Ensemble Estimation of Distributional Functionals via $k$-Nearest Neighbors

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Abstract

The problem of accurate nonparametric estimation of distributional functionals (integral functionals of one or more probability distributions) has received recent interest due to their wide applicability in signal processing, information theory, machine learning, and statistics. In particular, $k$-nearest neighbor (nn) based methods have received a lot of attention due to their adaptive nature and their relatively low computational complexity. We derive the mean squared error (MSE) convergence rates of leave-one-out $k$-nn plug-in density estimators of a large class of distributional functionals without boundary correction. We then apply the theory of optimally weighted ensemble estimation to obtain weighted ensemble estimators that achieve the parametric MSE rate under assumptions that are competitive with the state of the art. The asymptotic distributions of these estimators, which are unknown for all other $k$-nn based distributional functional estimators, are also presented which enables us to perform hypothesis testing.

I. INTRODUCTION

Information measures such as entropy, information divergence, and mutual information, are useful in many applications in signal processing, information theory, machine learning, and statistics. These information measures belong to a larger class of functionals known as distributional functionals, defined as integral functionals of one or more probability distributions. Distributional functionals have been used in applications such as Bayes error rate estimation [1]–[6], the two sample test [7], estimating the decay rates of error probabilities [8], clustering [9]–[11], intrinsic dimension estimation [12], [13], feature selection and classification [14]–[16], image segmentation [17], extending machine learning algorithms to distributional features [18]–[21], steganography [22], and structure learning [23], [24].

We consider the problem of nonparametric estimation of these distributional functionals from a finite population of i.i.d. samples drawn from each $d$-dimensional distribution without any knowledge of the boundary of the densities’ support set. We derive the mean squared error (MSE) convergence rates of leave-one-out $k$-nearest neighbor (nn) plug-in density estimators. We then apply the general theory of optimally weighted ensemble estimation developed in [25]–[27] to obtain weighted ensemble estimators that achieve the parametric MSE convergence rate of $O(1/N)$ when the densities are sufficiently smooth, where $N$ is the sample size. We also derive the asymptotic distribution of the weighted ensemble estimators.

For brevity, we focus on estimating functionals of two distributions (referred to as divergence functionals) in this paper. However, our methods can be easily extended to functionals of any finite number of distributions.

Several previous works have explored $k$-nn estimators for distributional functionals. Poczos and Schneider [18] proved that a fixed $k$-nn estimator with bias correction is weakly consistent for Renyi-$\alpha$ and other similar divergences. Wang et al [28] provided a $k$-nn based estimator for the Kullback-Leibler divergence while Gao et al [29] proved the consistency of local likelihood density estimators with $k$-nn bandwidths for polynomials of a single distribution. However, none of these works study the MSE convergence rates nor the asymptotic distribution of their estimators.

More recent work has focused on the convergence rates of $k$-nn based estimators of distributional functionals. Gao et al [30] showed that popular $k$-nn based Shannon entropy [31] and Shannon mutual information [32] estimators achieve the parametric MSE rate when the dimension of each of the random variables is less than 3. Singh and Poczos [33] derive the convergence rates for fixed $k$-nn estimators of specific distributional functionals where a bias correction term is known and when the densities’ support set contains no boundaries.

Ensemble techniques [25]–[27] have previously been applied to $k$-nn based estimators of some distributional functionals to obtain estimators that achieve the parametric rate when the densities are sufficiently smooth. Noshad et al [34] and Wisler et al [35] applied ensemble techniques to $k$-nn based direct estimators of $f$-divergence functionals. Moon and Hero [36] applied ensemble techniques to $k$-nn plug-in estimators of $f$-divergences and applied ensemble techniques to obtain an estimator that achieves the parametric rate when the densities’ support set is compact and contains no boundaries, or when boundary correction is applied. However, our assumptions on the smoothness of the densities are less strict than required for some of these estimators [34], [36] and we consider different boundary conditions on the densities’ support set. Additionally, our techniques can be applied to a larger class of distributional functionals which includes the $L^2$ divergence and general entropies whereas the work in

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is limited to $f$-divergence functionals (functionals of the likelihood ratio between two densities). Furthermore, while Moon and Hero \cite{37} derive the asymptotic distribution for the plug-in estimators defined in \cite{36}, the asymptotic distributions of the estimators in \cite{34}, \cite{35} are unknown. In contrast, we obtain the asymptotic distribution of our estimators under much less strict assumptions on the densities and the functional compared to the work in \cite{37}.

Many other approaches for distributional functional estimation have also been examined including methods based on kernel density estimators (KDE) \cite{25}, \cite{26}, \cite{38}–\cite{41} and convex risk minimization \cite{42}. While all of these works define estimators that can achieve the parametric MSE rate, these methods are generally more computationally intensive than $k$-nn based methods and some of them require explicit knowledge of the densities’ support set boundary \cite{27}, \cite{38}–\cite{41}.

Finally, Gao et al \cite{43} showed that $k$-nn or KDE based approaches underestimate the mutual information when the mutual information is large. As mutual information increases, the dependencies between random variables becomes more deterministic and some of them require explicit knowledge of the densities’ support set boundary \cite{27}, \cite{38}–\cite{41}.

\[ \sum_{i=1}^{N_2} g \left( \hat{f}_{1,k_1}(X_i), \hat{f}_{2,k_2}(X_i) \right) \].

B. Convergence Rates

We derive the MSE convergence rate of our estimators in terms of the Hölder condition:

**Definition 1** (Hölder Class). Let $\mathcal{X} \subset \mathbb{R}^d$ be a compact space. For $r = (r_1, \ldots, r_d)$, $r_i \in \mathbb{N}$, define $|r| = \sum_{i=1}^{d} r_i$ and $D^r = \sum_{i=1}^{d} \frac{\partial^{r_i}}{\partial x_i^{r_i}}$. The Hölder class $\Sigma(s, K)$ of functions on $L_2(\mathcal{X})$ consists of the functions $f$ that satisfy

\[ |D^r f(x) - D^r f(y)| \leq K \|x - y\|^{s - |r|}, \]

for all $x, y \in \mathcal{X}$ and for all $r$ s.t. $|r| \leq |s|$.

Consider the following assumptions:

- (B.1): Assume there exist constants $\epsilon_0, \epsilon_\infty$ such that $0 < \epsilon_0 \leq f_i(x) \leq \epsilon_\infty < \infty$, $\forall x \in S$.
- (B.2): Assume that the densities $f_i \in \Sigma(s, K)$ in the interior of $S$ with $s \geq 2$ and $r = |s|$.
- (B.3): Assume that $g$ has an infinite number of mixed derivatives.
- (B.4): Assume that $\frac{\partial^{\alpha}}{\partial x^\alpha \partial y^\beta} g(x,y)$, $k, l = 0, 1, \ldots$ are strictly upper bounded for $\epsilon_0 \leq x, y \leq \epsilon_\infty$.
- (B.5): Assume that the densities’ support set is $S = [0, 1]^d$.

These assumptions enable us to obtain the bias results for the $k$-nn plug in estimator $\hat{G}_{k_1,k_2}$. Assumption B.3 is used to obtain the bias convergence rates without knowledge of the boundary of the densities’ support set. This assumption is not
overly restrictive as most divergence functionals of interest are infinitely differentiable. Those functionals that are not infinitely differentiable are typically not differentiable everywhere (e.g. the total variation distance and the Bayes error) which violates the assumptions of current nonparametric estimators that achieve the parametric rate. Assumption 8.5 is used to handle the boundary bias of the k-nn estimators. In particular, the proof derives the bias contribution of points that are near the flat “walls” of the cube and near the corners. Thus our results still hold for rotated and stretched or compressed support sets. It is also likely that our results can be extended to other support sets with relatively smooth boundaries and some sharp corners. In contrast, the theory developed in [34]–[36] applies when the densities’ support set contains no boundaries (e.g. the surface of the hypersphere) [36], the densities decay to zero near the support set boundary [35], or the derivatives of the densities decay to zero near the support set boundary [34].

The following theorem on the bias of the plug-in estimator follows under assumptions 8.1 – 8.5. For simplicity, assume that $N_1 = N_2 = N$ and $k_1 = k_2 = k$.

**Theorem 2.** For general $g$, the bias of the plug-in estimator $\hat{G}_{k_1,k_2}$ is of the form

$$
\mathbb{E} \left[ \hat{G}_{k_1,k_2} \right] = \sum_{j=1}^{r} \left( c_{17,1,j} + \frac{c_{17,1,j,0}}{\sqrt{k_1}} \right) \left( \frac{k_1}{N_1} \right)^{\frac{d}{2}} + \left( c_{17,2,j} + \frac{c_{17,2,j,0}}{\sqrt{k_2}} \right) \left( \frac{k_2}{N_2} \right)^{\frac{d}{2}} \\
+ \sum_{j=0}^{r} \sum_{i=0}^{r} c_{18,i,j} \left( \frac{k_1}{N_1} \right)^{\frac{d}{2}} + \left( \frac{k_2}{N_2} \right)^{\frac{d}{2}} \\
+ O \left( \frac{1}{\sqrt{k_1 k_2}} + \frac{1}{k_1} + \frac{1}{k_2} + \max \left( \frac{k_1}{N_1}, \frac{k_2}{N_2} \right) \right).
$$

Furthermore, if $g(x,y)$ has $m$, $l$-th order mixed derivatives $\frac{\partial^{m+l} g(x,y)}{\partial x^m \partial y^l}$ that depend on $x,y$ only through $x^\alpha y^\beta$ for some $\alpha, \beta \in \mathbb{R}$, then for any positive integer $\nu \geq 0$, the bias is of the form

$$
\mathbb{E} \left[ \hat{G}_{k_1,k_2} \right] = \sum_{j=0}^{r} \sum_{i=0}^{r} c_{18,i,j} \left( \frac{k_1}{N_1} \right)^{\frac{d}{2}} + \left( \frac{k_2}{N_2} \right)^{\frac{d}{2}} + O \left( \max \left( \frac{k_1}{N_1}, \frac{k_2}{N_2} \right)^{\nu} \right) \\
+ \sum_{m=0}^{\nu} \sum_{j=0}^{r} \left( \frac{c_{20,1,j,m}}{k_1^{\nu+m}} \frac{k_1}{N_1} \right)^{\frac{d}{2}} + \left( \frac{c_{20,2,j,m}}{k_2^{\nu+m}} \frac{k_2}{N_2} \right)^{\frac{d}{2}} \\
+ \sum_{j=1}^{r} \left( c_{17,1,j} \left( \frac{k_1}{N_1} \right)^{\frac{d}{2}} + c_{17,2,j} \left( \frac{k_2}{N_2} \right)^{\frac{d}{2}} \right) \\
+ \sum_{m=0}^{\nu} \sum_{j=0}^{r} \sum_{n=0}^{\nu} \sum_{i=0}^{\nu} \frac{c_{18,i,j,m,n}}{k_1^{\nu+i} k_2^{\nu+j}} \left( \frac{k_1}{N_1} \right)^{\frac{d}{2}} + \left( \frac{k_2}{N_2} \right)^{\frac{d}{2}}.
$$

The following variance result requires much less strict assumptions:

**Theorem 3.** If the functional $g$ is Lipschitz continuous in both of its arguments with Lipschitz constant $C_g$, then the variance of $\hat{G}_{k_1,k_2}$ is

$$
\mathbb{V} \left[ \hat{G}_{k_1,k_2} \right] = O \left( \frac{1}{N_2^2} + \frac{N_1}{N_2^2} \right).
$$

From Theorems 2 and 3 it is clear that we require $k_i \to \infty$ and $k_i/N_i \to 0$ for $\hat{G}_{k_1,k_2}$ to be unbiased. For the variance to decrease to zero, we require $N_2 \to \infty$ and $N_1/N_2^2 \to 0$. The additional terms in (3) enable us to achieve the parametric MSE convergence rate when $s > d/2$ (similar to the estimators in [34]) for an appropriate choice of $k$ values whereas the terms in (2) require $s \geq d$ to achieve the same rate (similar to the estimators in [36], [36]). Moreover, the additional terms in (3) enable us to achieve the parametric rate for smaller values of $k$ which is more computationally efficient.

The Lipschitz condition on $g$ is comparable to other nonparametric estimators of distributional functionals [25], [38]–[41]. Specifically, assumption 8.1 ensures that functionals such as those for Shannon and Renyi divergences are Lipschitz on the space $c_0$ to $c_\infty$.

From Theorem 2 the dominating terms in the bias are $\Theta \left( \frac{k_1}{N_1} \right)^{\frac{d}{2}}$ and $\Theta \left( \frac{1}{k_1} \right)$. If no bias correction is made, the optimal choice of $k_i$ that minimizes the MSE is

$$
k_i^* = \Theta \left( N_i^{\frac{d}{2r}} \right).
$$
This results in a dominant bias term of order $O\left(\frac{1}{N}\right)$, which is large whenever $d$ is not small.

C. Proof Sketches of Theorems [2] and [3]

The proof of the bias result uses a conditioning argument on the $k$-nn distances by viewing the $k$-nn estimator as a kernel density estimator with uniform kernel and random bandwidth. This allows us to leverage some KDE plug-in estimator proof techniques. For fixed bandwidth (i.e. $k$-nn distance), we then consider separately the cases where the $k$-nn ball is contained within the support and when it intersects the boundary of the support. See Appendix [3] for the full proof.

The proof of the variance result uses the Efron-Stein inequality, which becomes complicated due to the dependencies between different $k$-nn neighborhoods. Thus we analyze the possible effects on the $k$-nn graph when one sample is allowed to differ in order to use the Efron-Stein inequality. See Appendix [3] for the full proof of Theorem [3].

III. Weighted Ensemble Estimation

The $k$-nn plug-in estimator $\hat{G}_{k_1,k_2}$ in Section III has slowly decreasing bias when the dimension of the data is not small. By applying the theory of optimally weighted ensemble estimation derived in [25], [26], we can take a weighted sum of an ensemble of estimators where the weights are chosen to reduce the bias.

We simplify the bias expressions in Theorem [2] by assuming that $N_1 = N_2 = N$ and $k_1 = k_2 = k$. Define $G_k := \hat{G}_{k,k}$.

**Corollary 4.** For general $g$, the bias of the plug-in estimator $\hat{G}_k$ is given by

$$B \left[ \hat{G}_k \right] = \sum_{j=1}^{r} \left( \frac{c_{21,1,j} + c_{21,2,j}}{\sqrt{k}} \right) \left( \frac{k}{N} \right)^{\frac{j}{2}} + O \left( \frac{1}{k} + \left( \frac{k}{N} \right)^{\frac{\min(\alpha,\beta)}{d}} \right).$$

If $g(x,y)$ has $m$, $l$-th order mixed derivatives $\frac{\partial^{m+l} g(x,y)}{\partial x^m \partial y^l}$ that depend on $x$, $y$ only through $x^\alpha y^\beta$ for some $\alpha, \beta \in \mathbb{K}$, then for any positive integer $\nu \geq 2$, the bias is of the form

$$B \left[ \hat{G}_k \right] = \sum_{j=1}^{r} \frac{c_{22,j}}{k} \left( \frac{k}{N} \right)^{\frac{j}{2}} + O \left( \frac{1}{k} + \left( \frac{k}{N} \right)^{\frac{\min(\alpha,\beta)}{d}} \right).$$

The corollary still holds if $N_1$ and $N_2$ are linearly related and if $k_1$ and $k_2$ are linearly related. An ensemble of estimators is formed by choosing different neighborhood sizes by choosing different values of $k$. Choose $L = \{l_1, \ldots, l_L\}$ to be real positive numbers that index $h(l_i)$. Define $w := \{w(l_1), \ldots, w(l_L)\}$ and $G_w := \sum_{l \in L} w(l) \hat{G}_{k(l)}$. The weights can be used to decrease the bias as before.

An ensemble of estimators is formed by choosing different neighborhood sizes by choosing different values of $k$. Choose $L = \{l_1, \ldots, l_L\}$ to be real positive numbers that index $k(l_i)$. Define $w := \{w(l_1), \ldots, w(l_L)\}$ and $G_w := \sum_{l \in L} w(l) \hat{G}_{k(l)}$. The weights can be used to decrease the bias as before. Consider the following assumptions on the ensemble of estimators $\{G_{k(l)}\}_{l \in L}$:

- **C.1** The bias is expressible as
  $$B \left[ \hat{G}_{k(l)} \right] = \sum_{i \in J} c_i \psi_i(l) \phi_i \left( \frac{1}{\sqrt{N}} \right) + O \left( \frac{1}{\sqrt{N}} \right),$$
  where $c_i$ are constants depending on the underlying density and are independent of $N$ and $l$, $J = \{i_1, \ldots, i_J\}$ is a finite index set with $I < L$, and $\psi_i(l)$ are basis functions depending only on the parameter $l$ and not on the sample size $N$.

- **C.2** The variance is expressible as
  $$\mathbb{V} \left[ \hat{G}_{k(l)} \right] = c_v \left( \frac{1}{N} \right) + o \left( \frac{1}{N} \right).$$

**Theorem 5.** [26] Assume conditions C.1 and C.2 hold for the ensemble of estimators $\{\hat{G}_{k(l)}\}_{l \in L}$. Then there exists a weight vector $w_0$ such that the MSE of the weighted ensemble estimator attains the parametric rate of convergence:

$$\mathbb{E} \left[ \left( \hat{G}_{w_0} - G(f_1, f_2) \right)^2 \right] = O \left( \frac{1}{N} \right).$$

The weight vector $w_0$ is the solution to the following offline convex optimization problem:

$$\min_w \quad \|w\|_2^2 \quad \text{subject to} \quad \sum_{l \in L} w(l) = 1, \quad \gamma_w(i) = \sum_{l \in L} w(l) \psi_i(l) = 0, \quad i \in J.$$  

(5)
To achieve the parametric rate $O(1/N)$ in MSE convergence, it is not necessary that $\gamma_w(i) = 0$, $i \in J$. The following convex optimization is also sufficient [26], [35]:

$$
\begin{align*}
\min_{w} & \quad \epsilon \\
\text{subject to} & \quad \sum_{\ell \in \ell} w(\ell) = 1, \\
& \quad |w|_2^2 \leq \eta, \\
& \quad |w_iN^{d/2} + \phi_{i,d}(N)| \leq \epsilon, \quad i \in \{1, \ldots, J\},
\end{align*}
$$

(6)

where the parameter $\eta$ is chosen to achieve a trade-off between bias and variance.

We now apply this theory to the plug-in $k$-nn estimators. For general $g$, let $k(l) = \ell / \sqrt{N}$. From Theorem 2, we have $\psi_2(l) = l^{i/d}$ for $i = 1, \ldots, d$. If $s \geq d$, then we have a $O\left(\frac{1}{\sqrt{N}}\right)$. We also include the function $\psi_{d+1}(l) = l^{-1}$. The bias of the resulting base estimator satisfies condition C.1 with $\phi_{i,d}(N) = N^{-i/(2d)}$ for $i = 1, \ldots, d$ and $\phi_{i,d+1}(N) = N^{-1/2}$. The variance also satisfies condition C.2. The optimal weight $w_0$ is found using (6) to obtain a plug-in divergence functional estimator $\hat{G}_{w_0,1}$ with an MSE convergence rate of $O\left(\frac{1}{\sqrt{N}}\right)$ as long as $s \geq d$. Otherwise, if $s < d$ we can only guarantee the MSE rate up to $O\left(\frac{1}{\sqrt{N}}\right)$. We refer to this estimator as the ODin1 $k$-nn estimator.

We can define another weighted ensemble estimator that achieves the parametric rate under less strict assumptions on the smoothness of the densities than $\phi_{i,d}(N)$ satisfies the assumption required for [3]. Let $\delta > 0$ and $k(l) = lN^{-\delta}$. From Theorem 2, the bias has terms proportional to $l^{-\delta}N^{-1/(1+\delta)} - N^{-1/2}$ where $j, q \geq 0$ and $j + \frac{q}{2} > 1$. Let $\psi_{j,q,d}(N) = N^{-j/(1+\delta)} - N^{-1/2}$ and $\psi_{j,q}(l) = l^{-\delta}$. Let

$$
J = \left\{\{j, q\} : 0 < \frac{(1-\delta)j}{d} + \frac{q\delta}{2} < \frac{1}{2}, \quad q \in \{0, 1, 2, \ldots, \nu\}, \quad j \in \{0, 1, 2, \ldots, r\}, \quad j + \frac{q}{2} > \frac{1}{2}\right\}
$$

Then the bias of the resulting base estimator satisfies condition C.1 and the variance satisfies condition C.2. If $L > |J|$, then the optimal weight can be found using (6). The resulting weighted ensemble estimator $\hat{G}_{w_0,2}$ achieves the parametric convergence rate if $\nu \geq 1/\delta$ and if $s \geq \frac{d}{\frac{1-\delta}{1-1/\delta}}$. Otherwise, if $s < d/(2(1 - \delta))$ we can only guarantee the MSE rate up to $O\left(\frac{1}{\sqrt{N}}\right)$. We refer to this estimator as the ODin2 $k$-nn estimator.

The parametric rate can be achieved with $\hat{G}_{w_0,2}$ under less strict assumptions on the smoothness of the densities than those required for $\hat{G}_{w_0,1}$. Since $\delta > 0$ can be arbitrary, it is theoretically possible to construct an estimator that achieves the parametric rate as long as $s > d/2$. However, $\hat{G}_{w_0,2}$ requires more parameters to implement the weighted ensemble estimator than $\hat{G}_{w_0,1}$ which may have an effect on the variance.

A. Central Limit Theorem

The following theorem shows that the appropriately normalized ensemble estimator $G_w$ converges in distribution to a normal random variable, which enables us to perform hypothesis testing on the divergence functional. The proof uses a lemma modified from [45] that gives sufficient conditions on an interchangeable process for a central limit theorem. The details are given in Appendix D.

**Theorem 6.** Assume that the mixed derivatives of $g$ of order 2 are bounded and $k(l) \to \infty$ as $N \to \infty$ for each $l \in \mathcal{L}$. Then for fixed $L$, and if $S$ is a standard normal random variable,

$$
\text{Pr}\left(\frac{\hat{G}_w - \mathbb{E}\left[\hat{G}_w\right]}{\sqrt{\text{Var}\left[\hat{G}_w\right]}} \leq t\right) \to \text{Pr}\left(S \leq t\right).
$$

IV. Numerical Validation

We validate our theory on the MSE convergence rates by estimating the Rényi-$\alpha$ divergence integral between two truncated multivariate Gaussian distributions with varying dimension and sample sizes. The densities have means $\bar{\mu}_1 = 0.7 * 1_d$, $\bar{\mu}_2 = 0.3 * 1_d$ and covariance matrices $0.1 * I_d$ where $1_d$ is a $d$-dimensional vector of ones, and $I_d$ is a $d \times d$ identity matrix. We used $\alpha = 0.5$ and restricted the Gaussians to the unit cube.

The left plot in Fig. I shows the MSE (200 trials) of the standard plug-in $k$-nn estimator where $k = \sqrt{N}$ and the two proposed optimally weighted estimators ODin1 and ODin2. We show the case where $d = 7$ and the sample size varies. For the ODin1 estimator, we chose $\mathcal{L}$ to be linearly spaced between 0.3 and 3 with $L = 50$. For the ODin2 estimator, we chose the minimum value of $\mathcal{L}$ to be 1.4 and then chose the next 24 values for $k$ (i.e. $L = 25$). Both ODin1 and ODin2 outperform both plug-in estimators which validates our theory.
In this chapter, we derived convergence rates for a $k$-nearest neighbor plug-in estimator of divergence functionals. We applied the generalized theory of optimally weighted ensemble estimation derived previously to derive an estimator that achieves the parametric rate when the densities belong to the Hölder smoothness class with smoothness parameter greater than $d/2$. The convergence rates we derive apply when the densities have support $[0,1]^d$ although the estimators do not require knowledge of the support. We also derived the asymptotic distribution of the estimator.

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We begin by focusing on points $x$ that are boundary points due to a single coordinate $x_i$ s.t. $x_i + u_i h \notin S$. Without loss of generality, assume that $x_i + u_i h > 1$. We focus first on the inner integral in (7). We will use the following lemma:
**Lemma 7.** Let $D_d(r)$ be a $d$-sphere with radius $d$ and let $\sum_{i=1}^{d} n_i = q$. Then

$$
\int_{D_d(r)} u_1^{n_1} u_2^{n_2} \ldots u_d^{n_d} du_1 \ldots du_d = C r^{d+q},
$$

where $C$ is a constant that depends on the $n_i$s and $d$.

**Proof:** We convert to $d$-dimensional spherical coordinates to handle the integration. Let $r$ be the distance of a point $u$ from the origin. We have $d - 1$ angular coordinates $\phi_i$ where $\phi_d$ ranges from 0 to $2\pi$ and all other $\phi_i$ range from 0 to $\pi$. The conversion from the spherical coordinates to Cartesian coordinates is then

$$
u_1 = r \cos(\phi_1)$$
$$
u_2 = r \sin(\phi_1) \cos(\phi_2)$$
$$
u_3 = r \sin(\phi_1) \sin(\phi_2) \cos(\phi_3)$$
$$\vdots$$
$$
u_{d-1} = r \sin(\phi_1) \cdots \sin(\phi_d) \cos(\phi_d-1)$$
$$
u_d = r \sin(\phi_1) \cdots \sin(\phi_d) \sin(\phi_d).$$

The spherical volume element is then

$$r^{d-1} \sin^{d-2}(\phi_1) \sin^{d-3}(\phi_1) \cdots \sin(\phi_{d-1}) \, d\phi_1 \, d\phi_2 \cdots d\phi_{d-1}.$$ Combining these results gives

$$
\int_{D_d(r)} u_1^{n_1} u_2^{n_2} \ldots u_d^{n_d} du_1 \ldots du_d
= \int_0^r \int_0^{2\pi} \cdots \int_0^{\pi} r^{q+d-1} \left[ \sin^{q-n_1-d-2}(\phi_1) \sin^{q-n_1-n_d-d-3}(\phi_2) \cdots \sin^{n_d+n_d-1}(\phi_{d-2}) \sin^{n_d}(\phi_{d-1}) \right] [\cos^{n_1}(\phi_1) \cdots \cos^{n_d}(\phi_{d-1})] \, d\phi_1 \cdots d\phi_{d-1} \, dr
= C r^{q+d}.
$$

The region of integration for the inner integral in (7) corresponds to a hyperspherical cap with radius 1 and height of $\frac{1-x}{h}$. The inner integral can be calculated using an approach similar to that used in [46] to calculate the volume of a hyperspherical cap. It is obtained by integrating the polynomial $p_x(u)$ over a $d-1$-sphere with radius $\sin \theta$ and height element $d \cos \theta$. This is done using Lemma [7]. We then integrate over $\theta$ which has a range of 0 to $\phi = \cos^{-1}\left(\frac{1-x}{h}\right)$. Thus we have

$$
\int_{\phi=0}^{\phi} sin^{n} \theta \cos^{m} \theta \, d\theta = -\frac{\sin^{n-1} \phi \cos^{m+1} \phi}{n + m} + \frac{n - 1}{n + m} \int_{\phi=0}^{\phi} sin^{n-2} \theta \cos^{m} \theta d\theta.\quad (9)
$$

If $n = 1$, then we get

$$
\int_{0}^{\phi} \sin \theta \cos^{m} \theta d\theta = \frac{1}{m + 1} - \frac{\cos^{m+1} \phi}{m + 1}.
$$

Since $\phi = \cos^{-1}\left(\frac{1-x}{h}\right)$, we have

$$
\cos \phi = \frac{1 - x}{h},
$$
$$
\sin \phi = \sqrt{1 - \left(\frac{1-x}{h}\right)^2}.
$$

Therefore, if $n$ is odd, we obtain

$$
\int_{0}^{\phi} \sin^{n} \theta \cos^{m} \theta d\theta = \sum_{\ell=0}^{(n-1)/2} c_{\ell} \left(\sqrt{1 - \left(\frac{1-x}{h}\right)^2}\right)^{2\ell} \left(\frac{1-x}{h}\right)^{m+1} + c,\quad (10)
$$
where the constants depend on $m$ and $n$.

If $n$ is even and $m > 0$, then the final term in the recursion in (9) reduces to

$$\int_0^\phi \cos^m \theta d\theta = \frac{\cos^{m-1} \phi \sin \phi}{m} + \frac{m-1}{m} \int_0^\phi \cos^{m-2} \theta d\theta.$$  

If $m = 2$, then

$$\int_0^\phi \cos^2 \theta d\theta = \frac{\phi}{2} + \frac{1}{4} \sin(2\phi) = \frac{\phi}{2} + \frac{1}{2} \sin \phi \cos \phi.$$  

Therefore, if $n$ and $m$ are both even, then this gives

$$\int_0^\phi \sin^n \theta \cos^m \theta d\theta = \sum_{\ell=0}^{(n-2)/2} c_\ell \left( \sqrt{1 - \left( \frac{1-x_i}{h} \right)^2} \right)^{2\ell+1} \left( \frac{1-x_i}{h} \right)^{m+1} + c \cos^{-1} \left( \frac{1-x_i}{h} \right),$$

On the other hand, if $n$ is even and $m$ is odd, we get

$$\int_0^\phi \sin^n \theta \cos^m \theta d\theta = \sum_{\ell=0}^{(n-2)/2} c_\ell \left( \sqrt{1 - \left( \frac{1-x_i}{h} \right)^2} \right)^{2\ell+1} \left( \frac{1-x_i}{h} \right)^{m+1} + \sum_{\ell=0}^{(m-1)/2} c_\ell \left( \sqrt{1 - \left( \frac{1-x_i}{h} \right)^2} \right)^{2\ell} \left( \frac{1-x_i}{h} \right)^m.$$  

If $d$ is odd, then combining (10) and (12) with (8) gives

$$\int_{u:|u|_2 \leq 1, x+uh \notin S} p_x(u) du = \sum_{m=0}^q \sum_{\ell=0}^{d+q} p_{m,\ell}(x) \left( \sqrt{1 - \left( \frac{1-x_i}{h} \right)^2} \right)^\ell \left( \frac{1-x_i}{h} \right)^m,$$

where the coefficients $p_{m,\ell}(x)$ are $r - q$ times differentiable wrt $x$. Similarly, if $d$ is even, then

$$\int_{u:|u|_2 \leq 1, x+uh \notin S} p_x(u) du = \sum_{m=0}^q \sum_{\ell=0}^{d+q} p_{m,\ell}'(x) \left( \sqrt{1 - \left( \frac{1-x_i}{h} \right)^2} \right)^\ell \left( \frac{1-x_i}{h} \right)^m + p'(x) \cos^{-1} \left( \frac{1-x_i}{h} \right),$$

where again the coefficients $p_{m,\ell}'(x)$ and $p'(x)$ are $r - q$ times differentiable wrt $x$. Raising (13) and (14) to the power of $t$ gives respective expressions of the form

$$\sum_{m=0}^{qt} \sum_{\ell=0}^{(d+q)t} \tilde{p}_{m,\ell}(x) \left( \sqrt{1 - \left( \frac{1-x_i}{h} \right)^2} \right)^\ell \left( \frac{1-x_i}{h} \right)^m,$$

$$\sum_{m=0}^{qt} \sum_{\ell=0}^{(d+q)t} \tilde{p}_{m,\ell,n}(x) \left( \sqrt{1 - \left( \frac{1-x_i}{h} \right)^2} \right)^\ell \left( \frac{1-x_i}{h} \right)^m \cos^{-1} \left( \frac{1-x_i}{h} \right)^n,$$

where the coefficients $\tilde{p}_{m,\ell}(x)$ and $\tilde{p}_{m,\ell,n}(x)$ are all $r - q$ times differentiable wrt $x$. Integrating (15) and (16) over all the coordinates in $x$ except for $x_i$ affects only the $\tilde{p}_{m,\ell}(x)$ and $\tilde{p}_{m,\ell,n}(x)$ coefficients, resulting in respective expressions of the form

$$\sum_{m=0}^{qt} \sum_{\ell=0}^{(d+q)t} \tilde{p}_{m,\ell}(x_i) \left( \sqrt{1 - \left( \frac{1-x_i}{h} \right)^2} \right)^\ell \left( \frac{1-x_i}{h} \right)^m,$$

(17)
boundary point case. Consider the case where two of the coordinates are near the boundary, e.g., where two other areas: a hyperspherical cap wrt $x_i$ and the remaining area (denoted, respectively, as $A_1$ and $A_2$). The remaining area $A_2$ can be decomposed further into two other areas: a hyperspherical cap wrt $x_2$ (denoted $B_1$) and a height chosen s.t. $B_1$ just intersects $A_1$ on their boundaries. Integrating over the remainder of $A_2$ is achieved by integrating along $x_2$ over $d - 1$-dimensional hyperspherical caps from the boundary of $B_1$ to the boundary of $A_2$. Thus integrating over these regions yields an expression similar to (18). Following a similar procedure will then yield the result.

**B. Multiple Coordinate Boundary Point**

The case where multiple coordinates of the point $x$ are near the boundary is a fairly straightforward extension of the single boundary point case. Consider the case where 2 of the coordinates are near the boundary, e.g., $x_1$ and $x_2$ with $x_1 + u_1 h > 1$ and $x_2 + u_2 h > 1$. The region of integration for the inner integral can be decomposed into two parts: a hyperspherical cap wrt $x_1$ and the remaining area (denoted, respectively, as $A_1$ and $A_2$). The remaining area $A_2$ can be decomposed further into two other areas: a hyperspherical cap wrt $x_2$ (denoted $B_1$) and a height chosen s.t. $B_1$ just intersects $A_1$ on their boundaries. Integrating over the remainder of $A_2$ is achieved by integrating along $x_2$ over $d - 1$-dimensional hyperspherical caps from the boundary of $B_1$ to the boundary of $A_2$. Thus integrating over these regions yields an expression similar to (18). Following a similar procedure will then yield the result.

**APPENDIX B**

**PROOF OF THEOREM 2 (BIAS)**

In this section, we prove the bias results in Thm. 2. The bias of the base $k$-nn plug-in estimator $\hat{G}_{k_1,k_2}$ can be expressed as

$$
\mathbb{E} [\hat{G}_{k_1,k_2}] = \mathbb{E} \left[ g \left( \hat{f}_{1,k_1}(Z), \hat{f}_{2,k_2}(Z) \right) - g \left( f_1(Z), f_2(Z) \right) \right]
$$

$$
= \mathbb{E} \left[ g \left( \hat{f}_{1,k_1}(Z), \hat{f}_{2,k_2}(Z) \right) - g \left( E_{Z,\rho_{1,k_1}}(Z) \hat{f}_{1,k_1}(Z), E_{Z,\rho_{2,k_2}}(Z) \hat{f}_{2,k_2}(Z) \right) \right]
$$

$$
+ \mathbb{E} \left[ g \left( E_{Z,\rho_{1,k_1}}(Z) \hat{f}_{1,k_1}(Z), E_{Z,\rho_{2,k_2}}(Z) \hat{f}_{2,k_2}(Z) \right) - g \left( f_1(Z), f_2(Z) \right) \right],
$$

where $Z$ is drawn from $f_2$ and $\rho_{i,k}(Z)$ is the $k_i$th nearest neighbor distance of $Z$ in the respective samples. For notational simplicity, let $\rho_{i,k}(Z) = \rho_i$. The $k$-nn density estimator can be viewed as a kernel density estimator. Let $K$ be the uniform kernel on the unit ball. That is,

$$
K(x) = \begin{cases} 
\frac{1}{cd}, & ||x|| < 1 \\
0, & \text{otherwise},
\end{cases}
$$

where $cd$ is the volume of the unit ball in $\mathbb{R}^d$. Then we have that

$$
\hat{f}_{1,k_1}(Z) = \frac{1}{N_1 \rho_{1,k_1}^{d_1}} \sum_{i=1}^{N_1} K \left( \frac{Z - Y_i}{\rho_{1,k_1}} \right),
$$

$$
\hat{f}_{2,k_2}(Z) = \frac{1}{N_2 \rho_{2,k_2}^{d_2}} \sum_{i=1}^{N_2} K \left( \frac{Z - X_i}{\rho_{2,k_2}} \right),
$$

and the remaining area is far away from the boundary, the coefficients are independent of $h$. For the integral wrt $x_i$ of (17), taking a Taylor series expansion of $\hat{p}_{m,t}(x_i)$ around $x_i = 1$ yields terms of the form

$$
\int_{1-h}^{1} \left( \sqrt{1 - \left( \frac{1-x_i}{h} \right)^2} \right)^{\ell} \left( \frac{1-x_i}{h} \right)^{m+j} h^d dx_i = h^{j+1} \int_0^1 \left( 1 - y_1 \right)^{\ell} y_1^{m+j-1} dy_i
$$

$$
= h^{j+1} \int_0^1 \left( 1 - y_1 \right)^{\ell} y_1^{m+j} \cos^{-1} \left( \frac{1-x_i}{h} \right)^n dy_i,
$$

where $0 \leq j \leq r - q, 0 \leq \ell \leq (d+q)t$, $0 \leq m \leq qt$, and $B(x,y)$ is the beta function. Note that the first step uses the substitution of $y_i = \left( \frac{1-x_i}{h} \right)^2$.

If $d$ is even (i.e., (18)), a simple closed-form expression is not easy to obtain due to the $\cos^{-1} \left( \frac{1-x_i}{h} \right)$ terms. However, by similarly applying a Taylor series expansion to $\hat{p}_{m,t,n}(x_i)$ and substituting $y_i = \frac{1-x_i}{h}$ gives terms of the form

$$
\int_{1-h}^{1} \left( \sqrt{1 - \left( \frac{1-x_i}{h} \right)^2} \right)^{\ell} \left( \frac{1-x_i}{h} \right)^{m+j} \cos^{-1} \left( \frac{1-x_i}{h} \right)^n h^d dx_i
$$

$$
= h^{j+1} \int_0^1 \left( 1 - y_1 \right)^{\ell} y_1^{m+j} \cos^{-1} \left( \frac{1-x_i}{h} \right)^n dy_i,
$$

for $0 \leq j \leq r - q, 0 \leq \ell \leq (d+q)t$, $0 \leq m \leq qt$, and $0 \leq n \leq t$. Combining terms results in the expansion $v_i(h) = \sum_{i=1}^{r-q} c_{i,q,d} h^i + o(h^{r-q}).$
The fact that the $k$-nn distances are random requires extra care. However, we can condition on these distances with these representations which enables us to use some of the same tools as in the KDE approach \cite{25}. Define
\[
S_{k_i}(Z) = \{X \in \mathbb{R}^d : \|X - Z\| < \rho_{i,k_i}\},
\]
\[
\Rightarrow \Pr(S_{k_i}(Z)) = \int_{S_{k_i}(Z)} f_i(x)dx.
\]

Note that from \cite{47}, we have that
\[
\mathbb{E}_{Z,\rho_{i,k_i}} \hat{f}_{i,k_i}(Z) = \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_{k_i}(Z))} \int_{S_{k_i}(Z)} K\left(\frac{Z - x}{\rho_{i,k_i}}\right) f_i(x)dx.
\]

The Taylor series expansion of $g\left(\mathbb{E}_{Z,\rho_{i,k_1}} \hat{f}_{i,k_1}(Z), \mathbb{E}_{Z,\rho_{2,k_2}} \hat{f}_{2,k_2}(Z)\right)$ around $f_1(Z)$ and $f_2(Z)$ is
\[
g\left(\mathbb{E}_{Z,\rho_{i,k_1}} \hat{f}_{i,k_1}(Z), \mathbb{E}_{Z,\rho_{2,k_2}} \hat{f}_{2,k_2}(Z)\right) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \delta^{i+j} \left(\frac{\partial^{i+j} g(x,y)}{\partial x^i \partial y^j}\right)_{x=f_1(Z)} \frac{1}{i! j!}
\]
\[
\times \mathbb{E}_{Z,\rho_{i,k_1}}^j \hat{f}_{i,k_1}(Z) \mathbb{E}_{Z,\rho_{2,k_2}}^j \hat{f}_{2,k_2}(Z),
\]
where $\mathbb{E}_{Z,\rho_{i,k_1}}^j \hat{f}_{i,k_1}(Z) = \left(\mathbb{E}_{Z,\rho_{i,k_1}} \hat{f}_{i,k_1}(Z) - f_i(Z)\right)^j$. We thus require an expression for $\mathbb{E}_{Z,\rho_{i,k_1}} \hat{f}_{i,k_1}(Z)$. Since we are conditioning on $\rho_{i,k_i}$, we can consider separately the cases when $Z$ is in the interior of the support $S$ or when $Z$ is near the boundary of the support. As before, a point $X \in S$ is defined to be in the interior of $S$ if for all $Y \notin S$, $K(\frac{X-Y}{\rho_i}) = 0$. A point $X \in S$ is near the boundary of the support if it is not in the interior. Denote the region in the interior and near the boundary wrt $\rho_{i,k_i}$ as $S_I$ and $S_B$, respectively. Recall that we assume that $S = [0,1]^d$, the unit cube.

Consider now $\int_{S_{k_i}(Z)} K\left(\frac{Z - x}{\rho_{i,k_i}}\right) f_i(x)dx$. Substituting $u = \frac{x - Z}{\rho_{i,k_i}}$ and then taking a Taylor series expansion of $f_i$ using multi-index notation gives
\[
\int_{S_{k_i}(Z)} K\left(\frac{Z - x}{\rho_{i,k_i}}\right) f_i(x)dx = \rho_{i,k_i}^d \int_{||u|| < 1} K(u) f_i(Z + u\rho_{i,k_i})du
\]
\[
= \sum_{|\alpha| \leq s} \left(\frac{D^{|\alpha|} f_i(Z)}{\alpha!}\right) \rho_{i,k_i}^{|\alpha|} \int_{u:Z + u\rho_{i,k_i} \in S} u^\alpha K(u)du, + O\left(\rho_{i,k_i}^{d+s}\right)
\]
\[
\Rightarrow \mathbb{E}_{Z,\rho_{i,k_1}} \hat{f}_{i,k_1}(Z) = \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_{k_i}(Z))}
\]
\[
\times \left(\sum_{|\alpha| \leq s} \left(\frac{D^{|\alpha|} f_i(Z)}{\alpha!}\right) \rho_{i,k_i}^{|\alpha|} \int_{u:Z + u\rho_{i,k_i} \in S} u^\alpha K(u)du, + O\left(\rho_{i,k_i}^{s}\right)\right).
\]

**Lemma 8.** Let $\gamma(x,y)$ be an arbitrary function satisfying $\sup_{x,y} |\gamma(x,y)| < \infty$. Let $S = [0,1]^d$ and let $f_1, f_2 \in \Sigma(s,L)$. Let $Z$ be a realization of the density $f_2$ independent of $\hat{f}_{i,k_i}$ for $i = 1, 2$. Then for any integer $\lambda \geq 0$,
\[
\mathbb{E}\left[\gamma(f_1(Z), f_2(Z)) \mathbb{E}_{Z,\rho_{i,k_1}} \hat{f}_{i,k_1}(Z)\right] = \sum_{j=1}^{s} c_{15,j,q} \left(\frac{k_i}{N_i}\right)^{\frac{1}{2}} + \sum_{m=0}^{\lambda} \sum_{j=0}^{s} \frac{c_{15,i,a,j,m}}{k_i^{\frac{1}{2}} \rho_{i,k_i}^{\frac{1}{2}}} \left(\frac{k_i}{N_i}\right)^{\frac{1}{2}}
\]
\[
+ O\left(\left(\frac{k_i}{N_i}\right)^{\frac{1}{2}} + \frac{1}{k_i^{s+1}}\right).
\]
Proof: We use the substitution $T_i = \Pr(S_i(Z))$ which is the $k$th order statistic of a uniform random variable \cite{47}. Therefore, $T_i$ has a beta distribution with parameters $k_i$ and $N_i - k_i + 1$. This gives
\[
\mathbb{E} \left[ \gamma(f_1(Z), f_2(Z)) \mathbb{E}_{Z,\rho_{i,k_i}} \left[ \hat{f}_{i,k_i}(Z) \right] \right] \\
= (k_i - 1) \left( \frac{N_i - 1}{k_i - 1} \right) \int_0^1 \int_0^1 t^{k-1}(1-t)^{n-k} \mathbb{E}_{Z,\rho_{i,k_i}} \left[ \hat{f}_{i,k_i}(Z) \right] dt f_i(Z) \gamma(f_1(Z), f_2(Z)) dZ \\
= (k_i - 1) \left( \frac{N_i - 1}{k_i - 1} \right) \int_0^1 \int_0^1 t^{k-1}(1-t)^{n-k} \mathbb{E}_{Z,\rho_{i,k_i}} \left[ \hat{f}_{i,k_i}(Z) \right] f_i(Z) \gamma(f_1(Z), f_2(Z)) dZ dt \\
= (k_i - 1) \left( \frac{N_i - 1}{k_i - 1} \right) \int_0^1 \int_0^1 t^{k-1}(1-t)^{n-k} \mathbb{E}_{Z,\rho_{i,k_i}} \left[ \hat{f}_{i,k_i}(Z) \right] f_i(Z) \gamma(f_1(Z), f_2(Z)) dZ dt \\
+ (k_i - 1) \left( \frac{N_i - 1}{k_i - 1} \right) \int_0^1 \int_0^1 t^{k-1}(1-t)^{n-k} \mathbb{E}_{Z,\rho_{i,k_i}} \left[ \hat{f}_{i,k_i}(Z) \right] f_i(Z) \gamma(f_1(Z), f_2(Z)) dZ dt.
\]

Note that $T_i$ monotonically increases with $\rho_{i,k_i}$ and is therefore invertible. Thus $\rho_{i,k_i}$ and $T_i$ are deterministically related and $\rho_{i,k_i}$ can be viewed as a function of $T_i$. Thus we can consider separately the cases where $Z$ is in $S_{i_1}$ and $S_{i_2}$ even after making the change of variables.

We first consider $Z \in S_{i_1}$. It is clear in this case by \cite{22} and the symmetry of $K(u)$ that
\[
\mathbb{E}_{Z,\rho_{i,k_i}} \left[ \hat{f}_{i,k_i}(Z) \right] = \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_k(Z))} \left( f_i(Z) + \sum_{j=1}^{[s/2]} c_{i,j}(Z) \rho_{i,k_i}^{j} + O\left( \rho_{i,k_i}^{s} \right) \right)
\]

For $q \geq 2$, we obtain by the binomial theorem,
\[
\left( \mathbb{E}_{Z,\rho_{i,k_i}} \hat{f}_{i,k_i}(Z) \right)^j = \left( \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_k(Z))} \right)^j \left( f_i(Z) + \sum_{n=1}^{[s/2]} c_{i,j,n}(Z) \rho_{i,k_i}^{n} + O\left( \rho_{i,k_i}^{s} \right) \right)^j \\
\mathbb{E}_{Z,\rho_{i,k_i}} \left[ f_{i,k_i}(Z) \right] = \sum_{j=0}^{q} \binom{q}{j} \left( \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_k(Z))} \right)^j \left( f_i(Z) + \sum_{n=1}^{[s/2]} c_{i,j,n}(Z) \rho_{i,k_i}^{n} + O\left( \rho_{i,k_i}^{s} \right) \right)^j \\
= \sum_{j=0}^{q} \binom{q}{j} \left( \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_k(Z))} \right)^j \left( f_i(Z) + \sum_{n=1}^{[s/2]} c_{i,j,n}(Z) \rho_{i,k_i}^{n} + O\left( \rho_{i,k_i}^{s} \right) \right)^j \\
\times \left( f_i(Z) + \sum_{n=1}^{[s/2]} c_{i,j,n}(Z) \rho_{i,k_i}^{n} + O\left( \rho_{i,k_i}^{s} \right) \right)^j.
\]

By applying concentration inequality arguments \cite{48}, it can be shown that with high probability,
\[
\left( \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_k(Z))} \right)^j = \frac{1}{\left( 1 + \frac{\sqrt{q}}{\sqrt{k_i}} \right)^j}.
\]

Then applying the binomial theorem in reverse gives (with high probability)
\[
\sum_{j=0}^{q} \binom{q}{j} \left( \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_k(Z))} \right)^j (-1)^j = \left( 1 - \frac{1}{1 + \frac{\sqrt{q}}{\sqrt{k_i}}} \right)^q \\
= \left( \frac{6}{k_i} \right)^q \left( 1 + \frac{\sqrt{q}}{\sqrt{k_i}} \right)^q \\
= \left( \frac{6}{k_i} \right)^q \sum_{j=0}^{\infty} \binom{-q}{j} (-1)^j \left( \frac{6}{k_i} \right)^j \\
= \sum_{j=0}^{\lambda - 1} \theta \left( \frac{1}{k_i} \right)^j + O\left( \frac{1}{k_i^{\lambda+1}} \right),
\]
where \( \lambda \) is any nonnegative integer. Thus

\[
E \left[ \sum_{j=0}^{q} \binom{q}{j} \left( \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_{k_i}(Z))} \right)^j (-1)^j f_i^q(Z) \right] = \sum_{j=0}^{\lambda-1} c_{3,i,j,q} \frac{1}{k_i^{s+1}} + O \left( \frac{1}{k_i^{s+\lambda}} \right).
\]

For \( q = 1 \), we have

\[
(k_i - 1) \left( \frac{N_i - 1}{k_i - 1} \right) \int_0^1 t^{k_i-2}(1-t)^{n-k_i} \int_{S_{k_i}} f_i(Z) f_2(Z) dZ dt - \int_{S_{k_i}} f_i(Z) f_2(Z) dZ = 0.
\]

For the terms that include \( \rho_{\lambda i,k_i} \) for some positive integer \( \lambda \), we have for \( Z \in S_{k_i} \) that

\[
E \left[ \rho_{\lambda i,k_i} \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_{k_i}(Z))} \right] = (k_i - 1) \left( \frac{N_i - 1}{k_i - 1} \right) \int_0^1 t^{k_i-2}(1-t)^{n-k_i} \int_{S_{k_i}} \rho_{\lambda i,k_i} f_2(Z) dZ dt.
\]

We now find an expression for \( \rho_{i,k_i} \) in terms of \( T_i \) when \( Z \in S_{k_i} \). Recall that \( T_i = \Pr(S_{k_i}(Z)) \). By Taylor series expansion,

\[
T_i = \int_{S_{k_i}(Z)} f_i(x) dx
\]

\[
= \rho_{i,k_i}^{d} \left( f_i(Z) c_d + \sum_{j=1}^{[s/2]} c_{4,i,j}(Z) \rho_{i,k_i}^{2j} + O \left( \rho_{i,k_i}^{s} \right) \right)
\]

\[
\Rightarrow \rho_{i,k_i} = \frac{T_i^{\frac{1}{d}}}{f_i(Z) c_d + \sum_{j=1}^{[s/2]} c_{4,i,j}(Z) \rho_{i,k_i}^{2j} + O \left( \rho_{i,k_i}^{s} \right)}.
\]

Note that as \( \rho_{i,k_i} \downarrow 0 \), we have that \( \left| \sum_{j=1}^{[s/2]} c_{4,i,j}(Z) \rho_{i,k_i}^{2j} + O \left( \rho_{i,k_i}^{s} \right) \right| < f_i(Z) c_d \) for sufficiently small \( \rho_{i,k_i} \) since we assume that \( f_i(x) \geq \varepsilon_0 > 0 \). Therefore, we can apply the generalized binomial theorem to obtain

\[
\left( f_i(Z) c_d + \sum_{j=1}^{[s/2]} c_{4,i,j}(Z) \rho_{i,k_i}^{2j} + O \left( \rho_{i,k_i}^{s} \right) \right)^{-\frac{1}{d}} = \sum_{m=0}^{\infty} \frac{(-1/d)^m}{m!} \left( f_i(Z) c_d \right)^{-1/d-m} \times \left( \sum_{j=1}^{[s/2]} c_{4,i,j}(Z) \rho_{i,k_i}^{2j} + O \left( \rho_{i,k_i}^{s} \right) \right)^m
\]

\[
= (f_i(Z) c_d)^{-1/d} + \sum_{j=1}^{[s/2]} c_{5,i,j}(Z) \rho_{i,k_i}^{2j} + O \left( \rho_{i,k_i}^{s} \right).
\]

Using this expression in (24) and resubstituting the LHS into the RHS gives that

\[
\rho_{i,k_i} = \left( \frac{T_i}{f_i(Z) c_d} \right)^\frac{1}{d} + \sum_{j=1}^{[s/2]} c_{6,i,j}(Z) T_i^{2j/d} + O \left( T_i^{s/d} \right),
\]

\[
\Rightarrow \rho_{\lambda i,k_i} = \left( \frac{T_i}{f_i(Z) c_d} \right)^\frac{1}{d} + \sum_{j=1}^{[s/2]} c_{7,i,j}(Z) T_i^{2j/d} + O \left( T_i^{s/d} \right).
\]

Therefore,

\[
E \left[ \rho_{\lambda i,k_i} \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_{k_i}(Z))} \right]
\]

\[
= (k_i - 1) \left( \frac{N_i - 1}{k_i - 1} \right) \int_0^1 t^{k_i-2+\lambda/d}(1-t)^{n-k_i} \int_{S_{k_i}} \frac{f_2(Z)}{f_i(Z) c_d} \frac{1}{\Pr(S_{k_i}(Z))} dZ dt
\]

\[
+ \sum_{j=1}^{[s/2]} (k_i - 1) \left( \frac{N_i - 1}{k_i - 1} \right) \int_0^1 t^{k_i-2+2j/\lambda/d}(1-t)^{n-k_i} \int_{S_{k_i}} f_2(Z) c_{7,i,j}(Z) dZ dt
\]

\[
= C_{7,i,0} \left( \frac{k_i}{N_i} \right)^{\lambda/d} + \sum_{j=1}^{[s/2]} C_{7,i,j} \left( \frac{k_i}{N_i} \right)^{2j/d} + O \left( \left( \frac{k_i}{N_i} \right)^{s/d} \right).
\]
Combining this result with (23) gives for \( q \geq 2 \) and any integer \( \lambda \geq 0 \)

\[
N_i \left( \frac{N_i - 1}{k_i - 1} \right) \int_0^1 t^{k_i - 2} (1 - t)^{N_i - k_i} \sum_{i=1}^{B_i} \mathbb{E}_{Z, p_{i,k_i}} \left[ \hat{f}_{i,k_i}(Z) \right] f_i(Z) \gamma (f_1(Z), f_2(Z)) dZ dt
\]

\[
= \sum_{j=0}^{\lambda-1} c_{3,i,j,q} \mathbb{E}_{Z, p_{i,k_i}} \left[ \hat{f}_{i,k_i}(Z) \right] f_i(Z) \gamma (f_1(Z), f_2(Z)) dZ dt
\]

Similarly, for \( q = 1 \),

\[
N_i \left( \frac{N_i - 1}{k_i - 1} \right) \int_0^1 t^{k_i - 2} (1 - t)^{N_i - k_i} \sum_{i=1}^{B_i} \mathbb{E}_{Z, p_{i,k_i}} \left[ \hat{f}_{i,k_i}(Z) \right] f_i(Z) \gamma (f_1(Z), f_2(Z)) dZ dt
\]

\[
= \sum_{j=0}^{\lambda-1} c_{7,i,j,m,q} \mathbb{E}_{Z, p_{i,k_i}} \left[ \hat{f}_{i,k_i}(Z) \right] f_i(Z) \gamma (f_1(Z), f_2(Z)) dZ dt
\]

We now consider the case where \( Z \in S_{B_1} \). In this case, we extend the density beyond the boundary. This gives

\[
\mathbb{E}_{Z, p_{i,k_i}} \left[ \hat{f}_{i,k_i}(Z) \right] = \frac{k_i - 1}{N_i} \frac{1}{\rho_{i,k_i}} \int_{S_{B_1}(Z) \cap S} K \left( \frac{Z - x}{\rho_{i,k_i}} \right) f_i(x) dx
\]

\[
= \frac{k_i - 1}{N_i} \frac{1}{\rho_{i,k_i}} \int_{S_{B_1}(Z)} K \left( \frac{Z - x}{\rho_{i,k_i}} \right) f_i(x) dx
\]

\[
= \frac{k_i - 1}{N_i} \frac{1}{\rho_{i,k_i}} \int_{x \in S} K \left( \frac{Z - x}{\rho_{i,k_i}} \right) f_i(x) dx
\]

\[
= T_1(Z, \rho_{i,k_i}) - T_2(Z, \rho_{i,k_i})
\]

The expression for \( T_1(Z, \rho_{i,k_i}) \) is identical to that when \( Z \in S_{B_i} \) and so taking the expectation gives the same results. Therefore, we focus on \( T_2(Z, \rho_{i,k_i}) \). As before, we substitute \( u = (Z - x)/\rho_{i,k_i} \) inside the integral and take a Taylor series expansion of \( f_i \) to get

\[
\sum_{|\alpha| \leq \lfloor s/2 \rfloor} D^\alpha f_i(Z) \rho_{i,k_i}^{\alpha} \int_{u \in S} u^\alpha K(u) du + O \left( \rho_{i,k_i}^s \right)
\]

As before, we can again substitute \( T_i = \text{Pr} \left( S_{B_1}(Z) \right) \). However, we need to find an expression for \( \rho_{i,k_i} \) in terms of \( T_i \), for \( Z \in S_{B_1} \). Note that

\[
T_i = \int_{z \in S_{B_1}(Z) \cap S} f_i(z) dz.
\]

\[
= \int_{z \in S_{B_1}(Z)} f_i(z) dz - \int_{z \in S_{B_1}(Z) \cap S^c} f(z) dz
\]

\[
= \rho_{i,k_i}^d \left( f_i(Z) c_d + \sum_{\alpha=1}^{\lfloor s/2 \rfloor} c_{4,i,j}^{s,i,j} f_i(Z) \rho_{i,k_i}^{2j} + O(\rho_{i,k_i}^s) \right)
\]

\[
- \int_{z \in S_{B_1}(Z) \cap S^c} \left( \sum_{|\alpha| \leq \lfloor s/2 \rfloor} (z - Z)^\alpha D^\alpha f_i(Z) + O ( (z - Z)^s ) \right) dz.
\]

We need to simplify the second integral in (25) before solving for \( \rho_{i,k_i} \). If we assume that the support \( S = [0,1]^d \), then we can use the techniques used in Appendix A.

Assume that \( d \) is odd as as the case for even \( d \) will be similar. We first consider the case where only a single coordinate \( Z_{(1)} \) is close to the boundary. Without loss of generality, we assume that \( Z_{(1)} \) is close to 1. Then for a given \( \alpha \), we can use (13) to obtain

\[
\int_{z \in S_{B_1}(Z) \cap S^c} (z - Z)^\alpha D^\alpha f_i(Z) dz = \rho_{i,k_i}^{d+|\alpha|} \sum_{\alpha=1}^{\lfloor s/2 \rfloor} \rho_{i,k_i}^{2j} \left( \sqrt{1 - \frac{1 - Z_{(1)}}{\rho_{i,k_i}}} \right)^j \times \left( \frac{1 - Z_{(1)}}{\rho_{i,k_i}} \right)^m.
\]

(26)
where \( p_{m,\ell,\alpha,i}(Z) \) is \( |s| - |\alpha| \) times differentiable wrt \( Z \). Now expand \( p_{m,\ell,\alpha,i}(Z) \) only in the \( Z_{(1)} \) coordinate at \( Z_{(1)} = 1 \) to get

\[
p_{m,\ell,\alpha,i}(Z) = \sum_{j=0}^{|s| - |\alpha|} \frac{\partial^j p_{m,\ell,\alpha,i}(1, Z_{(2)}, \ldots, Z_{(d)})}{\partial Z_{(1)}^j} (1 - Z_{(1)})^n.
\]

Substituting this into (26) and substituting \( W = \frac{1 - Z_{(1)}}{\rho_{i,k_i}} \) gives

\[
\sum_{m=0}^{d} \sum_{\ell=0}^{d+|\alpha|} \sum_{j=0}^{|s| - |\alpha|} \frac{\partial^j p_{m,\ell,\alpha,i}(1, Z_{(2)}, \ldots, Z_{(d)})}{\partial Z_{(1)}^j} \frac{1}{j!} \left( \sqrt{1 - \left( \frac{1 - Z_{(1)}}{\rho_{i,k_i}} \right)^2} \right)^{\ell} \left( \frac{1 - Z_{(1)}}{\rho_{i,k_i}} \right)^{m+j} \rho_{i,k_i}^{j+d+|\alpha|}.
\]

where \( Z' = (1, Z_{(2)}, \ldots, Z_{(d)}) \) and \( p_{m,\ell,\alpha,i}'(Z') = \frac{\partial^j p_{m,\ell,\alpha,i}(1, Z_{(2)}, \ldots, Z_{(d)})}{\partial Z_{(1)}^j} \). The variable \( W \) ranges from 0 to 1. Thus we have separated the dependence on \( \rho_{i,k_i} \). Substituting these results into (25) gives

\[
T_i = \rho_{i,k_i}^d \left( f_i(Z)c_d + \sum_{j=1}^{|s|/2} c_{4,i,j}(Z) \rho_{i,k_i}^{2j} + O(\rho_{i,k_i}^s) \right)
-
\rho_{i,k_i}^d \sum_{|\alpha| \leq |s|} \sum_{\ell=0}^{d+|\alpha|} \sum_{j=0}^{|s| - |\alpha|} p_{m,\ell,\alpha,i}(Z') \left( \sqrt{1 - W^2} \right)^\ell W^{m+j} \rho_{i,k_i}^{j+d+|\alpha|}.
\]

By substituting \( Z_{(1)} = 1 - W \rho_{i,k_i} \) in the first term and taking a Taylor series expansion of \( f_i(Z)^{-1/d} \) and \( c_{4,i,j}(Z) \) at \( Z_{(1)} = 1 \) gives

\[
\sum_{j=0}^{|s|} c_{8,i,j}(Z'') \rho_{i,k_i}^{j+d} + O \left( \rho_{i,k_i}^s \right).
\]

where \( Z'' = (W, Z_{(2)}, \ldots, Z_{(d)}) \). Thus we can write

\[
T_i = \rho_{i,k_i}^d \left( \sum_{j=0}^{|s|} c_{9,i,j}(Z'') \rho_{i,k_i}^j + O \left( \rho_{i,k_i}^s \right) \right)
\Rightarrow \rho_{i,k_i} = \frac{t^{\frac{1}{d}}}{\left( \sum_{j=0}^{|s|} c_{9,i,j}(Z'') \rho_{i,k_i}^j + O \left( \rho_{i,k_i}^s \right) \right)^{\frac{1}{d}}}.
\]

Then since \( \rho_{i,k_i} \downarrow 0 \), applying the generalized binomial theorem to the denominator gives

\[
\left( \sum_{j=0}^{|s|} c_{9,i,j}(Z'') \rho_{i,k_i}^j + O \left( \rho_{i,k_i}^s \right) \right)^{-\frac{1}{d}}
= \sum_{m=0}^\infty \left( -\frac{1}{d} \right)_m c_{9,i,0}(Z'')^{-\frac{1}{d} - m} \left( \sum_{j=1}^{|s|} c_{9,i,j}(Z'') \rho_{i,k_i}^j + O \left( \rho_{i,k_i}^s \right) \right)^m
= c_{9,i,0}(Z'')^{-\frac{1}{d}} + \sum_{j=1}^{|s|} c_{10,i,j}(Z'') \rho_{i,k_i}^j + O \left( \rho_{i,k_i}^s \right).
\]

Applying this result to (27) gives

\[
\rho_{i,k_i} = \left( \frac{T_i}{c_{9,i,0}(Z'')} \right)^{\frac{1}{d}} + T_i^{\frac{1}{d}} \sum_{j=1}^{|s|} c_{10,i,j}(Z'') \rho_{i,k_i}^j + O \left( T_i^{\frac{1}{d}} \rho_{i,k_i}^s \right).
\]
Resubstituting the LHS of (28) into the RHS multiple times then gives
\[
\rho_{i,k_i} = \sum_{j=1}^{[s]} c_{11,i,j}(Z') T_i^j + O\left(T_i^j\right)
\]
\[
\implies \rho_{i,k_i} = \sum_{j=1}^{[s]} c_{12,i,j,\lambda}(Z') T_i^{j\lambda} + O\left(T_i^{j\lambda}\right).
\]

Given these results and the fact that \(T_i\) has a beta distribution, we have that
\[
E\left[1_{\{Z \in S_{\lambda}\}} \mathbb{E}_{Z,\rho_{i,k_i}} \left[ \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_h(Z))\rho_{i,k_i}} \right] \right]
\]
\[
= \frac{k_i - 1}{N_i} \left(\frac{N_i - 1}{k_i - 1}\right) \int^1_0 t^{k_i-2}(1-t)^{N_i-k_i-1} \int_S \rho_{i,k_i}^j f_i(Z) dZ dt.
\]

Taking a Taylor series expansion of \(f_i\) at \(Z(1) = 1\) gives
\[
f_i(Z) = \sum_{j=0}^{[s]} \frac{\partial^j f_i(Z)}{\partial Z^j(1)} W^j \rho_{i,k_i}^j + O\left(\rho_{i,k_i}^s\right).
\]

Combining all of these results gives that
\[
E\left[1_{\{Z \in S_{\lambda}\}} \mathbb{E}_{Z,\rho_{i,k_i}} \left[ \frac{k_i - 1}{N_i} \frac{1}{\Pr(S_h(Z))\rho_{i,k_i}} \right] \right]
\]
has terms of the form of
\[
(k_i - 1)\left(\frac{N_i - 1}{k_i - 1}\right) \int^1_0 t^{k_i-2}(1-t)^{N_i-k_i-1} dt = \left(\frac{k_i}{N_i}\right)^{\frac{k_i+1}{2}} + O\left(\frac{k_i}{N_i}\right).
\]

Therefore,
\[
E\left[T_2(Z, \rho_{i,k_i})\right] = (k_i - 1)\left(\frac{N_i - 1}{k_i - 1}\right) \int^1_0 t^{k_i-2}(1-t)^{N_i-k_i-1} dt
\]
\[
\times \int_{S_{\lambda}} \left(\sum_{j=0}^{[s]} c_{13,i,j}(Z') t^{j\lambda} + O\left(t^{j\lambda}\right)\right) dZ' dt
\]
\[
= \sum_{j=1}^{[s]} c_{14,i,j} \left(\frac{k_i}{N_i}\right)^{j\lambda} + O\left(\frac{k_i}{N_i}\right)^{\min(s,d)/d}.
\]

For \(E[(T_1(Z, \rho_{i,k_i}) - T_2(Z, \rho_{i,k_i}))^q]\), we have by the binomial theorem that
\[
(T_1(Z, \rho_{i,k_i}) - T_2(Z, \rho_{i,k_i}))^q = \sum_{j=0}^{q} \binom{q}{j} T_1(Z, \rho_{i,k_i})^j T_2(Z, \rho_{i,k_i})^{q-j}.
\]

Applying a similar analysis gives similar results.

For the case when \(S_{\lambda}(Z)\) intersects multiple boundary points, a similar approach can be used as in Appendix A-B. This will yield a similar expression to (29). Combining all results with the fact that \(\gamma(x,y)\) is bounded finishes the proof.

**Lemma 9.** Let \(\gamma(x,y)\) be an arbitrary function satisfying \(\sup_{x,y} |\gamma(x,y)| < \infty\). Let \(Z\) be a realization of the density \(f_2\) independent of \(f_{i,k_i}\) for \(i = 1, 2\). Then for any integer \(\lambda \geq 0\)
\[
E\left[\gamma(f_1(Z), f_2(Z)) \mathbb{E}_{Z,\rho_{1,k_1}} \left[ f_{1,k_1}(Z) \right] \mathbb{E}_{Z,\rho_{2,k_2}} \left[ f_{2,k_2}(Z) \right] \right]
\]
\[
= \sum_{j=0}^{[s]} \sum_{i+j \neq 0} c_{16,i,j,q,t} \left(\frac{k_1}{N_1}\right)^{\frac{q}{2}} \left(\frac{k_2}{N_2}\right)^{\frac{q}{2}} + O\left(\max\left(\frac{k_1}{N_1}, \frac{k_2}{N_2}\right)^{\frac{\min(s,d)}{d}} + \frac{1}{\min(k_1, k_2)^{\frac{q}{2}}}ight)
\]
\[+
\sum_{m=0}^{\lambda} \sum_{n+i \neq 0} \sum_{n+1 \neq 0} c_{16,m,n,q,t} \frac{1}{k_1^{\frac{m}{2}}} \frac{1}{k_2^{\frac{n}{2}}} \left(\frac{k_1}{N_1}\right)^{\frac{q}{2}} \left(\frac{k_2}{N_2}\right)^{\frac{q}{2}}.
\]

**Proof:** Note that \(\rho_{1,k_1}\) and \(\rho_{2,k_2}\) are conditionally independent of each other given \(Z\). Applying similar techniques as in the proof of Lemma 8 yields the result.
Applying Lemmas 8 and 9 to (21) gives

\[
\mathbb{E} \left[ g \left( \mathbb{E}_{Z, \rho_{1,k_1}} (Z) \hat{f}_{1,k_1} (Z), \mathbb{E}_{Z, \rho_{2,k_2}} (Z) \hat{f}_{2,k_2} (Z) \right) - g (f_1 (Z), f_2 (Z)) \right] \\
= \sum_{j=0}^{s} \sum_{j=0}^{s} c_{18,i,j} \left( \frac{k_1}{N_1} \right)^{\frac{j}{2}} \left( \frac{k_2}{N_2} \right)^{\frac{j}{2}} + O \left( \max \left( \frac{k_1}{N_1}, \frac{k_2}{N_2} \right)^{\min(s,d)+1} + \frac{1}{\min(k_1, k_2)^{s+1}} \right) \\
+ \sum_{m=0}^{\lambda} \sum_{m=0}^{r} \left( \frac{c_{17.1,m}}{k_1^{1+m}} \left( \frac{k_1}{N_1} \right)^{\frac{j}{2}} + c_{17.2,m} \frac{k_2}{N_2} \right) \\
+ \sum_{j=1}^{r} \left( c_{17.1,j} \left( \frac{k_1}{N_1} \right)^{\frac{j}{2}} + c_{17.2,j} \left( \frac{k_2}{N_2} \right)^{\frac{j}{2}} \right) \\
+ \sum_{m=0}^{\lambda} \sum_{m=0}^{s} \sum_{n=0}^{\lambda} \sum_{n+i=0}^{s} \left( \frac{c_{18,i,j,m,n}}{k_1^{1+m} k_2^{1+n}} \left( \frac{k_1}{N_1} \right)^{\frac{j}{2}} \left( \frac{k_2}{N_2} \right)^{\frac{j}{2}} \right). 
\]

We now focus on the first term in (19). The truncated Taylor series expansion of \( g \left( \hat{f}_{1,k_1} (Z), \hat{f}_{2,k_2} (Z) \right) \) around \( \mathbb{E}_{Z, \rho_{1,k_1}} \hat{f}_{1,k_1} (Z) \) and \( \mathbb{E}_{Z, \rho_{2,k_2}} \hat{f}_{2,k_2} (Z) \) gives

\[
g \left( \hat{f}_{1,k_1} (Z), \hat{f}_{2,k_2} (Z) \right) = \sum_{i=0}^{r} \sum_{j=0}^{r} \frac{\partial^{i+j} g(x, y)}{\partial x^i \partial y^j} \left| x=\mathbb{E}_{Z, \rho_{1,k_1}} \hat{f}_{1,k_1} (Z), y=\mathbb{E}_{Z, \rho_{2,k_2}} \hat{f}_{2,k_2} (Z) \right| \frac{\hat{e}_{1,k_1}^i (Z) \hat{e}_{2,k_2}^j (Z)}{i! j!} + o \left( \hat{e}_{1,k_1}^i (Z) + \hat{e}_{2,k_2}^j (Z) \right), 
\]

where \( \hat{e}_{1,k_1} := \hat{f}_{1,k_1} (Z) - \mathbb{E}_{Z, \rho_{1,k_1}} \hat{f}_{1,k_1} (Z) \). We thus require expressions for \( \mathbb{E}_{Z, \rho_{1,k_1}} \left[ \hat{e}_{1,k_1}^q (Z) \right] \) to control this expression.

**Lemma 10.** Let \( Z \) be a realization of the density \( f_2 \) that is in the interior of the support \( \nu_{1,k_1} \) and is independent of \( \hat{f}_{1,k_1} \) for \( i = 1, 2 \). Let \( u(q) \) be the set of integer divisors of \( q \) including 1 but excluding \( q \). Then,

\[
\mathbb{E}_{Z, \rho_{1,k_1}} \left[ \hat{e}_{1,k_1}^q (Z) \right] = \begin{cases} \\
\frac{k_j-1}{N_1 \text{Pr}(S_q(Z))} \sum_{j \in u(q)} \frac{1}{(N_1 \rho_{1,k_1}^q)^{s}} \sum_{m=0}^{\lfloor s/2 \rfloor} c_{1,q,j,m} (Z) \rho_{1,k_1}^{2m} + O \left( \frac{\rho_{1,k_1}^2}{k_1} \right), & q \geq 2 \\
0, & q = 1 \\
\end{cases} 
\]

\[
\mathbb{E}_{Z, \rho_{1,k_1}, \rho_{2,k_2}} \left[ \hat{e}_{1,k_1}^q (Z) \hat{e}_{2,k_2}^l (Z) \right] = \\
\begin{cases} \\
\frac{k_j-1}{N_1 \text{Pr}(S_q(Z))} \sum_{j \in u(q)} \frac{1}{(N_1 \rho_{1,k_1}^q)} \sum_{m=0}^{\lfloor s/2 \rfloor} c_{1,q,j,m} (Z) \rho_{1,k_1}^{2m} \right) \times q \geq 2 \\
\left( \sum_{i \in u(l)} \frac{1}{(N_2 \rho_{2,k_2}^l)} \sum_{m=0}^{\lfloor s/2 \rfloor} c_{2,l,i,t} (Z) \rho_{2,k_2}^{2m} \right) + O \left( \frac{1}{N_1} + \frac{1}{N_2} \right), & q = 1 \text{ or } l = 1. \\
\end{cases} 
\]

**Proof:** Define the random variable \( V_i (Z) = K \left( \frac{X_i - Z}{\rho_{2,k_2}} \right) - \mathbb{E}_{Z, \rho_{2,k_2}} K \left( \frac{X_i - Z}{\rho_{2,k_2}} \right). \) Then

\[
\hat{e}_{2,k_2} (Z) = \frac{1}{N_2 \rho_{2,k_2}^l} \sum_{i=1}^{N_2} V_i (Z). 
\]

Note that \( \mathbb{E}_{Z, \rho_{2,k_2}} V_i (Z) = 0. \) From our previous results, we have for \( j \geq 1, \)

\[
\mathbb{E}_{Z, \rho_{2,k_2}} \left[ K^j \left( \frac{X_i - Z}{\rho_{2,k_2}} \right) \right] = \mathbb{E}_{Z, \rho_{2,k_2}} \left[ K \left( \frac{X_i - Z}{\rho_{2,k_2}} \right) \right] \\
= \frac{k_2-1}{N_2} \rho_{2,k_2}^l \sum_{m=0}^{\lfloor s/2 \rfloor} c_{2,m} (Z) \rho_{2,k_2}^{2m} + O \left( \rho_{2,k_2}^2 \right). 
\]
By the binomial theorem,
\[ 
\mathbb{E}_{z_{i,k_2}} \left[ V_i^j(z) \right] 
= \sum_{n=0}^{\infty} \binom{j}{n} \mathbb{E}_{z_{i,k_2}} \left[ K^j \left( \frac{X_i - Z}{\rho_{2,k_2}} \right) \right] \mathbb{E}_{z_{i,k_2}} \left[ K \left( \frac{X_i - Z}{\rho_{2,k_2}} \right) \right]^{j-n} 
= \sum_{n=0}^{\infty} \binom{j}{n} \left( \frac{\rho_{2,k_2}^j}{N_2} \mathbb{P}(S(Z)) \sum_{m=0}^{\infty} c_{2,m}(z) \rho_{2,k_2}^{2m} \right) O \left( \left( \frac{\rho_{2,k_2}^j}{N_2} \mathbb{P}(S(Z)) \right)^{j-n} \right) 
= \frac{k_2 - 1}{N_2} \sum_{m=0}^{\infty} c_{2,m}(z) \rho_{2,k_2}^{2m} + O \left( \left( \frac{\rho_{2,k_2}^j}{N_2} \mathbb{P}(S(Z)) \right)^{k_2 - 1} \right). 
\]

We can use these expressions to simplify \( \mathbb{E}_{z_{i,k_1}} \left[ \tilde{e}_{i,k_1}(z) \right] \). For example, let \( q = 2 \). Due to the independence of the \( X_i \)'s and the fact that with high probability
\[ 
\left( \frac{1}{\mathbb{P}(S_i(z))} \right)^2 = O \left( \frac{1}{k_1} \right), 
\]
we obtain
\[ 
\mathbb{E}_{z_{i,k_2}} \left[ \tilde{e}_{i,k_2}(z) \right] = \frac{1}{N_2 \rho_{2,k_2}^2} \mathbb{E}_{z_{i,k_2}} \left[ V_i^2(z) \right] 
= \frac{k_2 - 1}{N_2 \mathbb{P}(S(Z))} \frac{1}{N_2 \rho_{2,k_2}^2} \sum_{m=0}^{\infty} c_{2,m}(z) \rho_{2,k_2}^{2m} + O \left( \rho_{2,k_2}^j \right). 
\]

Similarly, for \( q = 3 \),
\[ 
\mathbb{E}_{z_{i,k_2}} \left[ \tilde{e}_{i,k_2}(z) \right] = \frac{1}{N_2 \rho_{2,k_2}^3} \mathbb{E}_{z_{i,k_2}} \left[ V_i^3(z) \right] 
= \frac{k_2 - 1}{N_2 \mathbb{P}(S(Z))} \left( \frac{1}{N_2 \rho_{2,k_2}^3} \right)^2 \sum_{m=0}^{\infty} c_{2,m}(z) \rho_{2,k_2}^{2m} + O \left( \rho_{2,k_2}^j \right), 
\]
and for \( q = 4 \),
\[ 
\mathbb{E}_{z_{i,k_2}} \left[ \tilde{e}_{i,k_2}(z) \right] = \frac{1}{N_2 \rho_{2,k_2}^4} \mathbb{E}_{z_{i,k_2}} \left[ V_i^4(z) \right] + \frac{N_2 - 1}{N_2 \rho_{2,k_2}^4} \left( \mathbb{E}_{z_{i,k_2}} \left[ V_i^2(z) \right] \right)^2 
= \frac{k_2 - 1}{N_2 \mathbb{P}(S(Z))} \left( \frac{1}{N_2 \rho_{2,k_2}^4} \right)^2 \sum_{m=0}^{\infty} c_{2,m}(z) \rho_{2,k_2}^{2m} + O \left( \rho_{2,k_2}^j \right). 
\]

It can then be seen that for \( q \geq 2 \), the pattern is given in the first expression in the lemma statement.

For any integer \( q \), the largest possible factor is \( q/2 \). Therefore, the smallest possible exponent on the \( N_2 \rho_{2,k_2}^j \) term is \( q/2 \). This increases as \( q \) increases. A similar expression for \( \mathbb{E}_{z_{i,k_1}} \left[ \tilde{e}_{i,k_1}(z) \right] \) for \( i = 1 \) can be proved using a similar technique. The second expression in the lemma statement then follows from the fact that \( \hat{e}_{1,k_1}(z) \) and \( \hat{e}_{2,k_2}(z) \) are conditionally independent given \( z \), \( \rho_{1,k_1} \), and \( \rho_{2,k_2} \).

For general \( g \), we can only say that
\[ 
\frac{\partial^{i+j} g(x,y)}{\partial x^i \partial y^j} \bigg|_{x = \mathbb{E}_{z_{i,k_1}} \tilde{e}_{i,k_1}(z), \quad y = \mathbb{E}_{z_{i,k_2}} \tilde{e}_{i,k_2}(z)} = O(1). 
\]

By applying similar techniques as in the proofs of Lemmas 8 and 9, it can then be shown with the application of Lemma 10 and the fact that with high probability
\[ 
\left( \frac{1}{\mathbb{P}(S_i(z))} \right)^j \left( \frac{1}{k_1} \right)^j = O \left( \frac{1}{k_1} \right), 
\]
the expected value of (31) reduces to
\[ 
\mathbb{E} \left[ g \left( \mathbb{E}_{z_{i,k_1}}(z) \tilde{e}_{1,k_1}(z), \mathbb{E}_{z_{i,k_2}}(z) \tilde{e}_{2,k_2}(z) \right) \right] + O \left( \frac{1}{k_1} + \frac{1}{k_2} \right). 
\]
If \( g(x, y) \) has mixed derivatives of the form \( x^\alpha y^\beta \) for \( \alpha, \beta \in \mathbb{R} \), we can apply the generalized binomial theorem prior to taking the expectation to show that

\[
\mathbb{E} \left[ g \left( \hat{f}_{1,k_1}(Z), \hat{f}_{2,k_2}(Z) \right) - g \left( \mathbb{E}_{Z_{p_1,k_1}}(Z), \mathbb{E}_{Z_{p_2,k_2}}(Z) \right) \right] = \sum_{j=1}^{\nu/2} \sum_{r=1}^{\nu/2} \sum_{i=1}^{j} \sum_{n=0}^{m} c_{19,1,i,m,n} \left( \frac{k_1}{N_1} \right)^{\frac{r}{2}} \left( \frac{k_2}{N_2} \right)^{\frac{r}{2}} + O \left( \frac{1}{k_1^{\nu/2}} + \frac{1}{k_2^{\nu/2}} + \left( \frac{k_1}{N_1} \right)^{\frac{\nu}{2}} + \left( \frac{k_2}{N_2} \right)^{\frac{\nu}{2}} \right).
\]

Combining (21) with either (32) or (33) completes the proof of Theorem 2.

APPENDIX C

PROOF OF THEOREM 3 (VARIANCE)

To bound the variance of the plug-in estimator \( \hat{G}_{k_1,k_2} \), we will again use the Efron-Stein inequality [49]:

**Lemma 11** (Efron-Stein Inequality). Let \( X_1, \ldots, X_n, X_1', \ldots, X_n' \) be independent random variables on the space \( S \). Then if \( f : S \times \cdots \times S \to \mathbb{R} \), we have that

\[
\mathbb{V} \left( f(X_1, \ldots, X_n) \right) \leq \frac{1}{2} \sum_{i=1}^{n} \mathbb{E} \left[ \left( f(X_1, \ldots, X_n) - f(X_1', \ldots, X_n') \right)^2 \right].
\]

Suppose we have samples \( \{X_1, \ldots, X_{N_2}, Y_1, \ldots, Y_{N_1}\} \) and \( \{X_1', \ldots, X_{N_2}, Y_1, \ldots, Y_{N_1}\} \) and denote the respective estimators as \( \hat{G}_{k_1,k_2} \) and \( \hat{G}'_{k_1,k_2} \). We have that

\[
\left| \hat{G}_{k_1,k_2} - \hat{G}'_{k_1,k_2} \right| \leq \frac{1}{N_2} \left| g \left( \hat{f}_{1,k_1}(X_1), \hat{f}_{2,k_2}(X_1) \right) - g \left( \hat{f}_{1,k_1}(X'_1), \hat{f}_{2,k_2}(X'_1) \right) \right| + \frac{1}{N_2} \sum_{j=2}^{N_2} \left| g \left( \hat{f}_{1,k_1}(X_j), \hat{f}_{2,k_2}(X_j) \right) - g \left( \hat{f}_{1,k_1}(X_j), \hat{f}_{2,k_2}(X_j) \right) \right|.
\]

Define \( P_{k_1}(X_j) = \Pr (S_{k_1}(X_j)) \). This is a random variable denoting the probability that a point drawn from \( f_i \) falls into the \( k_i \)th nearest neighbor ball of \( X_j \). As mentioned in Appendix B the distribution of \( P_{k_1}(X_j) \) is independent of \( X_j \) and \( f_i \) and is a beta random variable [50] with density

\[
f_{k_1}(p_{k_1}) = \frac{M_i!}{(k_i - 1)!(M_i - k_i)!} p_{k_1}^{k_i - 1} (1 - p_{k_1})^{M_i - k_i}.
\]

Define

\[
\tilde{f}_{i,k_1}(X_j) = f_i(X_j) \frac{k_i - 1}{M_i P_{k_1}(X_j)}.
\]

We then have that with high probability [48],

\[
\tilde{f}_{i,k_1}(X_j) = \tilde{f}_{i,k_1}(X_j) + O \left( \left( \frac{k_i}{M_i} \right)^{\frac{\nu}{2}} \right).
\]

The following lemma can be used to control the first term in (34):

**Lemma 12.**

\[
\mathbb{E} \left[ \left| g \left( \tilde{f}_{1,k_1}(X_1), \tilde{f}_{2,k_2}(X_1) \right) - g \left( \tilde{f}_{1,k_1}(X'_1), \tilde{f}_{2,k_2}(X'_1) \right) \right|^2 \right] = O(1).
\]

**Proof:** Since \( g \) is Lipschitz continuous with constant \( C_g \), we have

\[
\left| g \left( \tilde{f}_{1,k_1}(X_1), \tilde{f}_{2,k_2}(X_1) \right) - g \left( \tilde{f}_{1,k_1}(X'_1), \tilde{f}_{2,k_2}(X'_1) \right) \right| \leq C_g \left| \tilde{f}_{1,k_1}(X_1) - \tilde{f}_{1,k_1}(X'_1) \right| + C_g \left| \tilde{f}_{2,k_2}(X_1) - \tilde{f}_{2,k_2}(X'_1) \right|.
\]
From the triangle inequality, Jensen’s inequality, and (35), we get
\[
\mathbb{E} \left[ \left( \tilde{f}_{i,k_i}(X_i) - \tilde{f}_{i,k_i}(X_1) \right)^2 \right] \leq 2\mathbb{E} \left[ \left( \tilde{f}_{i,k_i}(X_1) \right)^2 \right] \\
\leq 4\mathbb{E} \left[ \left( \tilde{f}_{i,k_i}(X_1) \right)^2 \right] + O \left( \frac{(k_i)}{M_i} \right)^{\frac{3}{2}} \\
= 4\mathbb{E} \left[ f_i^2(X_1) \right] \frac{(k_i - 1)^2}{M_i^2} \cdot \frac{M_i(M_i - 1)}{(k_i - 1)(k_i - 2)} + O \left( \frac{(k_i)}{M_i} \right)^{\frac{3}{2}}.
\]
(37)

Combining (37) with (36) after applying Jensen’s inequality gives the result.

To control the second term in (34), consider the following events:

- \( A_1(X_i): X_i \) is strictly within the \( k_2\)-nn ball around \( X_i \) w.r.t the sample \( \{X_1, \ldots, X_{N_2}\} \setminus \{X_i\} \).
- \( A_2(X_i): X_i \) is the \( k_2\)th nearest neighbor of \( X_i \) w.r.t the sample \( \{X_1, \ldots, X_{N_2}\} \setminus \{X_i\} \).
- \( A_3(X_i): X_i \) is strictly outside of the \( k_2\)-nn ball around \( X_i \) w.r.t the sample \( \{X_1, \ldots, X_{N_2}\} \setminus \{X_i\} \).
- \( B_1(X_i): X_i \) is strictly within the \( k_2\)-nn ball around \( X_i \) w.r.t the sample \( \{X_1, X_2, \ldots, X_{N_2}\} \setminus \{X_i\} \).
- \( B_2(X_i): X_i \) is the \( k_2\)th nearest neighbor of \( X_i \) w.r.t the sample \( \{X_1, X_2, \ldots, X_{N_2}\} \setminus \{X_i\} \).
- \( B_3(X_i): X_i \) is strictly outside the \( k_2\)-nn ball around \( X_i \) w.r.t the sample \( \{X_1, X_2, \ldots, X_{N_2}\} \setminus \{X_i\} \).
- \( BE(X_i) = \left( A_1(X_i) \cap B_2(X_i) \right) \cup \left( A_3(X_i) \cap B_1(X_i) \right) \).
- \( BE_1(X_i, X_j) = BE(X_i) \cap \left( BE(X_j) \cup A_2(X_j) \right) \).
- \( BE_2(X_i, X_j) = A_2(X_i) \cap \left( A_2(X_j) \cup B_2(X_j) \right) \).
- \( BE_3(X_i, X_j) = B_2(X_i) \cap B_2(X_j) \).

Note that if neither \( BE_1(X_i, X_j) \), \( BE_2(X_i, X_j) \), nor \( BE_3(X_i, X_j) \) hold, then
\[
\left| g \left( \tilde{f}_{1,k_i}(X_i), \tilde{f}_{2,k_2}(X_i) \right) - g \left( \tilde{f}_{1,k_i}(X_i), \tilde{f}_{2,k_2}(X_i) \right) \right| = 0.
\]
(38)

since either \( \tilde{f}_{2,k_2}(X_i) = \tilde{f}_{2,k_2}(X_i) \) or \( \dot{f}_{2,k_2}(X_i) = \dot{f}_{2,k_2}(X_i) \). The same result holds if \( X_i \) or \( X_j \) are switched. Thus we only need to focus on the cases where these events are true. Note that since the samples are iid, the probability that \( A_2(X_i) \) occurs is \( 1/N_2 \). Similarly, the probability of \( B_2(X_i) \) is \( 1/N_2 \).

Claim 13. The following hold:

1. \( \Pr(BE_1(X_i, X_j)) = O \left( \frac{k_2}{M_2} \right)^2 \)
2. \( \Pr(BE_2(X_i, X_j)) = O \left( \frac{k_2}{M_2} \right)^2 \)
3. \( \Pr(BE_3(X_i, X_j)) = O \left( \frac{k_2}{M_2} \right)^2 \)

Proof: For the first expression, consider first the case \( BE(X_i) \cap BE(X_j) \). If \( X_i \) and \( X_j \) are far apart with disjoint \( k_2\)-nn balls, we can treat the probability of \( BE(X_i) \) and \( BE(X_j) \) separately within each ball which is \( O \left( \frac{k_2}{M_2} \right)^2 \) in each case. This gives a combined probability of \( O \left( \frac{k_2}{M_2} \right)^2 \) when the balls are disjoint. On the other hand, the probability that the \( k_2\)-nn balls intersect is \( O \left( \frac{k_2}{M_2} \right)^2 \). In this case, the probability of the event \( BE(X_i) \cap BE(X_j) \) is \( O \left( \frac{k_2}{M_2} \right)^2 \). Combining these facts proves the claim for \( BE(X_i) \cap BE(X_j) \).

Now consider \( BE(X_i) \cap A_2(X_j) \). In a similar manner as above, if the two \( k_2\)-nn balls are disjoint, we treat the probability of the two events separately within each ball giving a combined probability of \( O \left( \frac{k_2}{M_2} \right)^2 \). Again, the probability that the \( k_2\)-nn balls intersect is \( O \left( \frac{k_2}{M_2} \right)^2 \) and the resulting probability of \( BE(X_i) \cap A_2(X_j) \) is \( O \left( \frac{k_2}{M_2} \right)^2 \) giving a combined probability of \( O \left( \frac{k_2}{M_2} \right)^2 \). Similarly, \( \Pr(BE(X_i) \cap B_2(X_j)) = O \left( \frac{k_2}{M_2} \right)^2 \) which completes the proof for the first expression.

For the second and third expressions, note that since the points \( \{X_1, X_2, \ldots, X_{N_2}\} \) are all iid, \( A_2(X_i) \) is independent of \( A_2(X_j) \) and \( B_2(X_i) \) and \( B_2(X_j) \) is independent of \( B_2(X_j) \). Thus the probability of each of the intersecting events is \( 1/N_2^2 \) which completes the proof.

From the Lipschitz condition,
\[
\left| g \left( \tilde{f}_{1,k_i}(X_i), \tilde{f}_{2,k_2}(X_j) \right) - g \left( \tilde{f}_{1,k_i}(X_i), \tilde{f}_{2,k_2}(X_j) \right) \right|^2 \leq C_g \left| \tilde{f}_{2,k_2}(X_j) - \tilde{f}_{2,k_2}(X_j) \right|^2
\]
(39)
Now suppose that \( A_1(X_j) \cap B_3(X_j) \) occurs. In this case, \( \tilde{f}_{2,k_2}(X_j) = \frac{k_2 - 1}{k_2} \tilde{f}_{2,k_2+1}(X_j) \). To obtain a bound for \( \mathbb{E} \left[ \tilde{f}_{2,k_2}(X_j) - \tilde{f}_{2,k_2}^*(X_j) \right]^2 \), we need the joint distribution of \( \tilde{f}_{2,k_2}(X_j) \) and \( \tilde{f}_{2,k_2+1}(X_j) \) as

\[
\left| \tilde{f}_{2,k_2}(X_j) - \tilde{f}_{2,k_2}^*(X_j) \right|^2 \leq 2 \left| \tilde{f}_{2,k_2}(X_j) - \frac{k_2 - 1}{k_2} \tilde{f}_{2,k_2+1}(X_j) \right|^2 + O \left( \frac{k_2}{M_2} \right)^2. \tag{40}
\]

**Lemma 14.** The density function of the joint distribution of \( P_{k_2} \) and \( P_{k_2+1} \) is

\[
\tilde{f}_{P_{k_2},P_{k_2+1}}(p,q) = 1_{\{p \leq q\}} \frac{M_2!}{(k_2 - 1)! (M_2 - k_2 - 1)!} p^{k_2-1} (1 - q)^{M_2-k_2-1}. \tag{41}
\]

**Proof:** For \( P_{k_2} \), let \( r_{k_2} \) be the corresponding \( k \)-nn radius. Let \( \delta_p, \delta_q > 0 \). We are interested in the event \( \{ p \leq P_{k_2} \leq p + \delta_p, q \leq P_{k_2+1} \leq q + \delta_q \} \). Consider the following events:

- **C1:** There are \( k_2 - 1 \) points within the radius \( r_{k_2} \).
- **C2:** The \( k_2 \)th point is in the interval \( [r_{k_2}, r_{k_2} + \epsilon(\delta_p)] \).
- **C3:** The \( k_2 + 1 \)th point is in the interval \( [r_{k_2+1}, r_{k_2+1} + \epsilon(\delta_q)] \).
- **C4:** The remaining \( M_2 - k_2 - 1 \) points are outside the radius \( r_{k_2+1} + \epsilon(\delta_q) \).
- **C5:** \( r_{k_2} \leq r_{k_2+1} \)

We have that

\[
\Pr (p \leq P_{k_2} \leq p + \delta_p, q \leq P_{k_2+1} \leq q + \delta_q) = \Pr \left( \bigcap_{i=1}^{5} C_i \right).
\]

Of the \( M_2! \) different ways to permute the \( M_2 \) points, there are \( (k_2 - 1)! \) permutations for the points inside the \( k_2 \)-nn ball and \( (M_2 - k_2 - 1)! \) permutations for the points outside the \( (k_2 + 1) \)-nn ball. So the number of different point configurations with \( k_2 - 1 \) points inside \( r_{k_2} \) and \( M_2 - k_2 - 1 \) points outside \( r_{k_2+1} \) is \( \frac{M_2!}{(k_2 - 1)! (M_2 - k_2 - 1)!} \). This gives

\[
\Pr (p \leq P_{k_2} \leq p + \delta_p, q \leq P_{k_2+1} \leq q + \delta_q) = 1_{\{p \leq q\}} \frac{M_2!}{(k_2 - 1)! (M_2 - k_2 - 1)!} p^{k_2-1} (1 - q)^{M_2-k_2-1} \delta_p \delta_q. \tag{42}
\]

The \( p^{k_2-1} \) term is the probability that \( k_2 - 1 \) points fall within a ball of radius \( p \) (the coverage probability). The \( (1 - q)^{M_2-k_2-1} \) term is the probability that \( M_2 - k_2 - 1 \) points fall outside a ball of radius with coverage probability \( q \). The \( \delta_p \) and \( \delta_q \) terms correspond to the events that one point falls exactly at radius \( p \) and another point falls exactly at radius \( q \). The LHS of (42) is equal to the probability of these events. The combinatorial term then accurately accounts for the different possible combinations. From (42), we get the density in (41).

From Lemma 14,

\[
\mathbb{E} \left[ \tilde{f}_{2,k_2}(X_j) \tilde{f}_{2,k_2+1}(X_j) \right] = \mathbb{E} \left[ \frac{k_2(k_2 - 1)}{M_2^2 P_{k_2}(X_j) P_{k_2+1}(X_j)} \right] = \mathbb{E} \left[ \tilde{f}_2^2(X_j) \right] \frac{M_2 - 1}{k_2 (k_2 - 2)}.
\]

Then since \( \mathbb{E} \left[ P_{k_2}^{-2} \right] = \frac{M_2(M_2 - 1)}{(k_2 - 1)(k_2 - 2)} \), we obtain

\[
\mathbb{E} \left[ \left( \tilde{f}_{2,k_2}(X_j) - \frac{k_2 - 1}{k_2} \tilde{f}_{2,k_2+1}(X_j) \right)^2 \right] = \mathbb{E} \left[ \tilde{f}_2^2(X_j) \right] \frac{M_2 - 1}{M_2} \cdot \frac{2}{k_2 (k_2 - 2)} = O \left( \frac{1}{k_2^2} \right). \tag{43}
\]
A similar result follows if $A_3(X_i) \cap B_1(X_i)$ holds instead. Then (38) gives

$$
\mathbb{E} \left[ \sum_{j=2}^{N_2} g \left( \hat{f}_{1,k_1}(X_j), \hat{f}_{2,k_2}(X_j) \right) - g \left( \hat{f}_{1,k_1}(X_j), \hat{f}'_{2,k_2}(X_j) \right) \right]^2
$$

$$
= \sum_{i=2}^{N_2} \sum_{j=2}^{N_2} \mathbb{E} \left[ \left| g \left( \hat{f}_{1,k_1}(X_i), \hat{f}_{2,k_2}(X_i) \right) - g \left( \hat{f}_{1,k_1}(X_i), \hat{f}'_{2,k_2}(X_i) \right) \right| \times \left| g \left( \hat{f}_{1,k_1}(X_j), \hat{f}_{2,k_2}(X_j) \right) - g \left( \hat{f}_{1,k_1}(X_j), \hat{f}'_{2,k_2}(X_j) \right) \right| \right]
\leq \sum_{i=2}^{N_2} \sum_{j=2}^{N_2} 2\mathbb{E} \left[ \left| g \left( \hat{f}_{1,k_1}(X_i), \hat{f}_{2,k_2}(X_i) \right) - g \left( \hat{f}_{1,k_1}(X_i), \hat{f}'_{2,k_2}(X_i) \right) \right| \left| g \left( \hat{f}_{1,k_1}(X_j), \hat{f}_{2,k_2}(X_j) \right) - g \left( \hat{f}_{1,k_1}(X_j), \hat{f}'_{2,k_2}(X_j) \right) \right| \right]
\times \Pr \left( \bigcup_{\ell=1}^{3} B_{E_{\ell}}(X_i, X_j) \right)
$$

Combining the results from (44), (39), (40), (43), and Claim 13 with the Cauchy-Schwarz inequality gives

$$
\text{LHS (44)}
\leq 2M_2^2 \mathbb{E} \left[ \left| g \left( \hat{f}_{1,k_1}(X_i), \hat{f}_{2,k_2}(X_i) \right) - g \left( \hat{f}_{1,k_1}(X_i), \hat{f}'_{2,k_2}(X_i) \right) \right|^2 \left| B_{E_1}(X_i, X_j) \right| \right]
\times \Pr (B_{E_1}(X_i, X_j)) + O \left( \frac{M_2^2}{N_2^2} \right)
\leq 2M_2^2 C_g^2 \mathbb{E} \left[ \left| \hat{f}_{2,k_2}(X_j) - \hat{f}'_{2,k_2}(X_j) \right|^2 \left| B_{E_1}(X_i, X_j) \right| \Pr (B_{E_1}(X_i, X_j)) + O(1) \right)
\leq 4M_2^2 C_g^2 \mathbb{E} \left[ \left| \hat{f}_{2,k_2}(X_j) - \frac{k_2 - 1}{k_2} \hat{f}_{2,k_2+1}(X_j) \right|^2 \left| B_{E_1}(X_i, X_j) \right| \Pr (B_{E_1}(X_i, X_j)) \right]
\times \Pr (B_{E_1}(X_i, X_j)) + O \left( \frac{k_2}{M_2} \right) + 1
= O \left( \frac{k_2}{M_2} \left( \frac{k_2}{M_2} \right)^2 \right) + O \left( \frac{k_2}{M_2} \right) + 1
= O(1).
$$

Applying Jensen’s inequality to (34) and applying (55) and Lemma 12 gives

$$
\mathbb{E} \left[ \left| \hat{G}_{k_1,k_2} - \hat{G}'_{k_1,k_2} \right|^2 \right]
\leq 2 \mathbb{E} \left[ \left| g \left( \hat{f}_{1,k_1}(X_1), \hat{f}_{2,k_2}(X_1) \right) - g \left( \hat{f}_{1,k_1}(X_1), \hat{f}'_{2,k_2}(X_1) \right) \right|^2 \right]
\leq 2 \mathbb{E} \left[ \left| \sum_{j=2}^{N_2} g \left( \hat{f}_{1,k_1}(X_j), \hat{f}_{2,k_2}(X_j) \right) - g \left( \hat{f}_{1,k_1}(X_j), \hat{f}'_{2,k_2}(X_j) \right) \right|^2 \right]
\leq O \left( \frac{k_2}{M_2} \right)
.$$
Thus by similar arguments as was used to obtain (45),

\[
E \left[ \left| G_{k_1,k_2} - \hat{G}_{k_1,k_2} \right|^2 \right] \\
\leq \frac{1}{N^2} E \left[ \left( \sum_{j=1}^{N_2} g \left( \hat{f}_{1,k_1}(X_j), \hat{f}_{2,k_2}(X_j) \right) - g \left( \hat{f}_{1,k_1}(X_j), \hat{f}_{2,k_2}(X_j) \right) \right)^2 \right] \\
= O \left( \frac{1}{N^2} \right).
\]

Applying the Efron-Stein inequality gives

\[
\mathbb{V} \left[ G_{k_1,k_2} \right] = O \left( \frac{1}{N^2} + \frac{N_1}{N_2} \right).
\]

**APPENDIX D**

**PROOF OF THEOREM 6 (CLT)**

We use Lemma [15] which is adapted from [45]:

**Lemma 15.** Let the random variables \( \{ Y_{M,i} \}_{i=1}^{N} \) belong to a zero mean, unit variance, interchangeable process for all values of \( M \). Assume that \( \text{Cov}(Y_{M,1}, Y_{M,2}) \) and \( \text{Cov}(Y_{M,1}^2, Y_{M,2}^2) \) are \( o(1) \) as \( M \to \infty \). Then the random variable

\[
S_{N,M} = \frac{\sum_{i=1}^{N} Y_{M,i}}{\sqrt{\mathbb{V} \sum_{i=1}^{N} Y_{M,i}}} \tag{46}
\]

converges in distribution to a standard normal random variable.

The proof of this lemma is identical to that in [45] (See “Proof of Theorem 3.3 and Theorem 5.3” in [45]). The relaxed assumptions in Lemma [15] enable us to prove the central limit theorem under more relaxed conditions on the densities. Assume for simplicity that \( N_1 = N_2 = M \) and \( k_1(l) = k_2(l) = k(l) \). Define

\[
Y_{M,i} = \sum_{l \in \mathcal{I}} w(l) g \left( \hat{f}_{1,k(l)}(X_i), \hat{f}_{2,k(l)}(X_i) \right) - E \left[ \sum_{l \in \mathcal{I}} w(l) g \left( \hat{f}_{1,k(l)}(X_i), \hat{f}_{2,k(l)}(X_i) \right) \right]. \tag{47}
\]

This gives

\[
S_{N,M} = \frac{\hat{G}_w - E \left[ \hat{G}_w \right]}{\sqrt{\mathbb{V} \hat{G}_w}}.
\]

To bound the covariance between \( Y_{M,1} \) and \( Y_{M,2} \) and between \( Y_{M,1}^2 \) and \( Y_{M,2}^2 \), it is necessary to show that the denominator of \( Y_{M,i} \) converges to a nonzero constant or to zero sufficiently slowly. The numerator and denominator of \( Y_{M,i} \) are, respectively,

\[
\sum_{l \in \mathcal{I}} w(l) g \left( \hat{f}_{1,k(l)}(X_i), \hat{f}_{2,k(l)}(X_i) \right) - E \left[ \sum_{l \in \mathcal{I}} w(l) g \left( \hat{f}_{1,k(l)}(X_i), \hat{f}_{2,k(l)}(X_i) \right) \right] \\
= \sum_{l \in \mathcal{I}} w(l) \left( g \left( \hat{f}_{1,k(l)}(X_i), \hat{f}_{2,k(l)}(X_i) \right) - E \left[ g \left( \hat{f}_{1,k(l)}(X_i), \hat{f}_{2,k(l)}(X_i) \right) \right] \right),
\]

\[
\sqrt{\mathbb{V} \sum_{l \in \mathcal{I}} w(l) g \left( \hat{f}_{1,k(l)}(X_i), \hat{f}_{2,k(l)}(X_i) \right)}
\]

\[
= \sqrt{\sum_{l \in \mathcal{I}} \sum_{l' \in \mathcal{I}} w(l)w(l') \text{Cov} \left( g \left( \hat{f}_{1,k(l)}(X_i), \hat{f}_{2,k(l)}(X_i) \right), g \left( \hat{f}_{1,k(l')}(X_i), \hat{f}_{2,k(l')}(X_i) \right) \right)} \tag{48}.
\]

Thus we require bounds on \( \text{Cov} \left( g \left( \hat{f}_{1,k(l)}(X_i), \hat{f}_{2,k(l)}(X_i) \right), g \left( \hat{f}_{1,k(l')}(X_j), \hat{f}_{2,k(l')}(X_j) \right) \right) \) to bound the covariance between \( Y_{M,1} \) and \( Y_{M,2} \).
Define $\mathcal{M}(Z) := Z - \mathbb{E}Z$ and $\mathbf{e}_{z,k(l)}(Z) := \hat{f}_{z,k(l)}(Z) - \mathbb{E}_Z \hat{f}_{z,k(l)}(Z)$. A Taylor series expansion of $g \left( \hat{f}_{1,k(l)}(X_n), \hat{f}_{2,k(l)}(X_n) \right)$ around $\mathbb{E}_n \hat{f}_{1,k(l)}(X_n)$ and $\mathbb{E}_n \hat{f}_{2,k(l)}(X_n)$ gives

$$
g \left( \hat{f}_{1,k(l)}(X_n), \hat{f}_{2,k(l)}(X_n) \right) = \sum_{i=0}^1 \sum_{j=0}^1 \left( \frac{\partial^{i+j} g(x,y)}{\partial x^i \partial y^j} \bigg|_{x=\mathbb{E}_n \hat{f}_{1,k(l)}(X_n), y=\mathbb{E}_n \hat{f}_{2,k(l)}(X_n)} \right) \mathbf{e}_{i,k(l)}^1(X_n) \mathbf{e}_{j,k(l)}^2(X_n) + o \left( \mathbf{e}_{1,k(l)}^1(X_n) + \mathbf{e}_{2,k(l)}^1(X_n) + \mathbf{e}_{1,k(l)}^2(X_n) \mathbf{e}_{2,k(l)}^2(X_n) \right)
$$

Define

$$
p_n^{(l)} := \mathcal{M} \left( g \left( \mathbb{E}_n \hat{f}_{1,k(l)}(X_n), \mathbb{E}_n \hat{f}_{2,k(l)}(X_n) \right) \right), \quad q_n^{(l)} := \mathcal{M} \left( \frac{\partial}{\partial x} g \left( \mathbb{E}_n \hat{f}_{1,k(l)}(X_n), \mathbb{E}_n \hat{f}_{2,k(l)}(X_n) \right) \mathbf{e}_{1,k(l)}(X_n) \right),
$$

$$
r_n^{(l)} := \mathcal{M} \left( \frac{\partial}{\partial y} g \left( \mathbb{E}_n \hat{f}_{1,k(l)}(X_n), \mathbb{E}_n \hat{f}_{2,k(l)}(X_n) \right) \mathbf{e}_{2,k(l)}(X_n) \right),
$$

$$
s_n^{(l)} := \mathcal{M} \left( \frac{\partial^2}{\partial x \partial y} g \left( \mathbb{E}_n \hat{f}_{1,k(l)}(X_n), \mathbb{E}_n \hat{f}_{2,k(l)}(X_n) \right) \mathbf{e}_{1,k(l)}(X_n) \mathbf{e}_{2,k(l)}(X_n) \right),
$$

$$
t_n^{(l)} := \mathcal{M} \left( o \left( \mathbf{e}_{1,k(l)}(X_n) + \mathbf{e}_{2,k(l)}(X_n) + \mathbf{e}_{1,k(l)}(X_n) \mathbf{e}_{2,k(l)}(X_n) \right) \right).
$$

This gives

$$
\text{Cov} \left( g \left( \hat{f}_{1,k(l)}(X_i), \hat{f}_{2,k(l)}(X_j) \right), g \left( \hat{f}_{1,k(l')}(X_i), \hat{f}_{2,k(l')}(X_j) \right) \right) = \mathbb{E} \left[ \left( p_i^{(l)} + q_i^{(l)} + r_i^{(l)} + s_i^{(l)} + t_i^{(l)} \right) \left( p_j^{(l')} + q_j^{(l')} + r_j^{(l')} + s_j^{(l')} + t_j^{(l')} \right) \right].
$$

(49)

**Lemma 16.** Let $l, l' \in \mathbb{Z}$ be fixed and $k(l) \to \infty$ as $M \to \infty$ for each $l \in \mathbb{Z}$. Let $\gamma_1(x)$ and $\gamma_2(x)$ be arbitrary functions with $\sup_x |\gamma_i(x)| < \infty$, $i = 1, 2$. Then if $q + r \geq 1$ and $q' + r' \geq 1$,

$$
\text{Cov} \left( \gamma_1(X_i) \mathbf{e}_{i,k(l)}(X_i), \gamma_2(X_j) \mathbf{e}_{i,k(l')}(X_j) \right) = O \left( \frac{1}{\sqrt{k(l)k(l')}} \right),
$$

$$
\text{Cov} \left( \gamma_1(X_i) \mathbf{e}_{1,k(l)}^1(X_i) \mathbf{e}_{2,k(l')}^2(X_i), \gamma_2(X_j) \mathbf{e}_{1,k(l')}^1(X_j) \mathbf{e}_{2,k(l)}^2(X_j) \right) = O \left( \frac{1}{\sqrt{k(l)k(l')}} \right).
$$

**Proof:** These results follow from an application of Cauchy-Schwarz and Lemma 10.

**Lemma 17.** Let $l, l' \in \mathbb{Z}$ be fixed and $k(l) \to \infty$ as $M \to \infty$ for each $l \in \mathbb{Z}$. Then

$$
\text{Cov} \left( g \left( \hat{f}_{1,k(l)}(X_i), \hat{f}_{2,k(l)}(X_i) \right), g \left( \hat{f}_{1,k(l')}(X_j), \hat{f}_{2,k(l')}(X_j) \right) \right) = \begin{cases} 
\mathbb{E} \left[ p_i^{(l)} p_j^{(l')} \right] + O \left( \frac{1}{\sqrt{k(l)k(l')}} \right), & i = j \\
O \left( \frac{1}{\sqrt{k(l)k(l')}} \right) + o \left( \frac{1}{\sqrt{k(l)k(l')}} \right), & i \neq j.
\end{cases}
$$

**Proof:** Consider first $i = j$. Applying Lemma 16 to (49) gives

$$
\text{Cov} \left( g \left( \hat{f}_{1,k(l)}(X_i), \hat{f}_{2,k(l)}(X_i) \right), g \left( \hat{f}_{1,k(l')}(X_i), \hat{f}_{2,k(l')}(X_i) \right) \right) = \mathbb{E} \left[ p_i^{(l)} p_i^{(l')} \right] + O \left( \frac{1}{\sqrt{k(l)k(l')}} \right),
$$
When \( i \neq j \), \( \mathbb{E} \left[ p_l^{(i)} \left( p_j^{(i') \circ} + q_j^{(i')} + r_j^{(i')} + s_j^{(i')} + t_j^{(i')} \right) \right] = 0 \) since \( X_i \) and \( X_j \) are independent. A direct application of Lemma [16] gives

\[
\mathbb{E} \left[ q_l^{(i)} q_j^{(i')} \right] = O \left( \frac{1}{\sqrt{k(l)k(l')}} \right),
\]

\[
\mathbb{E} \left[ q_l^{(i)} r_j^{(i')} \right] = O \left( \frac{1}{\sqrt{k(l)k(l')}} \right),
\]

\[
\mathbb{E} \left[ q_l^{(i)} s_j^{(i')} \right] = O \left( \frac{1}{\sqrt{k(l)k(l')}^2} \right),
\]

\[
\mathbb{E} \left[ s_j^{(i)} s_j^{(i')} \right] = O \left( \frac{1}{k(l)k(l')} \right),
\]

\[
\mathbb{E} \left[ s_j^{(i)} r_j^{(i')} \right] = O \left( \frac{1}{\sqrt{k(l)k(l')}^2} \right),
\]

\[
\mathbb{E} \left[ r_j^{(i)} r_j^{(i')} \right] = O \left( \frac{1}{\sqrt{k(l)k(l')}} \right).
\]

To handle the implicit constants in the \( t_j^{(i)} \) terms, Cauchy-Schwarz can be applied with Lemma [16] to get

\[
\mathbb{E} \left[ q_l^{(i)} t_j^{(i')} \right] = o \left( \frac{1}{k(l)} \right),
\]

\[
\mathbb{E} \left[ r_j^{(i)} t_j^{(i')} \right] = o \left( \frac{1}{k(l')} \right),
\]

\[
\mathbb{E} \left[ s_j^{(i)} t_j^{(i')} \right] = o \left( \frac{1}{k(l)} \right),
\]

\[
\mathbb{E} \left[ t_j^{(i)} t_j^{(i')} \right] = o \left( \frac{1}{k(l)} \right).
\]

Combining these results with (49) completes the proof.

Since \( p_i(l) = \mathcal{M}(g(f_1(X_i), f_2(X_i))) + o(1) \), \( \mathbb{E} \left[ p_l^{(i)} p_i^{(i')} \right] \) is guaranteed to be a nonzero constant if

\[
\mathbb{E} \left[ g(f_1(X_i), f_2(X_i))^2 \right] \neq \mathbb{E} \left[ g(f_1(X_i), f_2(X_i))^2 \right].
\]

In this case, applying Lemma [17] to (47) gives \( \text{Cov}(Y_{M,1}, Y_{M,2}) = o(1) \) as long as \( k(l) \to \infty \) as \( M \to \infty \) for each \( l \in \tilde{I} \). Unfortunately, the condition in (50) does not hold for the important case of \( f \)-divergence functionals when the densities \( f_1 \) and \( f_2 \) are equal almost everywhere. However, we still have that the denominator in (47) converges more slowly to zero than the numerator as long as \( k(l), k(l') \to \infty \) at the same rate for each \( l, l' \in \tilde{I} \) as the \( \left( \frac{1}{k(l)} \right) \) goes to zero faster than \( O \left( \frac{1}{\sqrt{k(l)k(l')}} \right) \).

Thus we still get \( \text{Cov}(Y_{M,1}, Y_{M,2}) = o(1) \) in this case.

For the covariance between \( Y_{M,1}^2 \) and \( Y_{M,2}^2 \), we only need to focus on the numerator terms as the denominator terms will be similar as before. Thus the numerator of the covariance is

\[
\sum_{l \neq l'} \sum_{l' \neq l} \sum_{j \neq j'} \sum_{j' \neq j} \text{Cov} \left[ \left( p_1^{(l)} + q_1^{(l)} + r_1^{(l)} + s_1^{(l)} \right) \left( p_1^{(l')} + q_1^{(l')} + r_1^{(l')} + s_1^{(l')} \right), \right. \left. \left( p_2^{(j)} + q_2^{(j)} + r_2^{(j)} + s_2^{(j)} \right) \left( p_2^{(j')} + q_2^{(j')} + r_2^{(j')} + s_2^{(j')} \right) \right] .
\]

If \( l = l' \) and \( j = j' \), then the previous results apply and we get \( O \left( \frac{1}{n(l)} \right) + o \left( \frac{1}{k(l)} \right) \). For the general case, the terms with either \( p_1^{(l)} p_1^{(l')} \) in the left hand side or \( p_2^{(j)} p_2^{(j')} \) in the right hand side are zero due to independence. For the remaining terms, we use the proof of Lemma 10 in [37]. Under certain conditions, then for functions \( \gamma_1(x) \) and \( \gamma_2(x) \) under the same assumptions as in Lemma [16]

\[
\gamma_1(X_1) e_{1,(k,l)}(X_1) e_{2,(k,l)}(X_1) e_{2,(k,l')}^*(X_1) e_{1,(k,l')}^*(X_1),
\]

\[
\gamma_2(X_2) e_{1,(k,j)}(X_2) e_{2,(k,j)}(X_2) e_{2,(k,j')}^*(X_2) e_{1,(k,j')}^*(X_2)
\]

\[
= O \left( \frac{1}{k(l)k(l') k(j) k(j')} \right),
\]

(51)
As stated in [37], the conditions required for this expression to hold are “(1) There must be at least one positive exponent on both sides of the arguments in the covariance. (2) \( \{s + s' + t + t' \neq 1\} \cap \{q + q' + r + r' \neq 1\} \).” If neither of the conditions holds in condition (2), then the covariance in (51) reduces to the covariance with only one error term on each side. If only one of the conditions holds, then the covariance is zero. This means that if \( k(l), k(l') \to \infty \) at the same rate for each \( l, l' \in \hat{l} \), then (51) reduces to \( o \left( \frac{1}{k(l)} \right) \). Combining this result with the previous result on the denominator of \( Y_{M,i} \) gives that \( \text{Cov} \left( Y_{M,1}^2, Y_{M,2}^2 \right) = o(1) \). Then by Lemma [15] \( \hat{G}_w - \mathbb{E} [\hat{G}_w] \sqrt{\mathbb{V} \left[ \hat{G}_w \right]} \) converges in distribution to a standard normal random variable.