Efficient estimation of conditional covariance matrices for dimension reduction

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Abstract

We consider the problem of estimating a conditional covariance matrix in an inverse regression setting. We show that this estimation can be achieved by estimating a quadratic functional extending the results of Da Veiga & Gamboa (2008). We prove that this method provides a new efficient estimator whose asymptotic properties are studied.

1 Introduction

Consider the nonparametric regression

$$Y = \varphi(X) + \epsilon,$$

where $X \in \mathbb{R}^p$, $Y \in \mathbb{R}$ and $\mathbb{E}\left[\epsilon\right] = 0$. The main difficulty with any regression method is that, as the dimension of X becomes larger, the number of observations needed for a good estimator increases exponentially. This phenomena is usually called the *curse of dimensionality*. All the "classical" methods could break down, as the dimension p increases, unless we have at hand a very huge sample.

For this reason, there have been along the past decades a very large number of methods to cope with this issue. Their aim is to reduce the dimensionality of the problem, using just to name a few, the generalized linear model in Brillinger (1983), the additive models in Hastie & Tibshirani (1990), sparsity constraint models as Li (2007) and references therein.

Alternatively, Li (1991a) proposed the procedure of Sliced Inverse Regression (SIR) considering the following semiparametric model,

$$Y = \phi(\upsilon_1^\top X, \ldots, \upsilon_K^\top X, \epsilon)$$

where the υ's are unknown vectors in $\mathbb{R}^p$, ϵ is independent of X and ϕ is an arbitrary function in $\mathbb{R}^{K+1}$. This model can gather all the relevant information about the variable Y, with only the projection of X onto the $K \ll p$ dimensional subspace $(\upsilon_1^\top X, \ldots, \upsilon_K^\top X)$. In the case when K is small, it is possible to reduce the dimension by estimating the υ's efficiently. This method is also used to search nonlinear structures in data and to estimate the projection directions υ's. For a review on SIR methods, we refer to Li (1991a,b); Duan & Li (1991); Hardle & Tsybakov (1991) and references therein. The υ's define the effective dimension reduction (e.d.r) direction and the eigenvectors of $\mathbb{E}\big[\mathrm{Cov}\big(X|Y\big)\big]$ are the e.d.r. directions. Many estimators have been proposed in order to study the e.d.r directions in many different cases. For example, Zhu & Fang (1996) and Ferré & Yao (2005, 2003) use kernel estimators, Hsing (1999) combines nearest neighbor and SIR, Bura & Cook (2001) assume that $\mathbb{E}\big[X|Y\big]$ has some parametric form, Setodji & Cook (2004) use k-means and Cook & Ni (2005) transform SIR to least square form.

In this paper, we propose an alternate estimation of the matrix

$$\mathrm{Cov}\big(\mathbb{E}\big[X|Y\big]\big) = \mathbb{E}\big[\mathbb{E}\big[X|Y\big]\mathbb{E}\big[X|Y\big]^\top\big] - \mathbb{E}\big[X\big]\mathbb{E}\big[X\big]^\top,$$

using ideas developed by Da Veiga & Gamboa (2008), inspired by the prior work of Laurent (1996). More precisely since $\mathbb{E}\big[X\big]\mathbb{E}\big[X\big]^\top$ can be easily estimated with many usual methods, we will focus on finding an estimator of $\mathbb{E}\big[\mathbb{E}\big[X|Y\big]\mathbb{E}\big[X|Y\big]^\top\big]$. For this we will show that this estimation implies an estimation of a quadratic functional rather than plugging non parametric estimate into this form as commonly used. This method has the advantage of getting an efficient estimator in a semiparametric framework.

This paper is organized as follows. Section 2 is intended to motivate our investigation of $\mathrm{Cov}\big(\mathbb{E}\big[X|Y\big]\big)$ using a Taylor approximation. In Section 3.1 we set up notation and hypothesis. Section 3.2 is devoted to demonstrate that each coordinate of $\mathrm{Cov}\big(\mathbb{E}\big[X|Y\big]\big)$ converge efficiently. Also we find the normality asymptotic for the whole matrix. An asymptotic bound of the variance for the quadratic part for the Taylor's expansion of $\mathrm{Cov}\big(\mathbb{E}\big[X|Y\big]\big)$ is found in Section 4. All technical Lemmas and their proofs are postponed to Sections 6 and 5 respectively.

2 Methodology

Our aim is to estimate $\mathrm{Cov}\big(\mathbb{E}[X|Y]\big)$ efficiently when observing $X \in \mathbb{R}^p$, for $p\geq 1$, and $Y \in \mathbb{R}$. For this , write the matrix

$$\mathrm{Cov}\big(\mathbb{E}[X|Y]\big) = \mathbb{E}\big[\mathbb{E}[X|Y]\mathbb{E}[X|Y]^\top\big] - \mathbb{E}[X]\mathbb{E}[X]^\top,$$

where $A^\top$ means the transpose of A. If $\mathbb{E}[X]$ can be easily estimated by classical methods, the remainder term

$$\mathbb{E}\big[\mathbb{E}[X|Y]\mathbb{E}[X|Y]^\top\big] = \big(T^*_{ij}\big)_{i,j} \quad i,j = 1,\dots,p;$$

is a non linear term whose estimation is the main topic of this paper. Each term of this matrix can be written as

$$T^*_{ij} = \int \left(\frac{\int x_i f(x_i,x_j,y)dx_idx_j}{\int f(x_i,x_j,y)dx_idx_j}\right)\left(\frac{\int x_j f(x_i,x_j,y)dx_idx_j}{\int f(x_i,x_j,y)dx_idx_j}\right) f(x_i,x_j,y)dx_idx_jdy, \tag{1}$$

where $f(x_i,x_j,y)$ for i and j fixed, is the joint density of $\big(X_i,X_j,Y\big)$ $i,j=1,\dots,p$.

Hence, we focus on the efficient estimation of the corresponding non linear functional for $f \in \mathbb{L}(dx_i,dx_j,dy)$

$$f \mapsto T_{ij}(f) = \int \left(\frac{\int x_i f(x_i,x_j,y)dx_idx_j}{\int f(x_i,x_j,y)dx_idx_j}\right)\left(\frac{\int x_j f(x_i,x_j,y)dx_idx_j}{\int f(x_i,x_j,y)dx_idx_j}\right) f(x_i,x_j,y)dx_idx_jdy. \tag{2}$$

In the case $i = j$, this estimation has been considered in Da Veiga & Gamboa (2008); Laurent (1996). Here we extend their methodology to this case. Assume we have at hand an i.i.d sample $(X_i^{(k)}, X_j^{(k)}, Y^{(k)}),\ k = 1,\dots,n$ such that it is possible to build a preliminary estimator $\hat{f}$ of f with a subsample of size $n_1 < n$. Now, the main idea is to make a Taylor's expansion of $T_{ij}(f)$ in a neighborhood of $\hat{f}$ which will play the role of a suitable approximation of f. More precisely, define an auxiliar function $F : [0,1] \to \mathbb{R}$;

$$F(u) = T_{ij}(uf + (1-u)\hat{f})$$

with $u \in [0,1]$. The Taylor's expansion of F between 0 and 1 up to the third order is

$$F(1) = F(0) + F'(0) + \frac{1}{2}F''(0) + \frac{1}{6}F'''(\xi)(1-\xi)^3 \tag{3}$$

for some $\xi \in [0,1]$. Moreover, we have

$$F(1) = T_{ij}(f)$$

$$F(0) = T_{ij}(\hat{f}) = \int \left(\frac{\int x_i \hat{f}(x_i,x_j,y)dx_idx_j}{\int \hat{f}(x_i,x_j,y)dx_idx_j}\right)\left(\frac{\int x_j \hat{f}(x_i,x_j,y)dx_idx_j}{\int \hat{f}(x_i,x_j,y)dx_idx_j}\right) \hat{f}(x_i,x_j,y)dx_idx_jdy.$$

To simplify the notations, let

$$m_i(f_u,y) = \frac{\int x_i f_u(x_i,x_j,y)dx_idx_j}{\int f_u(x_i,x_j,y)dx_idx_j}$$

$$m_i(f_0,y) = m_i(\hat{f},y) = \frac{\int x_i \hat{f}(x_i,x_j,y)dx_idx_j}{\int \hat{f}(x_i,x_j,y)dx_idx_j},$$

where $f_u = uf + (1-u)\hat{f}, \quad \forall u \in [0,1]$. Then, we can rewrite $F(u)$ as

$$F(u) = \int m_i(f_u, y) m_j(f_u, y) f_u(x_i, x_j, y) dx_i dx_j dy.$$

The Taylor's expansion of $T_{ij}(f)$ is given in the next Proposition.

Proposition 1 (Linearization of the operator T)**.** *For the functional $T_{ij}(f)$ defined in* (2)*, the following decomposition holds*

$$\begin{aligned} T_{ij}(f) = & \int H_1(\hat{f}, x_i, x_j, y) f(x_i, x_j, y) dx_i dx_j dy \\ & + \int H_2(\hat{f}, x_{i1}, x_{j2}, y) f(x_{i1}, x_{j1}, y) f(x_{i2}, x_{j2}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy + \Gamma_n \end{aligned} \quad (4)$$

where

$$H_1(\hat{f}, x_i, x_j, y) = x_i m_j(\hat{f}, y) + x_j m_i(\hat{f}, y) - m_i(\hat{f}, y) m_j(\hat{f}, y) \quad (5)$$

$$H_2(\hat{f}, x_{i1}, x_{j2}, y) = \frac{1}{\int \hat{f}(x_i, x_j, y) dx_i dx_j} \big(x_{i1} - m_i(\hat{f}, y)\big)\big(x_{j2} - m_j(\hat{f}, y)\big) \quad (6)$$

$$\Gamma_n = \frac{1}{6} F'''(\xi)(1-\xi)^3, \quad (7)$$

for some $\xi \in]0,1[$.

This decomposition has the main advantage of separating the terms to be estimated into a linear functional of f, which can be easily estimated and a second part which is a quadratic functional of f. In this case, Section 4 will be dedicated to estimate this kind of functionals and specifically to control its variance. This will enable to provide an efficient estimator of $T_{ij}(f)$ using the decomposition of Proposition 1.

3 Main Results

In this section we build a procedure to estimate $T_{ij}(f)$ efficiently. Since we used $n_1 < n$ to build a preliminary approximation $\hat{f}$, we will use a sample of size $n_2 = n - n_1$ to estimate (5) and (6). Since (5) is a linear functional of the density f, it can be estimated by its empirical counterpart

$$\frac{1}{n_2} \sum_{k=1}^{n_2} H_1\big(\hat{f}, X_i^{(k)}, X_j^{(k)}, Y^{(k)}\big). \quad (8)$$

Since (6) is a nonlinear functional of f, the estimation is harder. Its estimation will be a direct consequence of the technical results presented in Section 4, where we build an estimator for the general functional

$$\theta(f) = \int \eta(x_{i1}, x_{j2}, y) f(x_{i1}, x_{j1}, y) f(x_{i2}, x_{j2}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy$$

where $\eta : \mathbb{R}^3 \to \mathbb{R}$ is a bounded function. The estimator $\hat{\theta}_n$ of $\theta(f)$ is an extension of the method developed in Da Veiga & Gamboa (2008).

3.1 Hypothesis and Assumptions

The following notations will be used throughout the paper. Let d_s and b_s for $s = 1, 2, 3$ be real numbers where $d_s < b_s$. Let, for i and j fixed, $\mathbb{L}^2(dx_i dx_j dy)$ be the squared integrable functions in the cube $[d_1, b_1] \times [d_2, b_2] \times [d_3, b_3]$. Moreover, let $(p_l(x_i, x_j, y))_{l\in D}$ be an orthonormal basis of $\mathbb{L}^2(dx_i dx_j dy)$, where D is a countable set. Let $a_l = \int p_l f$ denote the scalar product of f with p_l.

Furthermore, denote by $\mathbb{L}^2(dx_i dx_j)$ (resp. $\mathbb{L}^2(dy)$) the set of squared integrable functions in $[d_1, b_1] \times [d_2, b_2]$ (resp. $[d_3, b_3]$). If $\left(\alpha_{l_\alpha}(x_i, x_j)_{l_\alpha \in D_1}\right)$(resp. $\left(\beta_{l_\beta}(y)_{l_\beta \in D_2}\right)$) is an orthonormal basis of $\mathbb{L}^2(dx_i dx_j)$ (resp. $\mathbb{L}^2(dy)$) then $p_l(x_i, x_j, y) = \alpha_{l_\alpha}(x_i, x_j)\beta_{l_\beta}(y)$ with $l = (l_\alpha, l_\beta) \in D_1 \times D_2$.

We also use the following subset of $\mathbb{L}^2(dx_i dx_j dy)$

$$\mathcal{E} = \left\{ \sum_{l\in D} e_l p_l : \ (e_l)_{l\in D} \text{ is such that } \sum_{l\in D} \left| \frac{e_l}{c_l} \right|^2 < 1 \right\}$$

where $(c_l)_{l\in D}$ is a given fixed sequence.

Moreover assume that (X_i, X_j, Y) have a bounded joint density f on $[d_1, b_1] \times [d_2, b_2] \times [d_3, b_3]$ which lies in the ellipsoid $\mathcal{E}$.

In what follows, $X_n \xrightarrow{\mathcal{D}} X$ (resp. $X_n \xrightarrow{\mathcal{P}} X$) denotes the convergence *in distribution* or *weak* convergence (resp. convergence *in probability*) of X_n to X. Additionally, the support of f will be denoted by $\operatorname{supp} f$.

Let $(M_n)_{n\geq 1}$ denote a sequence of subsets D. For each n there exists M_n such that $M_n \subset D$. Let us denote by $|M_n|$ the cardinal of M_n.

We shall make three main assumptions:

Assumption 1. *For all $n \geq 1$ there is a subset $M_n \subset D$ such that $\left(\sup_{l\notin M_n} |c_l|^2\right)^2 \approx |M_n|/n^2$ ($A_n \approx B$ means $\lambda_1 \leq A_n/B \leq \lambda_2$ for some positives constants λ_1 and λ_2). Moreover, $\forall f \in \mathbb{L}^2(dxdydz)$, $\int (S_{M_n} f - f)^2 \, dxdydz \to 0$ when $n \to 0$, where $S_{M_n} f = \sum_{l\in M_n} a_l p_l$*

Assumption 2. $\operatorname{supp} f \subset [d_1, b_1] \times [d_2, b_2] \times [d_3, b_3]$ *and* $\forall (x, y, z) \in \operatorname{supp} f$*,* $0 < \alpha \leq f(x, y, z) \leq \beta$ *with* $\alpha, \beta \in \mathbb{R}$*.*

Assumption 3. *It is possible to find an estimator $\hat{f}$ of f built with $n_1 \approx n/\log(n)$ observations, such that for $\epsilon > 0$,*

$$\forall (x, y, z) \in \operatorname{supp} f, \ 0 < \alpha - \epsilon \leq \hat{f}(x, y, z) \leq \beta + \epsilon$$

and,

$$\forall \ 2 \leq q \leq +\infty, \ \forall l \in \mathbb{N}^*, \ \mathbb{E}_f \left\| \hat{f} - f \right\|_q^l \leq C(q, l) n_1^{-l\lambda}$$

for some $\lambda > 1/6$ and some constant $C(q, l)$ not depending on f belonging to the ellipsoid $\mathcal{E}$.

Assumption 1 is necessary to bound the bias and variance of $\hat{\theta}_n$. Assumption 2 and 3 allow to establish that the remainder term in the Taylor expansion is negligible, i.e $\Gamma_n = O(1/n)$. Assumption 3 depends on the regularity of the density function. For instance for $x \in \mathbb{R}^p$, $s > 0$ and $L > 0$, consider the class

$\mathcal{H}_q(s,L)$ of Nikol'skii of functions $f \in \mathbb{L}^q(dx)$ with partials derivatives up to order $r = \lfloor s \rfloor$ inclusive, and for each of these derivatives $g^{(r)}$

$$\left\| f^{(r)}(\cdot + h) - f^{(r)}(\cdot) \right\|_q \le L\,|h|^{s-r} \quad \forall h \in \mathbb{R}.$$

Then, Assumption 3 is satisfied for $f \in \mathcal{H}_q(s,L)$ with $s > \frac{p}{4}$.

3.2 Efficient Estimation of $T_{ij}(f)$

As seen in Section 2, $T_{ij}(f)$ can be decomposed as (4). Hence, using (8) and (14) we consider the following estimate

$$\widehat{T}_{ij}^{(n)} = \frac{1}{n_2}\sum_{k=1}^{n_2} H_1(\hat{f}, X_i^{(k)}, X_j^{(k)}, Y^{(k)})$$
$$+\frac{1}{n_2(n_2-1)}\sum_{l\in M}\sum_{k\neq k'=1}^{n_2} p_l\big(X_i^{(k)}, X_j^{(k)}, Y^{(k)}\big)\int p_l\big(x_i, x_j, Y^{(k')}\big) H_3\big(\hat{f}, x_i, x_j, X_i^{(k')}, X_j^{(k')}, Y^{(k')}\big)dx_i dx_j$$
$$-\frac{1}{n_2(n_2-1)}\sum_{l,l'\in M}\sum_{k\neq k'=1}^{n_2} p_l\big(X_i^{(k)}, X_j^{(k)}, Y^{(k)}\big)p_{l'}\big(X_i^{(k')}, X_j^{(k')}, Y^{(k')}\big)$$
$$\int p_l(x_{i1}, x_{j1}, y)p_{l'}(x_{i2}, x_{j2}, y)H_2\big(\hat{f}, x_{i1}, x_{j2}, y\big)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy.$$

where $H_3(f, x_{i1}, x_{j1}, x_{i2}, x_{j2}, y) = H_2(f, x_{i1}, x_{j2}, y) + H_2(f, x_{i2}, x_{j1}, y)$ and $n_2 = n - n_1$. The remainder Γ_n does not appear because we will prove that it is negligible when compared to the other error terms.

The asymptotic behavior of $\widehat{T}_{ij}^{(n)}$ for i and j fixed is given in the next Theorem.

Theorem 1. *Let Assumptions 1-3 hold and $|M_n|/n \to 0$ when $n \to \infty$. Then:*

$$\sqrt{n}\big(\widehat{T}_{ij}^{(n)} - T_{ij}(f)\big) \xrightarrow{\mathcal{D}} \mathcal{N}\left(0, C_{ij}(f)\right), \tag{9}$$

and

$$\lim_{n\to\infty} n\mathbb{E}\big[\widehat{T}_{ij}^{(n)} - T_{ij}(f)\big]^2 = C_{ij}(f), \tag{10}$$

where

$$C_{ij}(f) = \mathrm{Var}\big(H_1(f, X_i, X_j, Y)\big)$$

Note that, in Theorem 1, it appears that the asymptotic variance of $T_{ij}(f)$ depends only on $H_1(f, X_i, X_j, Y)$. Hence the asymptotic variance of $\widehat{T}_{ij}^{(n)}$ is explained only by the linear part of (4). This will entail that the estimator is naturally efficient as proved in the following.

Indeed, the semi-parametric Cramér-Rao bound is given in the next theorem.

Theorem 2 (Semi-parametric Cramér-Rao bound.). *Consider the estimation of*

$$T_{ij}(f) = \int\left(\frac{\int x_i f(x_i, x_j, y)dx_i dx_j}{\int f(x_i, x_j, y)dx_i dx_j}\right)\left(\frac{\int x_j f(x_i, x_j, y)dx_i dx_j}{\int f(x_i, x_j, y)dx_i dx_j}\right) f(x_i, x_j, y)dx_i dx_j dy$$

for a random vector $\big(X_i, X_j, Y\big)$ *with joint density* $f \in \mathcal{E}$*. Let* $f_0 \in \mathcal{E}$ *be a density verifying the assumptions of Theorem 1. Then, for all estimator* $\widehat{T}_{ij}^{(n)}$ *of* $T_{ij}(f)$ *and every family* $\{\mathcal{V}_r(f_0)\}_{r>0}$ *of neighborhoods of* f_0 *we have*

$$\inf_{\{\mathcal{V}_r(f_0)\}_{r>0}} \liminf_{n\to\infty} \sup_{f\in\mathcal{V}_r(f_0)} n\mathbb{E}\big[\widehat{T}_{ij}^{(n)} - T_{ij}(f_0)\big]^2 \geq C_{ij}(f_0)$$

where $\mathcal{V}_r(f_0) = \big\{f : \big\|f - f_0\big\|_2 < r\big\}$ *for* $r > 0$*.*

Consequently, the estimator $\widehat{T}_{ij}^{(n)}$ *is efficient.*

In the case of our estimate, its variance is $C_{ij}(f)$, which proves its asymptotically efficiency.

Remark that Theorem 1 proves asymptotic normality entry by entry of the matrix $\boldsymbol{T}(f) = (T_{ij}(f))_{p\times p}$. To extend the result for the whole matrix it is necessary to introduce the half-vectorization operator vech. This operator, stacks only the columns from the principal diagonal of a square matrix downwards in a column vector, that is, for an $p \times p$ matrix $\boldsymbol{A} = (a_{ij})$,

$$\mathrm{vech}(\boldsymbol{A}) = [a_{11}, \cdots, a_{p1}, a_{22}, \cdots, a_{p2}, \cdots, a_{33}, \cdots, a_{pp}]^\top .$$

Let define the estimator matrix $\widehat{\boldsymbol{T}}^{(n)} = \big(\widehat{T}_{ij}^{(n)}\big)$ and $\boldsymbol{H_1}(f)$ denote the matrix with entries $(H_1(f, x_i, x_j, y))_{i,j}$. Now we are able to state the following

Corollary 1. *Let Assumptions 1-3 hold and* $|M_n|/n \to 0$ *when* $n \to \infty$*. Then* $\widehat{\boldsymbol{T}}^{(n)}$ *has the following properties:*

$$\sqrt{n}\,\mathrm{vech}\big(\widehat{\boldsymbol{T}}^{(n)} - \boldsymbol{T}(f)\big) \xrightarrow{\mathcal{D}} \mathcal{N}\left(0, \boldsymbol{C}(f)\right), \tag{11}$$

$$\lim_{n\to\infty} n\mathbb{E}\big[\mathrm{vech}\big(\widehat{\boldsymbol{T}}^{(n)} - \boldsymbol{T}(f)\big)\,\mathrm{vech}\big(\widehat{\boldsymbol{T}}^{(n)} - \boldsymbol{T}(f)\big)^\top\big] = \boldsymbol{C}(f) \tag{12}$$

where

$$\boldsymbol{C}(f) = \mathrm{Cov}\big(\mathrm{vech}(\boldsymbol{H_1}(f))\big)$$

Previous results depend on the accurate estimation of the quadratic part of the estimator of $T_{ij}^{(n)}$, which is the issue of the following section.

4 Estimation of quadratic functionals

As pointed out in Section 2 the decomposition (4) has a quadratic part (6) that we want to estimate. To achieve this we will construct a general estimator of the form:

$$\theta = \int \eta(x_{i1}, x_{j2}, y) f(x_{i1}, x_{j1}, y) f(x_{i2}, x_{j2}, y) dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy,$$

for $f \in \mathcal{E}$ and $\eta : \mathbb{R}^3 \to \mathbb{R}$ a bounded function.

Given M_n a subset of D, consider the estimator

$$\hat{\theta}_n = \frac{1}{n(n-1)} \sum_{l \in M} \sum_{k \neq k'=1}^{n} p_l(X_i^{(k)}, X_j^{(k)}, Y^{(k)})$$
$$\int p_l(x_i, x_j, Y^{(k')}) \left(\eta(x_i, X_j^{(k')}, Y^{(k')}) + \eta(X_i^{(k')}, x_j, Y^{(k')}) \right) dx_i dx_j$$
$$- \frac{1}{n(n-1)} \sum_{l,l' \in M} \sum_{k \neq k'=1}^{n} p_l(X_i^{(k)}, X_j^{(k)}, Y^{(k)}) p_{l'}(X_i^{(k')}, X_j^{(k')}, Y^{(k')})$$
$$\int p_l(x_{i1}, x_{j1}, y) p_{l'}(x_{i2}, x_{j2}, y) \eta(x_{i1}, x_{j2}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy. \quad (13)$$

In order to simplify the presentation of the main Theorem, let $\psi(x_{i1}, x_{j1}, x_{i1}, x_{j2}, y) = \eta(x_{i1}, x_{j2}, y) + \eta(x_{i2}, x_{j1}, y)$ verifying

$$\int \psi(x_{i1}, x_{j1}, x_{i2}, x_{j2}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy = \int \psi(x_{i2}, x_{j2}, x_{i1}, x_{j1}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy.$$

With this notation we can simplify (13) in

$$\hat{\theta}_n = \frac{1}{n(n-1)} \sum_{l \in M} \sum_{k \neq k'=1}^{n} p_l(X_i^{(k)}, X_j^{(k)}, Y^{(k)}) \int p_l(x_i, x_j, Y^{(k')}) \psi(x_i, x_j, X_i^{(k')}, X_j^{(k')}, Y^{(k')}) dx_i dx_j$$
$$- \frac{1}{n(n-1)} \sum_{l,l' \in M} \sum_{k \neq k'=1}^{n} p_l(X_i^{(k)}, X_j^{(k)}, Y^{(k)}) p_{l'}(X_i^{(k')}, X_j^{(k')}, Y^{(k')})$$
$$\int p_l(x_{i1}, x_{j1}, y) p_{l'}(x_{i2}, x_{j2}, y) \eta(x_{i1}, x_{j2}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy. \quad (14)$$

Using simple algebra, it is possible to prove that this estimator has bias equal to

$$- \int (S_M f(x_{i1}, x_{j1}, y) - f(x_{i1}, x_{j1}, y))(S_M f(x_{i2}, x_{j2}, y) - f(x_{i2}, x_{j2}, y))$$
$$\eta(x_{i1}, x_{j2}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy \quad (15)$$

The following Theorem gives an explicit bound for the variance of $\hat{\theta}_n$.

Theorem 3. *Let Assumption 1 hold. Then if $|M_n|/n \to 0$ when $n \to 0$, then $\hat{\theta}_n$ has the following property*

$$\left| n\mathbb{E}\left[\left(\hat{\theta}_n - \theta \right)^2 \right] - \Lambda(f, \eta) \right| \leq \gamma \left[\frac{|M_n|}{n} + \left\| S_{M_n} f - f \right\|_2 + \left\| S_{M_n} g - g \right\|_2 \right], \quad (16)$$

where $g(x_i, x_j, y) = \int f(x_{i2}, x_{j2}, y) \psi(x_i, x_j, x_{i2}, x_{j2}, y) dx_{i2} dx_{j2}$ and

$$\Lambda(f, \eta) = \int g(x_i, x_j, y)^2 f(x_i, x_j, y) dx_i dx_j dy - \left(\int g(x_i, x_j, y) f(x_i, x_j, y) dx_i dx_j dy \right)^2,$$

where γ is constant depending only on $\|f\|_\infty$, $\|\eta\|_\infty$, and $\Delta_{x_i x_j} = (b_1 - a_1) \times (b_2 - a_2)$. Moreover, this constant is an increasing function of these quantities.

Note that equation (16) implies that

$$\lim_{n\to\infty} n\mathbb{E}\big[\hat{\theta}_n - \theta\big]^2 = \Lambda(f,\eta).$$

These results will be stated in order to control the term

$$Q = \int H_2(\hat{f}, x_{i1}, x_{j2}, y) f(x_{i1}, x_{j1}, y) f(x_{i2}, x_{j2}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy$$

which has the form of the quadratic functional θ with the particular choice $\eta(x_{i1}, x_{j2}, y) = H_2(\hat{f}, x_{i1}, x_{j2}, y)$. We point out that we also show that in this particular frame, we get $\Lambda(f,\eta) = 0$. This the reason why the asymptotic variance of the estimate $\widehat{T}_{ij}^{(n)}$ built in the previous section, is only governed by its linear part, yielding asymptotic efficiency.

5 Proofs

Proof of Proposition 1.

We need to calculate the three first derivatives of $F(u)$. In order to facilitate the calculation, we are going to differentiate $m_i(f_u, y)$:

$$\begin{aligned}
\frac{d}{du}\left(m_i(f_u,y)\right) &= \frac{d}{du}\left(\frac{\int x_i f_u(x_i,x_j,y)dx_i dx_j}{\int f_u(x_i,x_j,y)dx_i dx_j}\right)\\
&= \frac{\int x_i(f(x_i,x_j,y) - \hat{f}(x_i,x_j,y))dx_i dx_j}{\int f_u(x_i,x_j,y)dx_i dx_j}\\
&\quad - \frac{\int x_i f_u(x_i,x_j,y)dx_i dx_j \int f(x_i,x_j,y) - \hat{f}(x_i,x_j,y)dx_i dx_j}{\left(\int f_u(x_i,x_j,y)dx_i dx_j\right)^2},\\
&= \frac{\int x_i(f(x_i,x_j,y) - \hat{f}(x_i,x_j,y))dx_i dx_j}{\int f_u(x_i,x_j,y)dx_i dx_j}\\
&\quad - \frac{m_i(f_u,y)\int f(x_i,x_j,y) - \hat{f}(x_i,x_j,y)dx_i dx_j}{\int f_u(x_i,x_j,y)dx_i dx_j},\\
&= \frac{\int \big(x_i - m_i(f_u,y)\big)\big(f(x_i,x_j,y) - \hat{f}(x_i,x_j,y)\big)dx_i dx_j}{\int f_u(x_i,x_j,y)dx_i dx_j}.
\end{aligned} \tag{17}$$

Now, using (17) we first compute $F'(u)$,

$$\begin{aligned}
&\int \frac{d}{du}\left(m_i(f_u,y)\right) m_j(f_{u,},y) f_u(x_i,x_j,y) + m_i(f_u,y)\frac{d}{du}\left(m_j(f_u,y)\right) f_u(x_i,x_j,y)\\
&+ m_i(f_u,y)m_j(f_u,y)\frac{d}{du}\left(f_u(x_i,x_j,y)\right) dx_i dx_j dy,\\
&= \int \left[x_i m_j(f_u,y) + x_j m_i(f_u,y) - m_i(f_u,y)m_j(f_u,y)\right]\big(f(x_i,x_j,y) - \hat{f}(x_i,x_j,y)\big) dx_i dx_j dy.
\end{aligned}$$

Taking $u = 0$ we have

$$F'(0) = \int \Big[x_i m_j(\hat{f},y) + x_j m_i(\hat{f},y) - m_i(\hat{f},y)m_j(\hat{f},y)\Big]\big(f(x_i,x_j,y) - \hat{f}(x_i,x_j,y)\big) dx_i dx_j dy. \tag{18}$$

We derive now $m_i(f_u, y)m_j(f_u, y)$ to obtain

$$\frac{d}{du}\left(m_i(f_u, y)m_j(f_u, y)\right) = \frac{d}{du}\left(m_i(f_u, y)\right) m_j(f_u, y) + m_i(f_u, y)\frac{d}{du}\left(m_j(f_u, y)\right)$$
$$= m_j(f_u, y)\frac{\int \big(x_i - m_i(f_u, y)\big)(f(x_i, x_j, y) - \hat{f}(x_i, x_j, y))dx_i dx_j}{\int f_u(x_i, x_j, y)dx_i dx_j}$$
$$+ m_i(f_u, y)\frac{\int \big(x_j - m_j(f_u, y)\big)(f(x_i, x_j, y) - \hat{f}(x_i, x_j, y))dx_i dx_j}{\int f_u(x_i, x_j, y)dx_i dx_j}. \tag{19}$$

Following with $F''(u)$ and using (17) and (19) we get,

$$F''(u) = \int \Bigg[x_{i1}\frac{\int \big(x_{j2} - m_j(f_u, y)\big)(f(x_{i2}, x_{j2}, y) - \hat{f}(x_{i2}, x_{j2}, y))dx_{i2}dx_{j2}}{\int f_u(x_i, x_j, y)dx_i dx_j}$$
$$+ x_{j1}\frac{\int \big(x_{i2} - m_i(f_u, y)\big)(f(x_{i2}, x_{j2}, y) - \hat{f}(x_{i2}, x_{j2}, y))dx_{i2}dx_{j2}}{\int f_u(x_i, x_j, y)dx_i dx_j}$$
$$- m_j(f_u, y)\frac{\int \big(x_{i2} - m_i(f_u, y)\big)(f(x_{i2}, x_{j2}, y) - \hat{f}(x_{i2}, x_{j2}, y))dx_i dx_j}{\int f_u(x_i, x_j, y)dx_i dx_j}$$
$$- m_i(f_u, y)\frac{\int \big(x_{j2} - m_j(f_u, y)\big)(f(x_{i2}, x_{j2}, y) - \hat{f}(x_{i2}, x_{j2}, y))dx_{i2}dx_{j2}}{\int f_u(x_i, x_j, y)dx_i dx_j}\Bigg]$$
$$\big(f(x_{i1}, x_{j1}, y) - \hat{f}(x_{i1}, x_{j1}, y)\big)dx_{i1}dx_{j1}dy.$$

Simplifying the last expression we obtain

$$F''(u) =$$
$$\int \frac{1}{\int f_u(x_i, x_j, y)dx_i dx_j}\left\{\big(x_{i1} - m_i(f_u, y)\big)\big(x_{j2} - m_j(f_u, y)\big) + \big(x_{i2} - m_i(f_u, y)\big)\big(x_{j1} - m_j(f_u, y)\big)\right\}$$
$$\big(f(x_{i1}, x_{j1}, y) - \hat{f}(x_{i1}, x_{j1}, y)\big)\big(f(x_{i2}, x_{j2}, y) - \hat{f}(x_{i2}, x_{j2}, y)\big)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy.$$

Besides, when $u = 0$

$$F''(0) = \tag{20}$$
$$\int \frac{1}{\int \hat{f}(x_i, x_j, y)dx_i dx_j}\left\{\big(x_{i1} - m_i(\hat{f}, y)\big)\big(x_{j2} - m_j(\hat{f}, y)\big) + \big(x_{i2} - m_i(\hat{f}, y)\big)\big(x_{j1} - m_j(\hat{f}, y)\big)\right\}$$
$$\big(f(x_{i1}, x_{j1}, y) - \hat{f}(x_{i1}, x_{j1}, y)\big)\big(f(x_{i2}, x_{j2}, y) - \hat{f}(x_{i2}, x_{j2}, y)\big)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy$$
$$= \int \frac{2}{\int \hat{f}(x_i, x_j, y)dx_i dx_j}\big(x_{i1} - m_i(\hat{f}, y)\big)\big(x_{j2} - m_j(\hat{f}, y)\big)$$
$$\big(f(x_{i1}, x_{j1}, y) - \hat{f}(x_{i1}, x_{j1}, y)\big)\big(f(x_{i2}, x_{j2}, y) - \hat{f}(x_{i2}, x_{j2}, y)\big)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy. \tag{21}$$

Using the previous arguments we can finally find $F'''(u)$:

$$F'''(u) = \int \frac{-6}{\int f_u(x_i,x_j,y)dx_idx_j}\big(x_{i1}-m_j(f_u,y)\big)\big(x_{j2}-m_j(f_u,y)\big)$$
$$\big(f(x_{i1},x_{j1},y)-\hat{f}(x_{i1},x_{j1},y)\big)\big(f(x_{i2},x_{j2},y)-\hat{f}(x_{i2},x_{j2},y)\big)$$
$$\big(f(x_{i3},x_{j3},y)-\hat{f}(x_{i3},x_{j3},y)\big)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dx_{i3}dx_{j3}dy \quad (22)$$

Replacing (18), (21) and (22) into (3) we get the desired decomposition. □

Proof of Theorem 1.

We will first control the remaining term (7),

$$\Gamma_n = \frac{1}{6}F'''(\xi)(1-\xi)^3.$$

Remember that

$$F'''(\xi) = -6\int \frac{(x_{i1}-m_i(f_\xi,y))\,(x_{j2}-m_j(f_\xi,y))}{\left(\int f_\xi(x_i,x_j,y)dx_idx_j\right)^2}\left(f(x_{i1},x_{j1},y)-\hat{f}(x_{i1},x_{j1},y)\right)$$
$$\left(f(x_{i2},x_{j2},y)-\hat{f}(x_{i2},x_{j2},y)\right)\left(f(x_{i3},x_{j3},y)-\hat{f}(x_{i3},x_{j3},y)\right)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dx_{i3}dx_{j3}dy,$$

Assumptions 1 and 2 ensure that the first part of the integrand is bounded by a constant μ. Furthermore,

$$\begin{aligned}|\Gamma_n| \leq& \mu\int\left|f(x_{i1},x_{j1},y)-\hat{f}(x_{i1},x_{j1},y)\right|\left|f(x_{i2},x_{j2},y)-\hat{f}(x_{i2},x_{j2},y)\right|\\
&\left|f(x_{i3},x_{j3},y)-\hat{f}(x_{i3},x_{j3},y)\right|dx_{i1}dx_{j1}dx_{i2}dx_{j2}dx_{i3}dx_{j3}dy\\
=&\mu\int\left(\int\left|f(x_i,x_j,y)-\hat{f}(x_i,x_j,y)\right|dx_idx_j\right)^3dy\\
\leq&\mu\Delta^3_{x_ix_j}\int\left|f(x_{i1},x_{j1},y)-\hat{f}(x_{i1},x_{j1},y)\right|^3dx_idx_jdy\end{aligned}$$

by the Hölder inequality. Then $\mathbb{E}\left[\Gamma_n^2\right] = O(\mathbb{E}(\int|f-\hat{f}|^3)^2) = O(\mathbb{E}\|f-\hat{f}\|_3^6)$. Since $\hat{f}$ verifies Assumption 3, this quantity is of order $O(n_1^{-6\lambda})$. Since we also assume $n_1 \approx n/\log(n)$ and $\lambda > 1/6$, then $n_1^{-6\lambda} = o\left(\frac{1}{n}\right)$ .Therefore, we get $\mathbb{E}\left[\Gamma_n^2\right] = o(1/n)$ which implies that the remaining term Γ_n is negligible.

To prove the asymptotic normality of $\widehat{T}_{ij}^{(n)}$, we shall show that $\sqrt{n}\left(\widehat{T}_{ij}^{(n)} - T_{ij}(f)\right)$ and define

$$Z_{ij}^{(n)} = \frac{1}{n_2}\sum_{k=1}^{n_2} H_1\big(f,X_i^{(k)},X_j^{(k)},Y^{(k)}\big) - \int H_1(f,x_i,x_j,y)f(x_i,x_j,y))dx_idx_jdy \quad (23)$$

have the same asymptotic behavior. We can get for $Z_{ij}^{(n)}$ a classic central limit theorem with variance

$$\begin{aligned}C_{ij}(f) =& \operatorname{Var}\big(H_1(f,x_i,x_j,y)\big)\\
=&\int H_1(f,x_i,x_j,y)^2f(x_i,x_j,y))dx_idx_jdy - \left(\int H_1(f,x_i,x_j,y)f(x_i,x_j,y))dx_idx_jdy\right)^2\end{aligned}$$

which implies (9) and (10). In order to establish our claim, we will show that

$$R_{ij}^{(n)} = \sqrt{n}\left[\widehat{T}_{ij}^{(n)} - T_{ij}(f) - Z_{ij}^{(n)}\right] \tag{24}$$

has second-order moment converging to 0.

Define $\widehat{Z}_{ij}^{(n)}$ as $Z_{ij}^{(n)}$ with f replaced by $\hat{f}$. Let us note that $R_{ij}^{(n)} = R_1 + R_2$ where

$$R_1 = \sqrt{n}\left[\widehat{T}_{ij}^{(n)} - T_{ij}(f) - \widehat{Z}_{ij}^{(n)}\right]$$

$$R_2 = \sqrt{n}\left[\widehat{Z}_{ij}^{(n)} - Z_{ij}^{(n)}\right].$$

It only remains to state that $\mathbb{E}\left[R_1^2\right]$ and $\mathbb{E}\left[R_2^2\right]$ converges to 0. We can rewrite R_1 as

$$R_1 = -\sqrt{n}\left[\widehat{Q} - Q + \Gamma_n\right]$$

where we note that

$$Q = \int H_2(\hat{f}, x_{i1}, x_{j2}, y) f(x_{i1}, x_{j1}, y) f(x_{i2}, x_{j2}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy$$

$$H_2(\hat{f}, x_{i1}, x_{j2}, y) = \frac{1}{\int \hat{f}(x_i, x_j, y) dx_i dx_j}\left(x_{i1} - m_i(\hat{f}, y)\right)\left(x_{j2} - m_j(\hat{f}, y)\right)$$

has the form of a quadratic functional studied in Section 4 with $\eta(x_{i1}, x_{j2}, y) = H_2(\hat{f}, x_{i1}, x_{j2}, y)$. Hence such functional can be estimated as done in Section 4 and let $\widehat{Q}$ be its corresponding estimator. Since $\mathbb{E}\left[\Gamma_n^2\right] = o(1/n)$, we only have to control the term $\sqrt{n}(\widehat{Q} - Q)$ which is such that $\lim_{n\to\infty} n\mathbb{E}\left[\widehat{Q} - Q\right]^2 = 0$ by Lemma 7. This Lemma implies that $\mathbb{E}\left[R_1^2\right] \to 0$ as $n \to \infty$. For R_2 we have

$$\begin{aligned}\mathbb{E}\left[R_2^2\right] = \frac{n}{n_2}&\left[\int \left(H_1(f, x_i, x_j, y) - H_1(\hat{f}, x_i, x_j, y)\right)^2 f(x_i, x_j, y)) dx_i dx_j dy\right] \\ -\frac{n}{n_2}&\left[\int H_1(f, x_i, x_j, y) f(x_i, x_j, y)) dx_i dx_j dy - \int H_1(\hat{f}, x_i, x_j, y)^2 f(x_i, x_j, y)) dx_i dx_j dy\right]^2.\end{aligned}$$

The same arguments as the ones of Lemma 7 (mean value and Assumptions 2 and 3) show that $\mathbb{E}\left[R_2^2\right] \to 0$. □

Proof of Theorem 2 . To prove the inequality we will use the usual framework described in Ibragimov & Khas'minskii (1991). The first step is to calculate the Fréchet derivative of $T_{ij}(f)$ at some point $f_0 \in \mathcal{E}$. Assumptions 2 and 3 and equation (4), imply that

$$\begin{aligned}T_{ij}(f) - T_{ij}(f_0) = \int &\left(x_i m_j(f_0, y) + x_j m_i(f_0, y) - m_i(f_0, y) m_j(f_0, y)\right) \\ &\left(f(x_i, x_j, y) - f_0(x_i, x_j, y)\right) dx_i dx_j dy + O\left(\int (f - f_0)^2\right)\end{aligned}$$

where $m_i(f_0,y) = \int x_i f_0(x_i,x_j,y)dx_idx_jdy / \int f_0(x_i,x_j,y)dx_idx_jdy$. Therefore, the Fréchet derivative of $T_{ij}(f)$ at f_0 is $T'_{ij}(f_0)\cdot h = \langle H_1(f_0,\cdot), h\rangle$ with

$$H_1(f_0,x_i,x_j,y) = x_i m_j(f_0,y) + x_j m_i(f_0,y) - m_i(f_0,y)m_j(f_0,y).$$

Using the results of Ibragimov & Khas'minskii (1991), denote $H(f_0) = \left\{u \in \mathbb{L}^2(dx_idx_jdy), \int u(x_i,x_j,y)\sqrt{f_0(x_i,x_j,y)}dx_idx_jdy = 0\right\}$ the set of functions in $\mathbb{L}^2(dx_idx_jdy)$ orthogonal to $\sqrt{f_0}$, $\mathrm{Pr}_{H(f_0)}$ the projection onto $H(f_0)$, $A_n(t) = (\sqrt{f_0})t/\sqrt{n}$ and $P_{f_0}^{(n)}$ the joint distribution of $\left(X_i^{(k)}, X_j^{(k)}\right)$ $k = 1,\ldots,n$ under f_0. Since $\left(X_i^{(k)}, X_j^{(k)}\right)$ $k = 1,\ldots,n$ are i.i.d., the family $\left\{P_{f_0}^{(n)}, f \in \mathcal{E}\right\}$ is differentiable in quadratic mean at f_0 and therefore locally asymptotically normal at all points $f_0 \in \mathcal{E}$ in the direction $H(f_0)$ with normalizing factor $A_n(f_0)$ (see the details in Van der Vaart (2000)). Then, by the results of Ibragimov & Khas'minskii (1991) say that under these conditions, denoting $K_n = B_n\theta'(f_0)A_n\mathrm{Pr}_{H(f_0)}$ with $B_n = \sqrt{n}u$, if $K_n \xrightarrow{\mathcal{D}} K$ and if $K(u) = \langle t, u\rangle$, then for every estimator $\widehat{T}_{ij}^{(n)}$ of $T_{ij}(f)$ and every family $\mathcal{V}(f_0)$ of vicinities of f_0, we have

$$\inf_{\{\mathcal{V}(f_0)\}} \liminf_{n\to\infty} \sup_{f\in\mathcal{V}(f_0)} n\mathbb{E}\left[\widehat{T}_{ij}^{(n)} - T_{ij}(f_0)\right]^2 \geq \left\|t\right\|^2_{\mathbb{L}^2(dx_idx_jdy)}.$$

Here,

$$K_n(u) = \sqrt{n}T'(f_0)\cdot\frac{\sqrt{f_0}}{\sqrt{n}}\mathrm{Pr}_{H(f_0)}(u) = T'(f_0)\left(\sqrt{f_0}\left(u - \sqrt{f_0}\int u\sqrt{f_0}\right)\right),$$

since for any $u \in \mathbb{L}^2(dx_idx_jdy)$ we can write it as $u = \sqrt{f_0}\left\langle\sqrt{f_0}, u\right\rangle + \mathrm{Pr}_{H(f_0)}(u)$. In this case $K_n(u)$ does not depend on n and

$$\begin{aligned}K(h) &= T'(f_0)\cdot\left(\sqrt{f_0}\left(u - \sqrt{f_0}\int h\sqrt{f_0}\right)\right)\\ &= \int H_1(f_0,\cdot)\sqrt{f_0}u - \int H_1(f_0,\cdot)\sqrt{f_0}\int u\sqrt{f_0}\\ &= \langle t, u\rangle\end{aligned}$$

with

$$t(x_i,x_j,y) = H_1(f_0,x_i,x_j,y)\sqrt{f_0} - \left(\int H_1(f_0,x_i,x_j,y)f_0\right)\sqrt{f_0}.$$

The semi-parametric Cramér-Rao bound for this problem is thus

$$\left\|t\right\|_{\mathbb{L}^2(dx_i,dx_j,dy)} = \int H_1(f_0,x_i,x_j,y)^2 f_0dx_idx_jdy - \left(\int H_1(f_0,x_i,x_j,y)f_0dx_idx_jdy\right)^2 = C_{ij}(f_0)$$

and we recognize the expression $C_{ij}(f_0)$ found in Theorem 1. □

Proof of Corollary 1. The proof is based in the following observation. Employing equation (24) we have

$$\widehat{\boldsymbol{T}}^{(n)} - \boldsymbol{T}(f) = \boldsymbol{Z}^{(n)}(f) + \frac{\boldsymbol{R}^{(n)}}{\sqrt{n}}$$

where $\boldsymbol{Z}^{(n)}(f)$ and $\boldsymbol{R}^{(n)}$ are matrices with elements $Z_{ij}^{(n)}$ and $R_{ij}^{(n)}$, defined in (23) and (24), respectively.

Hence we have,

$$n\mathbb{E}\big[\|\text{vech}\left(\widehat{\boldsymbol{T}}^{(n)} - \boldsymbol{T}(f) - \boldsymbol{Z}^{(n)}(f)\right)\|^2\big] = \mathbb{E}\big[\|\text{vech}\left(\boldsymbol{R}^{(n)}\right)\|^2\big] = \sum_{i\leq j}\mathbb{E}\big[\left(R_{ij}^{(n)}\right)^2\big].$$

We see by Lemma 7 that $\mathbb{E}\big[R_{ij}^2\big] \to 0$ as $n \to 0$. It follows that

$$n\mathbb{E}\big[\|\text{vech}\left(\widehat{\boldsymbol{T}}^{(n)} - \boldsymbol{T}(f) - \boldsymbol{Z}^{(n)}(f)\right)\|^2\big] \to 0 \text{ as } n \to 0.$$

We know that if X_n, X and Y_n are random variables, then if $X_n \xrightarrow{\mathcal{D}} X$ and $(X_n - Y_n) \xrightarrow{\mathcal{P}} 0$, follows that $Y_n \xrightarrow{\mathcal{D}} X$.

Remember also that convergence in $\mathbb{L}^2$ implies convergence in probability, therefore

$$\sqrt{n}\,\text{vech}\left(\widehat{\boldsymbol{T}}^{(n)} - \boldsymbol{T}(f) - \boldsymbol{Z}^{(n)}(f)\right) \xrightarrow{\mathcal{P}} 0.$$

By the multivariate central limit theorem we have that $\sqrt{n}\,\text{vech}\left(\boldsymbol{Z}^{(n)}(f)\right) \xrightarrow{\mathcal{D}} \mathcal{N}\left(0, \boldsymbol{C}(f)\right)$. Therefore, $\sqrt{n}\,\text{vech}\left(\widehat{\boldsymbol{T}}^{(n)} - \boldsymbol{T}(f)\right) \xrightarrow{\mathcal{D}} \mathcal{N}\left(0, \boldsymbol{C}(f)\right)$. □

Proof of Theorem 3. For abbreviation, we write M instead of M_n and set $m = |M_n|$. We first compute the mean squared error of $\hat{\theta}_n$ as

$$\mathbb{E}\big[\hat{\theta}_n - \theta\big]^2 = \text{Bias}^2\big(\hat{\theta}_n\big) + \text{Var}\big(\hat{\theta}_n\big)$$

where $\text{Bias}\left(\hat{\theta}_n\right) = \mathbb{E}\big[\hat{\theta}_n\big] - \theta$.

We begin the proof by bounding $\text{Var}\big(\hat{\theta}_n\big)$. Let A and B be $m \times 1$ vectors with components

$$\begin{aligned}
a_l &= \int p_l(x_i, x_j, y) f(x_i, x_j, y)\, dx_i dx_j dy \quad l = 1, \ldots, m,\\
b_l &= \int p_l(x_{i1}, x_{j1}, y) f(x_{i2}, x_{j2}, y) \psi(x_{i1}, x_{j1}, x_{i2}, x_{j2}, y)\, dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy\\
&= \int p_l(x_i, x_j, y) g(x_i, x_j, y)\, dx_i dx_j dy \quad l = 1, \ldots, m
\end{aligned}$$

where $g(x_i, x_j, y) = \int f(x_{i2}, x_{j2}, y)\psi(x_i, x_j, x_{i2}, x_{j2}, y)dx_{i2}dx_{j2}$. Let Q and R be $m \times 1$ vectors of centered functions

$$\begin{aligned}
q_l(x_i, x_j, y) &= p_l(x_i, x_j, y) - a_l\\
r_l(x_i, x_j, y) &= \int p_l(x_{i2}, x_{j2}, y)\psi(x_i, x_j, x_{i2}, x_{j2}, y)\, dx_{i2} dx_{j2} - b_l
\end{aligned}$$

for $l = 1, \ldots, m$. Let C a $m \times m$ matrix of constants

$$c_{ll'} = \int p_l(x_{i1}, x_{j1}, y) p_{l'}(x_{i2}, x_{j2}, y) \eta(x_{i1}, x_{j2}, y)\, dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy \quad l, l' = 1, \ldots, m.$$

Let us denote by U_n the process

$$U_n h = \frac{1}{n(n-1)} \sum_{k \neq k'=1}^{n} h\big(X_i^{(k)}, X_j^{(k)}, Y^{(k)}, X_i^{(k')}, X_j^{(k')}, Y^{(k')}\big)$$

and P_n the empirical measure

$$P_n h = \frac{1}{n} \sum_{k=1}^{n} h\big(X_i^{(k)}, X_j^{(k)}, Y^{(k)}\big)$$

for some h in $\mathbb{L}^2(dx_i, dx_j, dy)$. With these notations, $\hat{\theta}_n$ has the Hoeffding's decomposition

$$\begin{aligned}
\hat{\theta}_n =& \frac{1}{n(n-1)} \sum_{l \in M} \sum_{k \neq k'=1}^{n} \big(q_l(X_i^{(k)}, X_j^{(k)}, Y^{(k)}) + a_l\big)\big(r_l(X_i^{(k')}, X_j^{(k')}, Y^{(k')}) + b_l\big) \\
&- \frac{1}{n(n-1)} \sum_{l,l' \in M} \sum_{k \neq k'=1}^{n} \big(q_l(X_i^{(k)}, X_j^{(k)}, Y^{(k)}) + a_l\big)\big(q_{l'}(X_i^{(k')}, X_j^{(k')}, Y^{(k')}) + a_{l'}\big) c_{ll'} \\
=& U_n K + P_n L + A^\top B - A^\top C A
\end{aligned}$$

where

$$\begin{aligned}
K\left(x_{i1}, x_{j1}, y_1, x_{i2}, x_{j2}, y_2\right) =& Q^\top(x_{i1}, x_{j1}, y_1) R(x_{i2}, x_{j2}, y_2) - Q^\top(x_{i1}, x_{j1}, y_1) C Q(x_{i2}, x_{j2}, y_2) \\
L(x_i, x_j, y) =& A^\top R(x_i, x_j, y) + B Q(x_i, x_j, y) - 2A^\top C Q(x_i, x_j, y).
\end{aligned}$$

Therefore $\mathrm{Var}\big(\hat{\theta}_n\big) = \mathrm{Var}\big(U_n K\big) + \mathrm{Var}\big(P_n L\big) - 2\,\mathrm{Cov}\big(U_n K, P_n L\big)$. These three terms are bounded in Lemmas 2 - 4, which gives

$$\mathrm{Var}\big(\hat{\theta}_n\big) \leq \frac{20}{n(n-1)} \big\|\eta\big\|_\infty^2 \big\|f\big\|_\infty^2 \Delta_{x_i x_j}^2 (m+1) + \frac{12}{n} \big\|\eta\big\|_\infty^2 \big\|f\big\|_\infty^2 \Delta_{x_i x_j}^2 .$$

For n enough large and a constant $\gamma \in \mathbb{R}$,

$$\mathrm{Var}\big(\hat{\theta}_n\big) \leq \gamma \big\|\eta\big\|_\infty^2 \big\|f\big\|_\infty^2 \Delta_{x_i x_j}^2 \left(\frac{m}{n^2} + \frac{1}{n}\right).$$

The term $\mathrm{Bias}\left(\hat{\theta}_n\right)$ is easily computed, as proven in Lemma 5, is equal to

$$\begin{aligned}
-\int \left(S_M f(x_{i1}, x_{j1}, y) - f(x_{i1}, x_{j1}, y)\right)\left(S_M f(x_{i2}, x_{j2}, y) - f(x_{i2}, x_{j2}, y)\right) \\
\eta(x_{i1}, x_{j1}, x_{i2}, x_{j2}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy.
\end{aligned}$$

From Lemma 5, the bias of $\hat{\theta}_n$ is bounded by

$$\left|\mathrm{Bias}\left(\hat{\theta}_n\right)\right| \leq \Delta_{x_i x_j} \big\|\eta\big\|_\infty \sup_{l \notin M} \left|c_l\right|^2 .$$

The assumption of $\left(\sup_{l \notin M} |c_i|^2\right)^2 \approx m/n^2$ and since $m/n \to 0$, we deduce that $\mathbb{E}\big[\hat{\theta}_n - \theta\big]^2$ has a parametric rate of convergence $O\left(1/n\right)$.

Finally to prove (16), note that

$$
\begin{aligned}
n\mathbb{E}\big[\hat{\theta}_n - \theta\big]^2 &= n\,\mathrm{Bias}^2\big(\hat{\theta}_n\big) + n\,\mathrm{Var}\big(\hat{\theta}_n\big) \\
&= n\,\mathrm{Bias}^2\big(\hat{\theta}_n\big) + n\,\mathrm{Var}\big(U_n K\big) + n\,\mathrm{Var}\big(P_n L\big).
\end{aligned}
$$

We previously proved that for some $\lambda_1, \lambda_2 \in \mathbb{R}$

$$
\begin{aligned}
n\,\mathrm{Bias}^2\big(\hat{\theta}_n\big) &\le \lambda_1 \Delta^2_{x_i x_j} \big\|\eta\big\|^2_\infty \frac{m}{n} \\
n\,\mathrm{Var}\big(U_n K\big) &\le \lambda_2 \Delta^2_{x_i x_j} \big\|f\big\|^2_\infty \big\|\eta\big\|^2_\infty \frac{m}{n}.
\end{aligned}
$$

Thus, Lemma 6 implies

$$
\big|n\,\mathrm{Var}\big(P_n L\big) - \Lambda(f,\eta)\big| \le \lambda\left[\big\|S_M f - f\big\|_2 + \big\|S_M g - g\big\|_2\right],
$$

where λ is a increasing function of $\big\|f\big\|^2_\infty$, $\big\|\eta\big\|^2_\infty$ and $\Delta_{x_i x_j}$. From all this we deduce (16) which ends the proof of Theorem 3. □

6 Technical Results

Lemma 1 (Bias of $\hat{\theta}_n$)**.** *The estimator $\hat{\theta}_n$ defined in* (14) *estimates θ with bias equal to*

$$
-\int \left(S_M f(x_{i1}, x_{j1}, y) - f(x_{i1}, x_{j1}, y)\right)\left(S_M f(x_{i2}, x_{j2}, y) - f(x_{i2}, x_{j2}, y)\right) \\
\eta(x_{i1}, x_{j2}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy.
$$

Proof. Let $\hat{\theta}_n = \hat{\theta}^1_n - \hat{\theta}^2_n$ where

$$
\hat{\theta}^1_n = \frac{1}{n(n-1)} \sum_{l\in M} \sum_{k\neq k'=1} p_l(X^{(k)}_i, X^{(k)}_j, Y^{(k)}) \int p_l(x_i, x_j, Y^{(k')}) \psi(x_i, x_j, X^{(k')}_i, X^{(k')}_j, Y^{(k')}) dx_i dx_j
$$

$$
\hat{\theta}^2_n = -\frac{1}{n(n-1)} \sum_{l,l'\in M} \sum_{k\neq k'=1}^{n} p_l(X^{(k)}_i, X^{(k)}_j, Y^{(k)}) p_{l'}(X^{(k')}_i, X^{(k')}_j, Y^{(k')}) \\
\int p_l(x_{i1}, x_{j1}, y) p_{l'}(x_{i2}, x_{j2}, y) \eta(x_{i1}, x_{j2}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy.
$$

Let us first compute $\mathbb{E}\big[\hat{\theta}_n^1\big]$.

$$\begin{aligned}\mathbb{E}\big[\hat{\theta}_n^1\big] =& \sum_{l\in M}\int p_l(x_{i1},x_{j1},y)f(x_{i1},x_{j1},y)dx_{i1}dx_{j1}dy\\
&\int p_l(x_{i1},x_{j1},y)\psi(x_{i1},x_{j1},x_{i2},x_{j2},y)f(x_{i2},x_{j2},y)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy\\
=&\sum_{l\in M}a_l\int p_l(x_{i1},x_{j1},y)\psi(x_{i1},x_{j1},x_{i2},x_{j2},y)f(x_{i2},x_{j2},y)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy\\
=&\int\left(\sum_{l\in M}a_lp_l(x_{i2},x_{j2},y)\right)\psi(x_{i1},x_{j1},x_{i2},x_{j2},y)f(x_{i2},x_{j2},y)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy\\
=&\int S_Mf(x_{i1},x_{j1},y)f(x_{i2},x_{j2},y)\eta(x_{i1},x_{j2},y)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy\\
&+\int S_Mf(x_{i2},x_{j2},y)f(x_{i1},x_{j1},y)\eta(x_{i1},x_{j2},y)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy\end{aligned}$$

Now for $\hat{\theta}_n^2$, we get

$$\begin{aligned}\mathbb{E}\big[\hat{\theta}_n^2\big] =& \sum_{l,l'\in M}\int p_l(x_i,x_j,y)f(x_i,x_j,y)dx_idx_jdy\int p_{l'}(x_i,x_j,y)f(x_i,x_j,y)dx_idx_jdy\\
&\int p_l(x_{i1},x_{j1},y)p_{l'}(x_{i2},x_{j2},y)\eta(x_{i1},x_{j2},y)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy\\
=&\sum_{l,l'\in M}a_la_{l'}\int p_l(x_{i1},x_{j1},y)p_{l'}(x_{i2},x_{j2},y)\eta(x_{i1},x_{j2},y)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy\\
=&\int\left(\sum_{l\in M}a_lp_l(x_{i1},x_{j1},y)\right)\left(\sum_{l'\in M}a_{l'}p_{l'}(x_{i2},x_{j2},y)\right)\eta(x_{i1},x_{j2},y)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy\\
=&\int S_Mf(x_{i1},x_{j1},y)S_Mf(x_{i2},x_{j2},y)\eta(x_{i1},x_{j2},y)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy.\end{aligned}$$

Arranging these terms and using

$$\text{Bias}\left(\hat{\theta}_n\right)=\mathbb{E}\big[\hat{\theta}_n\big]-\theta=\mathbb{E}\big[\hat{\theta}_n^1\big]-\mathbb{E}\big[\hat{\theta}_n^2\big]-\theta$$

we obtain the desire bias. □

Lemma 2 (Bound of $\text{Var}(U_nK)$). *Under the assumptions of Theorem 3, we have*

$$\text{Var}\big(U_nK\big)\leq\frac{20}{n(n-1)}\|\eta\|_\infty^2\|f\|_\infty^2\Delta_{x_ix_j}^2(m+1)$$

Proof. Note that U_nK is centered because Q and R are centered and $(X_i^{(k)},X_j^{(k)},Y^{(k)}),\ k=$

$1, \ldots, n$ is an independent sample. So $\mathrm{Var}\big(U_n K\big)$ is equal to

$$\mathbb{E}\big[U_n K\big]^2 = \mathbb{E}\Bigg(\frac{1}{\big(n(n-1)\big)^2}\sum_{k_1 \neq k_1'=1}^{n}\sum_{k_2 \neq k_2'=1}^{n} K\big(X_i^{(k_1)}, X_j^{(k_1)}, Y^{(k_1)}, X_i^{(k_1')}, X_j^{(k_1')}, Y^{(k_1')}\big)$$

$$K\big(X_i^{(k_2)}, X_j^{(k_2)}, Y^{(k_2)}, X_i^{(k_2')}, X_j^{(k_2')}, Y^{(k_2')}\big)\Bigg)$$

$$= \frac{1}{n(n-1)}\mathbb{E}\Bigg(K^2\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}, X_i^{(2)}, X_j^{(2)}, Y^{(2)}\big)$$

$$+K\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}, X_i^{(2)}, X_j^{(2)}, Y^{(2)}\big)K\big(X_i^{(2)}, X_j^{(2)}, Y^{(2)}, X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\Bigg)$$

By the Cauchy-Schwarz inequality, we get

$$\mathrm{Var}\big(U_n K\big) \leq \frac{2}{n(n-1)}\mathbb{E}\big[K^2\left(X_i^{(1)}, X_j^{(1)}, Y^{(1)}, X_i^{(2)}, X_j^{(2)}, Y^{(2)}\right)\big].$$

Moreover, using the fact that $2\left|\mathbb{E}\big[XY\big]\right| \leq \mathbb{E}\big[X^2\big] + \mathbb{E}\big[Y^2\big]$, we obtain

$$\mathbb{E}\big[K^2\left(X_i^{(1)}, X_j^{(1)}, Y^{(1)}, X_i^{(2)}, X_j^{(2)}, Y^{(2)}\right)\big] \leq 2\Bigg[\mathbb{E}\big[\big(Q^\top(X_i^{(1)}, X_j^{(1)}, Y^{(1)})R(X_i^{(2)}, X_j^{(2)}, Y^{(2)})\big)^2\big]$$

$$+\mathbb{E}\big[\big(Q^\top(X_i^{(1)}, X_j^{(1)}, Y^{(1)})CQ(X_i^{(2)}, X_j^{(2)}, Y^{(2)})\big)^2\big]\Bigg].$$

We will bound these two terms. The first one is

$$\mathbb{E}\big[\big(Q^\top(X_i^{(1)}, X_j^{(1)}, Y^{(1)})R(X_i^{(2)}, X_j^{(2)}, Y^{(2)})\big)^2\big]$$

$$= \sum_{l,l' \in M}\left(\int p_l(x_i, x_j, y)p_{l'}(x_i, x_j, y)f(x_i, x_j, y)dx_i dx_j dy - a_l a_{l'}\right)$$

$$\Bigg(\int p_l(x_{i2}, x_{j2}, y)p_{l'}(x_{i3}, x_{j3}, y)\psi(x_{i1}, x_{j1}, x_{i2}, x_{j2}, y)$$

$$\psi(x_{i1}, x_{j1}, x_{i3}, x_{j3}, y)f(x_{i1}, x_{j1}, y)dx_{i1}dx_{j1}dx_{i2}dx_{j2}dx_{i3}dx_{j3}dy - b_l b_{l'}\Bigg)$$

$$= W_1 - W_2 - W_3 + W_4$$

where

$$W_1 = \int \sum_{l,l' \in M} p_l(x_{i1}, x_{j1}, y) p_{l'}(x_{i1}, x_{j1}, y) p_l(x_{i2}, x_{j2}, y') p_{l'}(x_{i3}, x_{j3}, y') \psi(x_{i4}, x_{j4}, x_{i2}, x_{j2}, y')$$
$$\psi(x_{i4}, x_{j4}, x_{i3}, x_{j3}, y') f(x_{i1}, x_{j1}, y) f(x_{i4}, x_{j4}, y') dx_{i1} dx_{j1} dx_{i2} dx_{j2} dx_{i3} dx_{j3} dx_{i4} dx_{j4} dy dy'$$
$$W_2 = \int \sum_{l,l' \in M} b_l b_{l'} p_l(x_{i1}, x_{j1}, y) p_{l'}(x_{i1}, x_{j1}, y) f(x_{i1}, x_{j1}, y) dx_{i1} dx_{j1} dy$$
$$W_3 = \int \sum_{l,l' \in M} a_l a_{l'} p_l(x_{i2}, x_{j2}, y') p_{l'}(x_{i3}, x_{j3}, y')$$
$$\psi(x_{i4}, x_{j4}, x_{i2}, x_{j2}, y') \psi(x_{i4}, x_{j4}, x_{i3}, x_{j3}, y') f(x_{i4}, x_{j4}, y') dx_{i2} dx_{j2} dx_{i3} dx_{j3} dx_{i4} dx_{j4} dy'$$
$$W_4 = \sum_{l,l' \in M} a_l a_{l'} b_l b_{l'}.$$

W_2 and W_3 are positive, hence

$$\mathbb{E}\Big[\Big(2Q^\top(X_i^{(1)}, X_j^{(1)}, Y^{(1)}) R(X_i^{(2)}, X_j^{(2)}, Y^{(2)})\Big)^2\Big] \le W_1 + W_4.$$

$$W_1 = \int \sum_{l,l' \in M} p_l(x_{i1}, x_{j1}, y) p_{l'}(x_{i1}, x_{j1}, y) \Big(\int p_l(x_{i2}, x_{j2}, y') \psi(x_{i4}, x_{j4}, x_{i2}, x_{j2}, y') dx_{i2} dx_{j2}\Big)$$
$$\Big(\int p_{l'}(x_{i3}, x_{j3}, y') \psi(x_{i4}, x_{j4}, x_{i3}, x_{j3}, y') dx_{i3} dx_{j3}\Big) f(x_{i1}, x_{j1}, y) f(x_{i4}, x_{j4}, y') dx_{i1} dx_{j1} dx_{i4} dx_{j4} dy dy$$
$$\le \|f\|_\infty^2 \sum_{l,l' \in M} \int p_l(x_{i1}, x_{j1}, y) p_{l'}(x_{i1}, x_{j1}, y) dx_{i1} dx_{j1} dy$$
$$\int \Big(\int p_l(x_{i2}, x_{j2}, y') \psi(x_{i4}, x_{j4}, x_{i2}, x_{j2}, y') dx_{i2} dx_{j2}\Big)$$
$$\Big(\int p_{l'}(x_{i3}, x_{j3}, y') \psi(x_{i4}, x_{j4}, x_{i3}, x_{j3}, y') dx_{i3} dx_{j3}\Big) dx_{i2} dx_{j2} dx_{i4} dx_{j4} dy'$$

Since p_l's are orhonormal we have

$$W_1 \le \|f\|_\infty^2 \sum_{l \in M} \int \Big(\int p_l(x_{i2}, x_{j2}, y') \psi(x_{i4}, x_{j4}, x_{i2}, x_{j2}, y') dx_{i2} dx_{j2}\Big)^2 dx_{i4} dx_{j4} dy'.$$

Moreover by the Cauchy-Schwarz inequality and $\|\psi\|_\infty \le 2\|\eta\|_\infty$

$$\Big(\int p_l(x_{i2}, x_{j2}, y') \psi(x_{i4}, x_{j4}, x_{i2}, x_{j2}, y') dx_{i2} dx_{j2}\Big)^2 \le \int p_l(x_{i2}, x_{j2}, y')^2 dx_{i2} dx_{j2}$$
$$\int \psi(x_{i4}, x_{j4}, x_{i2}, x_{j2}, y')^2 dx_{i2} dx_{j2}$$
$$\le \|\psi\|_\infty^2 \Delta_{x_i x_j} \int p_l(x_{i2}, x_{j2}, y')^2 dx_{i2} dx_{j2}$$
$$\le 4\|\eta\|_\infty^2 \Delta_{x_i x_j} \int p_l(x_{i2}, x_{j2}, y')^2 dx_{i2} dx_{j2},$$

and then

$$\begin{aligned}
&\int\Big(\int p_l(x_{i2},x_{j2},y')\psi(x_{i4},x_{j4},x_{i2},x_{j2},y')dx_{i2}dx_{j2}\Big)^2 dx_{i4}dx_{j4}dy' \\
&\leq 4\|\eta\|_\infty^2\Delta_{x_ix_j}^2\int p_l(x_{i2},x_{j2},y')^2dx_{i2}dx_{j2}dy' \\
&= 4\|\eta\|_\infty^2\Delta_{x_ix_j}^2.
\end{aligned}$$

Finally,

$$W_1 \leq 4\|\eta\|_\infty^2\|f\|_\infty^2\Delta_{x_ix_j}^2 m.$$

For the term W_4 using the facts that $S_M f$ and $S_M g$ are projection and that $\int f = 1$, we have

$$W_4 = \left(\sum_{l\in M} a_l b_l\right)^2 \leq \sum_{l\in M} a_l^2 \sum_{l\in M} b_l^2 \leq \|f\|_2^2\|g\|_2^2 \leq \|f\|_\infty\|g\|_2^2.$$

By the Cauchy-Schwartz inequality we have $\|g\|_2^2 \leq 4\|\eta\|_\infty^2\|f\|_\infty\Delta_{x_ix_j}^2$ and then

$$W_4 \leq 4\|\eta\|_\infty^2\|f\|_\infty^2\Delta_{x_ix_j}^2$$

which leads to

$$\mathbb{E}\big[\big(Q^\top(X_i^{(1)},X_j^{(1)},Y^{(1)})R(X_i^{(2)},X_j^{(2)},Y^{(2)})\big)^2\big] \leq 4\|\eta\|_\infty^2\|f\|_\infty^2\Delta_{x_ix_j}^2(m+1). \quad (25)$$

The second term $\mathbb{E}\big[\big(Q^\top(X_i^{(1)},X_j^{(1)},Y^{(1)})CQ(X_i^{(2)},X_j^{(2)},Y^{(2)})\big)\big] = W_5 - 2W_6 + W_7$ where

$$\begin{aligned}
W_5 =& \int\sum_{l_1,l_1'}\sum_{l_2,l_2'} c_{l_1l_1'}c_{l_2l_2'}p_{l_1}(x_{i1},x_{j1},y)p_{l_2}(x_{i1},x_{j1},y)p_{l_1'}(x_{i2},x_{j2},y')p_{l_2'}(x_{i2},x_{j2},y') \\
& f(x_{i1},x_{j1},y)f(x_{i2},x_{j2},y')dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy'dy \\
W_6 =& \int\sum_{l_1,l_1'}\sum_{l_2,l_2'} c_{l_1l_1'}c_{l_2l_2'}a_{l_1}a_{l_2}p_{l_1'}(x_i,x_j,y)p_{l_2'}(x_i,x_j,y)dx_idx_jdy \\
W_7 =& \sum_{l_1,l_1'}\sum_{l_2,l_2'} c_{l_1l_1'}c_{l_2l_2'}a_{l_1}a_{l_1'}a_{l_2}a_{l_2'}.
\end{aligned}$$

Using the previous manipulation, we show that $W_6 \geq 0$. Thus

$$\mathbb{E}\big[\big(Q^\top(X_i^{(1)},X_j^{(1)},Y^{(1)})CQ(X_i^{(2)},X_j^{(2)},Y^{(2)})\big)\big] \leq W_5 + W_7.$$

First, observe that

$$
\begin{aligned}
W_5 =& \sum_{l_1,l_1'}\sum_{l_2,l_2'} c_{l_1 l_1'} c_{l_2 l_2'} \left(\int p_{l_1}(x_{i1},x_{j1},y) p_{l_2}(x_{i1},x_{j1},y) f(x_{i1},x_{j1},y) dx_{i1} dx_{j1} dy \right) \\
& \left(\int p_{l_1'}(x_{i2},x_{j2},y') p_{l_2'}(x_{i2},x_{j2},y') f(x_{i2},x_{j2},y') dx_{i2} dx_{j2} dy' \right) \\
\leq & \|f\|_\infty^2 \sum_{l_1,l_1'}\sum_{l_2,l_2'} c_{l_1 l_1'} c_{l_2 l_2'} \left(\int p_{l_1}(x_{i1},x_{j1},y) p_{l_2}(x_{i1},x_{j1},y) dx_{i1} dx_{j1} dy \right) \\
& \left(\int p_{l_1'}(x_{i2},x_{j2},y') p_{l_2'}(x_{i2},x_{j2},y') dx_{i2} dx_{j2} dy' \right) \\
=& \|f\|_\infty^2 \sum_{l,l'} c_{ll'}^2
\end{aligned}
$$

agin using the orthonormality of the the p_l's. Besides given the decomposition $p_l(x_i,x_j,y) = \alpha_{l_\alpha}(x_i,x_j)\beta_{l_\beta}(y)$,

$$
\begin{aligned}
\sum_{l,l'} c_{ll'}^2 = & \int \sum_{l_\beta,l_\beta'} \beta_{l_\beta}(y)\beta_{l_\beta'}(y)\beta_{l_\beta}(y')\beta_{l_\beta'}(y') \\
& \sum_{l_\alpha,l_\alpha'} \left(\int \alpha_{l_\alpha}(x_{i1},x_{j1}) \alpha_{l_\alpha'}(x_{i2},x_{j2}) \eta(x_{i1},x_{j2},y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} \right) \\
& \left(\int \alpha_{l_\alpha}(x_{i3},x_{j3}) \alpha_{l_\alpha'}(x_{i4},x_{j4}) \eta(x_{i3},x_{j4},y') dx_{i3} dx_{j3} dx_{i4} dx_{j4} \right) dy dy'
\end{aligned}
$$

But

$$
\begin{aligned}
& \sum_{l_\alpha,l_\alpha'} \left(\int \alpha_{l_\alpha}(x_{i1},x_{j1}) \alpha_{l_\alpha'}(x_{i2},x_{j2}) \eta(x_{i1},x_{j2},y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} \right) \\
& \left(\int \alpha_{l_\alpha}(x_{i3},x_{j3}) \alpha_{l_\alpha'}(x_{i4},x_{j4}) \eta(x_{i3},x_{j4},y') dx_{i3} dx_{j3} dx_{i4} dx_{j4} \right) \\
=& \sum_{l_\alpha,l_\alpha'} \int \alpha_{l_\alpha}(x_{i1},x_{j1}) \alpha_{l_\alpha'}(x_{i2},x_{j2}) \eta(x_{i1},x_{j2},y) \alpha_{l_\alpha}(x_{i3},x_{j3}) \\
& \alpha_{l_\alpha'}(x_{i4},x_{j4}) \eta(x_{i3},x_{j4},y') dx_{i1} dx_{j1} dx_{i2} dx_{j2} dx_{i3} dx_{j3} dx_{i4} dx_{j4} \\
=& \int \sum_{l_\alpha} \left(\int \alpha_{l_\alpha}(x_{i1},x_{j1}) \eta(x_{i1},x_{j2},y) dx_{i1} dx_{j1} \right) \alpha_{l_\alpha}(x_{i3},x_{j3}) \\
& \sum_{l_\alpha'} \left(\int \alpha_{l_\alpha'}(x_{i4},x_{j4}) \eta(x_{i3},x_{j4},y') dx_{i4} dx_{j4} \right) \alpha_{l_\alpha'}(x_{i2},x_{j2}) dx_{i2} dx_{j2} dx_{i3} dx_{j3} \\
\leq & \int \eta(x_{i3},x_{j3},x_{i2},x_{j2},y) \eta(x_{i3},x_{j2},y') dx_{i2} dx_{j2} dx_{i3} dx_{j3} \\
\leq & \Delta_{x_i x_j}^2 \|\eta\|_\infty^2
\end{aligned}
$$

using the orthonormality of the basis α_{l_α}. Then we get

$$\begin{aligned}\sum_{l,l'} c_{ll'}^2 &\leq \Delta_{x_ix_j}^2 \|\eta\|_\infty^2 \left(\int \sum_{l_\beta, l'_\beta} \beta_{l_\beta}(y)\beta_{l'_\beta}(y)\beta_{l_\beta}(y')\beta_{l'_\beta}(y')dydy' \right) \\ &= \Delta_{x_ix_j}^2 \|\eta\|_\infty^2 \sum_{l_\beta, l'_\beta} \left(\int \beta_{l_\beta}(y)\beta_{l'_\beta}(y)dy \right)^2 \\ &\leq \Delta_{x_ix_j}^2 \|\eta\|_\infty^2 \sum_{l_\beta} \left(\int \beta_{l_\beta}^2(y)dy \right)^2 \\ &\leq \Delta_{x_ix_j}^2 \|\eta\|_\infty^2 m\end{aligned}$$

since the β_{l_β} are orthonormal. Finally

$$W_5 \leq \|f\|_\infty^2 \|\eta\|_\infty^2 \Delta_{x_ix_j}^2 m.$$

Now for W_7 we first will bound,

$$\begin{aligned}\left| \sum_{l,l'} c_{ll'} a_l a_{l'} \right| &= \left| \int \sum_{l,l' \in M} a_l a_{l'} p_{l_2}(x_{i1}, x_{j1}, y) p_{l'_1}(x_{i2}, x_{j2}, y)\eta(x_{i1}, x_{j2}, y) dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy \right| \\ &\leq \int |S_M(x_{i1}, x_{j1}, y)S_M(x_{i2}, x_{j2}, y)\eta(x_{i1}, x_{j2}, y)| \, dx_{i1}dx_{j1}dx_{i2}dx_{j2}dy \\ &\leq \|\eta\|_\infty \int \left(\int |S_M(x_{i1}, x_{j1}, y)S_M(x_{i2}, x_{j2}, y)| \, dy \right) dx_{i1}dx_{j1}dx_{i2}dx_{j2}.\end{aligned}$$

Taking squares in both sides and using the Cauchy-Schwartz inequality twice, we get

$$\begin{aligned}\left(\sum_{l,l'} c_{ll'} a_l a_{l'} \right)^2 &= \|\eta\|_\infty^2 \left(\int \left(\int |S_M(x_{i1}, x_{j1}, y)S_M(x_{i2}, x_{j2}, y)| \, dy \right) dx_{i1}dx_{j1}dx_{i2}dx_{j2} \right)^2 \\ &\leq \|\eta\|_\infty^2 \Delta_{x_ix_j}^2 \int \left(\int |S_M(x_{i1}, x_{j1}, y)S_M(x_{i2}, x_{j2}, y)| \, dy \right)^2 dx_{i1}dx_{j1}dx_{i2}dx_{j2} \\ &\leq \|\eta\|_\infty^2 \Delta_{x_ix_j}^2 \int \left(\int S_M(x_{i1}, x_{j1}, y)^2 dy \right) \left(\int S_M(x_{i2}, x_{j2}, y')^2 dy' \right) dx_{i1}dx_{j1}dx_{i2}dx_{j2} \\ &= \|\eta\|_\infty^2 \Delta_{x_ix_j}^2 \int S_M(x_{i1}, x_{j1}, y)^2 S_M(x_{i1}, x_{j1}, y')^2 dx_{i1}dx_{j1}dx_{i2}dx_{j2}dydy' \\ &= \|\eta\|_\infty^2 \Delta_{x_ix_j}^2 \left(\int S_M(x_i, x_j, y)^2 dx_i dx_j dy \right) \\ &\leq \|\eta\|_\infty^2 \Delta_{x_ix_j}^2 \|f\|_\infty^2.\end{aligned}$$

Finally,

$$\mathbb{E}\left[\left(Q^\top(X_i^{(1)}, X_j^{(1)}, Y^{(1)}) C Q(X_i^{(2)}, X_j^{(2)}, Y^{(2)}) \right)^2 \right] \leq \|\eta\|_\infty^2 \|f\|_\infty^2 \Delta_{x_ix_j}^2 (m+1). \quad (26)$$

Collecting (25) and (26), we obtain

$$\mathrm{Var}\big(U_nK\big) \le \frac{20}{n(n-1)}\big\|\eta\big\|_\infty^2\big\|f\big\|_\infty^2\Delta_{x_ix_j}^2(m+1)$$

which concludes the proof of Lemma 2. □

Lemma 3 (Bound for $\mathrm{Var}\big(P_nL\big)$). *Under the assumptions of Theorem 3, we have*

$$\mathrm{Var}\big(P_nL\big) \le \frac{12}{n}\big\|\eta\big\|_\infty^2\big\|f\big\|_\infty^2\Delta_{x_ix_j}^2.$$

Proof. First note that given the independence of $\big(X_i^{(k)}, X_j^{(k)}, Y^{(k)}\big)$ $k = 1,\dots,n$ we have

$$\mathrm{Var}\big(P_nL\big) = \frac{1}{n}\mathrm{Var}\big(L\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\big)$$

we can write $L\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)$ as

$$\begin{aligned}
&A^\top R\left(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\right) + B^\top Q\left(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\right) - 2A^\top CQ\left(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\right)\\
=&\sum_{l\in M} a_l\left(\int p_l(x_i,x_j,Y^{(1)})\psi(x_i,x_j,X_i^{(1)},X_j^{(1)},Y^{(1)})dx_idx_j - b_l\right)\\
&+\sum_{l\in M} b_l\left(p_l(X_i^{(1)},X_j^{(1)},Y^{(1)}) - a_l\right) - 2\sum_{l,l'\in M} c_{ll'}a_{l'}\left(p_l(X_i^{(1)},X_j^{(1)},Y^{(1)}) - a_l\right)\\
=&\int\sum_{l\in M} a_lp_l(x_i,x_j,Y^{(1)})\psi(x_i,x_j,X_i^{(1)},X_j^{(1)},Y^{(1)})dx_idx_j\\
&+\sum_{l\in M} b_lp_l(X_i^{(1)},X_j^{(1)},Y^{(1)}) - 2\sum_{l,l'\in M} c_{ll'}a_{l'}p_l(X_i^{(1)},X_j^{(1)},Y^{(1)}) - 2A^tB - 2A^tCA.\\
=&\int S_Mf(x_i,x_j,Y^{(1)})\psi(x_i,x_j,X_i^{(1)},X_j^{(1)},Y^{(1)})dx_idx_j + S_Mg(X_i^{(1)},X_j^{(1)},Y^{(1)})\\
&-2\sum_{l,l'\in M} c_{ll'}a_{l'}p_l(X_i^{(1)},X_j^{(1)},Y^{(1)}) - 2A^\top B - 2A^\top CA.
\end{aligned}$$

Let $h(x_i,x_j,y) = \int S_Mf(x_{i2},x_{j2},y)\psi(x_i,x_j,x_{i2},x_{j2},y)dx_{i2}dx_{j2}$, we have

$$\begin{aligned}
&S_Mh(x_i,x_j,y)\\
=&\sum_{l\in M}\left(\int h(x_{i2},x_{j2},y)p_l(x_{i2},x_{j2},y)dx_{i2}dx_{j2}dy\right)p_l(x_i,x_j,y)\\
=&\sum_{l\in M}\left(\int S_Mf(x_{i3},x_{j3},y)\psi(x_{i2},x_{j2},x_{i3},x_{j3},y)p_l(x_{i2},x_{j2},y)dx_{i2}dx_{j2}dx_{i3}dx_{j3}dy\right)p_l(x_i,x_j,y)\\
=&\sum_{l,l'\in M}\left(\int a_{l'}p_{l'}(x_{i3},x_{j3},y)\psi(x_{i2},x_{j2},x_{i3},x_{j3},y)p_l(x_{i2},x_{j2},y)dx_{i2}dx_{j2}dx_{i3}dx_{j3}dy\right)p_l(x_i,x_j,y)\\
=&\,2\sum_{l,l'\in M}\left(\int a_{l'}p_{l'}(x_{i3},x_{j3},y)\eta(x_{i2},x_{j3},y)p_l(x_{i2},x_{j2},y)dx_{i2}dx_{j2}dx_{i3}dx_{j3}dy\right)p_l(x_i,x_j,y)\\
=&\,2\sum_{l,l'\in M} a_{l'}c_{ll'}p_l(x_i,x_j,y)
\end{aligned}$$

and we can write

$$\begin{aligned}L\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big) = & h\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big) + S_M g\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big) \\ & - S_M h\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big) - 2A^\top B - 2A^\top C A.\end{aligned}$$

Thus,

$$\begin{aligned}& \mathrm{Var}\big(L\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\big) \\ = & \mathrm{Var}\big(h\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big) + S_M g\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big) + S_M h\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\big) \\ \leq & \mathbb{E}\big[\big(h\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big) + S_M g\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big) + S_M h\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\big)^2\big] \\ \leq & \mathbb{E}\big[\big(h\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\big)^2 + \big(S_M g\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\big)^2 + \big(S_M h\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\big)^2\big].\end{aligned}$$

Each of these terms can be bounded

$$\begin{aligned}& \mathbb{E}\big[\big(h\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\big)^2\big] \\ = & \int \left(\int S_M f(x_{i2}, x_{j2}, y)\psi(x_{i1} x_{j2}, x_{i2}, x_{j2}, y) dx_{i2} dx_{j2}\right)^2 f(x_{i1}, x_{j1}, y) dx_{i1} dx_{j1} dy \\ \leq & \Delta_{x_i x_j} \int S_M f(x_{i2}, x_{j2}, y)^2 \psi(x_{i1} x_{j2}, x_{i2}, x_{j2}, y)^2 f(x_{i1}, x_{j1}, y) dx_{i1} dx_{j1} dx_{i2} dx_{j2} dy \\ \leq & 4\Delta_{x_i x_j}^2 \|f\|_\infty \|\eta\|_\infty^2 \int S_M f(x_i, x_j, y)^2 dx_i dx_j dy \\ = & 4\Delta_{x_i x_j}^2 \|f\|_\infty \|\eta\|_\infty^2 \|S_M f\|_2^2 \\ \leq & 4\Delta_{x_i x_j}^2 \|f\|_\infty \|\eta\|_\infty^2 \|f\|_2^2 \\ \leq & 4\Delta_{x_i x_j}^2 \|f\|_\infty^2 \|\eta\|_\infty^2\end{aligned}$$

and similar calculations are valid for the others two terms,

$$\begin{aligned}\mathbb{E}\big[\big(S_M g\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\big)^2\big] \leq \|f\|_\infty \|S_M g\|_2^2 \leq \|f\|_\infty \|g\|_2^2 \leq 4\Delta_{x_i x_j}^2 \|f\|_\infty^2 \|\eta\|_\infty^2 \\ \mathbb{E}\big[\big(S_M h\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\big)^2\big] \leq \|f\|_\infty \|S_M h\|_2^2 \leq \|f\|_\infty \|h\|_2^2 \leq 4\Delta_{x_i x_j}^2 \|f\|_\infty^2 \|\eta\|_\infty^2.\end{aligned}$$

Finally we get,

$$\mathrm{Var}\big(P_n L\big) \leq \frac{12}{n} \|\eta\|_\infty^2 \|f\|_\infty^2 \Delta_{x_i x_j}^2.$$

□

Lemma 4 (Computation of $\mathrm{Cov}\big(U_n K, P_n L\big)$)**.** *Under the assumptions of Theorem 3, we have*

$$\mathrm{Cov}\big(U_n K, P_n L\big) = 0.$$

Proof of Lemma 4. Since $U_n K$ and $P_n L$ are centered, we have

$$\begin{aligned}
&\operatorname{Cov}\big(U_n K, P_n L\big)\\
=&\,\mathbb{E}\big[U_n K P_n L\big]\\
=&\,\mathbb{E}\left[\frac{1}{n^2(n-1)}\sum_{k\neq k'=1}^{n} K\big(X_i^{(k)}, X_j^{(k)}, Y^{(k)}, X_i^{(k')}, X_j^{(k')}, Y^{(k')}\big)\sum_{k=1}^{n} L\big(X_i^{(k)}, X_j^{(k)}, Y^{(k)}\big)\right]\\
=&\,\frac{1}{n}\mathbb{E}\big[K\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}, X_i^{(2)}, X_j^{(2)}, Y^{(2)}\big)\big(L\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big) + L\big(X_i^{(2)}, X_j^{(2)}, Y^{(2)}\big)\big)\big]\\
=&\,\frac{1}{n}\mathbb{E}\big[\big(Q^\top(X_i^{(1)}, X_j^{(1)}, Y^{(1)})R(X_i^{(2)}, X_j^{(2)}, Y^{(2)}) - Q^\top(X_i^{(1)}, X_j^{(1)}, Y^{(1)})CQ(X_i^{(2)}, X_j^{(2)}, Y^{(2)})\big)\\
&\big(A^\top R(X_i^{(1)}, X_j^{(1)}, Y^{(1)}) + B^\top Q(X_i^{(1)}, X_j^{(1)}, Y^{(1)}) - 2A^\top CQ(X_i^{(1)}, X_j^{(1)}, Y^{(1)})\\
&+A^\top R(X_i^{(2)}, X_j^{(2)}, Y^{(2)}) + B^\top Q(X_i^{(2)}, X_j^{(2)}, Y^{(2)}) - 2A^\top CQ(X_i^{(2)}, X_j^{(2)}, Y^{(2)})\big)\big]\\
=&\,0.
\end{aligned}$$

Since K, L, Q and R are centered. □

Lemma 5 (Bound of $\operatorname{Bias}\big(\hat{\theta}_n\big)$)**.** *Under the assumptions of Theorem 3, we have*

$$\left|\operatorname{Bias}\big(\hat{\theta}_n\big)\right| \leq \Delta_{x_i x_j}\|\eta\|_\infty \sup_{l\notin M}|c_l|^2 .$$

Proof.

$$\begin{aligned}
\left|\operatorname{Bias}\big(\hat{\theta}_n\big)\right| &\leq \|\eta\|_\infty \int\left(\int |S_M f(x_{i1}, x_{j1}, y) - f(x_{i1}, x_{j1}, y)|\, dx_{i1}dx_{j1}\right)\\
&\qquad\left(\int |S_M f(x_{i2}, x_{j2}, y) - f(x_{i2}, x_{j2}, y)|\, dx_{i2}dx_{j2}\right) dy\\
&= \|\eta\|_\infty \int\left(\int |S_M f(x_i, x_j, y) - f(x_i, x_j, y)|\, dx_i dx_j\right)^2 dy\\
&\leq \Delta_{x_i x_j}\|\eta\|_\infty \int (S_M f(x_i, x_j, y) - f(x_i, x_j, y))^2\, dx_i dx_j dy\\
&= \Delta_{x_i x_j}\|\eta\|_\infty \sum_{l,l'\notin M} a_l a_{l'} \int p_l(x_i, x_j, y)p_{l'}(x_i, x_j, y)dx_i dx_j dy\\
&= \Delta_{x_i x_j}\|\eta\|_\infty \sum_{l\notin M}|a_l|^2 \leq \Delta_{x_i x_j}\|\eta\|_\infty \sup_{l\notin M}|c_l|^2 .
\end{aligned}$$

We use the Hölder's inequality and the fact that $f\in\mathcal{E}$ then $\sum_{l\notin M}|a_l|^2 \leq \sup_{l\notin M}|c_l|^2$. □

Lemma 6 (Asymptotic variance of $\sqrt{n}\big(P_n L\big)$.)**.** *Under the assumptions of Theorem 3, we have*

$$n\operatorname{Var}\big(P_n L\big) \to \Lambda(f, \eta)$$

where

$$\Lambda(f,\eta) = \int g(x_i, x_j, y)^2 f(x_i, x_j, y)dx_i dx_j dy - \left(\int g(x_i, x_j, y) f(x_i, x_j, y)dx_i dx_j dy\right)^2 .$$

Proof. We proved in Lemma 3 that

$$\begin{aligned}
&\operatorname{Var}\big(L\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\big) \\
=&\operatorname{Var}\big(h\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big) + S_M g\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big) + S_M h\big(X_i^{(1)}, X_j^{(1)}, Y^{(1)}\big)\big) \\
=&\operatorname{Var}\big(A_1 + A_2 + A_3\big) \\
=&\sum_{k,l=1}^{3} \operatorname{Cov}\big(A_k, A_l\big).
\end{aligned}$$

We claim that $\forall k, l \in \{1,2,3\}^2$, we have

$$\left|\operatorname{Cov}\big(A_k, A_l\big) - \epsilon_{kl}\left[\int g(x_i,x_j,y)^2 f(x_i,x_j,y)dx_i dx_j dy - \left(\int g(x_i,x_j,y) f(x_i,x_j,y)dx_i dx_j dy\right)^2\right]\right| \\ \leq \lambda\left[\|S_M f - f\|_2 + \|S_M g - g\|_2\right] \quad (27)$$

where

$$\epsilon_{kl} = \begin{cases} -1 & \text{if } k = 3 \text{ or } l = 3 \text{ and } k \neq l \\ 1 & \text{otherwise} \end{cases},$$

and where λ depends only on $\|f\|_\infty$, $\|\eta\|_\infty$and $\Delta_{x_i x_j}$. We will do the details only for the case $k = l = 3$ since the calculations are similar for others configurations.

$$\operatorname{Var}\big(A_3\big) = \int S_M^2 h\left(x_i,x_j,y\right) f(x_i,x_j,y)dx_i dx_j dy - \left(\int S_M h\left(x_i,x_j,y\right) f(x_i,x_j,y)dx_i dx_j dy\right)^2.$$

The computation will be done in two steps. We first bound the quantity by the Cauchy-Schwartz inequality

$$\begin{aligned}
&\left|\int S_M^2 h\left(x_i,x_j,y\right) f(x_i,x_j,y)dx_i dx_j dy - \int g(x_i,x_j,y)^2 f(x_i,x_j,y)dx_i dx_j dy\right| \\
\leq &\int \left|S_M^2 h\left(x_i,x_j,y\right) f(x_i,x_j,y) - S_M^2 g\left(x_i,x_j,y\right) f(x_i,x_j,y)\right| dx_i dx_j dy \\
&+ \int \left|S_M^2 g\left(x_i,x_j,y\right) f(x_i,x_j,y) - g(x_i,x_j,y)^2 f(x_i,x_j,y)\right| dx_i dx_j dy \\
\leq &\|f\|_\infty \|S_M h + S_M g\|_2 \|S_M h - S_M g\|_2 + \|f\|_\infty \|S_M g + g\|_2 \|S_M g - g\|_2.
\end{aligned}$$

Using several times the fact that since S_M is a projection, $\|S_M g\|_2 \leq \|g\|_2$, the sum is bounded by

$$\begin{aligned}
&\|f\|_\infty \|h + g\|_2 \|h - g\|_2 + 2\|f\|_\infty \|g\|_2 \|S_M g - g\|_2 \\
\leq &\|f\|_\infty \left(\|h\|_2 + \|g\|_2\right) \|h - g\|_2 + 2\|f\|_\infty \|g\|_2 \|S_M g - g\|_2.
\end{aligned}$$

We saw previously that $\|g\|_2 \leq 2\Delta_{x_i x_j} \|f\|_\infty^{1/2} \|\eta\|_\infty$ and $\|h\|_2 \leq 2\Delta_{x_i x_j} \|f\|_\infty^{1/2} \|\eta\|_\infty$. The sum is then bound by

$$4\Delta_{x_i x_j} \|f\|_\infty^{3/2} \|\eta\|_\infty \|h - g\|_2 + 4\Delta_{x_i x_j} \|f\|_\infty^{3/2} \|\eta\|_\infty \|S_M g - g\|_2.$$

We now have to deal with $\|h-g\|_2$:

$$
\begin{aligned}
&\|h-g\|_2^2 \\
=&\int\left(\int\left(S_M f(x_{i2},x_{j2},y)-f(x_{i2},x_{j2},y)\right)\psi(x_{i1},x_{j1},x_{i2},x_{j2},y)dx_{i2}dx_{j2}\right)^2 dx_{i1}dx_{j1}dy \\
\leq&\int\left(\int\left(S_M f(x_{i2},x_{j2},y)-f(x_{i2},x_{j2},y)\right)^2 dx_{i2}dx_{j2}\right)\left(\int \psi^2(x_{i1},x_{j1},x_{i2},x_{j2},y)dx_{i2}dx_{j2}\right)dx_{i1}dx_{j1}dy \\
\leq& 4\Delta_{x_ix_j}^2\|\eta\|_\infty^2\|S_M f-f\|_2^2.
\end{aligned}
$$

Finally this first part is bounded by

$$
\begin{aligned}
&\left|\int S_M^2 h\left(x_i,x_j,y\right)f(x_i,x_j,y)dx_idx_jdy-\int g(x_i,x_j,y)^2 f(x_i,x_j,y)dx_idx_jdy\right| \\
\leq& 4\Delta_{x_ix_j}\|f\|_\infty^{3/2}\|\eta\|_\infty\left(2\Delta_{x_ix_j}\|\eta\|_\infty\|S_M f-f\|_2+\|S_M g-g\|_2\right).
\end{aligned}
$$

Following with the second quantity

$$
\begin{aligned}
&\left|\left(\int S_M h\left(x_i,x_j,y\right)f(x_i,x_j,y)dx_idx_jdy\right)^2-\left(\int g(x_i,x_j,y)f(x_i,x_j,y)dx_idx_jdy\right)^2\right| \\
=&\left|\left(\int\left(S_M h\left(x_i,x_j,y\right)-g(x_i,x_j,y)\right)f(x_i,x_j,y)dx_idx_jdy\right)\right. \\
&\left.\left(\int\left(S_M h\left(x_i,x_j,y\right)+g(x_i,x_j,y)\right)f(x_i,x_j,y)dx_idx_jdy\right)\right|.
\end{aligned}
$$

By using the Cauchy-Schwartz inequality, it is bounded by

$$
\begin{aligned}
&\|f\|_2\|S_M h-g\|_2\|f\|_2\|S_M h+g\|_2 \\
\leq&\|f\|_2^2\left(\|h\|_2+\|g\|_2\right)\left(\|S_M h-S_M g\|_2+\|S_M g-g\|_2\right) \\
\leq&4\Delta_{x_ix_j}\|f\|_\infty^{3/2}\|\eta\|_\infty\left(\|h-g\|_2+\|S_M g-g\|_2\right) \\
\leq&4\Delta_{x_ix_j}\|f\|_\infty^{3/2}\|\eta\|_\infty\left(2\Delta_{x_ix_j}\|\eta\|_\infty\|S_M f-f\|_2+\|S_M g-g\|_2\right)
\end{aligned}
$$

using the previous calculations. Collecting the two inequalities gives (27) for $k=l=3$. Finally, since by assumption $\forall t\in\mathbb{L}^2(d\mu)$, $\|S_M t-t\|_2\to 0$ when $n\to\infty$ a direct consequence of (27) is

$$
\begin{aligned}
&\lim_{n\to\infty}\operatorname{Var}\left(L\left(X_i^{(1)},X_j^{(1)},Y^{(1)}\right)\right) \\
=&\int g^2(x_i,x_j,y)f(x_i,x_j,y)dx_idx_jdy-\left(\int g(x_i,x_j,y)f(x_i,x_j,y)dx_idx_jdy\right)^2 \\
=&\Lambda(f,\eta).
\end{aligned}
$$

We conclude by noting that $\operatorname{Var}\left(\sqrt{n}\left(P_nL\right)\right)=\operatorname{Var}\left(L\left(X_i^{(1)},X_j^{(1)},Y^{(1)}\right)\right)$. □

Lemma 7 (Asymptotics for $\sqrt{n}(\hat{Q}-Q)$). *Under the assumptions of Theorem 1, we have*

$$\lim_{n\to\infty} n\mathbb{E}\big[\hat{Q}-Q\big]^2 = 0.$$

Proof. The bound given in (16) states that if $|M_n|/n \to 0$ we have

$$\left| n\mathbb{E}\big[\big(\widehat{Q}-Q\big)^2|\hat{f}\big] - \left[\int \hat{g}(x_i,x_j,y)^2 f(x_i,x_j,y)dx_idx_jdy - \left(\int \hat{g}(x_i,x_j,y)f(x_i,x_j,y)dx_idx_jdy\right)^2\right]\right|$$
$$\leq \gamma\big(\|f\|_\infty, \|\eta\|_\infty, \Delta_{x_ix_j}\big)\left[\frac{|M_n|}{n} + \|S_Mf-f\|_2 + \|S_M\hat{g}-\hat{g}\|_2\right]$$

where $\hat{g}(x_i,x_j,y) = \int H_3(\hat{f},x_i,x_j,x_{i2},x_{j2},y)f(x_{i2},x_{j2},y)dx_{i2}dx_{j2}$, where we recall that $H_3(f,x_{i1},x_{j1},x_{i2},x_{j2},y) = H_2(f,x_{i1},x_{j2},y)+H_2(f,x_{i2},x_{j1},y)$ with $H_2(\hat{f},x_{i1},x_{j2},y) = \frac{1}{\int \hat{f}(x_i,x_j,y)dx_idx_j}\big(x_{i1}-m_i(\hat{f},y)\big)\big(x_{j2}-m_j(\hat{f},y)\big)$. By deconditioning we get

$$\left| n\mathbb{E}\big[\big(\widehat{Q}-Q\big)^2\big] - \mathbb{E}\left[\int \hat{g}(x_i,x_j,y)^2 f(x_i,x_j,y)dx_idx_jdy - \left(\int \hat{g}(x_i,x_j,y)f(x_i,x_j,y)dx_idx_jdy\right)^2\right]\right|$$
$$\leq \gamma\big(\|f\|_\infty, \|\eta\|_\infty, \Delta_{x_ix_j}\big)\left[\frac{|M_n|}{n} + \|S_Mf-f\|_2 + \mathbb{E}\big[\|S_M\hat{g}-\hat{g}\|_2\big]\right]$$

Note that

$$\begin{aligned}\mathbb{E}\big[\|S_{M_n}\hat{g}-\hat{g}\|_2\big] &\leq \mathbb{E}\big[\|S_M\hat{g}-S_Mg\|_2\big] + \mathbb{E}\big[\|\hat{g}-g\|_2\big] + \mathbb{E}\big[\|S_{M_n}g-g\|_2\big]\\ &\leq 2\mathbb{E}\big[\|\hat{g}-g\|_2\big] + \mathbb{E}\big[\|S_{M_n}g-g\|_2\big]\end{aligned}$$

where $g(x_i,x_j,y) = \int H_3(f,x_i,x_j,x_{i2},x_{j2},y)f(x_{i2},x_{j2},y)dx_{i2}dx_{j2}$. The second term converges to 0 since $g \in \mathbb{L}^2(dxdydz)$ and $\forall t \in \mathbb{L}^2(dxdydz)$, $\int (S_Mt-t)^2\, dxdydz \to 0$. Moreover

$$\begin{aligned}\|\hat{g}-g\|_2^2 &= \int [\hat{g}(x_i,x_j,y)-g(x_i,x_j,y)]^2\, dx_idx_jdy\\
&= \int\left[\int \Big(H_3(\hat{f},x_i,x_j,x_{i2},x_{j2},y) - H_3(f,x_i,x_j,x_{i2},x_{j2},y)\Big) f(x_{i2},x_{j2},y)dx_{i2}dx_{j2}\right]^2 dx_idx_jdy\\
&\leq \int\left[\int \Big(H_3(\hat{f},x_i,x_j,x_{i2},x_{j2},y) - H_3(f,x_i,x_j,x_{i2},x_{j2},y)\Big)^2 dx_{i2}dx_{j2}\right]\\
&\qquad \left[\int f(x_{i2},x_{j2},y)^2 dx_{i2}dx_{j2}\right] dx_idx_jdy\\
&\leq \Delta_{x_ix_j}\|f\|_\infty^2 \int \Big(H_2(\hat{f},x_i,x_j,x_{i2},x_{j2},y) - H_2(f,x_i,x_j,x_{i2},x_{j2},y)\Big)^2 dx_idx_jdx_{i2}dx_{j2}dy\\
&\leq \delta\Delta_{x_ix_j}^2\|f\|_\infty^2 \int \Big(\hat{f}(x_i,x_j,y) - f(x_i,x_j,y)\Big)^2 dx_idx_jdy\end{aligned}$$

for some constant δ that comes out of applying the mean value theorem to $H_3(\hat{f},x_i,x_j,x_{i2},x_{j2},y) - H_3(f,x_i,x_j,x_{i2},x_{j2},y)$. The constant δ was taken under Assumptions 1-3. Since $\mathbb{E}\big[\|f-\hat{f}\|_2\big] \to 0$ then $\mathbb{E}\big[\|g-\hat{g}\|_2\big] \to 0$. Now show that the expectation of

$$\int \hat{g}(x_i,x_j,y)^2 f(x_i,x_j,y)dx_idx_jdy - \left(\int \hat{g}(x_i,x_j,y)f(x_i,x_j,y)dx_idx_jdy\right)^2$$

converges to 0. We develop the proof for only the first term. We get

$$\begin{aligned}
&\left|\int \hat{g}(x_i,x_j,y)^2 f(x_i,x_j,y)dx_idx_jdy - \int g(x_i,x_j,y)^2 f(x_i,x_j,y)dx_idx_jdy\right| \\
\leq &\int \left|\hat{g}(x_i,x_j,y)^2 - g(x_i,x_j,y)^2\right| f(x_i,x_j,y)dx_idx_jdy \\
\leq &\lambda \int \left(\hat{g}(x_i,x_j,y) - g(x_i,x_j,y)\right)^2 dx_idx_jdy \\
= &\lambda \left\|\hat{g} - g\right\|_2^2
\end{aligned}$$

for some constant λ. By taking the expectation of both sides, we see it is enough to show that $\mathbb{E}\left[\left\|\hat{g} - g\right\|_2^2\right] \to 0$. Besides, we can verify

$$\begin{aligned}
g(x_i,x_j,y) = &\int H_3(f,x_i,x_j,x_{i2},x_{j2},y) f(x_{i2},x_{j2},y)dx_{i2}dx_{j2} \\
= &\frac{2}{\int f(x_i,x_j,y)dx_idx_j}\left(x_i - \hat{m}_i(y)\right) \\
&\left(\int x_{j2} f(x_{i2},x_{j2},y)dx_{i2}dx_{j2} - \hat{m}_j(y)\int f(x_{i2},x_{j2},y)dx_{i2}dx_{j2}\right) \\
= &0
\end{aligned}$$

which proves that the expectation of $\int \hat{g}(x_i,x_j,y)^2 f(x_i,x_j,y)dx_idx_j$ converges to 0. Similar computations shows that the expectation of $\left(\int \hat{g}(x_i,x_j,y)f(x_i,x_j,y)dx_idx_j\right)^2$ also converges to 0. Finally we have

$$\lim_{n\to\infty} n\mathbb{E}\left[\widehat{Q} - Q\right]^2 = 0.$$

□

References

Brillinger, D. R. (1983). A generalized linear model with" gaussian" regressor variables. *A Festschrift for Erich L. Lehmann in Honor of His Sixty-Fifth Birthday*, (pp. 97–114).

Bura, E. & Cook, R. D. (2001). Estimating the structural dimension of regressions via parametric inverse regression. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 63(2), 393–410.

Cook, R. D. & Ni, L. (2005). Sufficient dimension reduction via inverse regression. *Journal of the American Statistical Association*, 100(470), 410–428.

Da Veiga, S. & Gamboa, F. (2008). Efficient estimation of nonlinear conditional functionals of a density. *Submitted in The Annals of Statistics*. 42 pages 62G20, 62G06, 62G07, 62P30.

Duan, N. & Li, K. C. (1991). Slicing regression: a link-free regression method. *The Annals of Statistics*, (pp. 505–530).

Ferré, L. & Yao, A. F. (2003). Functional sliced inverse regression analysis. *Statistics*, 37(6), 475–488.

Ferré, L. & Yao, A.-F. (2005). Smoothed functional inverse regression. *Statist. Sinica*, 15(3), 665–683.

Hardle, W. & Tsybakov, A. B. (1991). Sliced inverse regression for dimension reduction: Comment. *Journal of the American Statistical Association*, 86(414), pp. 333–335.

Hastie, T. J. & Tibshirani, R. J. (1990). *Generalized Additive Models*. Monographs on Statistics and Applied Probability ;; 43. Chapman & Hall/CRC, 1st ed. edition.

Hsing, T. (1999). Nearest neighbor inverse regression. *The Annals of Statistics*, 27(2), 697–731.

Ibragimov, I. A. & Khas'minskii, R. Z. (1991). Asymptotically normal families of distributions and efficient estimation. *The Annals of Statistics*, (pp. 1681–1724).

Laurent, B. (1996). Efficient estimation of integral functionals of a density. *The Annals of Statistics*, 24(2), 659–681.

Li, K. C. (1991a). Sliced inverse regression for dimension reduction. *Journal of the American Statistical Association*, 86(414), 316–327.

Li, K. C. (1991b). Sliced inverse regression for dimension reduction: Rejoinder. *Journal of the American Statistical Association*, 86(414), pp. 337–342.

Li, L. (2007). Sparse sufficient dimension reduction. *Biometrika*, 94(3), 603.

Setodji, C. M. & Cook, R. D. (2004). K-means inverse regression. *Technometrics*, 46(4), 421–429.

Van der Vaart, A. W. (2000). *Asymptotic Statistics*. Cambridge Series on Statistical and Probabilistic Mathematics. Cambridge University Press.

Zhu, L. X. & Fang, K. T. (1996). Asymptotics for kernel estimate of sliced inverse regression. *The Annals of Statistics*, 24(3), 1053–1068.