the the coefficient $p_{(\xi, d_1, d_2, c)}$ in (90) is $P(\mathbf{R} = \xi|d_1, d_2, c)$. Then, denote a 6-dimension random variable $\mathbf{R}^* = (R_{0*}, R_{1*}, R_{2*}, R_{3*}, R_{4*}, R_{5*})$, taking all possible values of $\xi^*$ given $d_1, d_2, c$. By Bayesian rule,

$$P(\mathbf{R} = \xi|d_1, d_2, c) = P(\mathbf{R} = \xi|\mathbf{R}^* = \xi^*, d_1, d_2, c) P(\mathbf{R}^* = \xi^*|d_1, d_2, c).$$

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Since $S_1, S_2 \subset S_1^{(2k)}$, $S_3, S_4 \subset S_2^{(2k)}$ and $S_1^{(2k)}$ is independent from $S_2^{(2k)}$, $(R_{0*}, R_{1*}, R_{2*})$ are independent from $(R_{0*}, R_{1*}, R_{2*})$. Hence, we can further decompose $P(R^* = r^*|d_1, d_2, c)$ as $P(R_{0*} = r_{0*}, R_{1*} = r_{1*}, R_{2*} = r_{2*})|d_1, c) \cdot P(R_{0*} = r_{0*}, R_{1*} = r_{1*}, R_{2*} = r_{2*})|d_2, c)$. To simplify the notations, we denote

\[
p_{(d_1, d_2, c)} := P(R^* = r^*|d_1, d_2, c),
\]
\[
p_{(d, c)} := P(R = r|R^* = r^*, d_1, d_2, c),
\]
\[
p(r_{0*}, r_{1*}, r_{2*}, d_1, c) := P(R_{0*} = r_{0*}, R_{1*} = r_{1*}, R_{2*} = r_{2*})|d_1, c),
\]
\[
p(r_{0*}, r_{1*}, r_{2*}, d_2, c) := P(R_{0*} = r_{0*}, R_{1*} = r_{1*}, R_{2*} = r_{2*})|d_2, c).
\]

Given $R^*$, the distribution of $R$ does not depend on $d_1, d_2, c$ so we omit the subscript $d_1, d_2, c$ in $p_{(d, c)}$. We also remark that $\sum_{r^*} p_{(d, c)} = 1$ since $R|R^*$ can be viewed as a random variable. Based on these notations and (97), we can rewrite Equation (90) as

\[
\sum_{\text{feasible } r^*} \sum_{\text{feasible } d} p_{(d, c)} p(r_{0*}, r_{1*}, r_{2*}, d_1, c) p(r_{0*}, r_{1*}, r_{2*}, d_2, c) p^{(98)} = \sum_{\text{feasible } d} p_{(d, c)} p^{(99)}
\]

This justifies both Equations (91) and (93).

Secondly, we show Equation (92). Since $p(r_{0*}, r_{1*}, r_{2*}, d_1, c)$ and $p(r_{0*}, r_{1*}, r_{2*}, d_2, c)$ can be analyzed in the same way, our discussion focuses on $p(r_{0*}, r_{1*}, r_{2*}, d_1, c)$, which is boiled down to the distribution of $(R_{0*}, R_{1*}, R_{2*})$. Given $c$ and $d_1$, $c$ Influential Overlaps can fall into 4 different “boxes” in $S_1^{(2k)}$: $S_1 \cap S_2$, $S_1 \setminus S_2$, $S_2 \setminus S_1$, and $S_1^{(2k)} \setminus (S_1 \cup S_2)$, with “box size” as $d_1$, $k - d_1$, $k - d_1$, $d_1$ respectively. The number of samples in each “box” follows a hypergeometric distribution. This is illustrated by the following table.

| Index | 0 | 1 | 2 | 3 |
|-------|---|---|---|---|
| “box” | $S_1 \cap S_2$ | $S_1 \setminus S_2$ | $S_2 \setminus S_1$ | $S_1^{(2k)} \setminus (S_1 \cup S_2)$ |
| “box size” | $d_1$ | $k - d_1$ | $k - d_1$ | $d_1$ |
| # of Influential Overlaps | $r_{0*}$ | $r_{1*}$ | $r_{2*}$ | $c - r_{0*}$ |

Table 5: The distribution of Influential Overlaps in $S_1^{(2k)}$.

Hence, the probability mass function of $(R_{0*}, R_{1*}, R_{2*})$: $P(R_{0*} = r_{0*}, R_{1*} = r_{1*}, R_{2*} = r_{2*}|d_1, c)$ is

\[
p(r_{0*}, r_{1*}, r_{2*}, d_1, c) = \binom{d_1}{r_{0*}} \binom{k - d_1}{r_{1*}} \binom{k - d_1}{r_{2*}} \binom{c - r_{0*} - r_{1*} - r_{2*}}{d_1}^{-1}.
\]

It remains to show that $p(r_{0*}, r_{1*}, r_{2*}, d_1, c) = O(k^{r_{1*} + r_{2*} - c})$ for any fixed $c, d_1$. In the following, to simplify the notation, we denote $x_i = r_{i*}$ for $i = 0, 1, 2$ and $x_3 = c - r_{0*} - r_{1*} - r_{2*}$. Then Equation (92) can be
written as
\[
\frac{c!}{x_0!x_1!x_2!} \frac{d_1!}{(d_1 - x_0)!} \frac{(k - d_1)!}{(k - d_1 - x_1)!(k - d_1 - x_2)!} \frac{d_1!}{(d_1 - x_3)!} \frac{(k - d_1)!}{(2k)!} \frac{(2k)!}{(2k - c)!}.
\]
(99)

Before the formal justification, we remark that (99) looks similar to the probability mass function of a multinomial distribution:
\[
\frac{c!}{x_0!x_1!x_2!x_3!} \left( \frac{d_1}{2k} \right)^{x_0} \left( \frac{k-d_1}{2k} \right)^{x_1} \left( \frac{k-d_1}{2k} \right)^{x_2} \left( \frac{d_1}{2k} \right)^{x_3},
\]
which is obviously \(O(k^{x_1+x_2-c})\).

We decompose Equation (99) as a production of three parts, denoting Part I := \(\frac{c!}{x_0!x_1!x_2!x_3!} \frac{d_1!}{(d_1 - x_0)!} \frac{(k - d_1)!}{(k - d_1 - x_1)!(k - d_1 - x_2)!} \frac{d_1!}{(d_1 - x_3)!} \frac{(k - d_1)!}{(2k)!} \frac{(2k)!}{(2k - c)!}\). Part II := \(\frac{c!}{x_0!x_1!x_2!x_3!} \frac{d_1!}{(d_1 - x_0)!} \frac{(k - d_1)!}{(k - d_1 - x_1)!(k - d_1 - x_2)!} \frac{d_1!}{(d_1 - x_3)!} \frac{(k - d_1)!}{(2k)!} \frac{(2k)!}{(2k - c)!}\). Part III := \(\frac{(2k)!}{(2k - c)!}\). Since \(x_0, x_1, x_2, x_3, c\) are finite, Part I can be viewed as a constant in the asymptotic analysis. For Part II, again, \(\frac{d_1!}{(d_1 - x_0)!} \frac{d_1!}{(d_1 - x_3)!} \) does not depend on \(k\) and thus can be treated as a constant. For the rest part:
\[
\frac{(k - d_1)!}{(k - d_1 - x_1)!(k - d_1 - x_2)!} = \left[ \prod_{i=0}^{x_1-1} (k - d_1 - i) \right] \left[ \prod_{i=0}^{x_2-1} (k - d_1 - i) \right] \leq (k - d_1)^{x_1+x_2}.
\]

For Part III,
\[
\frac{(2k)!}{(2k - c)!} = c! \prod_{i=0}^{c-1} (2k - i) \geq k^c.
\]

Combining Part I, II, III, we have
\[
P(x_0, x_1, x_2, d_1, c) = O\left((k - d_1)^{x_1+x_2}/k^c\right) = O(k^{-c+x_1+x_2}).
\]

This completes the proof.

**Proof of Lemma H.4.** To show \(p(x_0, x_1, x_2, d, c) = O\left(\frac{1}{k}\right)\), we study two cases separately, where case I is \(x_1 + x_2 \leq c - 1\) and case II is \(x_1 + x_2 = c\). This is motivated by the conclusion of Proposition H.3, \(p(x_0, x_1, x_2, d, c) = O(k^{x_1+x_2-c})\).

We first study case I. For any finite \(c, d\), since \(x_1 + x_2 \leq c - 1\), by (92), \(p(x_0, x_1, x_2, d, c) = O(1/k)\). In particular, \(p(x_0, x_1, x_2, 0, c) = 0\). Therefore,
\[
p(x_0, x_1, x_2, d, c) - p(x_0, x_1, x_2, 0, c) = O\left(\frac{1}{k}\right) - 0 = O\left(\frac{1}{k}\right).
\]

Secondly, we study case II. For any finite \(c, d\), since \(x_1 + x_2 = c\), \(p(x_0, x_1, x_2, 0, c) \gg 1\) and \(p(x_0, x_1, x_2, 0, c) \gg 1\). Hence, we cannot conclude the order of \(p(x_0, x_1, x_2, d, c) - p(x_0, x_1, x_2, 0, c)\) directly from the order of each term. We need to study \(p(x_0, x_1, x_2, d, c) = \left(\frac{d}{x_0}\right)^{x_0} \left(\frac{k-d}{x_1}\right)^{x_1} \left(\frac{k-d}{x_2}\right)^{x_2} \left(\frac{1}{c}\right)^{x_3} \) a bit more carefully. It is equivalent to show that
\[
\left[ p(x_0, x_1, x_2, d, c) - p(x_0, x_1, x_2, 0, c) \right] / p(x_0, x_1, x_2, d, c) = O\left(\frac{1}{k}\right).
\]
To prove the above, we denote \( q(d) := p(x_0, x_1, x_2, d, c)/p(x_0, x_1, x_2, 0, c) \). It suffices to show that

\[
q(d) = p(x_0, x_1, x_2, d, c)/p(x_0, x_1, x_2, 0, c) = 1 + \mathcal{O}(\frac{1}{k}).
\]

Since \( x_0 + x_1 + x_2 + x_3 = c \) and \( x_1 + x_2 = c \), we have \( x_0 = x_3 = 0 \) in \( p(x_0, x_1, x_2, d, c) \). Therefore,

\[
q(d) = \frac{(d)(k-d)(k-d)\binom{d}{x_1}\binom{d}{x_2}}{\binom{2k}{x_1} \binom{2k}{x_2}} = \frac{(k-d)! (k-d)!}{(k-d-x_1)!x_1!(k-d-x_2)!x_2!} / \left[ \frac{k!}{(k-x_1)!x_1!(k-x_2)!x_2!} \right].
\] (100)

By direct cancellations of factorials, the above equation can be simplified as

\[
q(d) = \frac{\prod_{i=0}^{d-1} (k-x_1-i) \prod_{i=0}^{d-1} (k-x_2-i)}{\prod_{i=0}^{d-1} (k-i) \prod_{i=0}^{d-1} (k-i)} = \left[ \frac{\prod_{i=0}^{d-1} k-x_1-i}{k-i} \right] \left[ \frac{\prod_{i=0}^{d-1} k-x_2-i}{k-i} \right].
\] (101)

To upper bound these two products in Equation (101), we consider a general argument. For any integer \( b \geq a \geq x \geq 0 \), we have

\[
\frac{a-x}{b-x} \leq \frac{a-1}{b-1} \leq \frac{a}{b}.
\]

Therefore,

\[
\left( \frac{a-x}{b-x} \right)^x \leq \frac{a(a-1)\ldots(a-x+1)}{b(b-1)\ldots(b-x+1)} \leq \left( \frac{a}{b} \right)^x
\]

Hence, let \( a = k - x_1, b = k, x = d - 1 \), we can bound \( \prod_{i=0}^{d-1} \frac{k-x_1-i}{k-i} \) in Equation (101) as

\[
\left( \frac{k-d+1-x_1}{k-d+1} \right)^d \leq \prod_{i=0}^{d-1} \frac{k-x_1-i}{k-i} \leq \left( \frac{k-x_1}{k} \right)^d
\]

Similarly, we can bound \( \prod_{i=0}^{d-1} \frac{k-x_2-i}{k-i} \) in Equation (101) as \( \left( \frac{k-d+1-x_2}{k-d+1} \right)^d \leq \prod_{i=0}^{d-1} \frac{k-x_2-i}{k-i} \leq \left( \frac{k-x_2}{k} \right)^d \).

Therefore, the Equation (101) can be upper and lower bounded as

\[
\left( \frac{k-d+1-x_1}{k-d+1} \right)^d \left( \frac{k-d+1-x_2}{k-d+1} \right)^d \leq q(d) \leq \left( \frac{k-x_1}{k} \right)^d \left( \frac{k-x_2}{k} \right)^d.
\] (102)

We will show both LHS and RHS of Equation (102) is \( 1 + \mathcal{O}(\frac{1}{k}) \). First, consider the terms in the RHS of Equation (102). Recall that \( d, x_1 \) are finite compared to \( k \), by binomial theorem

\[
\left( \frac{k-x_1}{k} \right)^d = \left( 1 - \frac{x_1}{k} \right)^d = \sum_{i=0}^{d} \binom{d}{i} \left( -\frac{x_1}{k} \right)^i = 1 + \mathcal{O}(\frac{1}{k}).
\]

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Similarly, for the other term in the RHS of Equation (102), we achieve
\[
\left( \frac{k - x_2}{k} \right)^d = 1 + O\left( \frac{1}{k} \right).
\]
Similarly, for the two terms in the LHS of Equation (102), we have
\[
\left( \frac{k - x_1 - d + 1}{k - d + 1} \right)^d = 1 + O\left( \frac{1}{k - d + 1} \right) = 1 + O\left( \frac{1}{k} \right),
\]
\[
\left( \frac{k - x_2 - d + 1}{k - d + 1} \right)^d = 1 + O\left( \frac{1}{k - d + 1} \right) = 1 + O\left( \frac{1}{k} \right).
\]
Putting the above analysis together for Equation (102), we get
\[
\left[ 1 + O\left( \frac{1}{k} \right) \right] \left[ 1 + O\left( \frac{1}{k} \right) \right] \leq q(d) \leq \left[ 1 + O\left( \frac{1}{k} \right) \right] \left[ 1 + O\left( \frac{1}{k} \right) \right]
\]
\[
\implies \left[ 1 + O\left( \frac{1}{k} \right) \right] \leq q(d) \leq \left[ 1 + O\left( \frac{1}{k} \right) \right].
\]
This completes the proof.

H.6 Proof of Lemma G.6

Proof of Lemma G.6. By 27, given \( S_1^{(2k)}, S_2^{(2k)} \) s.t. \( |S_1^{(2k)} \cap S_2^{(2k)}| = c \),
\[
\eta_{c,2k}^2(d_1, d_2) = \text{Cov} \left[ \varphi_{d_1} \left( S_1^{(2k)} \right), \varphi_{d_2} \left( S_2^{(2k)} \right) \right] \leq \text{Cov} \left[ \varphi_{d_1} \left( S_1^{(2k)} \right), \varphi_{d_2} \left( S_2^{(2k)} \right) \right] + \text{Cov} \left[ \varphi_0 \left( S_1^{(2k)} \right), \varphi_0 \left( S_2^{(2k)} \right) \right],
\]
where the last inequality is by the non-negativity of \( \rho \). By the definition of \( \varphi_d \) in Equation (25), the RHS of above equation is upper bounded by
\[
2 \max_{S_1, S_2 \subset S_1^{(2k)}, s.t. |S_1 \cap S_2| \leq d_1, S_3, S_4 \subset S_2^{(2k)}, s.t. |S_3 \cup S_4| \leq d_2} \rho = O(F^{(k)}).
\]

H.7 Proof of Lemma G.8

Proof of Lemma G.8. We apply the strategies we used in the proof of Lemma G.4. The truncation parameter is \( T_2 = \lceil \frac{1}{\epsilon} \rceil + 1 \). Recall in Lemma G.4, \( \text{Var}(\bar{V}_u) = \sum_{c=1}^{2k} \binom{n}{c}^{-1} \binom{2k}{c} \binom{n-2k}{2k-c} \sigma_{c,2k}^2 \), where
\[
\sigma_{c,2k}^2 = \sum_{d_1=1}^{k} \sum_{d_1=1}^{k} w_{d_1} w_{d_2} \eta_{c,2k}^2(d_1, d_2), \text{ for } c = 1, 2, \ldots, T_1.
\]
We decompose $\sigma_{c,2k}^2$ into three parts:

$$
\sigma_{c,2k}^2 = \sum_{d_1=1}^{T_2} \sum_{d_2=1}^{T_2} w_{d_1} w_{d_2} \eta_{c,2k}^2(d_1, d_2) + 2 \sum_{d_1=1}^{T_2} \sum_{d_2=T_2+1}^{k} w_{d_1} w_{d_2} \eta_{c,2k}^2(d_1, d_2)
$$

$$
+ \sum_{d_1=T_2+1}^{k} \sum_{d_2=T_2+1}^{k} w_{d_1} w_{d_2} \eta_{c,2k}^2(d_1, d_2).
$$

Similarly, denote

$$
\tilde{A} := \tilde{\sigma}_{c,2k,(T_2)}^2 = \sum_{d_1=1}^{T_2} \sum_{d_2=1}^{T_2} w_{d_1} w_{d_2} \tilde{\eta}_{c,2k}^2(d_1, d_2),
$$

where $\tilde{\eta}_{c,2k}(d_1, d_2)$ is the upper bound given in Lemma G.5. To prove this lemma, it suffices to show

$$
\lim_{k \to \infty} \frac{2B + C}{A} = 0.
$$

It remains to bound $\tilde{A}, B, C$ as

$$
\tilde{A} = \Theta \left( \frac{w_d^2 F_c}{k^2} \right),
$$

$$
B = \mathcal{O} \left( w_1 \tilde{w}_{T_2+1} F_c \right),
$$

$$
C = \mathcal{O} \left( w_{T_2+1}^2 F_c \right),
$$

where $\tilde{w}_d = \mathcal{O}(\frac{k^{2d}}{d!n^{2d}})$ is the rough upper bound of $w_d$ in (26). We need to quantify two parts, the coefficients $w_{d_1} w_{d_2}$ and the covariance $\eta_{c,2k}^2(d_1, d_2)$. Let us fix one $c \leq T_1$ and first quantify $\eta_{c,2k}^2(d_1, d_2)$. By Lemma G.5 and G.6, we have

$$
\eta_{c,2k}^2(d_1, d_2) = \mathcal{O}(\frac{1}{k^2} F_c), \text{ for } c \leq T_1, d_1, d_2 \leq T_2,
$$

$$
\eta_{c,2k}^2(d_1, d_2) = \mathcal{O}(F_c), \text{ for } c \leq 2k, d_1, d_2 \leq k.
$$

By Proposition G.2, we have $A = \sigma_{c,2k,(T_2)}^2 = \mathcal{O}(\frac{k^2}{n^2} F_c)$. Since $\tilde{A}$ is the upper bound of $A$ given in Proposition G.2, $\tilde{A} = \mathcal{O}(\frac{k^2}{n^2} F_c)$. For $B, C$, we upper bound $\eta_{c,2k}^2(d_1, d_2)$ by $\mathcal{O}(F_c)$ in Equation (108). Hence, we can reduce the analysis for both coefficients and covariance to the analysis on only coefficients $w_d$, for

$$
B = \mathcal{O}(F_c) \left[ \sum_{d_1=1}^{T_2} w_{d_1} \right] \left[ \sum_{d_2=T_2+1}^{k} w_{d_2} \right]
$$

$$
C = \mathcal{O}(F_c) \left[ \sum_{d_1=T_2+1}^{k} w_{d_1} \right] \left[ \sum_{d_2=T_2+1}^{k} w_{d_2} \right].
$$
To be more specific, it remains to show that

$$\sum_{d=1}^{T_2} w_d = O(w_1), \quad \sum_{d=T_2+1}^{k} w_d = O(\tilde{w}_{T_2+1}).$$

where $\tilde{w}_d = O(\frac{k^2d}{n^2})$ is the rough upper bound of $w_d$ in (26).

For $\sum_{d=1}^{T_2} w_d$, by Equation (26), each $w_d = [1 + o(1)] \frac{k^2d}{d n^2} \leq [1 + o(1)] \frac{k^2d}{w^2}$. The common ratio of geometric decay is $k^2/n = o(1)$. Therefore, the first term $w_1$ dominates $\sum_{d=1}^{T_2} w_d$. For $\sum_{d=T_2+1}^{k} w_d$, by Equation (26), we have each $w_d = O(\frac{k^2d}{dn^2}) = O(\frac{k^2d}{n^2})$. Similarly, by geometric decay with common ratio $k^2/n$,

$$\sum_{d=T_2+1}^{k} w_d \leq \sum_{d=T_2+1}^{k} O(\frac{k^2d}{n^2}) = O\left(\frac{k^2}{n} (T_2+1)\right).$$

Hence we define $\tilde{w}_{T_2+1} = \Theta\left(\frac{k^2}{n} T_2+1\right)$. Then $\sum_{d=T_2+1}^{k} w_d = O(\tilde{w}_{T_2+1})$.

We have proved the bounds in Equation (106). Then plug Equation (106) into the LHS of Equation (105), we can conclude that

$$\frac{2B + C}{A} = O\left(\frac{k^2(w_1\tilde{w}_{T_2+1} + \tilde{w}_{T_2+1}^2)}{w_1^2}\right). \quad (109)$$

For (109), plugging in $T_2 = \lfloor 1/\epsilon \rfloor + 1$ and the upper bound of $w_d = [1 + o(1)] \frac{k^2d}{d n^2}$ and $\tilde{w}_d = O(\frac{k^2d}{n^2})$ from Equation (26) and (26), we conclude

$$\frac{2B + C}{A} = O\left(k^2n^{-2\epsilon(\lfloor 1/\epsilon \rfloor + 1)}\right) = O\left(k^2n^{-2\epsilon(\lfloor 1/\epsilon \rfloor + 1)}\right) = o(k^2n^{-2}) = o(1).$$

This completes the proof.

I Relaxation of Assumption 3 and According Proof

In this section, we first present Assumption 6 as a relaxation of Assumption 3. Then, we show that the technical lemmas can be proved under our relaxed assumption. Note that since $\rho$ will depend on all 11 DoF, we will use $\rho(\underline{r}, d_1, d_2)$ to denote $\rho$ throughout this section.

I.1 Assumption 6

Recall that Assumption 3 implies that $\rho(\underline{r}, d_1, d_2)$ only depends on $\underline{r}$, and thus has 9 DoF. Though Assumption 3 is valid in Example C.2, it is still too restrictive in practice. Our new assumption will allow $\rho(\underline{r}, d_1, d_2)$ have 11 DoF with some restriction on the impact from Non-influential Overlaps, i.e. samples not in $S_{1}^{(2k)} \cap S_{2}^{(2k)}$. 63
In the following Equation (110), we introduce a 9-DoF benchmark: \( \bar{\rho}(r) \), as the analogue to the \( \rho(r) \) (32). This is a bridge between 9 DoF and 11 DoF.

**Definition I.1** (\( \bar{\rho}(r) \)). ∀ feasible \( r \), we take \( d_1^* = r_0* = \sum_{j=0}^{2} r_{0j} \) and \( d_2^* = r_{*0} = \sum_{i=0}^{2} r_{i0} \). Then, we define

\[
\bar{\rho}(r) := \rho(r, d_1^*, d_2^*). \tag{110}
\]

Since \( r_{0*} = |(S_1 \cap S_2) \cap (S_3 \cup S_4)| \) (by (37)) and \( d_1 = |S_1 \cap S_2| \), we always have \( d_1 \geq r_{0*} \). Therefore, fixing \( r \), the constraint \( d_1 = r_{0*} \) in (110) means that the benchmark \( \bar{\rho}(r) \)'s \( d_1 \) already takes a smallest feasible value. Similarly, \( d_2 \) also takes a smallest feasible value. Since \( \bar{\rho}(r) \) is a “benchmark” of \( \rho(r, d_1, d_2) \) (given \( r \)), we impose the further relaxed assumption, where \( \rho(r, d_1, d_2) \) deviates from benchmark \( \bar{\rho}(r) \) based on its \( d_1 \) and \( d_2 \).

**Assumption 6** (Relaxation of Assumption 3). For any finite \( d_1, d_2 \geq 0 \), \( r \), s.t. \( d_1 \geq r_{0*}, d_2 \geq r_{*0} \), there exist constant \( B \) and \( B(r) \) s.t. \( B(r) \leq B < \infty, \)

\[
\rho(r, d_1, d_2) = \left[ 1 + B(r) \frac{d_1 - r_{0*} + d_2 - r_{*0}}{k} + O\left(\frac{1}{k^2}\right) \right] \bar{\rho}(r). \tag{111}
\]

Besides, for any \( d_1 \geq r_{0*}, d_2 \geq r_{*0} \),

\[
\rho(r, d_1, d_2) \leq B \bar{\rho}(r). \tag{112}
\]

In Equation (111), we refer the benchmark \( \bar{\rho}(r) \) as the main effect, capturing the overlapping between \( S_1^{(2k)} \) and \( S_2^{(2k)} \) while the rest \( O\left(\frac{1}{k}\right) \bar{\rho}(r) \) part as additional effect, capturing the overlapping within \( S_1^{(2k)} \) and \( S_2^{(2k)} \). We interpret this assumption as follows, where we mainly focus on \( d_1 = |S_1 \cap S_2| \). Similar analysis can be performed on \( d_1 \). First, \( S_1 \cup S_2 \) can be decomposed into two sets: \( A = (S_1 \cup S_2) \cap (S_1^{(2k)} \cap S_2^{(2k)}) \), i.e. the set of Influential Overlaps and \( B = (S_1 \cup S_2) \setminus (S_1^{(2k)} \cap S_2^{(2k)}) \). Moreover, \( B \) can be decomposed into two subsets \( B_1 = (S_1 \cap S_2) \setminus (S_1^{(2k)} \cap S_2^{(2k)}) \) and \( B_2 = ((S_1 \cup S_2) \setminus (S_1 \cap S_2)) \setminus (S_1^{(2k)} \cap S_2^{(2k)}) \). We note that \(|B_1| = 0\) for the benchmark \( \bar{\rho}(r) \). When we fix \( r \) while increase \( d_1 \), \( A \) does not change while \( |B_1| \) becomes larger and \( |B_2| \) becomes smaller. This causes \( \rho(r, d_1, d_2) \) deviates from \( \bar{\rho}(r) \). Secondly, since \( r \) is fixed and \( B \) does not involve any influential overlaps, we expect the change of \( B_1 \) and \( B_2 \) by increasing \( d_1 \) has a lower order, i.e. \( O\left(\frac{1}{k}\right) \), impact on \( \rho(r, d_1, d_2) \). Hence, fixing \( r \) for finite \( d_1 \), i.e \( d_1/k \to 0 \), the proportion of \( \rho(r, d_1, d_2) \)'s “deviation” from \( \bar{\rho}(r) \) is at a scale of

\[
[1 + o(1)]\frac{|B_1|}{|B|} = [1 + o(1)] \frac{|(S_1 \cap S_2) \setminus (S_1^{(2k)} \cap S_2^{(2k)})|}{|(S_1 \cup S_2)|} = [1 + o(1)] \frac{d_1^*}{k}. \tag{113}
\]

Similar analysis can also be performed on \( d_2 \) and \( S_3, S_4 \). In addition, Equation (112) bounds the additional effect up to the same order term as the main effect. Again, this is because \( \rho(r, d_1, d_2) \) should be dominated by the influential overlaps, i.e. the samples in \( S_1^{(2k)} \cap S_2^{(2k)} \). Note that in previous Example C.2, there is...
only the main effect, i.e., $B(\tau) \equiv 0$ and thus Assumption 6 degenerates to Assumption 3.

### I.2 Proof Under Assumption 6

In our previous proof, only two fundamental lemmas directly rely on Assumption 3: Lemma G.5 (the precise bound for $\eta_{c,2k}^2(d_1, d_2)$) and Lemma G.6 (the rough bound for $\eta_{c,2k}^2(d_1, d_2)$). Based on these two lemmas, we can derive the upper bounds of $\sigma_{c,2k}^2$ and hence upper bound $\text{Var}(\tilde{V}_u)$ (see the proof roadmap in Appendix D.1). Therefore, when Assumption 3 is relaxed to Assumption 6, it suffices to show the results in Lemma G.5 and G.6.

First, it is trivial to validate a relaxed Lemma G.6 under Assumption 6. Assumption 6 does not change the upper bound of $\rho(\tau, d_1, d_2)$, which is $F_c^{(k)} = \text{Cov}[h(S')^2, h(S'')]$ s.t. $|S' \cap S''| = c$ (34). The proof of Lemma G.6 in Appendix H.6 only requires the upper bound $F_c^{(k)}$, thus it still works.

Second, we need to adapt Proof of Lemma G.5 in Appendix H.5. $\rho(\tau, d_1, d_2)$ can no longer be represented as $\rho(\tau)$. Thus, $\rho(\tau, d_1, d_2) - \rho(\tau, d'_1, d'_2)$ is not necessary 0 for $(d_1, d_2) \neq (d'_1, d'_2)$.

**Proof of Lemma G.5 under Assumptions 1, 2, 4 - 6.** We adopt the beginning part of the proof in Appendix H.5 until Lemma H.3. We note that Lemma H.3 does not rely on Assumption 3. Hence, we still have Equation (91):

$$\text{Cov}\left[\varphi_d_1\left(S_1^{(2k)}\right), \varphi_d_2\left(S_2^{(2k)}\right)\right] = \sum_{\text{feasible } \tau^*} p_{r_0, r_1, r_2, d_1, c} p_{r_0, r_3, r_4, d_2, c} g(r^*, d_1, d_2),$$

where $g(r^*, d_1, d_2)$ is given in Equation (93). Since $\rho(\tau, d_1, d_2)$ in $g(r^*, d_1, d_2)$ (93) depends $d_1, d_2$, we cannot further simplify $g(r^*, d_1, d_2)$ as $G(r^*)$. Further we denote

$$\overline{pg}(r^*, d_1, d_2, c) := p_{r_0, r_1, r_2, d_1, c} p_{r_0, r_3, r_4, d_2, c} g(r^*, d_1, d_2, c);$$

$$\overline{\Delta pg}(r^*, d_1, d_2, c) := \overline{pg}(r^*, d_1, d_2, c) - \overline{pg}(r^*, 0, d_2, c) - \overline{pg}(r^*, d_1, 0, c) + \overline{pg}(r^*, 0, 0, c).$$

Then $\eta_{c,2k}^2(d_1, d_2)$ can be represented as

$$\eta_{c,2k}^2(d_1, d_2) = \sum_{(r_0, r_1, r_2))} \sum_{(r_0, r_3, r_4)} \overline{\Delta pg}(r^*, d_1, d_2, c). \tag{114}$$

We apply the strategy used in the proof of Lemma H.4, partitioning the summation as follows:

$$\eta_{c,2k}^2(d_1, d_2) = \left( \sum_{r_1 + r_2 = c} + \sum_{r_1 + r_2 \leq c - 1} \right) \left( \sum_{r_3 + r_4 = c} + \sum_{r_3 + r_4 \leq c - 1} \right) \overline{\Delta pg}(r^*, d_1, d_2, c). \tag{115}$$

There are 4 cases. Case A: $r_1 + r_2 = c$ and $r_3 + r_4 = c$ and $r_{1} + r_{2} \leq c - 1$; case B: $r_1 + r_2 = c$ and $r_3 + r_4 \leq c - 1$; case C: $r_1 + r_2 \leq c - 1$ and $r_3 + r_4 = c$; case D: $r_1 + r_2 \leq c - 1$ and $r_3 + r_4 \leq c - 1$. Since $c$ is finite, $r_i$’s and $r_j$’s are also finite. Thus, (115) is a finite summation. To show $\eta_{c,2k}^2(d_1, d_2) = O\left(\frac{1}{c^2} F_c^{(k)}\right)$, it suffices to show that the summand $\overline{\Delta pg}(r^*, d_1, d_2, c) = O\left(\frac{1}{c^2} F_c^{(k)}\right)$ in all 4 cases.
First, we study case A. For the \(g(r^*, d_1, d_2)\) defined in Equation (93), by approximation of \(\rho\) in Assumption 6: \(\rho(r, d_1, d_2) = \left[1 + B(r) \frac{d_1 + d_2}{k} + \mathcal{O}(\frac{1}{k^2})\right] \hat{\rho}(r)\), we have

\[
g(r^*, d_1, d_2) = \left[1 + \frac{d_1 + d_2}{k} \right] B(r) + \mathcal{O}(\frac{1}{k^2}) \] \(g(r^*, 0, 0),\)

Therefore, \(\Delta pg(r^*, d_1, d_2, c)\) can be simplified as

\[
\Delta pg(r^*, d_1, d_2, c) = g(r^*, 0, 0) \{ (p(r_0, r_1, r_2, d_1, c) - p_{(r_0, r_1, r_2, 0, c)}) (p(r_0, r_1, r_2, d_2, c) - p_{(r_0, r_1, r_2, 0, c)}),
\]

\[
+ \frac{d_1 B(r)}{k} \{ p(r_0, r_1, r_2, d_1, c) (p_{(r_0, r_1, r_2, 0, c)}) - p(r_0, r_1, r_2, d_1, c),
\]

\[
+ \frac{d_2 B(r)}{k} \{ p(r_0, r_1, r_2, d_2, c) (p_{(r_0, r_1, r_2, 0, c)}) - p(r_0, r_1, r_2, d_2, c),
\]

\[
+ \frac{1}{k^2} \mathcal{O}(\frac{1}{k^2})).
\]

By Lemma H.4, \(p_{(r_0, r_1, r_2, d_1, c)} - p_{(r_0, r_1, r_2, 0, c)} = \mathcal{O}(1/k)\), \(p_{(r_0, r_1, r_2, d_2, c)} - p_{(r_0, r_1, r_2, 0, c)} = \mathcal{O}(1/k)\). Besides, \(g(r^*, 0, 0, c) \leq F^k_c\). Thus, \(\Delta pg(r^*, d_1, d_2, c) = \mathcal{O}(\frac{1}{k^2} F^k_c)\).

Secondly, we study case B. Recall that \(p_{(r_0, r_1, r_2, 0, c)} = 0\) by (92). Therefore, \(\overline{pg}(r^*, d_1, 0, c) = \overline{pg}(r^*, 0, 0, c) = 0\). Hence, \(\Delta pg(r^*, d_1, d_2, c)\) can be simplified as

\[
\Delta pg(r^*, d_1, d_2, c) = \overline{pg}(r^*, d_1, d_2, c) - \overline{pg}(r^*, 0, d_2, c).
\]

By Assumption 6, we can approximate \(g(r^*, d_1, d_2)\) as

\[
g(r^*, d_1, d_2) = \left[1 + \frac{d_1 + d_2}{k} \right] B(r) + \mathcal{O}(\frac{1}{k^2}) g(r^*, 0, d_2).
\]

Then, plug the above approximation into Equation (116):

\[
\Delta pg(r^*, d_1, d_2, c) = g(r^*, 0, d_2) [p(r_0, r_1, r_2, d_1, c) (p(r_0, r_1, r_2, d_2, c) - p_{(r_0, r_1, r_2, 0, c)}),
\]

\[
+ \frac{d_1 B(r)}{k} \{ p(r_0, r_1, r_2, d_1, c) (p_{(r_0, r_1, r_2, 0, c)}) - p(r_0, r_1, r_2, d_1, c),
\]

\[
+ \frac{d_2 B(r)}{k} \{ p(r_0, r_1, r_2, d_2, c) (p_{(r_0, r_1, r_2, 0, c)}) - p(r_0, r_1, r_2, d_2, c) + \mathcal{O}(\frac{1}{k^2})).
\]

Similarly, we have \(p_{(r_0, r_1, r_2, d_1, c)} - p_{(r_0, r_1, r_2, 0, c)} = \mathcal{O}(1/k)\) and \(p_{(r_0, r_1, r_2, d_2, c)} - p_{0(c)} = \mathcal{O}(1/k)\). Besides, \(g(r^*, 0, d_2, c) \leq F^k_c\). Therefore, we conclude that \(\Delta pg(r^*, d_1, d_2, c) = \mathcal{O}(\frac{1}{k^2} F^k_c)\).

Thirdly, by a similarly analysis in case B, we can bound \(\Delta pg(r^*, d_1, d_2, c) = \mathcal{O}(\frac{1}{k^2} F^k_c)\) in case C.

Finally, we study case D. Since \(r_1 + r_2 \leq c - 1\) and \(r_1 + r_2 \leq c - 1\), \(p_{(r_0, r_1, r_2, 0, c)} = p_{(r_0, r_1, r_2, 0, c)} = 0\). Therefore,

\[
\Delta pg(r^*, d_1, d_2, c) = \mathcal{O}(\frac{1}{k^2} F^k_c)\) in case D.
\]

This completes the proof. \(\square\)
J  Low Order Kernel $h$ Illustration

As we have discussed in Section 4.5, we will present our 3-step analysis strategy under an oversimplified structure of kernel $h$. Moreover, issues for general kernel $h$ are presented and discussed in Appendix J.3, which motivates the development of the assumptions in Section B. One can go through Appendix J if they are interested in the motivations of the proof strategies.

J.1  Linear Average Kernel $h$

**Theorem J.1.** $X_1, X_2, \ldots, X_n \ iid$ distribution $F$, s.t. $E(X_1) = 0, \gamma^2 := \text{Var}(X_1) > 0$. Suppose kernel function $h(X_1, \ldots, X_k) = \frac{1}{k} \sum_{i=1}^{k} X_i$ Then, we have ratio consistency of the estimator,

$$\frac{\text{Var}(\hat{V}_u)}{(E(\hat{V}_u))} = \mathcal{O}(\frac{1}{n}).$$

To prove theorem J.1, it suffices to prove the following lemma.

**Lemma J.2.** Under the conditions in Theorem J.1, we have

$$E(\hat{V}_u) = \Omega(\frac{1}{n}), \text{ and } \text{Var}(\hat{V}_u) = \mathcal{O}(\frac{1}{n^3}),$$

where $\Omega$ indicates an asymptotic lower bound (see Table 4).

We remark that we are able to generalize Lemma J.2 from the linear average kernel $h$ to the intrinsic low order kernel $h$ (Definition J.5). After showing the proof of Lemma J.2, we will summarize the benefits from the low order structure of kernel $h$. Then, we present the potential difficulties and solutions when low order kernel assumption no longer holds.

**Proof.** **Part I: show** $E(\hat{V}_u) = \Omega(\frac{1}{n}).$

For linear average kernel, $U_n = \binom{n}{k}^{-1} \sum S_i h(S_i) = \frac{1}{n} \sum_{i=1}^{n} X_i$, $V_u$ is an unbiased estimator of $\text{Var}(U_u)$. Therefore,

$$E(\hat{V}_u) = \text{Var}(U_n) = \text{Var} \left( \frac{1}{n} \sum_{i=1}^{n} X_i \right) = \frac{1}{n} \text{Var}(X_1) = \frac{\gamma^2}{n} = \Theta(\frac{1}{n}).$$

**Part II: show** $\text{Var}(\hat{V}_u) = \mathcal{O}(\frac{1}{n^3}).$

We perform a 3-step analysis. By step 1 and 2, the order of $\hat{V}_u$ becomes $\mathcal{O}(\frac{k^2}{n \gamma^2}) = \mathcal{O}(\frac{1}{n})$. Further by the coefficient of leading variance in $\text{Var}(\hat{V}_u)$ in step 3, we can achieve $\text{Var}(\hat{V}_u) = \left[ \mathcal{O}(\frac{k^2}{n \gamma^2}) \right]^2 \mathcal{O}(\frac{1}{n}) = \mathcal{O}(\frac{1}{n^3})$. The rigorous analysis is presented as follows.

**Step 1: double U-statistic structure**
We reiterate the double U-statistic structure of \( \hat{V}_u \) (Proposition 4.3) as follows

\[
\hat{V}_u = \left( \frac{n}{2k} \right)^{-1} \sum_{S^{(2k)} \subseteq X_n} \psi(S^{(2k)}) = \sum_{d=1}^{k} w_d \left[ \varphi_d(S^{(2k)}) - \varphi_0(S^{(2k)}) \right],
\]

where \( w_1 = [1 + o(1)] \left( \frac{k^2}{n} \right) \), \( w_d = O \left( \frac{1}{d(\frac{k^2}{n})^2} \right), \forall d = 1, 2, \ldots, k \); \( \varphi_d \) is the asymptotic kernel U-stat defined in Equation (25). We observe that \( w_d \) decays with \( d \) fast. In the following analysis, we will show that the first summand in Equation (117) dominate the sum.

**Step 2: analyze** \( \varphi_d(S^{(2k)}) - \varphi_0(S^{(2k)}) \)

We further investigate the cancellation pattern \( \varphi_d(S^{(2k)}) - \varphi_0(S^{(2k)}) \) in Equation (117) by the following proposition.

**Proposition J.3.** Under linear average structure of \( h \), i.e., \( h(X_1, ..., X_k) = \frac{1}{k} \sum_{i=1}^{k} X_i \),

\[
\varphi_d(S^{(2k)}) - \varphi_0(S^{(2k)}) = \frac{d}{k^2} \left( \bar{X}^{(2k)} - \bar{Y}^{(2k)} \right),
\]

where \( \bar{X}^{(2k)} := \frac{1}{2k} \sum_{X_i \in S^{(2k)}} X_i^2 \) and \( \bar{Y}^{(2k)} := \frac{1}{2k(2k-1)} \sum_{X_i, X_j \notin S^{(2k)}, j \neq i} X_i X_j \).

Note that in Equation (118), the coefficient of \( \bar{X}^{(2k)} \) and \( \bar{Y}^{(2k)} \cdot \frac{d}{k^2} \), is resulting from the cancellation. The proof of above proposition is collected in Appendix J.4, by plugging the explicit form of \( h \) into \( \varphi(S^{(2k)}) \) (Equation (25)). Combining the results in Equation (117), (123) and (26), we have

\[
\psi(S^{(2k)}) = \frac{1}{k^2} \left( \bar{X}^{(2k)} - \bar{Y}^{(2k)} \right) \sum_{d=1}^{k} dw_d = [1 + o(1)] \frac{1}{n} \left( \bar{X}^{(2k)} - \bar{Y}^{(2k)} \right).
\]

**Step 3: show the leading variance term**

Based on Equation (119), we use classical approach in the U-statistic literature (Hoeffding, 1948), showing \( \sigma^2_{1,2k} \) dominating \( \text{Var}(\hat{V}_u) = \left( \frac{n}{2k} \right)^{-1} \sum_{c=1}^{2k} \binom{2k}{c} \binom{n-2k}{2k-c} \sigma^2_{c,2k} \), i.e.,

\[
\text{Var}(\hat{V}_u) = \left[ 1 + o(1) \right] \frac{4k^2}{n} \sigma^2_{1,2k}.
\]

To get our desired upper bound \( \text{Var}(\hat{V}_u) = O(\frac{1}{n^2}) \), it suffices to bound \( \sigma^2_{1,2k} \) by \( O(1/((k^2 n^2)) \) and further check \( \sigma^2_{2k,2k}/(2k \sigma^2_{1,2k}) = O(1) \) (DiCiccio and Romano, 2022). By Proposition J.7 in Appendix J.4 we have

\[
\text{Cov} \left( \bar{X}^{(2k)} - \bar{Y}^{(2k)} \right), \bar{X}^{(2k)} - \bar{Y}^{(2k)} = \begin{cases} \Theta(\frac{1}{k^2}) & \text{if } |S_{1}^{(2k)} \cap S_{2}^{(2k)}| = 1; \\
O(\frac{1}{k}) & \text{if } |S_{1}^{(2k)} \cap S_{2}^{(2k)}| = 2k. \end{cases}
\]

Thus, combining the above conclusion (120), the simplification form of \( \psi(S^{(2k)}) \) (119), and the definition of \( \sigma^2_{c,2k} \) (23), we can bound \( \sigma^2_{1,2k} \) and \( \sigma^2_{2k,2k} \) as \( \sigma^2_{1,2k} = \Theta(\frac{1}{n^2 k^2}) \), \( \sigma^2_{2k,2k} = O(\frac{1}{n^2 k}) \). This implies that
σ^2_{2k,2k}/(2kσ^2_{1,2k}) = O(1) Thus we conclude that

\[ \text{Var}(\hat{V}_u) = [1 + o(1)] \frac{4k^2}{n} \sigma^2_{1,2k} = O\left(\frac{1}{n^3}\right). \]

This completes the proof of Lemma J.2.

Remark J.4. An alternative approach to bound \(\text{Var}(\hat{V}_u)\) is by further simplifying \(\hat{V}_u\) as an order-2 U-statistic:

\[ \hat{V}_u = \left[1 + o\left(\frac{1}{n}\right)\right] (\bar{X}_2^{(n)} - \bar{Y}_2^{(n)}). \]

We present the analysis in Appendix J.4. The insight is that the lower-order structure of kernel \(k\) implies the low order structure of \(\hat{V}_u\).

The rest part of this section is organized as follows. In Section J.2, we discuss the generalization of this 3-step analysis for low order kernel \(h\) (see Definition J.5). In Section J.3 we show the issues to adapt this the 3-step analysis for a general kernel \(h\) (without any low order structure); then, we discuss the motivations of new tools to overcome this difficulty.

J.2 Kernel \(h\) with Low Order Structure

The analysis in step 1 depends on the double U-statistic structure of \(\hat{V}_u\). It definitely works with any kernel \(h\). To generalize theorem J.1, it remains to discuss the analysis in steps 2 and 3.

Definition J.5 (intrinsic low-order kernel). \(\exists L \in \mathbb{N}^+, \text{ which does not depend on } k\)

\[ h(X_1, ..., X_k) = \sum_{l=1}^{L} h^{(l)}(X_1, ..., X_k), \]

where \(h^{(l)}\) has lower order-\(l\) structure defined with the fixed order kernel \(g^{(l)}\):

\[ h^{(l)}(X_1, ..., X_k) = \binom{k}{l}^{-1} \sum_{i_1 < ... < i_l} g^{(l)}(X_{i_1}, ..., X_{i_l}). \]

For example, if we fix \(L = 1\) and \(g^{(1)}\) as identical map, then \(h\) becomes the linear average kernel we discussed in the last section: \(h(X_1, ..., X_k) = \frac{1}{k} \sum_{i=1}^{k} X_i\). Suppose \(h(X_1, ..., X_k)\) has the structure in Definition J.5. In step 2, similar to Equation (122) and (123), we can specify the form of \((\varphi_d - \varphi_0)(S^{(2k)})\) by plugging in \(h\)’s low order structure. Therefore, we are still able to have cancellations resulting in the order of \(\text{poly}\left(\frac{1}{n}\right)\). In step 3, additional \(O\left(\frac{1}{n}\right)\) rate comes from the variance of fixed order U-statistic. Similarly, since the summand in \(\hat{V}_u\) is in the form of \(h(S_1)h(S_2)\), we can verify that \(\hat{V}_u\) is a linear combination of U-statistic up to kernel order \(2L\), where \(L\) is the low order parameter in Definition J.5. Therefore, we reduce infinite order U-statistic to finite order U-statistic. Note that We only discussed the intrinsic low-order kernel cases without proof because they are trivial extensions of the previous arguments.
J.3 Discussion about General Kernel \( h \)

For general kernel \( h \) without low order structure, we show the difficulty in the 3-step analysis, which motivates our new strategies including the assumptions (Appendix C) and technical lemmas (Appendix G).

The first issue is that \( \varphi_d(S^{(2k)})(S^{(2k)}) \) no longer has a simple expression since \( h(S) \) does not have an explicit low order form. However, we still believe that a smaller \( d \) can imply a smaller difference between \( \varphi_d \) and \( \varphi_0 \). Our remedy is to quantify the implicit cancellation in covariance \( \eta_{c,2k}^2(d_1, d_2) := Cov[\varphi_{d_1}(S^{(2k)}_1) - \varphi_0(S^{(2k)}_1)], \varphi_{d_2}(S^{(2k)}_2) - \varphi_0(S^{(2k)}_2)] \) (see Equation (27)). The further decomposition of \( \eta_{c,2k}^2(d_1, d_2) \) involves the following covariance (31)

\[
\rho := Cov[h(S_1)h(S_2), h(S_3)h(S_4)].
\]

As demonstrated in Appendix B, \( \rho \) is determined by 11 free parameters. Assumption 3 reduce DoF from 11 to 9 of 11, which enables us to further reduce DoF to 6 in the proof of Lemma G.5 and bound \( \eta_{c,2k}^2(d_1, d_2) = \mathcal{O}(\frac{F_c(k)}{k^2}) \) for finite \( c, d_1, d_2 \). Note that a relaxation of Assumption 3 is presented in Appendix C.

The second issue is the difficulty to show that \( \sigma_{1,2k}^2 \) (or its upper bound) dominating \( \text{Var}(\hat{V}_u) \) (22). When we have low lower structure of \( h, \hat{V}_u \) can be simplified so it is easy to bound \( \sigma_{c,2k}^2 \). However, now \( h \) does not has a explicit form. Therefore, in our analysis, we provide one tight bound on \( \sigma_{c,2k} \) for \( c = 1, 2, ..., T_1 \) (Proposition G.2), which is finite number of terms. Then, we provide one loose bound on \( \sigma_{c,2k}^2 \) for \( c = T_1 + 1, ..., 2k \) (Proposition G.3). This is more challenging than only focusing on two terms: \( \sigma_{1,2k}^2 \) and \( \sigma_{2k,2k}^2 \). With the above results, it becomes easier to show that a upper bound of \( \sigma_{1,2k}^2 \) dominates our desired upper bound of \( \text{Var}(\hat{V}_u) \). Details are collected in Appendix D.1 and Appendix G.

J.4 Proof of the Propositions under Linear Average Kernel

Proof of Prop J.3. Consider \( S_1, S_2 \subset S^{(2k)} \), s.t. \( |S_1 \cap S_2| = d \). Recall \( \varphi_d(S^{(2k)}) = (S^{(2k)}) = \frac{1}{M_d} \sum_{S_1, S_2 \subset S^{(2k)}, |S_1 \cap S_2| = d} h(S_1)h(S_2) \), which is a U-stat with asymmetric kernel of \( h(S_1)h(S_2) \) s.t. \( |S_1, S_2| = d, S_1, S_2 \subset S^{(2k)} \). Let first investigate the form of \( h(S_1)h(S_2) \). Then \( \varphi_d(S^{(2k)}) \) will be an average.

Let \( S_1 = (X_1, ..., X_d, Y_1, ..., Y_{k-d}), S_2 = (X_1, ..., X_d, Z_1, ..., Z_{k-d}) \), where all \( X_i, Y_j, Z_j \in S^{(2k)}, i = 1, ..., d, j = 1, ..., k - d \) are independent.

\[
h(S_1)h(S_2) = \left[ \frac{1}{k} \left( \sum_{i=1}^{d} X_i + \sum_{i=1}^{k-d} Y_i \right) \right] \left[ \frac{1}{k} \left( \sum_{i=1}^{d} X_i + \sum_{i=1}^{k-d} Z_i \right) \right] = \frac{1}{k^2} \left( \sum_{i=1}^{d} X_i^2 + \sum_{i=1}^{d} \sum_{i=1}^{k-d} 2X_iX_j + \sum_{i=1}^{d} \sum_{j=1}^{k-d} X_iY_j + \sum_{i=1}^{d} \sum_{j=1}^{k-d} X_iZ_j + \sum_{i=1}^{d} \sum_{j=1}^{k-d} Y_iZ_j \right). \tag{121}
\]

In Equation (121), the proportion of squared terms \( X_i^2 \) is \( \frac{d}{k^2} \); the sum of proportions of cross terms \( X_iX_j, X_iY_j, X_iZ_j \) and \( Y_iZ_j \) is \( 1 - \frac{d}{k^2} \). Since \( \varphi(S^{(2k)}) \) is in the form of U-statistic, it can be viewed as an average. In this average, the proportion of squared terms and cross terms remain unchanged as \( \frac{d}{k^2} \) and \( 1 - \frac{d}{k^2} \).
WLOG, we denote $S^{(2k)} = (X_1, ..., X_{2k})$. We can derive the expression of $\varphi_d(S^{(2k)})$, for $d = 0, 1, 2, ..., k$:

$$
\varphi_d(S^{(2k)}) = \frac{d}{k^2} \left( \frac{1}{2k} \sum_{i=1}^{2k} X_i^2 \right) + \frac{k^2 - d}{k^2} \left( \frac{2}{2k(2k-1)} \sum_{i=1}^{2k} \sum_{j>i} X_i X_j \right).
$$

(122)

Then, by the above equation

$$
\varphi_d(S^{(2k)}) - \varphi_0(S^{(2k)}) = \frac{d}{k^2} \left[ \left( \frac{1}{2k} \sum_{i=1}^{2k} X_i^2 \right) - \left( \frac{2}{2k(2k-1)} \sum_{i=1}^{2k} \sum_{j>i} X_i X_j \right) \right],
$$

(123)

where $1 - \frac{d}{k^2}$ fraction of cross terms are cancelled.

**Proposition J.6.** Given the linear kernel structure: $h(X_1, ..., X_k) = \frac{1}{k} \sum_{i=1}^{k} X_i$, $\text{Var}(X^{(n)}_2 - \overline{XY}^{(n)}) = \mathcal{O}\left(\frac{1}{n}\right)$

**Proof.** Proof of Proposition J.6.

$$
\text{Var}(X^{(n)}_2 - \overline{XY}^{(n)}) = \text{Var}(X^{(n)}_2) + \text{Var}(\overline{XY}^{(n)}) - 2\text{Cov}(X^{(n)}_2, \overline{XY}^{(n)}).
$$

Since $E(X) = 0$ and $E(X_i X_j, X'_i X'_j) \neq 0$ iff $i = i', j = j'$, we it is trivial to verify that

$$
\text{Var}(X^{(n)}_2) = \frac{1}{n} \text{Var}(X_1^2), \quad \text{Var}(\overline{XY}^{(n)}) = \left(\frac{n}{2}\right)^{-1} \text{Var}^2(X_1), \quad \text{and} \quad \text{Cov}(X^{(n)}_2, \overline{XY}^{(n)}) = 0.
$$

Thus, $\text{Var}(X^{(n)}_2 - \overline{XY}^{(n)}) = \mathcal{O}\left(\frac{1}{n}\right)$.

In particular, we decompose $\text{Var}(\overline{XY}^{(n)})$ into $\binom{n}{2}$ pairs of covariance, where only $\binom{n}{2}$ pairs have non-zero. Besides, for $\text{Cov}(X^{(n)}_2, \overline{XY}^{(n)})$, every $\text{Cov}(X_i^2, X'_i X'_j) = E(X_i^2, X'_i X'_j) = 0$.

**Proposition J.7.**

$$
\text{Cov} \left( X^{(2k)}_2 - \overline{XY}^{(2k)}, \overline{X}^{(2k)} - \overline{XY}^{(2k)} \right) = \begin{cases} 
\Theta\left(\frac{1}{k^2}\right), & \text{when} \mid S_1^{(2k)} \cap S_2^{(2k)} \mid = 1; \\
\mathcal{O}\left(\frac{1}{k}\right), & \text{when} \mid S_1^{(2k)} \cap S_2^{(2k)} \mid = 2k,
\end{cases}
$$

(124)

where $\overline{X}^{(2k)} = \frac{1}{2k} \sum_{X_i \in S_1^{(2k)}} X_i^2$, $\overline{XY}^{(2k)} = \frac{1}{k(2k-1)} \sum_{X_i, X_j \in S_1^{(2k)}, i < j} X_i X_j$,

$$
\overline{X}^{(2k)} = \frac{1}{2k} \sum_{X_i \in S_2^{(2k)}} X_i^2, \quad \overline{XY}^{(2k)} = \frac{1}{k(2k-1)} \sum_{X_i, X_j \in S_2^{(2k)}, i < j} X_i X_j
$$

**Proof of Proposition J.7.** Under linear average structure of $h$, i.e., $h(X_1, ..., X_k) = \frac{1}{k} \sum_{i=1}^{k} X_i$,

$$
\text{Cov} \left( X^{(2k)}_2 - \overline{XY}^{(2k)}, \overline{X}^{(2k)} - \overline{XY}^{(2k)} \right).
$$
Part 1: $|S_1^{(2k)} \cap S_2^{(2k)}| = 1$

W.L.O.G, assume $S_1^{(2k)} = (X_1, X_2, \ldots, X_k), S_1^{(2k)} = (X_1, X_2, \ldots, X_k), S_1^{(2k)} \cap S_2^{(2k)} = X_1, X_1, \ldots, X_k, X_k', \ldots, X_k'$ are independent.

For Cov($A, B$), let us only consider $A, B$ have overlap; otherwise, it is 0. Therefore, three parts of covariance can be simplified as

\[
\text{Cov} \left( \overline{X}^{(2k)}, \overline{X}^{(2k)'} \right) = \frac{1}{4k^2} \text{Var}(X_1^2),
\]

\[
\text{Cov} \left( \overline{X}^{(2k)}Y^{(2k)}, \overline{X}^{(2k)'}Y^{(2k)'} \right) = \text{Cov} \left( \frac{2}{2k-1} \sum_{j=2}^{k} X_1 X_j, \frac{2}{2k-1} \sum_{j=2}^{2k} X_1 X'_j \right) = 0,
\]

\[
\text{Cov} \left( \overline{X}^{(2k)}, \overline{X}^{(2k)'} \right) = \text{Cov} \left( \frac{1}{4k^2} X_1^2, \frac{2}{2k-1} \sum_{j=2}^{2k} X_1 X'_j \right) = 0.
\]

Since $\text{Var}(X_1) > 0$, we have

\[
\text{Cov} \left( \overline{X}^{(2k)} - \overline{X}^{(2k)'} \right) = \Theta \left( \frac{1}{k^2} \right).
\]

Part 2: $|S_1^{(2k)} \cap S_2^{(2k)}| = 2k$

We borrow the proof of Proposition J.6 by replacing $n$ with $2k$. In other words, we get coefficient $O(\frac{1}{k})$ because this is the variance of a fixed-order kernel with $2k$-sample U-statistic. We have

\[
\text{Cov} \left( \overline{X}^{(2k)} - \overline{X}^{(2k)'}, \overline{X}^{(2k)} - \overline{X}^{(2k)'} \right) = \text{Var} \left( \overline{X}^{(2k)} - \overline{X}^{(2k)'} \right) = O(\frac{1}{k}).
\]

\[\square\]

## K Additional Simulation Results

### K.1 Ground Truth in the Simulation

As mentioned in Section 5.1, we simulate the ground truth of the expectation of forest predictions: $E(f(x^*))$ and the variance of forest predictions: $\text{Var}(f(x^*))$ by 10000 simulations. Since variance estimators are produced by different packages, we use the corresponding package to generate their ground truth. The result of the central testing sample (see Section 5) is presented in Table 6 and Table 7. We observe that there is a small difference between different packages though the similar tuning parameters are used to train random forests.

In addition, we present the “oracle” CI coverage rate in Table 8, which matches $1 - \alpha$. To construct these CIs, we still use the random forest prediction over 1000 simulations but replace the estimated variance with the “true variance”, $\text{Var}(f(x^*))$. This result also shows the normality of the random forest predictor.
Table 6: Ground Truth of $E(f(x^*))$ evaluated on central testing sample by 10000 simulations. The number in the bracket is the standard deviation of $E(f(x^*))$.

| Tree size | nTrees | MARS | MLR |
|-----------|--------|------|-----|
| $k = n/2$ | 2000   | 17.82 (0.01) | 18.18 (0.01) | 0.503 (0.004) | 0.498 (0.004) |
|           | 20000  | 17.82 (0.01) | 18.18 (0.01) | 0.503 (0.004) | 0.499 (0.004) |
| $k \leq n/2$ | $k = n/4$ | 2000 | 17.45 (0.01) | 18.00 (0.01) | 0.503 (0.003) | 0.468 (0.003) |
|           | 20000  | 17.45 (0.01) | 18.00 (0.01) | 0.503 (0.003) | 0.468 (0.003) |
| $k = n/8$ | 2000   | 17.41 (0.01) | 18.19 (0.01) | 0.503 (0.002) | 0.424 (0.002) |
|           | 20000  | 17.41 (0.01) | 18.18 (0.01) | 0.503 (0.002) | 0.424 (0.002) |
| $k > n/2$ | $k = 4n/5$ | 2000 | 18.21 (0.01) | 18.19 (0.01) | 0.499 (0.005) | 0.498 (0.005) |
|           | 20000  | 18.21 (0.01) | 18.19 (0.01) | 0.498 (0.005) | 0.498 (0.005) |

Table 7: Ground Truth of $\text{Var}(f(x^*))$ evaluated on the central testing sample by 10000 simulations.

| Tree size | nTrees | MARS | MLR |
|-----------|--------|------|-----|
| $k = n/2$ | 2000   | 0.859 | 0.814 | 0.130 | 0.132 |
|           | 20000  | 0.851 | 0.811 | 0.129 | 0.131 |
| $k \leq n/2$ | $k = n/4$ | 2000 | 0.523 | 0.527 | 0.075 | 0.077 |
|           | 20000  | 0.517 | 0.519 | 0.074 | 0.077 |
| $k = n/8$ | 2000   | 0.349 | 0.378 | 0.044 | 0.044 |
|           | 20000  | 0.342 | 0.370 | 0.043 | 0.044 |
| $k > n/2$ | $k = 4n/5$ | 2000 | 1.334 | 1.348 | 0.214 | 0.213 |
|           | 20000  | 1.331 | 1.341 | 0.213 | 0.212 |

Table 8: 90% CI Coverage Rate averaged on 50 testing samples, where the true variance is used in constructing the CI. The number in the bracket is the standard deviation of coverage over 50 testing samples. IJ estimator is performed by $\text{grf}$ package when $k \leq n/2$ and $\text{ranger}$ package when $k > n/2$.

| Tree size | nTrees | MARS | MLR |
|-----------|--------|------|-----|
| $k = n/2$ | 2000   | 90.12% (0.93%) | 90.00% (0.97%) | 89.97% (0.86%) | 90.04% (0.99%) |
|           | 20000  | 90.10% (0.96%) | 89.95% (0.97%) | 89.97% (0.88%) | 89.96% (1.00%) |
| $k \leq n/2$ | $k = n/4$ | 2000 | 89.87% (0.76%) | 89.69% (0.84%) | 90.07% (1.03%) | 90.06% (1.25%) |
|           | 20000  | 89.83% (0.78%) | 89.63% (0.82%) | 90.14% (1.04%) | 89.98% (1.21%) |
| $k = n/8$ | 2000   | 89.53% (0.78%) | 89.35% (0.85%) | 90.22% (1.13%) | 89.91% (1.17%) |
|           | 20000  | 89.38% (0.89%) | 89.28% (0.85%) | 90.20% (1.12%) | 89.78% (1.23%) |
| $k > n/2$ | $k = 4n/5$ | 2000 | 90.05% (0.94%) | 90.02% (0.97%) | 89.86% (1.05%) | 89.94% (0.98%) |
|           | 20000  | 90.05% (1.01%) | 90.00% (0.96%) | 89.88% (0.98%) | 89.86% (0.97%) |
K.2 Figures of MLR model

Figure 6 shows the performance of different methods on the MLR model. This is a counterpart of Figure 2 in Section 5.

![Figure 6: A comparison of different methods on MLR data. Each column of figure panel corresponds to one tree size: \( k = n/2, n/4, n/8 \). The first row: boxplots of relative variance estimators of the central test sample over 1000 simulations. The diamond symbol in the boxplot indicates the mean. The second row: boxplots of 90% CI coverage for 50 testing samples. For each method, three side-by-side boxplots represent \( nTrees \) as 2000, 10000, 20000. The third row: coverage rate averaged over 50 testing samples with 20000 \( nTrees \) and the confidence level (x-axis) from 80% to 95%. The black reference line \( y = x \) indicates the desired coverage rate.](image)

K.3 Smoothing Algorithm for Variance Estimation

In Algorithm 2, \( d(\cdot, \cdot) \) can be Euclidean distance for continuous covariates and other metrics for categorical covariates. In practice, one may pre-process data before fitting random forest models, such as performing standardization and feature selection.
Algorithm 2: Matched Sample Smoothing Variance Estimator \((k \leq n/2)\)

**Input:** \(n, k, M, B, \text{testing set } X_{\text{train}}, \text{testing sample } x^* \) and number of neighbors \(N\)

**Output:** Smooth Variance estimator \(\hat{\sigma}^2_{RF}(x^*)\)

1. Find the closed distance \(D_{\text{min}} = \min_{x \in X_{\text{train}}} d(x^*, x)\);
2. Randomly generate \(N\) neighbors \(x_1^*, ..., x_N^*\) that satisfy \(x : d(x, x^*) \leq D_{\text{min}}\) or \(x : d(x, x^*) = D_{\text{min}}\);
3. Obtain variance estimators \(\hat{\sigma}^2_{RF}(x^*), \hat{\sigma}^2_{RF}(x_1^*), ..., \hat{\sigma}^2_{RF}(x_N^*)\) by Algorithm 1;
4. \(\hat{\sigma}^2_{RF}(x^*) = \frac{1}{N+1}[\hat{\sigma}^2_{RF}(x^*) + \sum_{i=1}^{N} \hat{\sigma}^2_{RF}(x_i^*)](19)\).

### L Additional Information and Results on the Real Data

Table 9 describes the covariates of Airbnb data in Section 6. We use the samples with price falling in the interval \((0, 500]\) dollars. The missing values (NA) in rating score and bathroom number are replaced. The “having rating” covariate is created based on the “review number”.

| Covariate Name          | Description                                                                 |
|-------------------------|-----------------------------------------------------------------------------|
| latitude                | Latitude of the Airbnb unit.                                               |
| longitude               | Longitude of the Airbnb unit.                                              |
| room type               | Three types (with \# of samples): Entire home/apt (5547), Private room (1839) and Shared room (129). |
| bedroom number          | Number of bedrooms in this unit.                                           |
| bathroom number         | Number of bathrooms in this unit. NA values are replaced by 0.              |
| accommodates            | Maximum accommodates of this unit.                                         |
| reviews number          | The number of reviews of this unit.                                        |
| having a rating         | It is 1 if the number of reviews is greater than 0; and is 0 otherwise.      |
| rating score            | The average rating score. NA is replaced by the average score.              |

To train the random forest model, we set \(mtry\) (number of variables randomly sampled as candidates at each split) as 3, and set \(nodesize\) parameter as 36. Here we also present the details of testing samples. The latitude and longitude of SEA Airport, Seattle downtown, and Mercer Island are \((47.4502, -122.3088)\), \((47.6050, -122.3344)\), and \((47.5707, -122.2221)\) respectively. The “room type” “accommodates” and “having a rating” are fixed as “Entire home/apt”, the double of “bedroom numbers”, and 1 respectively. We use averages in the training data as the values of “reviews number” and “rating score”. 

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