ASYMPTOTICS OF ENTROPY-REGULARIZED OPTIMAL TRANSPORT
VIA CHAOS DECOMPOSITION

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Abstract. Consider the problem of estimating the optimal coupling (i.e., matching) between \( N \) i.i.d. data points sampled from two densities \( \rho_0 \) and \( \rho_1 \) in \( \mathbb{R}^d \). The cost of transport is an arbitrary continuous function that satisfies suitable growth and integrability assumptions. For both computational efficiency and smoothness, often a regularization term using entropy is added to this discrete problem. We introduce a modification of the commonly used discrete entropic regularization (Cuturi ’13) such that the optimal coupling for the regularized problem can be thought of as the static Schrödinger bridge with \( N \) particles. This paper is on the asymptotic properties of this discrete Schrödinger bridge as \( N \) tends to infinity. We show that it converges to the continuum Schrödinger bridge and derive the first two error terms of orders \( N^{-1/2} \) and \( N^{-1} \), respectively. This gives us functional CLT, including for the cost of transport, and second order Gaussian chaos limits when the limiting Gaussian variance is zero, extending similar recent results derived for finite state spaces and the quadratic cost. The proofs are based on a novel chaos decomposition of the discrete Schrödinger bridge by polynomial functions of the pair of empirical distributions as a first and second order Taylor approximations in the space of measures. This is achieved by extending the Hoeffding decomposition from the classical theory of U-statistics. The kernels corresponding to the first and second order chaoses are given by Markov operators which have natural interpretations in the Sinkhorn algorithm.

1. Introduction

Consider two probability densities \( \rho_0 \) and \( \rho_1 \) on \( \mathbb{R}^d \). Consider the Monge-Kantorovich optimal transport (OT) problem of transporting \( \rho_0 \) to \( \rho_1 \) with cost \( c \) [San15, Section 1.1]. The cost of transport is defined as

\[
C(\rho_0, \rho_1) = \inf_{\nu \in \Pi(\rho_0, \rho_1)} \int c(x, y) \nu(dx, dy),
\]

where the infimum is over the set \( \Pi(\rho_0, \rho_1) \) of couplings of \( (\rho_0, \rho_1) \), i.e., all joint probability distributions over \( \mathbb{R}^d \times \mathbb{R}^d \) with marginals given by \( \rho_0 \) and \( \rho_1 \). We will throughout assume \( c \) to be a continuous nonnegative function such that \( c(x, y) = 0 \) if and only if \( x = y \).

Suppose we have an i.i.d. sample \( \{(X_i, Y_i)\}_{i=1}^N \) from the product distribution \( \rho_0 \otimes \rho_1 \) and we would like to estimate \( C(\rho_0, \rho_1) \). It is natural to compute the discrete optimal matching cost [PC19, Section 2.2]

\[
\hat{C}_N := \min_{\sigma \in S_N} \frac{1}{N} \sum_{i=1}^N c(X_i, Y_{\sigma_i}),
\]

where now the infimum is over the set \( S_N \) of permutations of labels \( [N] := \{1, 2, \ldots, N\} \). The optimal matching is that permutation that attains the minimum value in (2). Rates of convergence of \( \hat{C}_N \) to \( C(\rho_0, \rho_1) \) and asymptotic distributions have been studied in combinatorics [AKT84], probability and statistics [Tal92, FG15, WB19, Lei20], and applied to economics [KY94, GS09]. This problem is also relevant in the statistical hypothesis testing [RGTC17] where one tests for the null hypothesis \( \rho_0 = \rho_1 \) by checking whether \( \hat{C}_N \approx 0 \). This, among other reasons, have spurred a more recent interest in the study of asymptotic distributions of \( \hat{C}_N \), properly scaled. Early works on the large sample behavior of the OT cost were focused on the well-behaved quadratic cost \( c(x, y) = |x - y|^2 \). The first two error terms of orders \( N^{-1/2} \) and \( N^{-1} \) are then called the Wasserstein-2 distance between...
\( \rho_0 \) and \( \rho_1 \) on the real line \( \mathbb{R} \). When \( \rho_0 \neq \rho_1 \), the optimal transportation cost \( \hat{C}_N - C(\rho_0, \rho_1) \) converges to a normal distribution at rate \( \sqrt{N} \) (see, e.g. [MC98]); while, when \( \rho_0 = \rho_1 \), with scaling \( N \), the limiting distribution is a weighted sum of chi-square distributions (see, e.g. [dBL19, dBGM99, dBGU05]). These results were built upon the explicit characterization, given by quantile functions, of the Wasserstein distances on measures supported on \( \mathbb{R} \). Beyond one dimension, similar results are rather challenging to obtain; see [AKT84, DY95] for almost sure convergence results. In [RRS16], the authors obtained the limiting law of Wasserstein distances between Gaussian distributions with parameters estimated from data by utilizing the \( \ell_2 \)-form representation in this special case. In the recent work [dBL19], normal distributional results have been generalized to \( \mathbb{R}^d \) in the case when \( \rho_0 \neq \rho_1 \). However, the limiting distribution for \( \rho_0 = \rho_1 \) is still missing. On the other hand, Wasserstein distances between discrete probability measures supported on a finite metric space have been investigated in [SM18], with the convergence results of Wasserstein distances between empirical measures for both \( \rho_0 = \rho_1 \) and \( \rho_0 \neq \rho_1 \). Let us also mention that the problem (2) is structurally similar to the classical random assignment problem [MP86, Ald01, Ste97, AS02] where there are no data points \( X \) and \( Y \), but instead there is an \( N \times N \) cost matrix with i.i.d. entries \( C_{i,j} \) and one considers \( \min_{\sigma \in \mathcal{S}_N} \sum_{i=1}^N C_{i,\sigma(i)} \).

An entropy-regularized formulation of (2) is particularly attractive both from a computational viewpoint [Cut13] and from a statistical viewpoint [RW18]. The Sinkhorn-Knopp algorithm, an alternating projection algorithm, is well suited to compute the entropy-regularized transport for large-scale problems [Cut13]. The usual way [PC19, Section 4.1] to do this is to consider \( \Pi(\tilde{\rho}_N^0, \tilde{\rho}_N^1) \) where \( \tilde{\rho}_N^0 = \frac{1}{N} \sum_{i=1}^N \delta_{X_i} \) and \( \tilde{\rho}_N^1 = \frac{1}{N} \sum_{i=1}^N \delta_{Y_i} \) are the two marginal empirical distributions, and \( \Pi(\tilde{\rho}_N^0, \tilde{\rho}_N^1) \) is the set of couplings of the two. Since the data points are sampled from densities, they are all distinct. In this case, any coupling between the two empirical distributions has a simple representation in terms of doubly stochastic matrices. In fact, if we forget the positions, both marginal mass functions are given by \( \frac{1}{N} \mathbf{1} \), where \( \mathbf{1} \) is the \( N \times 1 \) vector of all ones. In this case the matrix \( M \) belongs to the set of couplings \( \Pi(N^{-1} \mathbf{1}, N^{-1} \mathbf{1}) \) if and only if \( N \) is doubly stochastic. For such a matrix \( M \), the cost of transport is \( \langle C, M \rangle := \sum_{i=1}^N \sum_{j=1}^N c(X_i, Y_j) M_{ij} \).

Cuturi [Cut13] introduced the following entropic regularization; see also [FPPA14]. For an \((N \times N)\) doubly stochastic matrix \( M \), define its entropy as \( \text{Ent}_0(M) = \sum_{i=1}^N \sum_{j=1}^N M_{ij} \log(M_{ij}) \). For a regularization parameter \( \epsilon > 0 \), Cuturi’s entropy-regularized OT problem asks for

\[
\arg \min \left\{ \langle M, C \rangle + \epsilon \text{Ent}_0(M) \right\},
\]

where the minimization is now over all matrices \( M \) such that \( N \) is doubly stochastic. The solution, although non-explicit, can be efficiently computed due to the Sinkhorn algorithm [PC19, Section 4.2]. Let \( M_N^\epsilon \) denote the (unique) optimal solution to (3), then the regularized cost of transport is \( \langle C, M_N^\epsilon \rangle \), and, again, its asymptotic distribution, both as \( N \to \infty \) and \( \epsilon \) either fixed or decreasing to zero, becomes important. For finite state spaces and \( c(x, y) = \|x - y\|^p \), for \( p \geq 1 \), this has been taken up in [BCP19]. Actually, their result is for the slightly different but related concept of Sinkhorn divergence [FSV+19], but we will not bother with the distinction here. More importantly, the main idea in [BCP19] is to use the so-called delta-method [vdV00, Chapter 3] and the established differentiability of entropy regularized cost on finite spaces to identify the first and second order terms in a Taylor expansion around \((\rho_0, \rho_1)\).

We introduce a different entropic regularization for which the solution is explicit. For a permutation \( \sigma \in \mathcal{S}_N \), let \( A_\sigma \) denote the permutation matrix corresponding to \( \sigma \in \mathcal{S}_N \). By Birkhoff’s Theorem every doubly stochastic matrix can be written as a convex combination of permutation matrices. Thus, every coupling \( M \) can be expressed as \( M = \sum_{\sigma \in \mathcal{S}_N} q_M(\sigma) \frac{1}{N} A_\sigma \), where \( q_M(\sigma) \geq 0 \) and \( \sum_{\sigma \in \mathcal{S}_N} q_M(\sigma) = 1 \). Such convex combinations are generally not unique. Nevertheless, for any probability \( q \) on \( \mathcal{S}_N \), we can get an element in \( \Pi(N^{-1} \mathbf{1}, N^{-1} \mathbf{1}) \) by defining \( M_q := \sum_{\sigma \in \mathcal{S}_N} q(\sigma) \frac{1}{N} A_\sigma \). Define the cost for each permutation \( c_\sigma := \frac{1}{N} \sum_{i=1}^N c(X_i, Y_{\sigma(i)}) \), \( \sigma \in \mathcal{S}_N \). Then, for every doubly stochastic matrix \( M_q \), \( \langle M_q, C \rangle = \sum_{\sigma \in \mathcal{S}_N} q(\sigma) c_\sigma \).

For a probability \( q \) on \( \mathcal{S}_N \) define the entropy of \( q \) as \( \text{Ent}(q) := \sum_{\sigma \in \mathcal{S}_N} q(\sigma) \log(q(\sigma)) \). For a positive parameter \( \epsilon > 0 \), define the modified entropic regularization of the OT problem as

\[
\arg \min \left\{ \langle M_q, C \rangle + \frac{\epsilon}{N} \text{Ent}(q) \right\},
\]

where the minimization is now over probabilities \( q \) on \( \mathcal{S}_N \). The solution to (4) can be explicitly described. For \( \sigma = (\sigma_1, \ldots, \sigma_N) \in \mathcal{S}_N \), let \( c(X, Y_\sigma) := \sum_{i=1}^N c(X_i, Y_{\sigma(i)}) \). Define the weights \( w(\sigma) := \exp\left( -\frac{\epsilon}{N} c(X, Y_\sigma) \right) \).
The Gibbs probability distribution on $S_N$,

$$q_\epsilon^*(\sigma) := \frac{w(\sigma)}{\sum_{\tau \in S_N} w(\tau)} = \frac{\exp \left(-\frac{1}{\epsilon} c(X, Y_\sigma) \right)}{\sum_{\tau \in S_N} \exp \left(-\frac{1}{\epsilon} c(X, Y_\tau) \right)}, \quad \sigma \in S_N,$$

is the unique solution to (4) (see Lemma 6 below), and corresponds to a coupling of $\hat{\rho}_0^N$ and $\hat{\rho}_1^N$ given by the mixture

$$\hat{\mu}_\epsilon^N := \sum_{\sigma \in S_N} q_\epsilon^*(\sigma) \frac{1}{N} \sum_{i=1}^N \delta(x_i, y_{\sigma_i}).$$

One can think of every permutation $\sigma$ corresponding to a discrete Monge map that transports atom $X_i$ to atom $Y_{\sigma_i}$. Thus $\hat{\mu}_\epsilon^N$ is a convex combination of these extremal measures where permutations get exponentially small weights if the cost of transport is relatively high. Note that the statistic is a function solely of the pair of marginal empirical distributions $(\hat{\rho}_0^N, \hat{\rho}_1^N)$ that is symmetric under the permutations of the atoms in each.

$\hat{\mu}_\epsilon^N$ can also be thought of as the (static) Schrödinger bridge [Sch32, Föll88, Léo12] between the two discrete empirical distributions. Suppose we are given two probability measures $\mu_0$ and $\mu_1$ in $\mathbb{R}^d$. Assume that the following Markov transition kernel density is well-defined:

$$p_\epsilon(x, y) = \frac{1}{Z_\epsilon(x)} \exp \left[ -\frac{1}{\epsilon} c(x, y) \right], \quad y \in \mathbb{R}^d,$$

where $Z_\epsilon(x)$ is the normalizing constant. This defines a Markov chain. Suppose $(X_0, X_1)$ is distributed according to this Markov chain, “conditioned to have $X_0 \sim \mu_0$ and $X_1 \sim \mu_1$.” Then the joint law of $(X_0, X_1)$ is called the Schrödinger bridge joining $\mu_0$ to $\mu_1$ at temperature $\epsilon$. The quoted statement is not an event and is non-trivial to make precise. In continuum, when $\mu_0 = \rho_0$ and $\mu_1 = \rho_1$ are densities, it can be made precise as the solution of the continuum counterpart of (3) [Léo14]:

$$\arg \min_{\nu \in \Pi(\rho_0, \rho_1)} \left[ \int c(x, y) \nu(dx) dy + \epsilon \text{Ent}(\nu) \right],$$

where $\text{Ent}(\nu)$ is the entropy of $\nu$ defined as $\text{Ent}(\nu) = \int \nu(x, y) \log \nu(x, y) dx dy$, if $\nu$ is a density, and infinity otherwise. The solution to (8) is typically not explicit. However, it is known, due to [Csi75, RT93] that it has the following form. There exist two measurable functions $a_\epsilon$ and $b_\epsilon$ to be called the Schrödinger potentials, such that if $\xi(x, y) = \exp \left(-\frac{1}{\epsilon} (c(x, y) - a_\epsilon(x) - b_\epsilon(y)) \right)$, then

$$\mu_\epsilon(x, y) = \xi(x, y) \rho_0(x) \rho_1(y)$$

is a joint density on $\mathbb{R}^d \times \mathbb{R}^d$ that belongs to $\Pi(\rho_0, \rho_1)$ and is the unique solution to (8). We will call (9) the (law of the) static Schrödinger bridge connecting $\rho_0$ to $\rho_1$ at temperature $\epsilon$.

However, Schrödinger’s original lazy gas experiment was stated in terms of discrete gas particles. The particles were assumed to be Brownian, i.e., the cost is $c(x, y) = ||x - y||^2$. He assumed that the empirical distribution of the particles at an initial time is approximately $\rho_0$ and at a terminal time it is approximately $\rho_1$. If the temperature $\epsilon \approx 0$, Schrödinger inquired about the likely path of each particle. As Föllmer shows in [Föll88], the paths are determined by first solving for the static Schrödinger bridge and then connecting the two end points $(X_0, X_1)$ by a Brownian bridge with diffusion $\epsilon$. For a general cost function, the dynamic problem might not make sense, but the static Schrödinger bridge continues to exist.

Let us explain why $\hat{\mu}_\epsilon^N$ in (6) recovers Schrödinger’s original discrete set-up as the Schrödinger bridge connecting the two empirical distributions $\hat{\rho}_0^N$ and $\hat{\rho}_1^N$ at temperature $\epsilon$. Let $X_i = x_i, i \in [N]$, and $Y_j = y_j, j \in [N]$. Then $\hat{\rho}_0^N$ and $\hat{\rho}_1^N$ are given discrete distributions each supported on exactly $N$ atoms. Imagine $N$ independent Markov chains (or particles) $X(1), \ldots, X(N)$, starting from positions $X_0(i) = x_i, i \in [N]$, make jumps according to the Markov kernel $p_\epsilon(x_i, \cdot)$, respectively. Let $L^N_1 := \frac{1}{N} \sum_{i=1}^N X_1(i)$ denote the empirical distribution of their terminal values and let $L^N_0(0, 1) := \frac{1}{N} \sum_{i=1}^N \delta_{X_0(i), X_1(i)}$ denote the joint empirical distribution at two time points. What is the distribution of $L^N_1(0, 1)$, given $L^N_0(0, 1) = \hat{\rho}_1^N$? Since $\hat{\rho}_0^N \approx \rho_0$ and $\hat{\rho}_1^N \approx \rho_1$ by the Law of Large Numbers, this is one way to make sense of Schrödinger’s problem.
The event \( \{ L^N(1) = \hat{\rho}_N^1 \} \) is a union of \( N! \) disjoint events \( E_\sigma := \{ X_1(i) = y_{\sigma(i)}, \, i \in [N] \} \) for \( \sigma \in S_N \). The infinitesimal probability of \( E_\sigma \) is (informally)

\[
\prod_{i=1}^N \rho_\epsilon(x_i, y_{\sigma(i)}) \, dy_1 \ldots dy_N = \frac{1}{\prod_{i=1}^N Z_\epsilon(x_i)} \exp \left( -\frac{1}{\epsilon} c(x, y_\sigma) \right) \, dy_1 \ldots dy_N.
\]

Taking union over all these disjoint events for various permutations, and treating these densities as probabilities over infinitesimally small balls, we get that the infinitesimal probability of \( \{ L^N(1) = \hat{\rho}_N^1 \} \) is

\[
\frac{1}{\prod_{i=1}^N Z_\epsilon(x_i)} \sum_{\sigma \in S_N} \exp \left( -\frac{1}{\epsilon} c(x, y_\sigma) \right) \, dy_1 \ldots dy_N.
\]

Thus the conditional probability of \( E_\sigma \), given \( L^N(1) = \mu_1 \), is \( q^*_\epsilon(\sigma) \), for all \( \sigma \in S_N \). However, on the event \( E_\sigma \), \( L^N(0, 1) = \frac{1}{\epsilon} \sum_{i=1}^N \delta(x_i, y_{\sigma(i)}) \). Hence, the law of \( L^N(0, 1) \), given \( L^N(1) = \hat{\rho}_N^1 \), is given by the mixture formula \( \hat{\mu}_\epsilon \) in (6) (given \( X_i = x_i, \, Y_i = y_i, \, i \in [N] \)). The argument can be made rigorous by considering a disintegration of the joint law of \( L^N(0, 1) \), given \( L^N(1) \), but is standard and skipped in the interest of space. In this interpretation \( \hat{\mu}_\epsilon \) first appeared in [PW20] for a particular cost function (see [PW16, PW18, Won18, WY19] for related work). It was additionally shown that, under suitable assumptions, as \( N \to \infty \) and \( \epsilon = \epsilon_N \downarrow 0 \) at suitable rate, \( \hat{\mu}_\epsilon \) converges in a suitable sense to the optimal Monge coupling of \( (\rho_0, \rho_1) \), assumed to exist.

1.1. **Main results.** Our main results are regarding functional limits of the random measure \( \hat{\rho}_N^\epsilon \) as \( N \to \infty \) while \( \epsilon > 0 \) is kept fixed. Given a probability measure \( \nu \) and \( p \geq 1 \), let \( L^p(\nu) \) be the space of functions that have finite \( p \)th norm under \( \nu \). We follow the standard abuse of keeping the same notation for an absolutely continuous measure and its density.

**Assumption 1.** All the results stated below hold under the following assumptions.

1. \( c \) is a nonnegative continuous cost function such that \( c(x, y) = 0 \) if and only if \( x = y \), and satisfies the following asymptotic growth bound: for some \( a, b > 0 \) and for some \( p \geq 1 \),

\[
c(x, y) \leq a + b(|x|^p + |y|^p), \quad \text{as } |x|, |y| \to \infty.
\]

2. \( \rho_0 \) and \( \rho_1 \) have finite \( p \)th moment. Consequently, \( \int c(x, y) \, d\mu_\epsilon < \infty \).

3. The Schrödinger potentials are integrable, i.e., \( a_\epsilon \in L^1(\rho_0) \) and \( b_\epsilon \in L^1(\rho_1) \). See [RT93] for sufficient conditions.

Let \( \eta \) be any function on \( \mathbb{R}^d \times \mathbb{R}^d \) integrable under \( \mu_\epsilon \). Let \( T_N = T_N(\eta) := \int \eta(x, y) \, d\hat{\rho}_N^\epsilon \) and let \( \theta = \int \eta(x, y) \, d\mu_\epsilon \). Explicitly, \( T_N = \sum_{\sigma \in S_N} q^*_\epsilon(\sigma) \frac{1}{N} \sum_{i=1}^N \eta(X_i, Y_{\sigma(i)}) \) from (9),

\[
T_N = \frac{1}{N} \sum_{\sigma \in S_N} q^*_\epsilon(\sigma) \frac{1}{N} \sum_{i=1}^N \eta(X_i, Y_{\sigma(i)}) = \frac{1}{N} \sum_{\sigma \in S_N} \sum_{i=1}^N \eta(X_i, Y_{\sigma(i)}) \exp \left( -\frac{1}{\epsilon} c(X, Y_\sigma) \right) \sum_{\sigma \in S_N} \exp \left( -\frac{1}{\epsilon} c(X, Y_\sigma) \right)
\]

\[
= \frac{1}{N} \sum_{\sigma \in S_N} \sum_{i=1}^N \eta(X_i, Y_{\sigma(i)}) \exp \left( -\frac{1}{\epsilon} c(X, Y_\sigma) \right) \prod_{i=1}^N \exp \left( (a_\epsilon(X_i) + b_\epsilon(Y_i)) \right)
\]

\[
= \frac{1}{N} \sum_{\sigma \in S_N} \sum_{i=1}^N \eta(X_i, Y_{\sigma(i)}) \prod_{i=1}^N \xi(X_i, Y_{\sigma(i)}) = \frac{1}{N} \sum_{\sigma \in S_N} \eta(X, Y_\sigma) \xi^{\otimes}(X, Y_\sigma)
\]

where \( \xi^{\otimes}(X, Y_\sigma) := \prod_{i=1}^N \xi(X_i, Y_{\sigma(i)}) \). A particularly important example is when \( \eta = c \) is the cost function in which case \( T_N(\epsilon) \) is the optimal cost of transport for the regularized problem (4).

**Theorem 1.** *(Consistency.)* As \( N \to \infty \), \( T_N \) converges in probability to \( \theta \) for all \( \eta \in L^1(\mu_\epsilon) \).

In fact, Theorem 12 shows that, as \( N \to \infty \), \( \hat{\mu}_\epsilon \) converges weakly to \( \mu_\epsilon \), in probability.

Before we state the distributional results, let us define some operators on various \( L^2 \) spaces.

**Definition 1.** Define linear operators \( A : L^2(\rho_0) \to L^2(\rho_1) \) and its adjoint \( A^* : L^2(\rho_1) \to L^2(\rho_0) \) by

\[
(Af)(y) = \int f(x) \xi(x, y) \rho_0(x) \, dx, \quad (A^*g)(x) = \int g(y) \xi(x, y) \rho_1(y) \, dy.
\]
Call $A(x, y) := \xi(x, y)\rho_0(x)$ the kernel of $A$ and $A^*(x, y) := \xi(x, y)\rho_1(y)$ the kernel of $A^*$.

We will prove in Lemma 13 that $A$ is a well-defined linear operator, and $A^*A$ and $AA^*$ are two Markov operators defined on $L^2(\rho_0)$ and $L^2(\rho_1)$, respectively. Moreover, they can be rewritten as two conditional expectations: $(Af)(y) = E[f(X) \mid Y(y)]$ and $(A^*g)(x) = E[g(Y) \mid X(x)]$ where $(X, Y) \sim \mu_\nu$. We denote by $I_0 : L^2(\nu) \to L^2(\nu)$ the identity operator on $L^2(\nu)$, and, by definition, its kernel is given by the Dirac delta function. When the context is clear, we will write $I$ for short. We further make the following assumptions.

**Assumption 2.** All the results stated below hold under the following additional assumptions.

1. $\xi \in L^2(\rho_0 \otimes \rho_1)$, $\eta \in L^2(\mu_\nu)$ and $\eta \xi \in L^2(\rho_0 \otimes \rho_1)$.
2. The operator $A$ is compact. Then the operators $A^*A$ and $AA^*$ admit eigenvalue decomposition $A^*A \alpha_k = s_k^2 \alpha_k$ and $AA^* \beta_k = s_k^2 \beta_k$ for all $k \geq 0$ with $s_0 = 1$, $\alpha_0 = \beta_0 = 1$ and $0 \leq s_k \leq 1$ for all $k \geq 0$. Moreover, it holds that $A\alpha_k = s_k \beta_k$ and $A^* \beta_k = s_k \alpha_k$; see [GGK90, Chapter 6.1]. We call $\{s_k\}_{k \geq 0}$ the singular values of $A$ and $A^*$, and call $\{\alpha_k\}_{k \geq 0}$ and $\{\beta_k\}_{k \geq 0}$ the singular functions.
3. The operators $A^*A$ and $AA^*$ have positive eigenvalue gap, i.e., $s_k \leq s_1 < 1$ for all $k \geq 1$. By Jentzsch’s Theorem [Rug10, Theorem 7.2], a sufficient condition is that $\xi$ is bounded.

**Theorem 2. (First order chaos)** Recall $\theta := \int \eta(x, y) d\mu_\nu$. Define

\[ \kappa_{1,0}(x) := \int [\eta(x, y) - \theta] \xi(x, y) \rho_1(y) dy \quad \text{and} \quad \kappa_{0,1}(y) := \int [\eta(x, y) - \theta] \xi(x, y) \rho_0(x) dx. \]

Then, $T_N - \theta = L_1 + o_p(1/\sqrt{N})$, where

\[ L_1 := \frac{1}{N} \sum_{i=1}^{N} [(I - A^*A)^{-1}(\kappa_{1,0} - A^* \kappa_{0,1})(X_i) + (I - AA^*)^{-1}(\kappa_{0,1} - A \kappa_{1,0})(Y_i)]. \]

We call $L_1$ the first order chaos of $T_N$.

**Corollary 3. (Functional CLT for $\mu_\nu^N$)** For any $\eta$ satisfying Assumption 2, as $N \to \infty$, the sequence $\sqrt{N}(T_N - \theta)$ converges in law to $N(0, \varsigma^2 \nu)$, where $\varsigma^2 = \varsigma^2(\eta)$, as a function of $\eta$, is given by

\[ \varsigma^2 = \int \left((I - A^*A)^{-1}(\kappa_{1,0} - A^* \kappa_{0,1})(x)) \right)^2 \rho_0(x) dx + \int \left((I - AA^*)^{-1}(\kappa_{0,1} - A \kappa_{1,0})(y) \right)^2 \rho_1(y) dy. \]

When $\varsigma^2$ in Corollary 3 is zero for certain $\eta$, the Gaussian limit is trivial and we need to consider a higher order expansion. This is true, for example, when we subtract off from $T_N - \theta$ its first order chaos. That is, consider

\[ \overline{\eta}(x, y) := \eta(x, y) - \theta - (I - A^*A)^{-1}(\kappa_{1,0} - A^* \kappa_{0,1})(x) - (I - AA^*)^{-1}(\kappa_{0,1} - A \kappa_{1,0})(y). \]

By linearity, the corresponding statistic follows from Theorem 2 by subtracting the first order terms:

\[ T_N(\overline{\eta}) = T_N(\eta) - \theta - \frac{1}{N} \sum_{i=1}^{N} [(I - A^*A)^{-1}(\kappa_{1,0} - A^* \kappa_{0,1})(X_i) + (I - AA^*)^{-1}(\kappa_{0,1} - A \kappa_{1,0})(Y_i)]. \]

In this case both $T_N(\overline{\eta}) \to 0$ in probability and $\varsigma^2(\overline{\eta}) = 0$. Thus we need a higher order expansion.

For that purpose, define operators on bivariate functions via the notion of tensor product. Let $A_1 \in \{A, A^*, I_{\rho_0}, I_{\rho_1}\}$ be an operator mapping from $L^2(\nu_1)$ to $L^2(\gamma_1)$ with kernel $A_1$. And define $A_2, A_2$ similarly. The tensor product $A_1 \otimes A_2 : L^2(\nu_1 \otimes \nu_2) \to L^2(\gamma_1 \otimes \gamma_2)$ is defined by, for all $f \in L^2(\nu_1 \otimes \nu_2)$,

\[ (A_1 \otimes A_2)f(v_1, v_2) = \int \int f(v_1', v_2') A_1(v_1', v_1) A_2(v_2', v_2) dv_1' dv_2'. \]

For instance, $I_{\rho_0} \otimes A : L^2(\rho_0 \otimes \rho_0) \to L^2(\rho_0 \otimes \rho_0)$ is defined by

\[ (I_{\rho_0} \otimes A)f(v_1, v_2) = \int \int f(v_1', v_2') \delta_{v_1}(v_1') \xi(v_2', v_2) \rho_0(v_2') dv_1' dv_2' = \int \int f(v_1, v_2') \xi(v_2, v_2) \rho_0(v_2') dv_2', \]

or as a conditional expectation: $(I_{\rho_0} \otimes A)f(v_1, v_2) = E[f(X', Y) | X, Y](v_1, v_2)$ where $(X, Y) \sim \mu_\nu$. In particular, when $f := f_1 \oplus f_2$, we have $(A_1 \otimes A_2)(f_1 \oplus f_2)(v_1, v_2) = A_1 f_1(v_1) + A_2 f_2(v_2)$. Finally, define the swap operator $T$ by $T f(u, v) = f(v, u)$ for any $f$ on $\mathbb{R}^d \times \mathbb{R}^d$. It is easy to see that $T(A_1 \otimes A_2) = (A_2 \otimes A_1) T$. 

5
Definition 2. Define the following operators on the space $L^2(\rho_0 \otimes \rho_1)$:

$$B := T(A \otimes A^*) = (A^* \otimes A)^T \quad \text{and} \quad C := (I - A^* A) \otimes (I - A A^*).$$

Remark 1. In terms of this new operator $B$ the first order chaos of $T_N$ can be alternatively expressed (see Corollary 17) as:

$$L_1 = \frac{1}{N} \sum_{i=1}^N (I + B)^{-1}(\kappa_{1,0} \otimes \kappa_{0,1})(X_i, Y_i).$$

Both expression come from the following system of linear equations. Assume the first order chaos in Theorem 2 is given by $\frac{1}{N} \sum_{i=1}^N [f(X_i) + g(Y_i)]$, then $f$ and $g$ are (almost surely) solutions to:

$$\kappa_{1,0}(x) = f(x) + A^* g(x), \quad \kappa_{0,1}(y) = Af(y) + g(y).$$

Assumption 3. The following results hold under the additional assumptions that $\xi \in L^{2p}(\rho_0 \otimes \rho_1)$ and $C^{-1}(\eta \xi) \in L^{2p/(v-2)}(\rho_0 \otimes \rho_1)$ for some $1 \leq p \leq 2$, $\infty$.

Let $\kappa_{2,0} := -(I \otimes A)^* C^{-1}(\eta \xi)$, $\kappa_{0,2} := -(A \otimes I \rho_1) C^{-1}(\eta \xi)$, and $\kappa_{1,1} := (I + B) C^{-1}(\eta \xi)$.

Theorem 4. (Second order chaos) Assume, for some $\eta \in L^2(\mu_\varepsilon)$, $\xi^2 = 0$ in Corollary 3. Let $\theta_{1,1'} := \int \int \kappa_{1,1'}(x, y) \mu_\varepsilon(x, y) dx dy$. Then

$$T_N - \theta + \frac{\theta_{1,1'}}{N} = \frac{1}{N(N-1)} \sum_{i \neq j} \left( \kappa_{2,0}(X_i, X_j) + \kappa_{0,2}(Y_i, Y_j) + \sum_{i,j=1}^N \kappa_{1,1}(X_i, Y_j) \right) + o_p(N^{-1}).$$

The term $\theta_{1,1'}/N$ should be interpreted as an $O(1/N)$ estimate of the bias since we show later in Theorem 11 that $T_N$ may not be an unbiased estimator of $\theta$, i.e., $E[T_N]$ may not be $\theta$.

Corollary 5. (Second order functional convergence) Assume, for some $\eta \in L^2(\mu_\varepsilon)$, $\xi^2 = 0$ in Corollary 3. Suppose that the function $(\eta - \theta)\xi$ has a spectral expansion in $L^2(\rho_0 \otimes \rho_1)$ with respect to the orthonormal basis $\{ \alpha_k \otimes \beta_l \}_{k, l \geq 0}$ of $L^2(\rho_0 \otimes \rho_1)$ with coefficients $(\gamma_{kl}, k, l \geq 0)$, i.e., $(\eta - \theta)\xi = \sum_{k, l \geq 0} \gamma_{kl} \alpha_k \otimes \beta_l$.

Then, as $N \to \infty$, the sequence of random variables $N(T_N - \theta + \theta_{1,1'})$ converges in law to a zero-mean standard normal random variable

$$\sum_{k, l \geq 1} \frac{\gamma_{kl}}{(1 - s_k^2)(1 - s_l^2)} \{ U_k V_l + s_k s_l U_l V_k - s_l(U_k U_l - 1 \{ k = l \}) - s_k(V_k V_l - 1 \{ k = l \}) \},$$

where $\{ U_k, \ k \geq 1 \}$ and $\{ V_l, \ l \geq 1 \}$ are a pair of independent sequences of i.i.d. standard normal random variables.

1.2. An abstract Taylor expansion and a conjectured universality. Consider the Schrödinger bridge $\mu_\varepsilon$ as a function of the input $(\rho_0, \rho_1)$ (and $\varepsilon$, which is kept fixed). Hence, over a suitable space of pairs of probability distributions on $\mathbb{R}^d$ we get a function $(\rho_0, \rho_1) \mapsto \mu_\varepsilon(\rho_0, \rho_1)$. This space of probability distributions is assumed to be convex in the usual sense. How can one define gradients or variations of this map?

It seems natural to take a class of test functions and consider the real-valued map $(\rho_0, \rho_1) \mapsto \theta(\rho_0, \rho_1) := \int \eta d\mu_\varepsilon$. Suppose, formally, one can take the gradient $\nabla \theta(\rho_0, \rho_1)$ and the Hessian $\nabla^2 \theta(\rho_0, \rho_1)$ of this function at $(\rho_0, \rho_1)$. Then, a formal Taylor approximation around $(\rho_0, \rho_1)$ would give us

$$\theta(\hat{\rho}_0, \hat{\rho}_1) = \theta(\rho_0, \rho_1) + \nabla \theta(\rho_0, \rho_1) \cdot (\hat{\rho}_0 - \rho_0, \hat{\rho}_1 - \rho_1) + \frac{1}{2} \left( \nabla^2 \theta(\rho_0, \rho_1) \cdot (\hat{\rho}_0 - \rho_0, \hat{\rho}_1 - \rho_1) \right) + o_p \left( \| (\hat{\rho}_0 - \rho_0, \hat{\rho}_1 - \rho_1) \|^2 \right).$$

Here $\nabla \theta(\rho_0, \rho_1)$ and $\nabla^2 \theta(\rho_0, \rho_1)$ are linear operators on the pair of measures $(\hat{\rho}_0 - \rho_0, \hat{\rho}_1 - \rho_1)$. Linear operators on measures can be identified with integrals of functions. Hence, one would expect a representation

---

1. We will show in Lemma 18 that $C^{-1}(\eta \xi)$ is a well-defined element in $L^2(\rho_0 \otimes \rho_1)$. When $p = 2$, we assume $\xi \in L^2(\rho_0 \otimes \rho_1)$ and $C^{-1}(\eta \xi) \in L^2(\rho_0 \otimes \rho_1)$; when $p = \infty$, we only assume $\xi \in L^\infty(\rho_0 \otimes \rho_1)$, i.e., $\xi$ is bounded.

2. We will prove in Lemma 16 that $\{ \alpha_k \otimes \beta_l \}_{k, l \geq 0}$ is indeed an orthonormal basis of $L^2(\rho_0 \otimes \rho_1)$. 

---
of the form
\[
\text{grad } \theta(\rho_0, \rho_1) \cdot (\hat{\rho}_0^N - \rho_0, \hat{\rho}_1^N - \rho_1) = \int f(x) (\hat{\rho}_0^N - \rho_0) \, (dx) + \int g(y) (\hat{\rho}_1^N - \rho_1) \, (dy) \\
= \frac{1}{N} \sum_{i=1}^N \tilde{f}(X_i) + \frac{1}{N} \sum_{j=1}^N \tilde{g}(Y_j),
\]
for some functions \( f \) and \( g \) and their centered versions \( \tilde{f} \) and \( \tilde{g} \) obtained by subtracting off their expectations. Similarly, one would expect a functional representation for the Hessian as a quadratic function:
\[
\langle (\hat{\rho}_0^N - \rho_0, \hat{\rho}_1^N - \rho_1), \text{Hess } \theta(\rho_0, \rho_1) \cdot (\hat{\rho}_0^N - \rho_0, \hat{\rho}_1^N - \rho_1) \rangle = \int \int f_{2,0}(x,u) (\hat{\rho}_0^N - \rho_0) (dx) (\hat{\rho}_0^N - \rho_0) (du) \\
+ \int \int f_{1,1}(x,y) (\hat{\rho}_0^N - \rho_0) (dx) (\hat{\rho}_1^N - \rho_1) (dy) + \int \int f_{0,2}(v,y) (\hat{\rho}_1^N - \rho_1) (dv) (\hat{\rho}_1^N - \rho_1) (dy) \\
= \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N \tilde{f}_{2,0}(X_i, X_j) + \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N \tilde{f}_{1,1}(X_i, Y_j) + \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N \tilde{f}_{0,2}(Y_i, Y_j),
\]
for some functions \( f_{2,0}, f_{1,1}, f_{0,2} \) and their suitably centered versions. For example,
\[
\tilde{f}_{1,1}(x,y) = f_{1,1}(x,y) - \int f_{1,1}(x,y) \rho_0(x) \, dx - \int f_{1,1}(x,y) \rho_1(y) \, dy + \int \int f_{1,1}(x,y) \rho_0(x) \rho_1(y) \, dx \, dy.
\]
Moreover, due to the Central Limit Theorem, \( \sqrt{N} (\tilde{\rho}_0^N - \rho_0, \tilde{\rho}_1^N - \rho_1) \) is a tight family of random measures and has a limiting Gaussian distribution. Thus, we’d expect
\[
(1) \quad \sqrt{N} \text{grad } \theta(\rho_0, \rho_1) \cdot (\hat{\rho}_0^N - \rho_0, \hat{\rho}_1^N - \rho_1) \text{ to converge to a mean zero Gaussian with a variance given by a norm square of the gradient } \text{grad } \theta(\rho_0, \rho_1).
\]
\[
(2) \quad N \langle (\hat{\rho}_0^N - \rho_0, \hat{\rho}_1^N - \rho_1), \text{Hess } \theta(\rho_0, \rho_1) \cdot (\hat{\rho}_0^N - \rho_0, \hat{\rho}_1^N - \rho_1) \rangle \text{ converges to an element in the Gaussian second order chaos, which is comprised of linear combinations of central chi-squares and products of independent mean-zero Gaussians. The coefficients of the combinations will be given by the operator } \text{Hess } \theta(\rho_0, \rho_1).
\]
\[
(3) \quad o_p \left( \| (\hat{\rho}_0^N - \rho_0, \hat{\rho}_1^N - \rho_1) \|^2 \right) = o_p \left( N^{-1} \right).
\]
In fact, this method of Taylor expansion has been made rigorous for finite spaces and for \( c(x,y) = \|x - y\|^p \) in [BCP19] who go on to derive similar distributional limits. The linear terms can also be related to mean elements in abstract spaces [Mou53]. In [FSV†19], the authors show how the entropy-regularized transport as a divergence between second order chaos, which is comprised of linear combinations of central chi-squares and products of independent mean-zero Gaussians. The coefficients of the combinations will be given by the operator \( \text{Hess } \theta(\rho_0, \rho_1) \).

Our main results, Theorems 2 and 4 and the respective Corollaries 3 and 5, establish the representations (16) and (17) and the three limits without a differential structure by devising a chaos expansion similar to the classical Hoeffding decomposition [vdV00, Section 11.4] in the theory of U-statistics [vdV00, Chapter 12]. Turning the tables around, the kernels appearing in Theorems 2 and 4 therefore suggest the linear operators \( \text{grad } \theta(\rho_0, \rho_1) \) and \( \text{Hess } \theta(\rho_0, \rho_1) \). In a formal sense we have derived the first and second order variations of the map \( (\rho_0, \rho_1) \mapsto \mu_\epsilon(\rho_0, \rho_1) \) in terms of the Markov operators appearing in those theorems. Hence, we conjecture that the same limiting distributions (up to constant multiples) would appear for any other sequence of statistics of the form \( F(\hat{\rho}_0^N, \hat{\rho}_1^N) \) that asymptotically converges in probability to \( \theta(\rho_0, \rho_1) \).

Conjecture. The distributional limits for fixed \( \epsilon \) of Corollaries 3 and 5 continue to hold (up to constant multiples) for the cost \( \langle C, M_N^\epsilon \rangle \), where \( M_N^\epsilon \) is the solution to regularized OT problem (3) for i.i.d. data.

1.3. **Outline of the paper.** Arguably, the most difficult part of analyzing \( T_N \) is its denominator. We start in Section 2 by showing that \( T_N \) has a natural interpretation as a conditional expectation if we assume that the data \( (X_i, Y_i), \ i \in [N], \) are i.i.d. sample points from the Schrödinger bridge \( \mu_\epsilon \). For the rest of the paper we do the above useful change of measure which brings in a more natural analysis. However, to pull back
the results to our set-up, we prove in Section 2 a novel contiguity result for the sequence of pairs of empirical distributions under the two models.

Next in Section 3 we derive the first and (approximate) second order chaoses under the change of measure. \( T_N \) is a function of the pair of empirical distributions. Hence, it is invariant under permutations of the X or the Y data points, separately. The successive terms in the chaos expansions are polynomial functions of the empirical distributions \((\hat{\rho}_0^N, \hat{\rho}_1^N)\). Hence they are also symmetric under permutations. Thus, we derive symmetric projections on subspaces of \( L^2 \) spaces when \( X_i \) and \( Y_i \), under the change of measure \( \mu_\epsilon \), are not independent. In fact, the derivations in this section has nothing to do with optimal transport and holds for any probability \( \mu \) independent of \( N \), the size of the data. However, in our case, \( T_N \) is not a finite order polynomial. We show that the error terms are determined by the variance of a polynomial function of order \( N \) of the pair empirical distributions \((\hat{\rho}_0^N, \hat{\rho}_1^N)\). So this section develops yet another new extension of Hoeffding decomposition to handle polynomial functions of empirical distributions of growing order.

Section 5 puts together all these different ingredients to prove the main results and the corollaries. Finally, Appendix A is a collection of technical results on the closeness of subspaces and the existence of symmetric \( L^2 \) projections that get used in the other proofs.

2. Schrödinger bridges and contiguity

Lemma 6. The unique solution to (4) is given by (5).

Proof. For any probability \( q \) on \( S_N \), consider the relative entropy \( H(q \mid q^*_{\epsilon}) \) of \( q \) with respect to \( q^*_{\epsilon} \):

\[
H(q \mid q^*_{\epsilon}) = \sum_{\sigma \in S_N} q(\sigma) \log \frac{q(\sigma)}{q^*_{\epsilon}(\sigma)} = \sum_{\sigma \in S_N} q(\sigma) \log \left( \frac{q(\sigma) \sum_{\tau \in S_N} w(\tau)}{w(\sigma)} \right)
\]

\[
= \text{Ent}(q) + \sum_{\tau \in S_N} w(\tau) \sum_{\sigma \in S_N} q(\sigma) + \frac{1}{\epsilon} \sum_{\sigma \in S_N} c(X, Y_\epsilon)q(\sigma) = \frac{N}{\epsilon} \langle M_q, C \rangle + \text{Ent}(q) + \sum_{\tau \in S_N} w(\tau).
\]

Hence, (4) is equivalent to minimizing \( H(q \mid q^*_{\epsilon}) \), which is, of course, uniquely minimized at \( q = q^*_{\epsilon} \). \( \square \)

The expression for \( T_N \) in (11) is complicated. However, it has a rather simple structure under a change of measure. Instead of assuming that \( \{(X_i, Y_i)\}_{i=1}^N \) is a.i.d. sample from the product measure \( \rho_0 \otimes \rho_1 \), we assume that \( \{(X_i, Y_i)\}_{i=1}^N \) is a.i.d. sample from the Schrödinger bridge \( \mu_\epsilon \). As Theorem 11 shows below, under this change of measure, \( T_N \) is a simple conditional expectation and an unbiased estimator for the parameter \( \theta = \int \eta(x, y) d\mu_\epsilon \). Hence, it is natural to ask if there is a way to extract information ignoring the change of measure. The law of the entire i.i.d. sequence \( (X_i, Y_i), i = 1, 2, \ldots \), under the two models \( \rho_0 \otimes \rho_1 \) and \( \mu_\epsilon \) are obviously singular. But \( T_N \) is a function of only \((\hat{\rho}_0^N, \hat{\rho}_1^N)\). Restricted to the \( \sigma \)-algebra generated by these marginal empirical distributions, we show that the two models are contiguous in the sense of Le Cam [vdV00, Chapter 6]. This allows us to do a more natural analysis under the changed measure \( \mu_\epsilon \) and then use contiguity to prove our main results.

We first set-up a measure-theoretic framework. Consider the sample space of \((\mathbb{R}^d \times \mathbb{R}^d)^N\) with the usual topology of pointwise convergence. Let \( P^\infty \) denote the joint product measure \( \otimes_{i=1}^\infty (\rho_0 \otimes \rho_1) \) over \((\mathbb{R}^d \times \mathbb{R}^d)^N\). Let \( Q^\infty \) denote the corresponding measure \( \otimes_{i=1}^\infty (\mu_\epsilon) \). Let \( P^N, Q^N \) denote the corresponding joint distributions for the finite sequence \((X_i, Y_i), i \in [N]\). Let \( R^N \) and \( S^N \) denote the law of \((\hat{\rho}_0^N, \hat{\rho}_1^N)\) under \( P^\infty \) and \( Q^\infty \), respectively. Let \( F_N \) denote the \( \sigma \)-algebra generated by \((X_i, Y_i), i \in [N]\). Let \( G_N \) denote the sub-\( \sigma \)-algebra of \( F_N \) generated by the pair of random variables \((\hat{\rho}_0^N, \hat{\rho}_1^N)\). Clearly the two measures \( P^\infty \) and \( Q^\infty \) are mutually absolutely continuous when restricted to \( F_N \), and, hence, also when restricted to \( G_N \).
Theorem 7. Under Assumption 2, the sequence \((R^N, N \geq 1)\) is contiguous with respect to \((S^N, N \geq 1)\), i.e., \(R^N \Rightarrow S^N, N \geq 1\). Explicitly, if \((A_N \in \mathcal{G}_N, N \geq 1)\) is a sequence of events such that \(\lim_{N \to \infty} S^N(A_N) = 0\) then \(\lim_{N \to \infty} R^N(A_N) = 0\).

The proof follows after a sequence of relevant lemmas. Suppose \(\{x_1, \ldots, x_N\}\) and \(\{y_1, \ldots, y_N\}\) are two sets of \(N\) vectors. Given two permutations \(\sigma, \zeta \in \mathcal{S}_N\), consider the corresponding matchings:

\[
\hat{\rho}(\sigma) := \frac{1}{N} \sum_{i=1}^{N} \delta(x_i, y_{\sigma_i}), \quad \hat{\rho}(\zeta) := \frac{1}{N} \sum_{i=1}^{N} \delta(x_i, y_{\zeta_i}).
\]

For any other permutation \(\tau \in \mathcal{S}_N\), let \(\tau \sigma\) denote the product permutation that sends \(i \mapsto \tau_{\sigma_i}, i = 1, 2, \ldots, N\). Consider

\[
\hat{\rho}(\tau \sigma) := \frac{1}{N} \sum_{i=1}^{N} \delta(x_i, y_{\tau_{\sigma_i}}), \quad \hat{\rho}(\tau \zeta) := \frac{1}{N} \sum_{i=1}^{N} \delta(x_i, y_{\tau_{\zeta_i}}).
\]

Lemma 8. Consider the \(p \geq 1\) from Assumption 2. Let \(W_p(\mu, \nu)\) denote the \(p\)-th Wasserstein distance between two probability distributions \(\mu\) and \(\nu\). Then,

\[
W_p(\hat{\rho}(\sigma), \hat{\rho}(\zeta)) = W_p(\hat{\rho}(\tau \sigma), \hat{\rho}(\tau \zeta)).
\]

Proof. By relabeling \(\{y_1, \ldots, y_N\}\), we can take \(\zeta = \text{id}\), the identity permutation. Hence, we need to show that for all \(\tau, \zeta \in \mathcal{S}_N, W_p(\hat{\rho}(\text{id}), \hat{\rho}(\zeta)) = W_p(\hat{\rho}(\tau \text{id}), \hat{\rho}(\tau \zeta))\). In fact, it is enough to show that, for all \(\tau, \zeta, \)

\[
W_p(\hat{\rho}(\text{id}), \hat{\rho}(\zeta)) \geq W_p(\hat{\rho}(\tau \text{id}), \hat{\rho}(\tau \zeta)).
\]

since then \(W_p(\hat{\rho}(\sigma'), \hat{\rho}(\zeta')) \geq W_p(\hat{\rho}(\tau' \sigma'), \hat{\rho}(\tau' \zeta'))\) for all \(\sigma', \tau', \zeta' \in \mathcal{S}_N\) and the reverse inequality of (18) then follows by symmetry between \(\sigma' = \tau, \tau' = \tau^{-1}\) and \(\zeta' = \tau \zeta\).

To prove (18), note that since \(\hat{\rho}(\text{id})\) and \(\hat{\rho}(\zeta)\) are discrete measures with finitely many atoms, its optimal \(W_p\) coupling is given by yet another matching/permutation of the \(N\) atoms of the two measures. Thus, \(\exists \gamma \in \mathcal{S}_N\) such that the optimal coupling takes the atom \((x_i, y_i)\) to \((x_{\gamma_i}, y_{(\tau \gamma_i)})\). This induces a coupling of \(\hat{\rho}(\tau)\) and \(\hat{\rho}(\tau \zeta)\) where the atom \((x_i, y_{\tau \zeta_i})\) of \(\hat{\rho}(\tau)\) is transported to the atom \((x_{\gamma_i}, y_{(\tau \gamma \zeta_i)})\) of \(\hat{\rho}(\tau \zeta)\). Hence, by definition of the \(W_p\) distance,

\[
W_p(\hat{\rho}(\tau), \hat{\rho}(\tau \zeta)) \leq \frac{1}{N} \sum_{i=1}^{N} \| (x_i, y_{\tau_i}) - (x_{\gamma_i}, y_{(\tau \gamma \zeta_i)}) \|^p = \frac{1}{N} \sum_{i=1}^{N} \| x_i - x_{\gamma_i} \|^p + \frac{1}{N} \sum_{i=1}^{N} \| y_{\tau_i} - y_{(\tau \gamma \zeta_i)} \|^p
\]

\[
= \frac{1}{N} \sum_{i=1}^{N} \| x_i - x_{\gamma_i} \|^p + \frac{1}{N} \sum_{i=1}^{N} \| y_{\tau_i} - y_{(\tau \gamma \zeta_i)} \|^p = W_p(\hat{\rho}(\text{id}), \hat{\rho}(\zeta)).
\]

This proves (18) and hence our claim.

Lemma 9. Suppose \((X_i, Y_i), i \geq 1\), are i.i.d. \(\rho_0 \otimes \rho_1\). Under assumption 2, almost surely, the following set of probability measures is pre-compact in the \(W_p\) topology:

\[
\mathcal{M} = \left\{ \frac{1}{N} \sum_{i=1}^{N} \delta(X_i, Y_{\sigma_i}), \sigma \in \mathcal{S}_N, N \geq 1 \right\}.
\]

Proof. It suffices to show that, almost surely, \(\mathcal{M}\) is pre-compact in the topology of weak convergence and that the set of \(p\)th moments of elements of \(\mathcal{M}\) are uniformly bounded. This is because convergence in \(W_p\) is equivalent to convergence in the weak topology plus the convergence of \(p\)th moments [San15, Theorem 5.2.3], and hence, under the previous statement, \(\mathcal{M}\) is sequentially pre-compact. However, almost surely, by the Law of Large Numbers, the set of marginal empirical distributions \(\left\{ \frac{1}{N} \sum_{i=1}^{N} \delta X_i, N \geq 1 \right\}\) and \(\left\{ \frac{1}{N} \sum_{i=1}^{N} \delta Y_i, N \geq 1 \right\}\) are pre-compact in the weak topology. Since every probability measure in \(\mathcal{M}\) have marginals in the above sets, \(\mathcal{M}\) is also pre-compact in the weak topology. To check uniform boundedness of the \(p\)th moment, note that, for any \(N\) and any \(\sigma \in \mathcal{S}_N\),

\[
\int \| z \|^p \, d\hat{\rho}(\sigma) = \frac{1}{N} \sum_{i=1}^{N} (\| X_i \|^p + \| Y_{\sigma_i} \|^p) = \frac{1}{N} \sum_{i=1}^{N} \| X_i \|^p + \frac{1}{N} \sum_{i=1}^{N} \| Y_i \|^p.
\]
Due to assumption 2 and the Law of Large Numbers, almost surely,
\[
\lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \|X_i\|^p = \int \|x\|^p \rho_0(x) dx, \quad \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \|Y_i\|^p = \int \|y\|^p \rho_1(y) dy.
\]

Hence, \( \{ \int \|z\|^p \, d\tilde{\rho}(\sigma), \ \sigma \in \mathcal{S}_N, \ N \geq 1 \} \) is uniformly bounded, completing the argument. \( \square \)

Let
\[
D_\varepsilon(x,y) := -\log \xi(x,y) = \frac{1}{\varepsilon} (c(x,y) - a_\varepsilon(x) - b_\varepsilon(y)),
\]
according to the notation in (9). We will use this notation for the rest of this section.

**Lemma 10.** There is a positive constant \( c_1 \) such that, almost surely,
\[
\lim_{N \to \infty} \min_{\sigma \in \mathcal{S}_N} \frac{1}{N} \sum_{i=1}^{N} D_\varepsilon(X_i, Y_{\sigma_i}) < -c_1.
\]

**Proof of Lemma 10.** Consider the OT problem with cost \( D_\varepsilon(x,y) \) transporting \( \rho_0 \) to \( \rho_1 \). Let \( \nu_\varepsilon \) denote the optimal coupling. Since \( D_\varepsilon(x,y) = \frac{1}{\varepsilon}c(x,y) \) plus terms involving only \( x \) or \( y \), it follows that \( \nu_\varepsilon \) is simply the optimal Monge-Kantorovich coupling for cost \( c \) (and, in fact, does not depend on \( \varepsilon \)). Since \( c \) is nonnegative and continuous, \( \nu_\varepsilon \) exists [San15, Theorem 1.7].

Since \( \mu_\varepsilon \) is another coupling of \( (\rho_0, \rho_1) \), it follows that
\[
\int D_\varepsilon(x,y) d\nu_\varepsilon \leq \int D_\varepsilon(x,y) d\mu_\varepsilon = \int D_\varepsilon(x,y) \exp ( -D_\varepsilon(x,y) ) \rho_0(x) \rho_1(y) dxdy = -H(\mu_\varepsilon \mid \rho_0 \otimes \rho_1) < 0.
\]

Hence, the optimal cost of transport is negative, i.e., \( \inf_{\nu \in \Pi(\rho_0, \rho_1)} \int D_\varepsilon(x,y) d\nu(x,y) < 0 \).

Now, almost surely, \( \rho_0^N \to \rho_0 \) and \( \sigma^N \to \sigma_1 \) and
\[
\inf_{\nu \in \Pi(\rho_0^N, \sigma^N)} \int D_\varepsilon(x,y) d\nu(x,y) = \min_{\sigma \in \mathcal{S}_N} \frac{1}{N} \sum_{i=1}^{N} D_\varepsilon(X_i, Y_{\sigma_i}).
\]

We claim that, almost surely, the optimal transport cost converges:
\[
\lim_{N \to \infty} \inf_{\nu \in \Pi(\rho_0^N, \sigma^N)} \int D_\varepsilon(x,y) d\nu(x,y) = \int D_\varepsilon(x,y) d\nu_\varepsilon < 0.
\]

This would prove the lemma for \( c_1 = -\frac{1}{2} H(\mu_\varepsilon \mid \rho_0 \otimes \rho_1) \), say.

To see (19), recall from the proof of Lemma 9 that \( \mathcal{M} \) is pre-compact in the \( W_p \) topology and \( \mu \mapsto \int cd\mu \) is \( W_p \) continuous. The optimal plan \( \nu^N \) for each \( N \) has a limit in \( W_p \) which must be \( \nu_\varepsilon \) (see [San15, Theorem 1.50]). By continuity of \( c \), \( \int d\nu^N \to \int d\nu_\varepsilon \), and Assumptions 2 and the Law of Large Numbers, the integrals of the two Schrödinger potentials also converge to their respective limits, almost surely. This gives (19). \( \square \)

**Proof of Theorem 7.** Start by deriving an explicit expression for \( L_N := \frac{dS^N}{d\mathcal{G}^N} = \frac{dQ^N}{d\mathcal{G}^N} \mid \mathcal{G}_N \). Obviously, the Radon-Nikodym derivative of \( Q^N \) with respect to \( P^N \) on \( \mathcal{F}_N \) is given by
\[
f_N = \prod_{i=1}^{N} \exp (-D_\varepsilon(x_i, y_i)) = \exp \left( -\sum_{i=1}^{N} D_\varepsilon(x_i, y_i) \right), \quad \text{on } (\mathbb{R}^d \times \mathbb{R}^d)^N.
\]

Hence, \( dQ^N/dP^N \) on \( \mathcal{G}_N \) is given by \( P^N [ f_N \mid \mathcal{G}_N ] \), where \( P^N [ \cdot \mid \mathcal{G}_N ] \) refers to the conditional expectation under measure \( P^N \) given the \( \sigma \)-algebra \( \mathcal{G}_N \). On the event \( \tilde{\rho}_0^N = \frac{1}{N} \sum_{i=1}^{N} \delta_{x_i} \) and \( \tilde{\rho}_1^N = \frac{1}{N} \sum_{j=1}^{N} \delta_{y_j} \), for some sets \( \{ x_1, \ldots, x_N \} \) and \( \{ y_1, \ldots, y_N \} \) of \( N \) distinct values, it follows from exchangeability under \( P^N \) that
\[
P^N [ f_N \mid \mathcal{G}_N ] = \frac{1}{N!} \sum_{\sigma \in \mathcal{S}_N} \exp \left( -\sum_{i=1}^{N} D_\varepsilon(x_i, y_{\sigma_i}) \right) = \frac{1}{N!} \sum_{\sigma \in \mathcal{S}_N} \exp (-D_\varepsilon(X, Y_{\sigma})).
\]

Hence, \( L_N = L_N (\tilde{\rho}_0^N, \tilde{\rho}_1^N) = \frac{1}{N!} \sum_{\sigma \in \mathcal{S}_N} \exp (-D_\varepsilon(X, Y_{\sigma})). \)

According to Le Cam’s first lemma [vdV00, page 88], \( R^N \circ S^N, \ N \geq 1 \), if and only if the following holds. If \( L_N \), under \( R^N \) (or, under \( P^N \)), converges weakly to \( U \), along a subsequence, then \( P(U > 0) = 1 \). We prove below this alternative characterization. In the following argument, the generic notation \( P \) will refer
to probabilities calculated under $P^\infty$, i.e., we work under the assumption that $X_i, Y_i$ are independent and i.i.d. from their respective marginal distributions.

By Portmanteau lemma, for any $\delta > 0$, through the convergent subsequence, \( \liminf_{N \to \infty} P(L_N < \delta) \geq P(U < \delta) \). Hence, to prove our result, it is enough to show that, for any $\epsilon' > 0$, there is a $\delta > 0$ such that \( \limsup_{N \to \infty} P(L_N < \delta) \leq \epsilon' \). Then \( P(U = 0) \leq P(U < \delta) \leq \epsilon' \), for all $\epsilon' > 0$, proving our claim.

Towards that aim, using Lemma 10, assume that $N$ is large enough such that there exists a permutation $\sigma^N$ such that

\[
-c_1 > \frac{1}{N} \sum_{i=1}^{N} D_\epsilon(X_i, Y_{\sigma^N_i}) - \frac{1}{N} \sum_{i=1}^{N} a_\epsilon(X_i) - \frac{1}{N} \sum_{i=1}^{N} b_\epsilon(Y_i),
\]

for some $c_1 > 0$.

Under the growth condition (10), the function $\mu \mapsto \int cd\mu$, where $\mu$ is a probability on $\mathbb{R}^d$, is continuous under the $W_p$ metric. Hence, there is a $\delta > 0$ such that, if $\tau \in S_N$ is such that $W_p(\hat{\rho}(\tau), \hat{\rho}(\sigma^N)) < \delta$, then

(21) \[
\frac{1}{N} \sum_{i=1}^{N} D_\epsilon(X_i, Y_{\tau_i}) = -\sum_{i=1}^{N} D_\epsilon(x_i, y_{\tau_i}) - \frac{1}{N} \sum_{i=1}^{N} a_\epsilon(X_i) - \frac{1}{N} \sum_{i=1}^{N} b_\epsilon(Y_i) < -\frac{c_1}{2}.
\]

By the pre-compactness of $\mathcal{M}$ in the $W_p$ topology proved in Lemma 9, there are finitely many $W_p$ balls of radius $\delta/2$ that covers the $W_p$ closure of $\mathcal{M}$. Let this number be $M_\delta$ (which depends on the samples). Now, for any $N \geq M_\delta$, and any $\sigma, \tau \in S_N$, consider them equivalent $\sigma \equiv \tau$ if $W_p(\hat{\rho}(\sigma), \hat{\rho}(\tau)) < \delta$. Clearly, there are at most $M_\delta$ many such equivalent classes. By Lemma 8, each of these equivalent classes have the same number of permutations. Hence, by the union bound, the number of permutations in each equivalent class is at least $N!/M_\delta$. Hence, from (21) there are at least $N!/M_\delta$ many permutations $\tau$ such that $\frac{1}{N} \sum_{i=1}^{N} D_\epsilon(X_i, Y_{\tau_i}) < -\frac{c_1}{2}$. Hence, almost surely, for all $N$ large enough,

\[
L_N \geq \frac{1}{N} \sum_{\tau \equiv \sigma^N} \exp \left( -\sum_{i=1}^{N} D_\epsilon(x_i, y_{\tau_i}) \right) \geq \frac{1}{M_\delta} e^{Nc_1/2}.
\]

Thus, almost surely, $\lim_{N \to \infty} 1 \{L_N < \delta\} = 0$. By the Dominated Convergence Theorem, $\lim_{N \to \infty} P(L_N < \delta) = 0$, and we are done.

Recall $T_N = T_N(\eta)$ from (11). It can be alternatively expressed as

\[
T_N = \frac{\frac{1}{N} \sum_{\sigma \in S_N} \eta(X, Y_\sigma) \exp(-D_\epsilon(X, Y_\sigma))}{\sum_{\sigma \in S_N} \exp(-D_\epsilon(X, Y_\sigma))}.
\]

**Theorem 11.** $T_N = Q^N(\eta(X_1, Y_1) \mid \mathcal{G}_N)$. Moreover, under $Q^\infty$, $T_N$ is an unbiased, asymptotically consistent estimator of $\theta = \int \eta d\mu_*$. That is, $\mathbb{E}(T_N) = \theta$ for all $N$ and $\lim_{N \to \infty} T_N = \theta$, $Q^\infty$ almost surely.

**Proof of Theorem 11.** By exchangeability and independence, $Q^N(\eta(X_1, Y_1) \mid \mathcal{F}_N) = \frac{1}{N} \sum_{i=1}^{N} \eta(X_i, Y_i)$. Denote it by $\tilde{\eta}_N(X, Y)$. By the tower property of conditional expectations,

\[
h_N := Q^N[\eta(X_1, Y_1) \mid \mathcal{G}_N] = Q^N[Q^N(\eta(X_1, Y_1) \mid \mathcal{F}_N) \mid \mathcal{G}_N] = Q^N[\tilde{\eta}_N(X, Y) \mid \mathcal{G}_N].
\]

By definition, the final expression is the unique (almost surely) $\mathcal{G}_N$ measurable function such that for any bounded measurable $\phi \in \mathcal{G}_N$, $Q^N(\tilde{\eta}_N(X, Y)\phi) = Q^N(h_N \phi)$. Since $\tilde{\eta}_N(x, y) \in \mathcal{F}_N$, by a change of measure (20), one can write

\[
Q^N[\tilde{\eta}_N(X, Y)\phi] = P^N[f_N \tilde{\eta}_N(X, Y)\phi] = P^N[P^N(f_N \tilde{\eta}_N(X, Y) \mid \mathcal{G}_N) \phi]
\]

\[
= Q^N \left[ \frac{dR^N}{dS^N} P^N(f_N \tilde{\eta}_N(X, Y) \mid \mathcal{G}_N) \phi \right].
\]

Hence, again by using exchangeability,

\[
h_N = \frac{dR^N}{dS^N} P^\infty(f_N \tilde{\eta}_N(X, Y) \mid \mathcal{G}_N) = \frac{1}{L_N} \frac{1}{N} \sum_{\sigma \in S_N} \frac{1}{N} \eta(X, Y_\sigma) \exp(-\frac{1}{\epsilon} D_\epsilon(X, Y_\sigma)) = T_N.
\]

Hence, unbiasedness of $T_N$ under $Q^\infty$ follows by the tower property of conditional expectations. Now consider the reverse $\sigma$-algebra $\mathcal{G}_N = \sigma(\mathcal{G}_N, (X_i, Y_i), i \geq N + 1)$. By the i.i.d. property of the data under $Q^\infty$,
$T_N$ is also equal to $Q^\infty(c(X_1,Y_1) \mid \mathcal{G}_N)$. Hence $(T_N, \mathcal{G}_N)_{N \geq 1}$ is a reverse martingale. Thus $T_N$ converges almost surely to $Q^\infty(c(X_1,Y_1)) = \theta$. This proves asymptotic consistency. 

Proof of Theorem 1. As shown in Theorem 11, $T_N \to \theta$ under $Q^\infty$. But each $T_N$ is measurable with respect to $\mathcal{G}_N$. Using contiguity from Theorem 7, it then follows that $T_N \to \theta$ under $P^\infty$. 

In fact, a much stronger result holds.

**Theorem 12.** As $N \to \infty$, $\hat{\mu}_\nu^N$, in (6), converges weakly, almost surely under $Q^\infty$ and in probability under $P^\infty$, to $\mu_\nu$.

Proof. Theorem 11 holds for any bounded continuous function $\eta$. Thus, except for a null set, the convergence in Theorem 11 holds for a countable collection of bounded continuous functions. By separability of $\mathbb{R}^d$, almost sure weak convergence follows [Var58, Theorem 3.1] by choosing such a countable collection judiciously. This shows almost sure weak convergence under $Q^\infty$. Weak convergence in probability under $P^\infty$ now follows from contiguity (Theorem 7).

3. A chaos decomposition for paired samples

In this section, we obtain the first and (approximate) second order chaoses of $T_N$ under the measure $\mu^N$. In other words, we change the measure so that $(X_1,Y_1), \ldots, (X_N,Y_N)$ i.i.d. $\mu_\nu$, where $\mu_\nu(x,y) := \xi(x,y)\rho_0(x)p_1(y)$. We will write $E$ for the expectation under $\mu_\nu$. We fix $N$ throughout this section.

**Definition 3.** Let $\nu$ be a probability measure. Let $X_{[N]}$ and $Y_{[N]}$ be two sequences of random vectors on $\mathbb{R}^d$. Let $T := T(X_A,Y_B) \in \mathbb{L}^2(\nu)$ where $A,B \subset [N]$. We say $T$ is permutation symmetric in $X$ if $T(X_{\sigma A},Y_B) = T(X_A,Y_B)$ for every $\sigma \in S_N$ almost surely, where $X_{\sigma i} := (X_{\sigma i})_{i \in A}$. We define permutation symmetry in $Y$ similarly. We will say $T$ is permutation symmetric if it is permutation symmetric in both $X$ and $Y$. If, for some strict subset $A' \subset A$, $T(X_{\sigma A},Y_B) = T(X_A,Y_B)$ for every $\sigma \in S_N$ such that $\sigma_i = i$ for each $i \in A \setminus A'$, then we say $T$ is permutation symmetric in $X_{A'}$.

**Definition 4.** Let $0 < a' \leq a$ be two positive integers. Let $f : \times_{i=1}^a \mathbb{R}^d \rightarrow \mathbb{R}$. If $f$ satisfies $f(x_{\sigma[a]}) = f(x_{[a]})$ for all $\{x_i\}_{i \in [a]} \subset \mathbb{R}^d$ and every $\sigma \in S_a$ such that $\sigma_i = i$ for $a'+1 \leq i \leq a$, we say the function $f$ is symmetric in its first $a'$ arguments. In particular, if $a' = a$, we say $f$ is symmetric.

Let $H_0 \subset \mathbb{L}^2(\mu_\nu)$ be the space of constant functions. For each $k \geq 1$, let $H_k \subset \mathbb{L}^2(\mu_\nu)$ be a subspace spanned by functions of the type

\[
\sum_{a+b=k \atop a,b \in \mathbb{N}_+} \sum_{1 \leq i_1 < \cdots < i_a \leq N} \sum_{1 \leq j_1 < \cdots < j_b \leq N} f_{a,b}(X_{i_1}, \ldots, X_{i_a}, Y_{j_1}, \ldots, Y_{j_b}),
\]

and is orthogonal to $\oplus_{i=0}^{k-1} H_i$, where $f_{a,b}$ is symmetric in the first $a$ and the last $b$ arguments when $a > 0$ and $b > 0$, respectively. When, for instance, $a = 0$, we view $f_{0,b}$ as a function of $(Y_{j_1}, \ldots, Y_{j_b})$. It is clear that the (orthogonal) projection (see Appendix A) of $T_N$ onto $H_0$ is given by $\text{Proj}_{H_0}(T_N) = \theta$. We will compute the projections of $T_N$ onto $H_1$ and $H_2$, which we refer to as first and second order chaos. Note that the elements in $\mathbb{L}^2$ spaces are only defined up to zero-measure sets (or equivalent classes). For two elements $f$ and $g$ in $\mathbb{L}^2$, $f = g$ should be understood as $f$ equals $g$ up to equivalent classes.

3.1. First-order chaos. Given a probability measure $\nu$ on $\mathbb{R}^d$, let $L_0^0(\nu)$ be the subspace of $L^2(\nu)$ consisting of mean-zero functions. We first argue that $(I - A^*A)^{-1}$ and $(I - AA^*)^{-1}$ are well-defined on $L_0^0(\rho_0)$ and $L_0^0(\rho_1)$, respectively.

**Lemma 13.** Under Assumption 2, the operators $A$ and $A^*$ has the following properties:

(a) Let $(X,Y) \sim \mu_\nu$. For any $f \in L^2(\rho_0)$ and $g \in L^2(\mu_\nu)$, it holds $E[f(X) \mid Y](y) = Af(y)$ and $E[g(Y) \mid X](x) = A^*g(x)$. In particular, $Af \in L^2(\rho_1)$ and $A^*g \in L^2(\rho_0)$.

(b) The largest eigenvalue of $A$ and $A^*$ is $1$, and $A1 = A^*1 = 1$.

(c) The operator $A$ maps $L_0^0(\rho_0)$ to $L_0^0(\rho_1)$, and $A^*$ maps $L_0^0(\rho_1)$ to $L_0^0(\rho_0)$.

(d) The operator $(I - A^*A)^{-1} : L_0^0(\rho_0) \rightarrow L_0^0(\rho_0)$ is well-defined, and $(I - AA^*)^{-1}$ similarly.
(e) It holds that \( A(I - A^* A)^{-1} = (I - AA^*)^{-1} A \) and \( A^*(I - AA^*)^{-1} = (I - A^* A)^{-1} A^* \) on their domains defined above. Moreover, for any \( f \in L^2_0(\rho_0) \) and \( g \in L^2_0(\rho_1) \), we have, with \( (X, Y) \sim \mu_e \),
\[
\begin{align*}
\text{E} \left[ (I - A^* A)^{-1}(f - A^* g)(X) + (I - AA^*)^{-1}(g - Af)(Y) \mid X \right] &= f(X) \\
\text{E} \left[ (I - A^* A)^{-1}(f - A^* g)(X) + (I - AA^*)^{-1}(g - Af)(Y) \mid X \right] &= g(Y).
\end{align*}
\]

Proof of Lemma 13. (a) The conditional density of \( X \) given \( Y \) is \( p(x \mid y) = \mu_x(x, y) / \rho_1(y) = \xi(x, y) \rho_0(x) \).

Therefore,
\[
\text{E}[f(X) \mid Y](y) = \int f(x)p(x \mid y)dx = \int f(x)\xi(x, y)\rho_0(x)dx = Af(y).
\]

It follows from Jensen’s inequality that
\[
\|Af\|^2_{L^2(\rho_1)} = \text{E}[(Af)^2(Y)] = \text{E}[\text{E}[f(X) \mid Y]^2] \leq \text{E}[f^2(X)] = \|f\|^2_{L^2(\rho_0)} < \infty,
\]
which implies \( Af \in L^2(\rho_1) \). A similar argument holds for \( A^* g \).

(b) Since \( \mu_e \in \Pi(\rho_0, \rho_1) \), we get, for any \( y \in \mathbb{R}^d \),
\[
A1(y) = \int 1(x)\xi(x, y)\rho_0(x)dx \overset{a.s.}{=} 1.
\]

This implies \((1, 1)\) is a (eigenvalue, eigenvector) pair of \( A \). It then follows from (24) that 1 is the largest eigenvalue of \( A \).

(c) For any \( f \in L^2_0(\rho_0) \), it holds
\[
\int Af(y)\rho_1(y)dy = \int \rho_1(y)dy \int f(x)\xi(x, y)\rho_0(x)dx = \int f(x)\rho_0(x)dx = 0.
\]

It then follows that \( Af \in L^2_0(\rho_1) \).

(d) From (b) and (c) we know \( A^* A \) maps from \( L^2_0(\rho_0) \) to \( L^2_0(\rho_0) \) with the largest eigenvalue being \( 1 \). Recall that we assume \( A^* A \) has positive eigenvalue gap, in other words, \( 1 \) is the only eigenfunction corresponds to the eigenvalue \( 1 \). Given \( f, g \in L^2_0(\rho_0) \), if \( (I - A^* A)f = (I - A^* A)g \), then \( f - g = c1 \) for some constant \( c \). Since \( f - g \in L^2_0(\rho_0) \) is orthogonal to \( 1 \), it holds that \( f = g \) and thus \( I - A^* A \) is injective on \( L^2_0(\rho_0) \). Moreover, for every \( f \in L^2_0(\rho_0) \),
\[
\bar{f} := \left[ I + \sum_{k \geq 1}(A^* A)^k \right] f
\]
converges in \( L^2(\rho_0) \) and \( (I - A^* A)\bar{f} = f \). It follows that \( I - A^* A \) is also surjective. Therefore, \((I - A^* A)^{-1}f \) is well-defined and is equal to \( f \).

(e) From (d) we get, for any \( f \in L^2_0(\rho_0) \),
\[
A(I - A^* A)^{-1}f = A \left[ I + \sum_{k \geq 1}(A^* A)^k \right] f = \left[ I + \sum_{k \geq 1}(AA^*)^k \right] Af = (I - AA^*)^{-1}Af.
\]

This implies \( A(I - A^* A)^{-1} = (I - AA^*)^{-1}A \). The other identity can be proved analogously. Finally, we prove the first equation in (23). In fact,
\[
\begin{align*}
\text{E} \left[ (I - A^* A)^{-1}(f - A^* g)(X) + (I - AA^*)^{-1}(g - Af)(Y) \mid X \right] \\
= (I - A^* A)^{-1}(f - A^* g)(X) + A^*(I - AA^*)^{-1}(g - Af)(X) \\
= (I - A^* A)^{-1}(f - A^* g)(X) + (I - A^* A)^{-1}A^*(g - Af)(X) = f(X),
\end{align*}
\]
by a simple algebra.

Now we are ready to give the first order chaos of \( T_N \), i.e., \( \text{Proj}_{H_1}(T_N) \). Recall that
\[
\kappa_{1,0}(x) := \int [\eta(x, y) - \theta] \xi(x, y)\rho_1(y)dy \quad \text{and} \quad \kappa_{0,1}(y) := \int [\eta(x, y) - \theta] \xi(x, y)\rho_0(x)dx,
\]
where \( \theta := \iint \eta(x, y)\mu_e(x, y)dxdy \).
Proposition 14. Under Assumption 2, the first order chaos of the statistic $T_N$ in (11) is given by

\begin{equation}
\mathcal{L}_1^i := \frac{1}{N} \sum_{i=1}^{N} [(I - \mathcal{A}^* \mathcal{A})^{-1} (\kappa_{1,0} - \mathcal{A}^* \kappa_{0,1})(X_i) + (I - \mathcal{A} \mathcal{A}^*)^{-1} (\kappa_{0,1} - \mathcal{A} \kappa_{1,0})(Y_i)].
\end{equation}

Proof of Proposition 14. By the definition of orthogonal projection, it suffices to show that, for any $i \in [N],$

\[ \mathbb{E}[T_N - \theta - \mathcal{L}_1 | X_i] = 0 \quad \text{and} \quad \mathbb{E}[T_N - \theta - \mathcal{L}_1 | Y_i] = 0 \]

almost surely. We will prove it for $X_1$, and the rest of them can be proved similarly. Note that $\kappa_{1,0} \in \mathbb{L}_0^2(\rho_0)$ and $\kappa_{0,1} \in \mathbb{L}_0^2(\rho_1)$. By (c) and (d) in Lemma 13, we know

\[ \mathbb{E}[(I - \mathcal{A}^* \mathcal{A})^{-1} (\kappa_{1,0} - \mathcal{A}^* \kappa_{0,1})(X_1) + (I - \mathcal{A} \mathcal{A}^*)^{-1} (\kappa_{0,1} - \mathcal{A} \kappa_{1,0})(Y_1)] = 0, \quad \text{for every} \quad i \in [N]. \]

It then follows from (23) that

\[ \mathbb{E}[(T_N - \theta) \sum_{i=1}^{N} \phi(X_i)] = \sum_{i=1}^{N} \mathbb{E}[(T_N - \theta) \phi(X_i)] = N \mathbb{E}[h(X_1) \phi(X_1)]. \]

Recall from Theorem 11 that $T_N = \mathbb{E}[\eta(X_1, Y_1) | \mathcal{G}_N]$. Since $\sum_{i=1}^{N} \phi(X_i)$ is $\mathcal{G}_N$ measurable, by the tower property of conditional expectation, we get

\[ \mathbb{E}[(T_N - \theta) \sum_{i=1}^{N} \phi(X_i)] = \mathbb{E}[(\eta(X_1, Y_1) - \theta) \sum_{i=1}^{N} \phi(X_i)] = \mathbb{E}[(\kappa_{1,0}(X_1) \phi(X_1)). \]

It follows that $\mathbb{E}[\kappa_{1,0}(X_1) \phi(X_1)] = N \mathbb{E}[h(X_1) \phi(X_1)].$ Since $\phi$ is arbitrary, we have $h(X_1) = \frac{1}{N} \kappa_{1,0}(X_1).$ \hfill \Box

We then prove some properties of $\mathcal{B} := T(\mathcal{A} \otimes \mathcal{A}^*)$ in the following lemma.

Lemma 15. Under Assumption 2, the operator $\mathcal{B}$ has the following properties:

(a) Let $(X_1, Y_1), (X_2, Y_2) \overset{i.i.d.}{\sim} \mu_e$. It holds $\mathbb{E}[f(X_1, Y_2) | X_2, Y_1](x, y) = \mathcal{B} f(x, y)$ for any $f \in \mathbb{L}_2^2(\rho_0 \otimes \rho_1)$. In particular, $\mathcal{B} f \in \mathbb{L}_2^2(\rho_0 \otimes \rho_1)$.

(b) The operator $\mathcal{B}$ maps $\mathbb{L}_0^2(\rho_0 \otimes \rho_1)$ to $\mathbb{L}_0^2(\rho_0 \otimes \rho_1)$.

(c) For any $f \otimes g \in \mathbb{L}_2^2(\rho_0 \otimes \rho_1)$, we have $\mathcal{B}(f \otimes g) = \mathcal{A}^* g \otimes \mathcal{A} f$.

(d) The operator $(I + \mathcal{B})^{-1}$ is well-defined on $\mathbb{L}_0^2(\rho_0 \otimes \rho_1)$.

(e) For any $f \in \mathbb{L}_0^2(\rho_0)$ and $g \in \mathbb{L}_0^2(\rho_1)$, it holds that

\begin{equation}
(I + \mathcal{B})^{-1}(f \otimes g) = [(I - \mathcal{A}^* \mathcal{A})^{-1}(f - \mathcal{A}^* g)] \otimes [(I - \mathcal{A} \mathcal{A}^*)^{-1}(g - \mathcal{A} f)].
\end{equation}

Proof of Lemma 15. (a) Let $f \in \mathbb{L}_2^2(\rho_0 \otimes \rho_1)$. By the definition of $\mathcal{B}$, we have

\[ \mathcal{B} f(x, y) = \int \int f(x', y') \xi(x', y) \xi(x, y') \rho_0(x') \rho_1(y') dx' dy'. \]

On the other hand, since the conditional density of $(X_1, Y_2)$ given $(X_2, Y_1)$ is

\[ p(x_1, y_2 | x_2, y_1) = \frac{\xi(x_1, y_1) \rho_0(x_1) \rho_1(y_1) \xi(x_2, y_2) \rho_0(x_2) \rho_1(y_2)}{\rho_0(x_2) \rho_1(y_1)} = \xi(x_1, y_1) \xi(x_2, y_2) \rho_0(x_1). \]

Therefore,

\[ \mathbb{E}[f(X_1, Y_2) | X_2, Y_1](x, y) = \int \int f(x', y') p(x', y' | x, y) dx' dy' = \mathcal{B} f(x, y). \]

It follows from Jensen’s inequality that $\|\mathcal{B} f\|^2_{\mathbb{L}_2^2(\rho_0 \otimes \rho_1)} = \mathbb{E}[\mathcal{B} f(X_1, Y_2) | X_2, Y_1]^2 \leq \mathbb{E}[f^2(X_1, Y_2)] < \infty$, and thus $\mathcal{B} f \in \mathbb{L}_2^2(\rho_0 \otimes \rho_1)$.

(b) Take any $f \in \mathbb{L}_0^2(\rho_0 \otimes \rho_1)$, we have, by (a),

\[ \mathbb{E}_\mu[\mathcal{B} f(X, Y)] = \mathbb{E}[\mathcal{B} f(X_2, Y_1)] = \mathbb{E}[\mathbb{E}[f(X_1, Y_2) | X_2, Y_1]] = \mathbb{E}[f(X_1, Y_2)] = 0, \]
and thus $Bf \in L^2_0(\rho_0 \otimes \rho_1)$.

(c) Recall $B = T(A \otimes A^*)$. Take any $f \oplus g \in L^2(\rho_0 \otimes \rho_1)$, we have

$$B(f \oplus g)(x,y) = (A \otimes A^*)(f \oplus g)(y,x) = Af(y) + A^*g(x) = (A^*g \oplus Af)(x,y).$$

(d) Recall from Assumption 2 that $A$ admits a singular value decomposition: $A\alpha_k = s_k\beta_k$ and $A^*\beta_k = s_k\alpha_k$ for all $k \geq 0$ with $s_0 = 1$ and $\alpha_0 = \beta_0 = 1$, where $\{\alpha_k\}$ and $\{\beta_k\}$ are orthonormal bases of $L^2(\rho_0)$ and $L^2(\rho_1)$, respectively. Take any $f \in L^2_0(\rho_0 \otimes \rho_1)$, we get, by Lemma 16, that $f$ has an expansion

$$f = \sum_{i,j \geq 0, i+j > 0} \gamma_{ij}(\alpha_i \otimes \beta_j),$$

where $\sum_{i,j \geq 0, i+j > 0} \gamma_{ij}^2 < \infty$. Define a function

$$\bar{f} := \sum_{i,j \geq 0, i+j > 0} \frac{\gamma_{ij}}{1 + s_is_j}(\alpha_i \otimes \beta_j).$$

Since $s_k \geq 0$ for all $k \geq 0$, it holds that $\bar{f} \in L^2(\rho_0 \otimes \rho_1)$. Furthermore, we have $(\rho_0 \otimes \rho_1)[\bar{f}] = 0$ as $\alpha_i \in L^2_0(\rho_0)$ and $\beta_i \in L^2_0(\rho_1)$ for all $i > 0$. This implies $\bar{f} \in L^2_0(\rho_0 \otimes \rho_1)$. Moreover, we have

$$(I + B)\bar{f} = \sum_{i,j \geq 0, i+j > 0} \frac{\gamma_{ij}}{1 + s_is_j}(\alpha_i \otimes \beta_j) + \sum_{i,j \geq 0, i+j > 0} \frac{\gamma_{ij}}{1 + s_is_j}s_is_j(\alpha_i \otimes \beta_j) = f,$$

and thus $I + B : L^2_0(\rho_0 \otimes \rho_1) \to L^2_0(\rho_0 \otimes \rho_1)$ is a surjective. On the other hand, if $(I + B)f = 0$ for some $f \in L^2_0(\rho_0 \otimes \rho_1)$, then we must have $(Bf, \bar{f})_{L^2_0(\rho_0 \otimes \rho_1)} = -\|f\|_{L^2_0(\rho_0 \otimes \rho_1)}$. However, we also know $\langle Bf, \bar{f} \rangle_{L^2_0(\rho_0 \otimes \rho_1)} = \sum_{i,j \geq 0, i+j > 0} s_is_j\gamma_{ij}^2 \geq 0$. Consequently, it holds $f \equiv 0$ and thus $I + B$ is also an injective. Hence, the inverse operator $(I + B)^{-1}$ is well-defined on $L^2_0(\rho_0 \otimes \rho_1)$.

(e) Take any $f \oplus g \in L^2_0(\rho_0 \otimes \rho_1)$, it follows from (d) that $(I + B)^{-1}(f \oplus g)$ exists. It then suffices to verify

$$(I + B) [(I - A^*A)^{-1}(f - A^*g) \oplus (I - AA^*)^{-1}(g - Af)] = f \oplus g.$$

By (c), we know

$$B [(I - A^*A)^{-1}(f - A^*g) \oplus (I - AA^*)^{-1}(g - Af)] = A^*(I - AA^*)^{-1}(g - Af) \oplus A(I - A^*A)^{-1}(f - A^*g) = (I - AA^*)^{-1}A^*(g - Af) \oplus (I - A^*A)^{-1}A(f - A^*g),$$

where the last equality follows from (e) in Lemma 13. Consequently,

$$(I + B) [(I - A^*A)^{-1}(f - A^*g) \oplus (I - AA^*)^{-1}(g - Af)] = f \oplus g.$$

The next lemma shows that $\{\alpha_i \otimes \beta_j\}_{i,j \geq 0}$ forms an orthonormal basis of $L^2(\rho_0 \otimes \rho_1)$; see Appendix A for a proof.

**Lemma 16.** Let $\nu_0$ and $\nu_1$ be two probability measures on $\mathbb{R}^d$. Let $\{\alpha_i^{(0)}\}_{i \geq 0}$ and $\{\alpha_i^{(1)}\}_{i \geq 0}$ be orthonormal bases of $L^2(\nu_0)$ and $L^2(\nu_1)$, respectively. Then $\{\alpha_i^{(0)} \otimes \alpha_i^{(1)}\}_{i,j \geq 0}$ is an orthonormal basis of $L^2(\nu_0 \otimes \nu_1)$.

According to the identity (26), the first order chaos $L_1$ admits a more compact representation using the operator $B$.

**Corollary 17.** The first order chaos of $T_N$ admits an alternative expression $L_1 = \frac{1}{N} \sum_{i=1}^N (I + B)^{-1}(\kappa_{1,0} \otimes \kappa_{0,1})(X_i, Y_i)$.

**Remark 2.** Note that the above expression of $L_1$ is permutation symmetric, i.e., $\sum_{i=1}^N (I + B)^{-1}(\kappa_{1,0} \otimes \kappa_{0,1})(X_i, Y_i) = \sum_{i=1}^N (I + B)^{-1}(\kappa_{0,1} \otimes \kappa_{1,0})(X_i, Y_i)$ for all $\sigma \in S_N$.

**Remark 3.** Another way to see this is: assume the first order chaos is given by $\sum_{i=1}^N [f(X_i) + g(Y_i)]$, then we must have

$$\frac{1}{N} \kappa_{1,0}(X_i) = \mathbb{E}\{T_N - \theta \mid X_i\} = \mathbb{E}\{f(X_i) + g(Y_i) \mid X_i\} = f(X_i) + A^*g(X_i)$$

$$\frac{1}{N} \kappa_{0,1}(Y_i) = \mathbb{E}\{T_N - \theta \mid Y_i\} = \mathbb{E}\{f(X_i) + g(Y_i) \mid Y_i\} = Af(Y_i) + g(Y_i).$$
This implies \( \frac{1}{\kappa_{1,0} + \kappa_{0,1}} = f + g + A^*g \oplus A f = (I + B)(f \oplus g) \).

3.2. Second-order chaos. Recall that we have defined the operator \( C := (I - A^*A) \otimes (I - AA^*) \). Again, let us prove its inverse is well-defined. Given a measure \( \nu \) on \( \mathbb{R}^d \times \mathbb{R}^d \), let
\[
L^2_{0,0}(\nu) := \{ f \in L^2(\nu) : \mathbb{E}[f(X, Y) \mid Y]^* \mathbb{E}[f(X, Y) \mid X] \mathbb{P} 0 \text{ for all } (X, Y) \sim \nu \}.
\]
For \( f \in L^2_{0,0}(\nu) \), we say \( f \) is degenerate with respect to \( \nu \). For example, we will show in the next lemma that the function \( \overline{\eta} \) defined in (14),
\[
\overline{\eta}(x, y) := \eta(x, y) - \theta (I - A^*A)^{-1}(\kappa_{1,0} - A^*\kappa_{1,0})(x) - (I - AA^*)^{-1}(\kappa_{0,1} - A\kappa_{1,0})(y),
\]
belongs to \( L^2_{0,0}(\mu) \), and then, by Assumption 2, \( \overline{\eta} \in L^2_{0,0}(\rho_0 \otimes \rho_1) \).

**Lemma 18.** Under Assumption 2, the inverse operator \( C^{-1} : L^2_{0,0}(\rho_0 \otimes \rho_1) \to L^2_{0,0}(\rho_0 \otimes \rho_1) \) is well-defined. Moreover, it is equal to \( (I - A^*A)^{-1} \otimes (I - AA^*)^{-1} \). In particular, \( \overline{\eta} \in L^2_{0,0}(\rho_0 \otimes \rho_1) \) so that \( C^{-1}(\overline{\eta}) \) is well-defined.

**Proof of Lemma 18.** We will prove that \( C : L^2_{0,0}(\rho_0 \otimes \rho_1) \to L^2_{0,0}(\rho_0 \otimes \rho_1) \) is bijective. On the one hand, take any \( f \in L^2_{0,0}(\rho_0 \otimes \rho_1) \), by Lemma 16, we know \( f \) must admit the following expansion:
\[
f = \sum_{i,j \geq 1} \gamma_{ij} \alpha_i \otimes \beta_j, \quad \text{where} \sum_{i,j \geq 1} \gamma_{ij}^2 < \infty.
\]
Note that we have assumed \( s_k < 1 \) for all \( k \geq 1 \). Define
\[
\tilde{f} := \sum_{i,j \geq 1} \frac{\gamma_{ij}}{(1 - s_i^2)(1 - s_j^2)} \alpha_i \otimes \beta_j,
\]
then, similar to (27), we have \( C \tilde{f} = f \) and \( \tilde{f} \in L^2_{0,0}(\rho_0 \otimes \rho_1) \). Hence, \( C \) is surjective. On the other hand, if \( Cf = 0 \), then \( Cf = \sum_{i,j \geq 1} (1 - s_i^2)(1 - s_j^2)\gamma_{ij} \alpha_i \otimes \beta_j = 0 \). It follows that \( \gamma_{ij} = 0 \) for all \( i,j \geq 1 \), and thus \( C \) is injective.

By (23) we get
\[
\mathbb{E}[(I - A^*A)^{-1}(\kappa_{1,0} - A^*\kappa_{1,0})(X_1) + (I - AA^*)^{-1}(\kappa_{0,1} - A\kappa_{1,0})(Y_1) \mid X_1] = \kappa_{1,0}(X_1).
\]
By definition, \( \kappa_{1,0}(X_1) = \int [\eta(X_1, y) - \theta \xi(X_1, y)]\rho_1(y)dy = \mathbb{E}[\eta(X_1, Y_1) - \theta \mid X_1] \). This yields \( \mathbb{E}[\overline{\eta}(X_1, Y_1) \mid X_1] = 0 \). Similarly, \( \mathbb{E}[\overline{\eta}(X_1, Y_1) \mid Y_1] = 0 \). We obtain \( \overline{\eta} \in L^2_{0,0}(\mu_\nu) \), and then, by Assumption 2, \( \overline{\eta} \in L^2_{0,0}(\rho_0 \otimes \rho_1) \) since
\[
0 = \mathbb{E}[\overline{\eta}(X_1, Y_1) \mid X_1](x) = \int \overline{\eta}(x, y)\xi(x, y)\rho_1(y)dy
\]
\[
0 = \mathbb{E}[\overline{\eta}(X_1, Y_1) \mid Y_1](y) = \int \overline{\eta}(x, y)\xi(x, y)\rho_0(x)dx.
\]
\[\square\]

From Lemma 18 we know \( C \) preserves the degeneracy with respect to \( \rho_0 \otimes \rho_1 \). The following lemma verifies similar properties for other operators under consideration.

**Lemma 19.** Let \( A_k \in \{ A, A^*, I_{\rho_0}, I_{\rho_1} \} \) be an operator mapping from \( L^2(\nu_\nu) \) to \( L^2(\nu_\nu') \) for \( k \in \{ 1, 2 \} \). Then \( A_1 \otimes A_2 \) maps \( L^2_{0,0}(\nu_{\nu'}) \) to \( L^2_{0,0}(\nu_{\nu''}) \), and in particular, the operator \( B \) maps \( L^2_{0,0}(\rho_0 \otimes \rho_1) \) to \( L^2_{0,0}(\rho_0 \otimes \rho_1) \).

**Proof.** We prove the claim for \( A_1 = A : L^2(\rho_0) \to L^2(\rho_1) \) and \( A_2 = A^* : L^2(\rho_1) \to L^2(\rho_0) \). The rest follows similarly. Take any \( f \in L^2_{0,0}(\rho_0 \otimes \rho_1) \), we know \( (A \otimes A^*)f(Y_1, X_2) = \mathbb{E}[f(X_1, Y_2) \mid X_2, Y_1] \). Hence, by the tower property, it holds that
\[
\mathbb{E}[(A \otimes A^*)f(Y_1, X_2) \mid X_2] = \mathbb{E}[f(X_1, Y_2) \mid X_2] = \mathbb{E}[(A \otimes A^*)f(X_1, Y_2) \mid X_2, Y_1].
\]
Analogously, \( \mathbb{E}[(A \otimes A^*)f(Y_1, X_2) \mid Y_1] = 0 \). This implies \( (A \otimes A^*)f(Y_1, X_2) \in L^2_{0,0}(\rho_1 \otimes \rho_0) \), and the claim follows. Now, observe that \( (A \otimes A^*)f(Y_1, X_2) \in L^2_{0,0}(\rho_1 \otimes \rho_0) \) yields \( T(A \otimes A^*)f(X_2, Y_1) = \mathbb{E}[f(X_1, Y_2) \mid X_2, Y_1] \), and \( B = T(A \otimes A^*) \), we get \( B \) maps \( L^2_{0,0}(\rho_0 \otimes \rho_1) \) to \( L^2_{0,0}(\rho_0 \otimes \rho_1) \). \( \square \)
Unlike the first order chaos, we will give an approximation to the second order chaos, i.e., the projection onto $H_2$, of $T_N$. According to Lemma 18, we know $\tilde{\eta}_B \in L^2_{0,0}(\rho_0 \otimes \rho_1)$ and $C^{-1}(\tilde{\eta}_B)$ is well-defined. Let

(29) \[ \kappa_{2,0} := -(I_{\rho_0} \otimes A^*)C^{-1}(\tilde{\eta}_B), \kappa_{0,2} := -(A \otimes I_{\rho_1})C^{-1}(\tilde{\eta}_B), \quad \text{and} \quad \kappa_{1,1'} := (I + B)C^{-1}(\tilde{\eta}_B). \]

We define

(30) \[ L_2 := \frac{1}{N(N-1)} \left\{ \sum_{i \neq j} \kappa_{2,0}(X_i, X_j) + \kappa_{0,2}(Y_i, Y_j) + \sum_{i,j=1}^N \kappa_{1,1'}(X_i, Y_j) - \sum_{i=1}^N \kappa_{1,1'}(X_i, Y_i) \right\}, \]

where $\kappa_{1,1'}(X_1, Y_1)$ is an affine function such that $\kappa_{1,1'} \in L^2_0(\mu_e)$. We will show in the next lemma that $\kappa_{1,1'} \in L^2_0(\mu_e)$, so $\kappa_{1,1'}$ can be derived the same way we obtain $\tilde{\eta}_B$. Note that $L_2$ is permutation symmetric due to affineness of $\kappa_{1,1'}$.

**Lemma 20.** The functions $\kappa_{2,0}$, $\kappa_{0,2}$ and $\kappa_{1,1'}$ are degenerate, i.e., $\kappa_{2,0} \in L^2_0(\rho_0 \otimes \rho_0)$, $\kappa_{0,2} \in L^2_0(\rho_1 \otimes \rho_1)$ and $\kappa_{1,1'} \in L^2_0(\rho_0 \otimes \rho_1)$. Under Assumption 3, the function $\kappa_{1,1'}$ also belongs to $L^2_0(\mu_e)$, and thus $L_2 \in H_2$. Moreover, the following identities hold:

\[ (I + T)[\kappa_{2,0} + (A^* \otimes A^*)\kappa_{0,2} + (I_{\rho_0} \otimes A^*)\kappa_{1,1'}] = 0 \]

\[ (I + T)[(A \otimes A)\kappa_{1,1'} + (A \otimes I_{\rho_1})\kappa_{1,1'}] = 0 \]

\[ (I_{\rho_0} \otimes A)(I + T)\kappa_{2,0} + (A^* \otimes I_{\rho_1})(I + T)\kappa_{0,2} + (I + B)\kappa_{1,1'} = \tilde{\eta}_B. \]

**Proof.** Since $\tilde{\eta}_B \in L^2_0(\rho_0 \otimes \rho_1)$, we know from Lemma 18 and Lemma 19 that $\kappa_{2,0} \in L^2_0(\rho_0 \otimes \rho_0)$, $\kappa_{0,2} \in L^2_0(\rho_1 \otimes \rho_1)$ and $\kappa_{1,1'} \in L^2_0(\rho_0 \otimes \rho_1)$. Let $f := C^{-1}(\tilde{\eta}_B)$. Recall from Assumption 3 that $f \in L^{2p}(\rho_0 \otimes \rho_1)$ and $f \in L^{2p/(p-2)}(\rho_0 \otimes \rho_1)$. As a result,

(31) \[ \mu_e [f^2]^{\text{Hölder}} \leq \left[ \int f^{2p}(x, y)\rho_0(x)\rho_1(y)dx dy \right]^{\frac{p-1}{p}} \left[ \int \xi^p(x, y)\rho_0(x)\rho_1(y)dx dy \right]^{\frac{1}{p}} < \infty. \]

Furthermore,

\[ \left( \int (B f)^{2p}(x, y)\rho_0(x)\rho_1(y)dx dy \right)^{\frac{1}{2p}} \leq \left( \int \left( \int f^{2p}(x', y')\xi(x, y)\xi(x, y')\rho_0(x')\rho_1(y')dx'\right)^{\frac{2p}{p-1}} \rho_0(x)\rho_1(y)dx dy \right)^{\frac{1}{2p}} \leq \left( \int \left( \int f^{2p}(x', y')\xi(x, y)\xi(x, y')\rho_0(x')\rho_1(y')\rho_0(x)\rho_1(y)dx'\right)^{\frac{2p}{p-1}} dx' \right)^{\frac{1}{2p}} \]

\[ \leq \left( \int f^{2p}(x', y')\rho_0(x')\rho_1(y')dx' \right)^{\frac{1}{2p}} < \infty, \]

where (i) follows from $\int f(x', y')\rho_0(y')dx' \leq \int \xi(x, y')\rho_0(x)dx$. Similar to (31), it then holds that

\[ \mu_e [B f^2]^{\frac{1}{2}} \leq \left( \int (B f)^{2p}(x, y)\rho_0(x)\rho_1(y)dx dy \right)^{\frac{1}{2p+1}} \left( \int \xi^p(x, y)\rho_0(x)\rho_1(y)dx dy \right)^{\frac{1}{p}} < \infty. \]

This yields that $\kappa_{1,1'} := (I + B)f \in L^2_0(\mu_e)$. Now, by the degeneracy (28) of $\kappa_{2,0}$, $\kappa_{0,2}$ and $\kappa_{1,1'}$, we obtain $L_2 \in H^+_0 \cap H^+_1$. It then follows from the permutation symmetry of $L_2$ that $L_2 \in H_2$. Notice that $(A^* \otimes A^*)\kappa_{0,2} = -(A^* A \otimes A^*)C^{-1}(\tilde{\eta}_B)$ and

\[ (I_{\rho_0} \otimes A^*)\kappa_{1,1'} = [(I_{\rho_0} \otimes A^*) + (I_{\rho_0} \otimes A^*)B]C^{-1}(\tilde{\eta}_B) \]

\[ = -(\kappa_{2,0} + \kappa_{0,2} + (A \otimes I_{\rho_1})\kappa_{1,1'}) \]

where we have used $B = T(A \otimes A^*)$ in (i). It then follows that

\[ (I + T)[\kappa_{2,0} + (A^* \otimes A^*)\kappa_{0,2} + (I_{\rho_0} \otimes A^*)\kappa_{1,1'}] = (I + T)(T - I)(A^* A \otimes A^*)C^{-1}(\tilde{\eta}_B) \equiv 0, \]

since $(I + T)(T - I) = T - I + T T - T = 0$. Similarly, $(I + T)[(A \otimes A)\kappa_{1,1'} + (A \otimes I_{\rho_1})\kappa_{1,1'}] \equiv 0$.

Let us verify the last identity in the statement of Lemma 20. Note that

\[ (I_{\rho_0} \otimes A)(I + T)\kappa_{2,0} = [(I_{\rho_0} \otimes A) + T(A \otimes I_{\rho_0})]\kappa_{2,0} = -[(I_{\rho_0} \otimes A A^*) + T(A \otimes A^*)]C^{-1}(\tilde{\eta}_B) \]

\[ = -[(I_{\rho_0} \otimes A A^*) + B]C^{-1}(\tilde{\eta}_B). \]
Analogously, \((A^* \otimes I_{\rho_1})(I + T)\kappa_{0,2} = -[(A^*A \otimes I_{\rho_1}) + B]C^{-1}(\bar{\eta}\xi)\) and
\((I + B)\kappa_{1,1'} = (I + B)(I + B)C^{-1}(\bar{\eta}\xi) = |I + 2B + (A^* \otimes A)TT(A \otimes A^*)|C^{-1}(\bar{\eta}\xi)\).

Hence,
\[
(I_{\rho_0} \otimes A)(I + T)\kappa_{2,0} + (A^* \otimes I_{\rho_1})(I + T)\kappa_{0,2} + (I + B)\kappa_{1,1'}
= [I - (I_{\rho_0} \otimes AA^*) - (A^*A \otimes I_{\rho_1}) + (A^*A \otimes AA^*)]C^{-1}(\bar{\eta}\xi) = \bar{\eta}\xi,
\]
where the last equality follows from \(C := (I - A^*A) \otimes (I - AA^*) = I - I_{\rho_0} \otimes AA^* - A^*A \otimes I_{\rho_1} + A^*A \otimes AA^*\).

The next proposition shows that \(L_2\) is equal to the second order chaos of \(T_N\) up to an \(o_p(N^{-1})\) term.

**Proposition 21.** Suppose Assumption 3 holds. Let the second order chaos of \(T_N\) be \(^3\text{Proj}_{H_2}(T_N)\). Then we have \(\text{Proj}_{H_2}(T_N) = L_2 + o_p(N^{-1})\) under the measure \(\mu_\nu\).

**Proof of Proposition 21.** Define
\[
\tilde{L}_2 := \frac{1}{N(N - 1)} \sum_{i \neq j} [\kappa_{2,0}(X_i, X_j) + \kappa_{0,2}(Y_i, Y_j) + \kappa_{1,1'}(X_i, Y_j)].
\]

It follows from LLN that \(L_2 - \tilde{L}_2 = o_p(N^{-1})\). It then suffices to show \(\tilde{L}_2 - \text{Proj}_{H_2}(T_N) = o_p(N^{-1})\).

According to the degeneracy in Lemma 20, we know \(E[\tilde{L}_2] = 0\) and \(E[\tilde{L}_2 \mid X_i] = E[\tilde{L}_2 \mid Y_i] = 0\) for all \(i \in [N]\), which implies \(\tilde{L}_2 \in H^+ \cap H^\perp\). Note that \(\tilde{L}_2\) is not permutation symmetric since it lacks the diagonal terms \(\kappa_{1,1'}(X_i, Y_i)\), so it is not in \(H_2\). Moreover, we have
\[
E[\tilde{L}_2 \mid X_i, Y_i] = 0, \quad \text{for all } i \in [N].
\]

**Step 1.** We show \(\text{Proj}_{H_2}(T_N) = \text{Proj}_{H_2}(\tilde{T}_N)\), where
\[
\tilde{T}_N := \frac{1}{N} \sum_{i=1}^N [\eta(X_i, Y_i) - \theta] - L_1 = \frac{1}{N} \sum_{i=1}^N \bar{\eta}(X_i, Y_i).
\]

In fact, since \(\theta \perp H_2\) and \(L_1 \perp H_2\), we have, for any \(U \in H_2\),
\[
E[(\tilde{T}_N - T_N)U] = E \left[ \left( \frac{1}{N} \sum_{i=1}^N \eta(X_i, Y_i) - T_N \right) U \right].
\]

By the exchangeability of \(\{(X_i, Y_i)\}_{i \in [N]}\), it holds that \(E \left[ \frac{1}{N} \sum_{i=1}^N \eta(X_i, Y_i)U \right] = E[\eta(X_i, Y_i)U]\), and thus
\[
E[(\tilde{T}_N - T_N)U] = E[\eta(X_1, Y_1)U] - E[T_NU] = E[\eta(X_1, Y_1)U] - E[E[\eta(X_1, Y_1)U \mid G_N]] = 0,
\]
where (i) follows from the tower property. Hence, \(\tilde{T}_N - T_N \in H^+ \cap H^\perp\) and thus the claim follows. Moreover, since \(\bar{\eta} \in L^2_{0,0}(\mu_\nu)\), we have \(\tilde{T}_N \in H^+ \cap H^\perp\),
\[
E[\tilde{T}_N \mid X_i, Y_i] = \frac{1}{N} \sum_{k=1}^N E[\bar{\eta}(X_k, Y_k) \mid X_i, Y_i] = \frac{1}{N} \bar{\eta}(X_i, Y_i), \quad \text{for all } i \in [N],
\]
and
\[
E[\tilde{T}_N \mid X_i, X_j] = E[\tilde{T}_N \mid Y_i, Y_j] = E[\tilde{T}_N \mid X_i, Y_j] = 0, \quad \text{for all } i \neq j.
\]

**Step 2.** We show \(\text{Proj}_{H_2}(T_N) = \text{Proj}_{H_2}(\tilde{L}_2)\). By Step 1, it suffices to prove \(\tilde{T}_N - \tilde{L}_2 \in H^\perp\). We will prove \(E[(\tilde{T}_N - \tilde{L}_2)U] = 0\) for every
\[
U := \sum_{i < j} [f_{2,0}(X_i, X_j) + f_{0,2}(Y_i, Y_j)] + \sum_{i,j=1}^N f_{1,1}(X_i, Y_j) \in L^2(\mu_\nu).
\]

\(^3\text{We show in Proposition 41 in Appendix A that the subspace } H_2 \text{ is closed, so the second order chaos exists.}\)
We first compute $E[\bar{T}_N - \bar{L}_2 \mid X_1, X_2]$. Since $\kappa_{2,0} \in L^2_{0,0}(\rho_0 \otimes \rho_0)$, so it holds

$$E \left[ \sum_{i \neq j} \kappa_{2,0}(X_i, X_j) \mid X_1, X_2 \right] = E \left[ \sum_{(i,j) \neq (1,2)} \kappa_{2,0}(X_i, X_j) \mid X_1, X_2 \right] = (I + \mathcal{T})\kappa_{2,0}(X_1, X_2).$$

(37)

Since $\kappa_{0,2} \in L^2_{0,0}(\rho_1 \otimes \rho_1)$ and $E[f(Y_1, Y_2) \mid X_1, X_2] = (A^* \otimes A^*)f(X_1, X_2)$ for any $f \in L^2(\rho_1 \otimes \rho_1)$, we get

$$E \left[ \sum_{i \neq j} \kappa_{0,2}(Y_i, Y_j) \mid X_1, X_2 \right] = (I + \mathcal{T})(A^* \otimes A^*)\kappa_{0,2}(X_1, X_2).$$

(38)

Furthermore, since $E[f(X_1, Y_2) \mid X_1, X_2] = (I_{\rho_0} \otimes A^*)f(X_1, X_2)$, we have

$$E \left[ \sum_{i \neq j} \kappa_{1,1'}(X_i, Y_j) \mid X_1, X_2 \right] = (I + \mathcal{T})(I_{\rho_0} \otimes A^*)\kappa_{1,1'}(X_1, X_2).$$

(39)

Putting (37), (38) and (39) together, we get $E[\bar{L}_2 \mid X_1, X_2] = 0$ by the first identity in Lemma 20. Consequently, by (36),

$$E[\bar{T}_N - \bar{L}_2 \mid X_1, X_2] = E[\bar{T}_N \mid X_1, X_2] = 0.$$

By the exchangeability of $\{(X_i, Y_i)\}_{i=1}^N$, we obtain $E[\bar{T}_N - \bar{L}_2 \mid X_i, X_j] = 0$ for all $i \neq j$. Similarly, $E[\bar{T}_N - \bar{L}_2 \mid Y_i, Y_j] = 0$ for all $i \neq j$. Hence, we only need to prove

$$E \left[ (\bar{T}_N - \bar{L}_2) \sum_{i,j} f_{1,1}(X_i, Y_j) \right] = 0.$$

For that purpose, we will compute $E[\bar{L}_2 \mid X_i, Y_j]$. We have shown in (33) that $E[\bar{L}_2 \mid X_i, Y_i] = 0$ for all $i \in [N]$. For $(i, j) = (1, 2)$, it holds that

$$E \left[ \sum_{i \neq j} \kappa_{2,0}(X_i, X_j) \mid X_1, Y_2 \right] = (I_{\rho_0} \otimes A)(I + \mathcal{T})\kappa_{2,0}(X_1, Y_2)$$

$$E \left[ \sum_{i \neq j} \kappa_{0,2}(Y_i, Y_j) \mid X_1, Y_2 \right] = (A^* \otimes I_{\rho_1})(I + \mathcal{T})\kappa_{0,2}(X_1, Y_2)$$

$$E \left[ \sum_{i \neq j} \kappa_{1,1'}(X_i, Y_j) \mid X_1, Y_2 \right] = (I + \mathcal{B})\kappa_{1,1'}(X_1, Y_2).$$

It then follows from the third identity in Lemma 20 that

$$E[\bar{L}_2 \mid X_1, Y_2] = \frac{1}{N(N-1)}\bar{\eta}(X_1, Y_2)\xi(X_1, Y_2).$$

By the exchangeability of $\{(X_i, Y_i)\}_{i=1}^N$ again, we get

$$E \left[ \bar{L}_2 \sum_{i,j=1}^N f_{1,1}(X_i, Y_j) \right] = \sum_{i \neq j} E[\bar{L}_2 f_{1,1}(X_i, Y_j)] = E[\bar{\eta}(X_1, Y_2)\xi(X_1, Y_2)f_{1,1}(X_1, Y_2)]$$

$$= E \left[ \bar{\eta}(X_1, Y_1)f_{1,1}(X_1, Y_1) \right],$$

since $\xi$ is the Radon-Nikodym derivative of $\mu_\epsilon$ with respect to $\rho_0 \otimes \rho_1$ under $E$. On the other hand, we also have, by (35) and (36),

$$E \left[ \bar{T}_N \sum_{i,j=1}^N f_{1,1}(X_i, Y_j) \right] = N E[\bar{T}_N f_{1,1}(X_1, Y_1)] = E[\bar{\eta}(X_1, Y_1)f_{1,1}(X_1, Y_1)].$$

Hence, $E \left[ (\bar{T}_N - \bar{L}_2) \sum_{i,j=1}^N f(X_i, Y_j) \right] = 0$ and the claim follows.
Step 3. We control the variance of \( \text{Proj}_{H_2}(T_N) - \tilde{L}_2 \). From Step 2 we know \( \text{Proj}_{H_2}(\tilde{L}_2) = \text{Proj}_{H_2}(T_N) \). By the definition of \( L^2 \) projection, it holds
\[
E[(\text{Proj}_{H_2}(T_N) - \tilde{L}_2)^2] = E[(\text{Proj}_{H_2}(\tilde{L}_2) - \tilde{L}_2)^2] = \min_{V \in H_2} E[(\tilde{L}_2 - V)^2] \leq E[(\tilde{L}_2 - L_2)^2],
\]
since \( L_2 \in H_2 \). Note that
\[
L_2 - \tilde{L}_2 = \frac{1}{N(N-1)} \sum_{i=1}^{N} [\kappa_{1,i}(X_i, Y_i) - \ell_{1,i}(X_i, Y_i)].
\]
By independence, we get
\[
E[(\tilde{L}_2 - L_2)^2] = \frac{1}{N^2(N-1)^2} \sum_{i=1}^{N} E[(\kappa_{1,i}(X_i, Y_i) - \ell_{1,i}(X_i, Y_i))^2] = O(N^{-3}).
\]
It follows that \( \tilde{L}_2 = \text{Proj}_{H_2}(T_N) + o_p(N^{-1}) \).

4. Control of higher-order remainders

We denote \( R_1 := T_N - \theta - L_1 \) and \( R_2 := R_1 - L_2 \) the first and second order remainders, respectively. Recall that \( L_1 \) and \( L_2 \) are defined in (25) and (30), respectively. The goal in this section is to show \( R_1 = o_p(N^{-1/2}) \) and \( R_2 = o_p(N^{-1}) \) under \( \mu_\nu^N \). Let
\[
U_N := \frac{1}{N \cdot N!} \sum_{\sigma \in S_N} \tilde{\eta}(X, Y) \xi^{\otimes}(X, Y) \quad \text{and} \quad D_N := \frac{1}{N!} \sum_{\sigma \in S_N} \xi^{\otimes}(X, Y). \tag{40}
\]
Recall from (15) that
\[
R_1 = E[\tilde{\eta}(X_1, Y_1) \mid G_N] = \frac{\sum_{\sigma \in S_N} \frac{1}{N} \tilde{\eta}(X, Y, \sigma) \xi^{\otimes}(X, Y, \sigma)}{\sum_{\sigma \in S_N} \xi^{\otimes}(X, Y, \sigma)} = \frac{U_N}{D_N}.
\]
By a change of measure,
\[
E[||R_1||] = \mu_\nu^N ||R_1|| = (\rho_0 \otimes \rho_1)^N \left[ \frac{d\mu_\nu^N}{d(\rho_0 \otimes \rho_1)^N} ||R_1|| \right] = (\rho_0 \otimes \rho_1)^N \left[ \frac{||\xi^{\otimes}(X, Y) \mid G_N||}{D_N} \right] \leq \sqrt{E[U^2_N]},
\]
where \( E \) is the expectation under the measure \( P^N \). Consequently, it suffices to show \( E[U^2_N] = o(N^{-1}) \). A similar argument shows that \( E[||U_N - L_2 D_N||^2] = o(N^{-2}) \) is enough to imply \( R_2 = o_P(N^{-1}) \) under \( \mu_\nu^N \).

Hence, in what follows, we shall work with the original model assuming that \((X_1, Y_1), \ldots, (X_N, Y_N) \overset{i.i.d.}{\sim} \rho_0 \otimes \rho_1 \) and prove
\[
E[U^2_N] = o(N^{-1}) \quad \text{and} \quad E[(U_N - L_2 D_N)^2] = o(N^{-2}). \tag{41}
\]

4.1. Hoeffding decomposition under the product measure.

**Definition 5.** Given \( A, B \subseteq [N] \), we denote by \( H_{AB} \) the subspace of \( L^2((\rho_0 \otimes \rho_1)^N) \) spanned by functions of the form \( f(X_A, Y_B) \) such that
\[
E[f(X_A, Y_B) \mid X_C, Y_D] \overset{a.s.}{=} 0, \quad \text{for all} \quad C \subset A, D \subset B \quad \text{and} \quad |C| + |D| < |A| + |B|.
\]

We say such an \( f(X_A, Y_B) \) is completely degenerate. By definition, for distinct choices of the pair \((A, B)\), the subspaces \( H_{AB} \) are orthogonal. Take an arbitrary mean-zero statistic \( T \in L_0^2((\rho_0 \otimes \rho_1)^N) \). If \( T \) can be decomposed as
\[
T = \sum_{A, B \subseteq [N]} T_{AB}, \quad \text{with} \quad T_{AB} \in H_{AB}, \tag{43}
\]
then we call it the **Hoeffding decomposition** of \( T \) [vdV00, Chapter 11]. In particular, its variance can be computed as \( E[T^2] = \sum_{A, B \subseteq [N]} E[T_{AB}^2] \).
For example, both $\xi(X_1, Y_1) - 1$ and $h(X_1, Y_1) := \eta(X_1, Y_1)\xi(X_1, Y_1)$ are completely degenerate since they are both elements in $L^2_{0,0}(\rho_0 \otimes \rho_1)$. To see that $\xi - 1 \in L^2_{0,0}(\rho_0 \otimes \rho_1)$, note that $\mathbb{E}[\xi(X_i, Y_j) | X_i] \overset{\text{a.s.}}{=} \mathbb{E}[\xi(X_i, Y_j) | Y_j]^{\otimes 1}$ for all $i, j \in [N]$. And $h \in L^2_{0,0}(\rho_0 \otimes \rho_1)$ has been shown in Lemma 18.

**Definition 6.** Let $r > 0$ be an integer. We say a statistic $T := T(X_{[N]}, Y_{[N]})$ is $r$-degenerate if
\[
\mathbb{E}[T | X_A, Y_B] \overset{\text{a.s.}}{=} 0, \quad \text{for all } A, B \subset [N] \text{ such that } |A| + |B| = r.
\]
If $T$ is $(r - 1)$-degenerate, and $L \in \oplus_{|A|+|B|=r} H_{AB}$ such that $T - L$ is $r$-degenerate, then we call $L$ the $r$-th order term of $T$.

**Lemma 22.** Let $A_1, A_2, B_1, B_2 \subset [N]$ such that $A_1 \cap A_2 = B_1 \cap B_2 = \emptyset$. Assume $T_1 := f_1(X_{A_1}, Y_{B_1}) \in L^2((\rho_0 \otimes \rho_1)^N)$ and $T_2 := f_2(X_{A_2}, Y_{B_2}) \in L^2((\rho_0 \otimes \rho_1)^N)$ are completely degenerate. Then $T_1 T_2 \in L^2((\rho_0 \otimes \rho_1)^N)$ is also completely degenerate.

**Proof.** Take any $A' \subset A_1 \cup A_2$ and $B' \subset B_1 \cup B_2$ such that $|A'| + |B'| < |A_1| + |A_2| + |B_1| + |B_2|$. Let $A'_1 := A' \cap A_1$, $A'_2 := A' \cap A_2$, $B'_1 := B' \cap B_1$ and $B'_2 := B' \cap B_2$. Then $A' = A'_1 \cup A'_2$ and $B' = B'_1 \cup B'_2$. Furthermore, without loss of generality, we may assume $|A'_1| + |B'_1| < |A_1| + |B_1|$. By independence, we have
\[
\mathbb{E}[T_1 T_2 | X_{A'}, Y_{B'}] = \mathbb{E}[T_1 | X_{A'_1}, Y_{B'_1}] \mathbb{E}[T_2 | X_{A'_2}, Y_{B'_2}] = 0,
\]
since $\mathbb{E}[T_1 | X_{A'_1}, Y_{B'_1}] = 0$. \hfill $\square$

**Lemma 23.** Let $A \subset [N]$ be a subset. For any $\sigma \in S_N$, the following identity holds:
\[
\prod_{i \in A} \xi(X_i, Y_{\sigma_i}) = \sum_{C \subset A} \prod_{i \in C} \xi(X_i, Y_{\sigma_i}) - 1,
\]
where $\prod_{i \in \emptyset} [\xi(X_i, Y_{\sigma_i}) - 1] := 1$. Moreover, (44) gives the Hoeffding decomposition of $\prod_{i \in A} \xi(X_i, Y_{\sigma_i})$.

**Proof.** By Lemma 22, $\prod_{i \in C} [\xi(X_i, Y_{\sigma_i}) - 1]$ is completely degenerate for each $C \subset A$. It then suffices to prove the identity (44). Without loss of generality, we prove it for $A = [N]$ by induction. For $N = 1$, the identity reduces to $\xi(X_1, Y_1) = 1 + [\xi(X_1, Y_1) - 1]$. Assume the identity holds for $N - 1$. Consequently, we have
\[
\prod_{i=1}^{N} [\xi(X_i, Y_{\sigma_i}) - 1] = \sum_{C \subset [N-1]} \prod_{i \in C} \xi(X_i, Y_{\sigma_i}) - 1 \times \xi(X_N, Y_{\sigma_N})
\]
\[
= \sum_{C \subset [N], N \in C} \prod_{i \in C} \xi(X_i, Y_{\sigma_i}) - 1 + \sum_{C \subset [N-1]} \prod_{i \in C} \xi(X_i, Y_{\sigma_i}) - 1
\]
\[
= \sum_{C \subset [N]} \prod_{i \in C} \xi(X_i, Y_{\sigma_i}) - 1.
\]
Thus, the identity holds for $N$. \hfill $\square$

4.2. **Variance bound for $U_N$.** Let us derive the Hoeffding decomposition of $U_N$ as defined in (30). For any $A, B \subset [N]$ such that $|A| = |B| > 0$, let $U_{AB} := \sum_{\sigma \in S_N : \sigma_A = B} \sum_{i \in A \setminus \{i\}} h(X_i, Y_{\sigma_i}) \prod_{j \in A \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1]$, where $\sigma_A := \{\sigma_i : i \in A\}$.

**Lemma 24.** The following Hoeffding decomposition holds:
\[
U_N = \frac{1}{N \cdot N!} \sum_{A, B \subset [N]} U_{AB}.
\]
Moreover,
\[
\mathbb{E}[U_N^2] = \frac{1}{N^2} \sum_{r=1}^{N} p_r \sum_{\sigma \in S_r} \sum_{i=1}^{r} \mathbb{E} \left[ h(X_1, Y_1) \prod_{j=2}^{r} [\xi(X_j, Y_j) - 1] h(X_i, Y_{\sigma_i}) \prod_{j \in [r] \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1] \right].
\]
Proof. By definition,
\[
U_N:= \frac{1}{N \cdot N!} \sum_{\sigma \in S_N} \sum_{i=1}^{N} h(X_i, Y_{\sigma_i}) \prod_{j \in [N] \setminus \{i\}} \xi(X_j, Y_{\sigma_j})
\]
\[
= \frac{1}{N \cdot N!} \sum_{\sigma \in S_N} \sum_{i=1}^{N} h(X_i, Y_{\sigma_i}) \sum_{C \subset [N] \setminus \{i\}} \prod_{j \in C} [\xi(X_j, Y_{\sigma_j}) - 1], \quad \text{by Lemma 23.}
\]
Take \(A, B \subset [N]\) such that \(|A| = |B| > 0\). We will write \(U_N\) as a sum of terms that only contain \(X_A := (X_i)_{i \in A}\) and \(Y_B := (Y_i)_{i \in B}\). The terms corresponding to \(X_A\) in the above decomposition are
\[
\frac{1}{N \cdot N!} \sum_{\sigma \in S_N} \sum_{i \in A} h(X_i, Y_{\sigma_i}) \prod_{j \in A \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1].
\]
Consequently, the terms corresponding to \((X_A, Y_B)\) are
\[
\frac{1}{N \cdot N!} \sum_{\sigma \in S_N: \sigma_A = B} \sum_{i \in A} h(X_i, Y_{\sigma_i}) \prod_{j \in A \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1] = \frac{1}{N \cdot N!} U_{AB}.
\]
Hence, the identity (45) follows. Moreover, since \(h \in L^2_{\rho_0 \rho_1}(\rho_0 \otimes \rho_1)\), we get, by Lemma 22, that
\[
h(X_i, Y_{\sigma_i}) \prod_{j \in A \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1] \in H_{AB}, \quad \text{for any } i \in A \text{ and } \sigma \in S_N \text{ such that } \sigma_A = B.
\]
This implies \(U_{AB} \in H_{AB}\), and thus (45) is the Hoeffding decomposition of \(U_N\).

Let us compute \(\mathbb{E}[U_N^2]\). For any \(A, B \subset [N]\) such that \(|A| = |B| = r > 0\), we get, by the exchangeability of \(X_{[N]}\) and \(Y_{[N]}\) under the measure \((\rho_0 \otimes \rho_1)^N\), \(\mathbb{E}[U_{AB}^2] = \mathbb{E}[U_{[r][r]}^2]\). Furthermore, since there are \((N-r)!\) permutations that map \(r\) to \([r]\), we get
\[
\mathbb{E}[U_{[r][r]}^2] = (N-r)!^2 \mathbb{E}\left[ \sum_{\sigma \in S_r} \sum_{i=1}^{r} h(X_i, Y_{\sigma_i}) \prod_{j \in [r] \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1] \right]^2.
\]
As a result, \(\mathbb{E}[U_{[r][r]}^2]\) is equal to
\[
(N-r)!^2 \sum_{r \in S_N} \sum_{\tau \in S_N} \mathbb{E}\left[ \sum_{k \in [r] \setminus \{i\}} h(X_i, Y_{\tau_k}) \prod_{k \in [r] \setminus \{i\}} [\xi(X_k, Y_{\tau_k}) - 1] \sum_{\sigma \in S_r} \sum_{i=1}^{r} h(X_i, Y_{\sigma_i}) \prod_{j \in [r] \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1] \right]
\]
By symmetry, the contribution from every \(r\) is the same, so
\[
\mathbb{E}[U_{[r][r]}^2] = (N-r)!^2 \mathbb{E}\left[ \sum_{i=1}^{r} h(X_i, Y_i) \prod_{k \in [r] \setminus \{i\}} [\xi(X_k, Y_k) - 1] \sum_{\sigma \in S_r} \sum_{i=1}^{r} h(X_i, Y_{\sigma_i}) \prod_{j \in [r] \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1] \right]
\]
\[
= (N-r)!^2 \mathbb{E}\left[ \sum_{i=1}^{r} h(X_i, Y_i) \prod_{k=2}^{r} [\xi(X_k, Y_k) - 1] \sum_{\sigma \in S_r} \sum_{i=1}^{r} h(X_i, Y_{\sigma_i}) \prod_{j \in [r] \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1] \right],
\]
where the last equality follows from the exchangeability of \(\{(X_i, Y_i)\}_{i \in [N]}\). It then follows that
\[
\mathbb{E}[U_N^2] = \frac{1}{N^2(N)!^2} \sum_{r=1}^{N} \sum_{|A|=|B|=r} \mathbb{E}[U_{AB}^2] = \frac{1}{N^2(N)!^2} \sum_{r=1}^{N} \binom{N}{r}^2 \mathbb{E}[U_{[r][r]}^2]
\]
\[
= \frac{1}{N^2} \sum_{r=1}^{N} \frac{r}{r!} \sum_{\sigma \in S_r} \sum_{i=1}^{r} \mathbb{E}\left[ h(X_i, Y_i) \prod_{j=2}^{r} [\xi(X_k, Y_k) - 1] h(X_i, Y_{\sigma_i}) \prod_{j \in [r] \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1] \right].
\]
We then bound the variance of \(U_N\) using the spectral gap of operators \(A\) and \(A^*\). Assumption 2 guarantees that such spectral gaps do exist. Before that, let us prove a contraction property.
Lemma 25. Recall $s_1$ from Assumption 2. For any $f \in L^2_{0,0}((\rho_0 \otimes \rho_0))$, we have $(I_{\rho_0} \otimes A)f \in L^2_{0,0}((\rho_0 \otimes \rho_1))$ and $\| (I_{\rho_0} \otimes A)f \|_{L^2((\rho_0 \otimes \rho_1))} \leq s_1 \| f \|_{L^2((\rho_0 \otimes \rho_0))}$. Similar results hold for $I_{\rho_0} \otimes A^*$, $A \otimes I_{\rho_1}$, and $A^* \otimes I_{\rho_1}$.

Proof. Take an arbitrary $f \in L^2_{0,0}((\rho_0 \otimes \rho_0))$. According to Lemma 19, we know $(I_{\rho_0} \otimes A)f \in L^2_{0,0}((\rho_0 \otimes \rho_1))$. Now, by Lemma 16, $f$ admits the following expansion:

$$f = \sum_{i,j \geq 1} \gamma_{ij} \alpha_i \otimes \alpha_j,$$

where $\sum_{i,j \geq 1} \gamma_{ij} < \infty$.

It then follows that

$$\| (I_{\rho_0} \otimes A)f \|_{L^2((\rho_0 \otimes \rho_1))}^2 = \left\| \sum_{i,j \geq 1} \gamma_{ij} \beta_i \otimes \beta_j \right\|_{L^2((\rho_0 \otimes \rho_1))}^2 = \sum_{i,j \geq 1} \gamma_{ij}^2 s_j^2 \leq s_1^2 \| f \|_{L^2((\rho_0 \otimes \rho_0))}^2.$$

In order to bound the expectation on the right hand side of (46), we decompose a permutation into disjoint cycles. By independence, the expectation then equals the product of expectations with respect to each cycle. We give a simple example before we prove the general result.

Example 1. Consider the case when $r = 3$, $i = 3$, and $\sigma$ is given by $\sigma_1 = 2$, $\sigma_2 = 1$ and $\sigma_3 = 3$. We are interested in bounding the following expectation:

$$E[h(X_1, Y_1)]\|X_2, Y_2\| \|X_3, Y_3\| - \|X_2, Y_2\| \|X_3, Y_3\|.$$

By construction, $\sigma$ contains two cycles, $1 \to 2 \to 1$ and $3 \to 3$, and the above expectation reads

$$E[h(X_1, Y_1)]\|X_2, Y_2\| \|X_3, Y_3\| - \|X_2, Y_2\| \|X_3, Y_3\|.$$

By the Cauchy-Schwarz inequality, the second expectation is upper bounded by $\| h \|_{L^2((\rho_0 \otimes \rho_1))} \| \xi - 1 \|_{L^2((\rho_0 \otimes \rho_1))}$. It then suffices to bound the first expectation. We simply this expectation by iteratively integrating with respect to a single variable, while keeping the rest being fixed. We first integrate with respect to $X_1$ given $X_2, Y_1, Y_2$. This gives us

$$E[h(X_1, Y_1)]\|X_2, Y_2\| \|X_3, Y_3\| - \|X_2, Y_2\| \|X_3, Y_3\|.$$

where we have used $E[h(X_1, Y_1)]\|X_3, Y_3\| - \|X_2, Y_2\| \|X_3, Y_3\| = E[h(X_1, Y_1)]\|X_1, Y_2\| \|X_2, Y_1\| = (A \otimes I_{\rho_1})h(Y_2, Y_1).$

We then integrate with respect to $Y_2$ given $X_2$ and $Y_1$. This yields

$$E[(A \otimes I_{\rho_1})h(Y_2, Y_1)]\|X_3, Y_3\| - \|X_2, Y_2\| \|X_3, Y_3\|.$$

By the Cauchy-Schwarz inequality and Lemma 25, its expectation is upper bounded by

$$E[(A \otimes I_{\rho_1})]h(Y_2, Y_1)]\|X_3, Y_3\| - \|X_2, Y_2\| \|X_3, Y_3\|.$$

Hence, the expectation in (47) is upper bounded by $s_1^2 \| h \|_{L^2((\rho_0 \otimes \rho_1))} \| \xi - 1 \|_{L^2((\rho_0 \otimes \rho_1))}^2$.

The following lemma generalizes this example by taking an arbitrary cycle $k_1 \to k_2 \to \cdots \to k_l \to k_1$.

Lemma 26. Assume Assumption 2 holds. Let $f, g \in L^2_{0,0}((\rho_0 \otimes \rho_1))$. Define $\gamma_t := \| g \|_{L^2((\rho_0 \otimes \rho_1))}$ and $s_t := \| f \|_{L^2((\rho_0 \otimes \rho_1))}$. For any $l > 0$ and $l$ distinct indices $\{k_1, \ldots, k_l\} \subset [N]$, we have, for all $t, t' \in [l]$, $t \neq t'$

$$E\left[ f(X_{k_t}, Y_{k_t})g(X_{k_{t'}}, Y_{k_{t'+1}}) \prod_{i \in t} \xi(X_{k_i}, Y_{k_i}) - 1 \prod_{j \in t} \xi(X_{k_j}, Y_{k_{j+1}}) - 1 \right] \leq s_1^{2(l-1)} \gamma_t s_t.$$

Proof. There are two cases to consider: $t = t'$ and $t \neq t'$. We only prove it for $t = t'$. The other case follows from a similar argument. By exchangeability, it suffices to consider $t = t' = 1$. The strategy is again to iteratively take expectation with respect to one variable, while keeping the rest being fixed. Note that

$$E[f(X_{k_1}, Y_{k_1})] \xi(X_{k_1}, Y_{k_1}) - 1 \right] \leq E[f(X_{k_1}, Y_{k_1})] \xi(X_{k_1}, Y_{k_1}) \right] \leq (I_{\rho_0} \otimes A^*)f(X_{k_1}, X_{k_1}).$$
Taking expectation with respect to $Y_{k_1}$ in (48), while keeping others being fixed, we get
\[
E \left[ E[f(X_{k_1}, Y_{k_1}) | \xi(X_{k_1}, Y_{k_1}) - 1 \mid X_{k_1}, X_{k_1}] g(X_{k_1}, Y_{k_2}) \prod_{i=2}^{\ell} [\xi(X_{k_i}, Y_{k_i}) - 1] \prod_{i=2}^{l-1} [\xi(X_{k_i}, Y_{k_{i+1}}) - 1] \right]
\]
\[
= E \left[ (I_{\rho_0} \otimes A^*) f(X_{k_1}, X_{k_2}) g(X_{k_1}, Y_{k_2}) \prod_{i=2}^{l} [\xi(X_{k_i}, Y_{k_i}) - 1] \prod_{i=2}^{l-1} [\xi(X_{k_i}, Y_{k_{i+1}}) - 1] \right].
\]
Now taking expectation with respect to $X_{k_1}$, while keeping others being fixed, we get
\[
E \left[ (I_{\rho_0} \otimes A^*) f(X_{k_1}, X_{k_2}) g(X_{k_1}, Y_{k_2}) \prod_{i=2}^{l-1} [\xi(X_{k_i}, Y_{k_i}) - 1] [\xi(X_{k_i}, Y_{k_{i+1}}) - 1] \right],
\]
since
\[
E[ (I_{\rho_0} \otimes A^*) f(X_{k_1}, X_{k_1}) | \xi(X_{k_1}, Y_{k_1}) - 1 \mid X_{k_1}, Y_{k_1}]
\]
\[
= E[(I_{\rho_0} \otimes A^*) f(X_{k_1}, X_{k_1}) | X_{k_1}, Y_{k_1}] - E[(I_{\rho_0} \otimes A^*) f(X_{k_1}, X_{k_1}) | X_{k_1}]
\]
\[
= (I_{\rho_0} \otimes A^*) f(X_{k_1}, Y_{k_1}).
\]
Keep repeating this argument, we ultimately get
\[
E \left[ f(X_{k_1}, Y_{k_1}) g(X_{k_1}, Y_{k_2}) \prod_{i=2}^{l} [\xi(X_{k_i}, Y_{k_i}) - 1] [\xi(X_{k_i}, Y_{k_{i+1}}) - 1] \right]
\]
\[
\leq \| (I_{\rho_0} \otimes A^*)^{l-1} f \|_{L^2(\rho_0 \otimes \rho_1)} \| g \|_{L^2(\rho_0 \otimes \rho_1)} \leq s_1^{2(l-1)} \xi_s \zeta_s.
\]

**Lemma 27.** Assume Assumption 2 holds. Let $s_0 := \| \xi - 1 \|_{L^2(\rho_0 \otimes \rho_1)}$ and $\zeta := \| h \|_{L^2(\rho_0 \otimes \rho_1)} = \| \eta \xi \|_{L^2(\rho_0 \otimes \rho_1)}$. For any $N \in \mathbb{N}_+$, $\sigma \in S_N$ and $i \in [N]$, we have
\[
(49) \quad E \left[ h(X_1, Y_1) \prod_{j=2}^{N} [\xi(X_j, Y_j) - 1] h(X_i, Y_{\sigma_i}) \prod_{j \in [N] \setminus \{i\}} [\xi(X_j, Y_j) - 1] \right] \leq s_1^{2(N-\# \sigma)} \zeta_s^{2(\# \sigma - 1)},
\]
where $\# \sigma$ is the number of cycles of the permutation $\sigma$.

**Proof.** We first consider the case when $i \neq 1$. It is well-known that any permutation can be decomposed as disjoint cycles. Take a cycle $k_1 \rightarrow k_2 \rightarrow \cdots \rightarrow k_l \rightarrow k_1$ of $\sigma$. If this cycle contains both 1 and $i$, then we assume, w.l.o.g., $k_1 = 1$ and $k_2 = i$. Consequently, all the terms that involve $X_{k_{1j}}$ and $Y_{k_{1j}}$ are
\[
h(X_1, Y_1) h(X_i, Y_{\sigma_i}) \prod_{j=2}^{l} [\xi(X_{k_j}, Y_{k_j}) - 1] \prod_{j \in [l] \setminus \{2\}} [\xi(X_{k_j}, Y_{k_{j+1}}) - 1].
\]
Using Lemma 26 with $f = h$ and $g = h$, it holds that
\[
E \left[ h(X_1, Y_1) h(X_i, Y_{\sigma_i}) \prod_{j=2}^{l} [\xi(X_{k_j}, Y_{k_j}) - 1] \prod_{j \in [l] \setminus \{2\}} [\xi(X_{k_j}, Y_{k_{j+1}}) - 1] \right] \leq s_1^{2(l-1)} \zeta_s^2.
\]
If this cycle only contains 1, then a similar argument gives
\[
E \left[ h(X_1, Y_1) \prod_{j=2}^{l} [\xi(X_{k_j}, Y_{k_j}) - 1] \prod_{j=1}^{l} [\xi(X_{k_j}, Y_{k_{j+1}}) - 1] \right] \leq s_1^{2(l-1)} \zeta_s s_0.
\]
If this cycle only contains $i$, with $k_1 = i$, then we have

$$E \left[ h(X_i, Y_{\sigma_i}) \prod_{j=1}^{l} [\xi(X_{k_j}, Y_{k_j}) - 1] \prod_{j=2}^{l} [\xi(X_{k_{j-1}}, Y_{k_{j-1}+1}) - 1] \right] \leq s_1^{2(l-1)} \xi \varsigma_0.$$  

Finally, if this cycle does not contain either 1 or $i$, then it holds

$$E \left[ \prod_{j=1}^{l} [\xi(X_{k_j}, Y_{k_j}) - 1][\xi(X_{k_{j-1}}, Y_{k_{j-1}+1}) - 1] \right] \leq s_1^{2(l-1)} \xi \varsigma_0^2.$$  

Here we are invoking Lemma 26 with $f = g = \xi - 1$. Putting all together, we obtain

$$E \left[ h(X_1, Y_1) \prod_{j=2}^{N} [\xi(X_j, Y_j) - 1]h(X_i, Y_{\sigma_i}) \prod_{j \in [N] \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1] \right] \leq s_1^{2(N-\#\sigma)} \xi \varsigma_0^2(\#\sigma-1).$$  

When $i \neq 1$, we can again invoke Lemma 26 to get the same bound, since we allow $t = t'$ in this lemma. \hfill $\square$

Now we are ready to give an upper bound for the variance of $U_N$.

**Proposition 28.** Assume Assumption 2 holds. Let $s_0 := \|\xi - 1\|_{L^2(\rho_0 \otimes \rho_1)}$ and $\varsigma := \|h\|_{L^2(\rho_0 \otimes \rho_1)} = \|\tilde{\eta}_0\|_{L^2(\rho_0 \otimes \rho_1)}$. Then, with $\#\sigma$ being the number of cycles of $\sigma$,

$$E[U_N^2] \leq \frac{1}{N^2} \sum_{r=1}^{N} \frac{r^2}{r!} \sum_{\sigma \in S_r} s_1^{2(r-\#\sigma)} \varsigma_0^{2(\#\sigma-1)} \varsigma^2.$$  

In particular, $E[U_N^2] = O(N^{-2})$ and thus $R_1 := T_N - \theta - L_1 = o_p(N^{-1/2})$ under the measure $\mu_{\tilde{\eta}}^N$.

**Proof.** Recall from (46) that

$$E[U_N^2] = \frac{1}{N^2} \sum_{r=1}^{N} \frac{r^2}{r!} \sum_{\sigma \in S_r} \sum_{i=1}^{r} \left[ h(X_1, Y_1) \prod_{j=2}^{r} [\xi(X_j, Y_j) - 1]h(X_i, Y_{\sigma_i}) \prod_{j \in [N] \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1] \right].$$

By Lemma 27, we know

$$E[U_N^2] \leq \frac{1}{N^2} \sum_{r=1}^{N} \frac{r^2}{r!} \sum_{\sigma \in S_r} s_1^{2(r-\#\sigma)} \varsigma_0^{2(\#\sigma-1)} \varsigma^2.$$  

Now, let $\sigma^*$ be a random permutation uniformly sampled from $S_r$. It is well-known [ABT03, Chapter 1] that the moment generating function of $\sigma^*$ is given by $E[u^{\sigma^*}] = \prod_{i=1}^{r} (1 - \frac{1}{i} + \frac{s_2}{i^2})$. Thus,

$$\frac{r^2}{r!} \sum_{\sigma \in S_r} s_1^{2(r-\#\sigma)} \varsigma_0^{2(\#\sigma-1)} = r^2 \mathbb{E} \left[ s_1^{2(r-\#\sigma^*)} \varsigma_0^{2(\#\sigma^*-1)} \right] = r^2 s_1^{2} \varsigma_0^{2} \sum_{i=1}^{r} \left( 1 - \frac{1}{i} + \frac{s_2}{i^2} \right).$$

Let $m := \lfloor \varsigma_0^2 / s_1^2 - 1 \rfloor$. Then, for every $r \geq m$,

$$\prod_{i=1}^{r} \left( 1 - \frac{1}{i} + \frac{s_2}{i^2} \right) \leq \prod_{i=1}^{r} \left( 1 + m/i \right) = \prod_{i=1}^{r} (1 + m/i) = \frac{\prod_{i=m+1}^{r} (i + m)}{m!} = \frac{\prod_{i=m+1}^{r} (i + m)}{m!} \leq \frac{(r + m)^m}{m!},$$

and thus

$$\sum_{r=1}^{N} \frac{r^2}{r!} \sum_{\sigma \in S_r} s_1^{2(r-\#\sigma)} \varsigma_0^{2(\#\sigma-1)} \leq \sum_{r=1}^{m} \frac{1}{m!} r^2 (r + m)^m s_1^{2r} \varsigma_0^2.$$  

converges as $N \to \infty$. It follows from (51) that $E[U_N^2] = O(N^{-2}).$ \hfill $\square$
4.3. Variance bound for $U_N - L_2 D_N$. Recall from Proposition 21

\[
L_2 := \frac{1}{N(N-1)} \left\{ \sum_{i \neq j, \sigma \in S_N} [\kappa_{2,0}(X_i, X_j) + \kappa_{2,0}(Y_i, Y_j)] + \sum_{i,j=1}^N \kappa_{1,1'}(X_i, Y_j) - \sum_{i=1}^N \delta_{1,1'}(X_i, Y_i) \right\}.
\]

is an approximate second order chaos of $T_N$. We will decompose $L_2 D_N$ into manageable pieces. Let $K_{2,0}(x,x',y,y') := \kappa_{2,0}(x,x')\xi(x,y)\xi(x',y')$ and $K_{2,0}(x,x',y,y') := \kappa_{2,0}(y,y')\xi(x,y)\xi(x',y')$. Then we have

\[
\sum_{i \neq j} \kappa_{2,0}(X_i, X_j) D_N = \frac{1}{N^2} \sum_{i \neq j, \sigma \in S_N} K_{2,0}(X_i, X_j, Y_{\sigma_i}, Y_{\sigma_j}) \prod_{k \in [N] \setminus \{i,j\}} \xi(X_k, Y_{\sigma_k})
\]

\[
\sum_{i \neq j} \kappa_{0,2}(Y_i, Y_j) D_N = \frac{1}{N^2} \sum_{i \neq j, \sigma \in S_N} K_{0,2}(Y_i, Y_j) \xi(x_{\sigma_i-1}, Y_i)\xi(x_{\sigma_i-1}, Y_j) \prod_{k \in [N] \setminus \{\sigma_i^{-1}, \sigma_j^{-1}\}} \xi(X_k, Y_{\sigma_k})
\]

(52)

Furthermore, let $K_{1,1'}(x,x',y,y') := \kappa_{1,1'}(x,y')\xi(x,y)\xi(x',y')$, then

\[
\sum_{i,j=1}^N \kappa_{1,1'}(X_i, Y_j) \xi^{\otimes}(X, Y) = \frac{1}{N^2} \sum_{i,j=1}^N \kappa_{1,1'}(X_i, Y_j) \xi^{\otimes}(X, Y) = \frac{1}{N^2} \sum_{i,j=1}^N \kappa_{1,1'}(X_i, Y_j) \xi^{\otimes}(X, Y).
\]

(53)

Note that $\sum_{i=1}^N \xi_{1,1'}(X_i, Y_i) = \sum_{i=1}^N \xi_{1,1'}(X_i, Y_i)$ by affineness, and

\[
\frac{1}{N^2} \sum_{i,j=1}^N \xi_{1,1'}(X_i, Y_j) \xi^{\otimes}(X, Y) = \frac{1}{N^2} \sum_{i=1}^N \sum_{\sigma \in S_N} \kappa_{1,1'}(X_i, Y_j) \xi^{\otimes}(X, Y).
\]

(54)

It follows that

\[
\frac{1}{N^2} \sum_{i,j=1}^N \kappa_{1,1'}(X_i, Y_j) \xi^{\otimes}(X, Y) - \sum_{i=1}^N \xi_{1,1'}(X_i, Y_i) D_N = \frac{1}{N^2} \sum_{\sigma \in S_N} (\kappa_{1,1'} - \xi_{1,1'})(X_i, Y_i) \xi^{\otimes}(X, Y).
\]

(55)

Repeating the argument in Proposition 28 for $\tilde{\eta}$ replaced by $\kappa_{1,1'} - \xi_{1,1'} \in L_2^2(\mu_N)$ gives

\[
\frac{1}{N(N-1)} \frac{1}{N!} \sum_{i,j=1}^N \kappa_{1,1'}(X_i, Y_j) \xi^{\otimes}(X, Y) - \sum_{i=1}^N \xi_{1,1'}(X_i, Y_i) D_N = O(N^{-2}).
\]

Here we say a random variable $\phi_N = O(N^{-2})$ if $\text{Var}(\phi_N) = O(N^{-4})$. Putting (52), (53), (54) and (55) together, we obtain

\[
L_2 D_N = \frac{1}{N(N-1)} \frac{1}{N!} \sum_{\sigma \in S_N} \sum_{i,j=1}^N (K_{2,0} + K_{0,2} + K_{1,1'})(X_i, X_j, Y_{\sigma_i}, Y_{\sigma_j}) \prod_{k \in [N] \setminus \{i,j\}} \xi(X_k, Y_{\sigma_k}) + O(N^{-2}).
\]

Recall the definition of $r$-degeneracy and $r$-th order term in Definition 6. In the following, we further decompose $K_{2,0} + K_{0,2} + K_{1,1'}$ into second, third and fourth order terms using Hoeffding decomposition, and show that the second order terms cancel out $U_N$ and the rest of the terms are negligible.

The following lemma gives the second order terms of $K_{2,0}$, $K_{0,2}$ and $K_{1,1'}$.

**Lemma 29.** Let

\[
k_{2,0}(x,x',y,y') := \kappa_{2,0}(x,x') + (A \otimes A)\kappa_{2,0}(y,y') + (I_{\rho_0} \otimes A)\kappa_{2,0}(x,y') + (I_{\rho_0} \otimes A)\kappa_{2,0}(x',y),
\]

\[
k_{0,2}(x,x',y,y') := (A^* \otimes A)\kappa_{0,2}(x,x') + \kappa_{0,2}(y,y') + (A^* \otimes I_{\rho_1})\kappa_{0,2}(x,y') + (A^* \otimes I_{\rho_1})\kappa_{0,2}(x',y),
\]

\[
k_{1,1'}(x,x',y,y') := (I_{\rho_0} \otimes A^*)\kappa_{1,1'}(x,x') + T(A \otimes I_{\rho_1})\kappa_{1,1'}(y,y') + \kappa_{1,1'}(x,y') + B_{\kappa_{1,1'}}(x',y).
\]

For any $i \neq i'$ and $j \neq j'$, the function $\tilde{K}_I(X_i, X_{i'}, Y_j, Y_{j'}) := (K_I - k_I)(X_i, X_{i'}, Y_j, Y_{j'})$ is 2-degenerate for every $I = \{2,0\}, \{0,2\}, \{1,1\}$. 

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Proof. We only prove the claim for $I = \{2, 0\}$. Recall that $K_{2,0}(x, x', y, y') := \kappa_{2,0}(x, x') \xi(x, y) \xi(x', y')$. Conditioning on $X_i, X_{i'}$, we have

$$\mathbb{E}[K_{2,0}(X_i, X_{i'}, Y_j, Y_{j'}) \mid X_i, X_{i'}] = \kappa_{2,0}(X_i, X_{i'}) \mathbb{E}[\xi(X_i, Y_j) \mid X_i] \mathbb{E}[\xi(X_{i'}, Y_{j'}) \mid X_{i'}] = \kappa_{2,0}(X_i, X_{i'}).$$

It then follows from degeneracy that $\mathbb{E}[(K_{2,0} - k_{2,0})(X_i, X_{i'}, Y_j, Y_{j'}) \mid X_i, X_{i'}] = 0$. Conditioning on $X_i, Y_j$, we have

$$\mathbb{E}[K_{2,0}(X_i, X_{i'}, Y_j, Y_{j'}) \mid X_i, Y_j] = \xi(X_i, Y_j) \mathbb{E}[\kappa_{2,0}(X_i, X_{i'}) \xi(X_{i'}, Y_{j'}) \mid X_i, Y_j] = 0 = \mathbb{E}[k_{2,0}(X_i, X_{i'}, Y_j, Y_{j'}) \mid X_i, Y_j].$$

Conditioning on $X_i, Y_{j'}$, we have

$$\mathbb{E}[K_{2,0}(X_i, X_{i'}, Y_j, Y_{j'}) \mid X_i, Y_{j'}] = \mathbb{E}[\kappa_{2,0}(X_i, X_{i'}) \xi(X_{i'}, Y_{j'}) \mid X_i, Y_{j'}] = (I_{p_0} \otimes \mathcal{A}) \kappa_{2,0}(X_i, Y_{j'}) = \mathbb{E}[k_{2,0}(X_i, X_{i'}, Y_j, Y_{j'}) \mid X_i, Y_{j'}].$$

The rest follows analogously. \hfill \Box

Now, we get

$$\mathcal{L}_2 D_N = W_N + V_N + O(N^{-2}),$$

where

$$W_N := \frac{1}{N(N - 1) N!} \sum_{\sigma \in S_N} \sum_{i \neq j} \kappa_{2,0} + \kappa_{1,1'}(X_i, X_j, Y_{\sigma_i}, Y_{\sigma_j}) \prod_{k \in [N] \setminus \{i, j\}} \xi(X_k, Y_{\sigma_k})$$

and

$$V_N := \frac{1}{N(N - 1) N!} \sum_{\sigma \in S_N} \sum_{i \neq j} \kappa_{2,0} + k_{0,2} + k_{1,1'}(X_i, X_j, Y_{\sigma_i}, Y_{\sigma_j}) \prod_{k \in [N] \setminus \{i, j\}} \xi(X_k, Y_{\sigma_k}).$$

We will show that $\mathbb{E}[(U_N - V_N)^2] = O(N^{-4})$ and $\mathbb{E}[W_N^2] = O(N^{-4})$. As a result, $\mathbb{E}[(U_N - \mathcal{L}_2 D_N)^2] = O(N^{-4})$, which implies $R_2 := R_1 - \mathcal{L}_2 = o_p(N^{-1})$ under the measure $\mu^N$.

**Lemma 30.** The following algebraic identity holds:

$$V_N = \frac{1}{N(N - 1) N!} \sum_{i,j=1}^{N} \sum_{\sigma \neq j} \eta(x_i, y_j) \xi(x_i, y_j) \prod_{k \in [N] \setminus \{i, \sigma_j^{-1}\}} \xi(x_k, y_{\sigma_k}).$$

Moreover, under Assumption 2, $\mathbb{E}[(U_N - V_N)^2] = O(N^{-4})$.

Proof. We consider the terms involving $(X_i, X_j)$ and $(Y_{\sigma_i}, Y_{\sigma_j})$ in $\sum_{i \neq j} (k_{2,0} + k_{0,2} + k_{1,1'})(X_i, X_j, Y_{\sigma_i}, Y_{\sigma_j})$. By Lemma 20, we get

$$\sum_{i \neq j} [\kappa_{2,0}(X_i, X_j) + (A^* \otimes A^*) \kappa_{0,2}(X_i, X_j) + (I_{p_0} \otimes A^*) \kappa_{1,1'}(X_i, X_j)] = 0$$

and

$$\sum_{i \neq j} [(A \otimes A) \kappa_{2,0}(Y_{\sigma_i}, Y_{\sigma_j}) + \kappa_{0,2}(Y_{\sigma_i}, Y_{\sigma_j}) + (A \otimes I_{p_1}) \kappa_{1,1'}(Y_{\sigma_i}, Y_{\sigma_j})] = 0.$$

We then consider the terms involving $(X_i, Y_{\sigma_j})$ and $(X_j, Y_{\sigma_j})$. Notice that

$$\sum_{i \neq j} \sum_{\sigma \in S_N} (I_{p_0} \otimes A) \kappa_{2,0}(X_i, Y_{\sigma_j}) \prod_{k \in [N] \setminus \{i, j\}} \xi(x_k, y_{\sigma_k})$$

$$= \sum_{i \neq j} \sum_{j'=1}^{N} \sum_{\sigma \neq j'} (I_{p_0} \otimes A) \kappa_{2,0}(X_i, Y_{j'}) \prod_{k \in [N] \setminus \{i, j\}} \xi(x_k, y_{\sigma_k})$$

$$= \sum_{i \neq j} \sum_{j'=1}^{N} \sum_{\sigma \neq j'} (I_{p_0} \otimes A) \kappa_{2,0}(X_i, Y_{j'}) \prod_{k \in [N] \setminus \{i, \sigma_j^{-1}\}} \xi(x_k, y_{\sigma_k}).$$
A similar argument gives
\[
\sum_{i \neq j} \sum_{\sigma \in S_N} (I_{\rho_0} \otimes A) \mathcal{T}_2 \kappa_2(\sigma)(X_j, Y_{\sigma}) \prod_{k \in [N] \setminus \{i, j\}} \xi(X_k, Y_{\sigma_k})
\]
\[
= \sum_{i, j = 1}^{N} (I_{\rho_0} \otimes A) \mathcal{T}_2 \kappa_2(X_j, Y_{\sigma}) \prod_{k \in [N] \setminus \{i, j\}} \xi(X_k, Y_{\sigma_k}).
\]

Hence
\[
\sum_{i \neq j} \sum_{\sigma \in S_N} [(I_{\rho_0} \otimes A) \mathcal{T}_2 \kappa_2(X_i, Y_{\sigma}) + (I_{\rho_0} \otimes A) \mathcal{T}_2 \kappa_2(X_j, Y_{\sigma})] \prod_{k \in [N] \setminus \{i, j\}} \xi(X_k, Y_{\sigma_k})
\]
\[
= \sum_{i, j = 1}^{N} (I_{\rho_0} \otimes A)(I + \mathcal{T}) \kappa_2(X_i, Y_j) \prod_{k \in [N] \setminus \{i, j\}} \xi(X_k, Y_{\sigma_k}).
\]

Analogously,
\[
\sum_{i \neq j} \sum_{\sigma \in S_N} [(A^* \otimes I_{\rho_1}) \kappa_0(X_i, Y_{\sigma}) + (A^* \otimes I_{\rho_1}) \mathcal{T}_2 \kappa_0(X_j, Y_{\sigma})] \prod_{k \in [N] \setminus \{i, j\}} \xi(X_k, Y_{\sigma_k})
\]
\[
= \sum_{i, j = 1}^{N} (A^* \otimes I_{\rho_1})(I + \mathcal{T}) \kappa_0(X_i, Y_j) \prod_{k \in [N] \setminus \{i, j\}} \xi(X_k, Y_{\sigma_k}),
\]

and
\[
\sum_{i \neq j} \sum_{\sigma \in S_N} [\kappa_{1, 1}(X_i, Y_{\sigma}) + B \kappa_{1, 1}(X_j, Y_{\sigma})] \prod_{k \in [N] \setminus \{i, j\}} \xi(X_k, Y_{\sigma_k})
\]
\[
= \sum_{i, j = 1}^{N} (I + B) \kappa_{1, 1}(X_i, Y_j) \prod_{k \in [N] \setminus \{i, j\}} \xi(X_k, Y_{\sigma_k}).
\]

Hence, the identity (59) follows from the third identity in Lemma 20.

Let us compute \(E([U_N - V_N]^2)\). Denote \(h := \tilde{\eta} \xi\). Recall from (40) that
\[
U_N := \frac{1}{N!} \sum_{\sigma \in S_N} \frac{1}{N} \sum_{i = 1}^{N} \tilde{\eta}(X_i, Y_{\sigma}) \xi(X, Y) = \frac{1}{N!} \sum_{i, j = 1}^{N} \sum_{\sigma = \emptyset}^{N} h(X_i, Y_j) \prod_{k \in [N] \setminus \{i\}} \xi(X_k, Y_{\sigma_k}).
\]

By Lemma 23, we get
\[
U_N = \frac{1}{N^2 N!} \sum_{i, j = 1}^{N} \sum_{\sigma = \emptyset}^{N} h(X_i, Y_j) \sum_{A \subset [N] \setminus \{i\}} \prod_{k \in A} [\xi(X_k, Y_{\sigma_k}) - 1].
\]

Similarly,
\[
V_N = \frac{1}{N(N - 1) N!} \sum_{i, j = 1}^{N} \sum_{\sigma = \emptyset}^{N} h(X_i, Y_j) \sum_{A \subset [N] \setminus \{i, j\}} \prod_{k \in A} [\xi(X_k, Y_{\sigma_k}) - 1].
\]

Define the set of sequences of length \(r\) to be
\[
S_{N, r} := \{(k_i)_{i = 1}^{r} : k_i \in [N], |\{k_1, \ldots, k_r\}| = r\}, \quad \text{for } r \in [N].
\]

Take \(r \in [N]\) and \((k_i)_{i = 1}^{r}, (k_i')_{i = 1}^{r} \in S_{N, r}\). Let us count the number of times the term
\[
h(X_{k_1}, Y_{k_1}) \prod_{s = 2}^{r} [\xi(X_{k_s}, Y_{k_s}) - 1]
\]
appears in (63) and (64), respectively. In order to get this term, we must have $i = k_1$, $j = k'_1$, $A = \{k_2, \ldots, k_r\}$ and $\sigma_k = k'_s$ for all $s \in \{2, \ldots, r\}$. Note that $\sigma_1 = j$ in (63), so there are $(N - r)!$ such terms in (63). Similarly, there are $(N - r)(N - r)!$ such terms in (64). Hence, the coefficient of this term in $U_N - V_N$ is

$$C_{N,r} = \frac{(N - r)!}{N \cdot N!} \cdot \frac{(N - r)(N - r)!}{N(N - 1) \cdot N!} = \frac{r - 1}{N - 1} (N - r)!.$$

We claim that

$$U_N - V_N = \frac{1}{N(N - 1)} \sum_{r=1}^{N} \frac{N(N - 1)}{N!} \sum_{|A|=|B|=r} \sum_{\sigma \in S_N: \sigma A = B} \sum_{i \in A \setminus \{i\}} h(X_i, Y_{\sigma_i}) \prod_{j \in A \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1].$$

To see this, we only need to prove that the coefficient of the term (65) on the right hand side of (66) is exactly $C_{N,r}$. In other words, it appears $(N - r)!$ times in the following sum:

$$\sum_{|A|=|B|=r} \sum_{\sigma \in S_N: \sigma A = B} \sum_{i \in A \setminus \{i\}} h(X_i, Y_{\sigma_i}) \prod_{j \in A \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1].$$

To get this term, we must have $A = \{k_1, \ldots, k_r\}$, $B = \{k'_1, \ldots, k'_r\}$, $i = k_1$ and $\sigma_k = k'_s$ for all $s \in \{r\}$. There are $(N - r)!$ permutations satisfy this condition, and thus it appears $(N - r)!$ times.

A derivation analogous to the one for (46) implies that $\mathbb{E}[(U_N - V_N)^2]$ is equal to

$$\frac{1}{N^2(N - 1)^2} \sum_{r=1}^{N} \frac{N(N - 1)}{N!} \sum_{|A|=|B|=r} \sum_{\sigma \in S_N: \sigma A = B} \sum_{i \in A \setminus \{i\}} h(X_i, Y_{\sigma_i}) \prod_{j \in A \setminus \{i\}} [\xi(X_j, Y_{\sigma_j}) - 1].$$

Repeating the argument in Proposition 28, we know $\mathbb{E}[(U_N - V_N)^2] = O(N^{-4})$. 

Before we bound $\mathbb{E}[W_N^2]$, let us give a result similar to Lemma 26 for functions with 3 and 4 arguments. Let $\phi \in \mathbb{L}^2(\rho_0 \otimes \rho_0 \otimes \rho_1 \otimes \rho_1)$ and $\psi \in \mathbb{L}^2(\rho_0 \otimes \rho_0 \otimes \rho_1)$ such that $\phi(X_1, X_2, Y_1, Y_2)$ and $\psi(X_1, X_2, Y_1)$ are completely degenerate under the measure $(\rho_0 \otimes \rho_1)^N$. Recall $p$ from Assumption 3 and let $q := p/(p - 1)$.

**Lemma 31.** Assume $\|\phi\|_{\mathbb{L}^2(\rho_0 \otimes \rho_0 \otimes \rho_1 \otimes \rho_1)} < \infty$ and $\|\psi\|_{\mathbb{L}^2(\rho_0 \otimes \rho_0 \otimes \rho_1)} < \infty$. Under Assumption 2 and Assumption 3, there exists a constant $C$ such that, for any $\sigma \in S_N$ and $i \neq j \in [N]$,

$$\mathbb{E} \left[ \phi(X_1, X_2, Y_1, Y_2) \prod_{k=3}^{N} [\xi(X_k, Y_k) - 1] \phi(X_i, X_j, Y_{\sigma_i}, Y_{\sigma_j}) \prod_{k=3}^{N} [\xi(X_k, Y_{\sigma_k}) - 1] \right] \leq s_1^{2(N - \#\sigma - 2)} C^{\#\sigma}$$

and

$$\mathbb{E} \left[ \psi(X_1, X_2, Y_1) \prod_{k=3}^{N} [\xi(X_k, Y_k) - 1] \psi(X_i, X_j, Y_{\sigma_i}, Y_{\sigma_j}) \prod_{k=3}^{N} [\xi(X_k, Y_{\sigma_k}) - 1] \right] \leq s_1^{2(N - \#\sigma - 2)} C^{\#\sigma},$$

where $\#\sigma$ is the number of cycles of $\sigma \in S_N$.

The proof of Lemma 31 is similar to Lemma 26—we iteratively take expectation with respect to a single variable, while keeping the rest being fixed. In consideration of the space, we only give an example here.

**Example 2.** Consider $N = 4$, $i = 2$, $j = 3$ and $\sigma$ given by $\sigma_i = i + 1$ for $i \in [3]$. By construction, $\sigma$ only has one cycle $1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 1$. The expectation of interest then reads

$$\mathbb{E} [\phi(X_1, X_2, Y_1, Y_2) [\xi(X_3, Y_3) - 1] [\xi(X_4, Y_4) - 1] \phi(X_2, X_3, Y_3, Y_4) [\xi(X_1, Y_2) - 1] [\xi(X_4, Y_1) - 1]].$$

Let $A_4$ be a shorthand notation for $I_{\rho_0} \otimes I_{\rho_0} \otimes I_{\rho_1} \otimes \mathcal{A}$, and $A_4^*$ similarly. Taking expectation with respect to $Y_4$, while keeping others being fixed, we get

$$\mathbb{E} [\phi(X_1, X_2, Y_1, Y_2) [\xi(X_3, Y_3) - 1] (A_4^* \phi)(X_2, X_3, Y_3, Y_4) [\xi(X_1, Y_2) - 1] [\xi(X_4, Y_1) - 1]],$$

since

$$\mathbb{E} [\phi(X_2, X_3, Y_3, Y_4) [\xi(X_4, Y_4) - 1] | X_2, X_3, X_4, Y_3] = \mathbb{E} [\phi(X_2, X_3, Y_3, Y_4) [\xi(X_4, Y_4) | X_2, X_3, X_4, Y_3] \phi(X_2, X_3, Y_3, Y_4)]$$

(67)
Now taking expectation with respect to $X_4$, while keeping others being fixed, we get
\[
\mathbb{E}\left[\phi(X_1, X_2, Y_1, Y_2)|\xi(X_3, Y_3) - 1\right](A_4A_3^*)\phi(X_2, X_3, Y_3, Y_1)|\xi(X_1, Y_2) - 1\right]
\]
Now, both $X_1$ and $Y_2$ in $\xi(X_1, Y_2) - 1$ appears in $\phi(X_1, X_2, Y_1, Y_2)$, and both $X_3$ and $Y_3$ in $\xi(X_3, Y_3) - 1$ appears in $\phi(X_2, X_3, Y_3, Y_1)$, so we stop here and use the Cauchy-Schwarz inequality to get an upper bound
\[
(68) \quad \sqrt{\mathbb{E}[\phi^2(X_2, X_3, Y_3, Y_1)]} \times \mathbb{E}[\phi^2(X_1, X_2, Y_1, Y_2)|\xi(X_3, Y_3) - 1|^2]\xi(X_1, Y_2) - 1|2^2].
\]
Notice that $\mathbb{E}\left[\phi^2(X_1, X_2, Y_1, Y_2)|\xi(X_3, Y_3) - 1|^2\xi(X_1, Y_2) - 1|2^2]\right]$ is equal to
\[
\mathbb{E}\left[\phi^2(X_1, X_2, Y_1, Y_2)|\xi(X_1, Y_2) - 1|^2\right] \|\xi - 1\|^2 L^2(\rho_0 \otimes \rho_1)
\]
Hölder
\[
\leq \mathbb{E}\left[\phi^2(X_1, X_2, Y_1, Y_2)\right]^{1/6} \mathbb{E}\left[\left|\xi(X_1, Y_2) - 1\right|^{2p}\right]^{1/6} \|\xi - 1\|^2 L^2(\rho_0 \otimes \rho_1).
\]
Hence, (68) can be further bounded above by
\[
\|A_4A_3^*)\phi\|L^2(\rho_0 \otimes \rho_0 \otimes \rho_1) \|\phi\|L^2(\rho_0 \otimes \rho_0 \otimes \rho_1) \leq C s^2,
\]
where $C := \|\phi\|L^2(\rho_0 \otimes \rho_0 \otimes \rho_1) \|\phi\|L^2(\rho_0 \otimes \rho_1) \|\xi - 1\|^2 L^2(\rho_0 \otimes \rho_1).

For the expectation associated with $\psi$, we view $\psi$ as a function with four arguments such that it is constant in its fourth argument and then repeat the argument for $\phi$. It only makes a difference at places where we apply $A_4$ or $A_3^*$ to $\phi$—instead of applying this operator, the expectation is exactly zero, and thus the bound holds trivially. To be more specific, in the first step of the above example, where we take expectation with respect to $Y_4$, we should have, in (67), that
\[
\mathbb{E}[\psi(X_2, X_3, Y_3)|\xi(X_4, Y_4) - 1] = \psi(X_2, X_3, Y_3) \mathbb{E}[\xi(X_4, Y_4) - 1 | X_4] \equiv 0.
\]
Recall from (57) that
\[
W_N := \frac{1}{N(N - 1)} \frac{1}{N!} \sum_{i \in S_N \setminus \{\xi\}} \sum_{j \in S_N \setminus \{\xi\}} (K_{2,0} + \bar{K}_{0,2} + \bar{K}_{1,1})(X_i, X_j, Y_\sigma, Y_\sigma) \prod_{k \in [N] \setminus \{i,j\}} \xi(X_k, Y_\sigma).
\]
To prove $\mathbb{E}[W_N^2] = O(N^{-4})$, we again use Hoeffding decomposition. From Lemma 29 we know $(K_{2,0} + \bar{K}_{0,2} + \bar{K}_{1,1})(X_i, X_j, Y_\sigma, Y_\sigma)$ is 2-degenerate, so each term in its Hoeffding decomposition should contain at least 3 variables. We assume it is given by the following form:
\[
\phi(X_i, X_j, Y_\sigma, Y_\sigma) + \psi_0(X_i, X_j, Y_\sigma) + \psi_1(X_i, X_j, Y_\sigma) + \psi_2(X_i, Y_\sigma, Y_\sigma) + \psi_3(X_j, Y_\sigma, Y_\sigma).
\]
Define
\[
W_N^\phi := \frac{1}{N(N - 1)} \frac{1}{N!} \sum_{i \in S_N \setminus \{\xi\}} \sum_{j \in S_N \setminus \{\xi\}} \phi(X_i, X_j, Y_\sigma, Y_\sigma) \prod_{k \in [N] \setminus \{i,j\}} \xi(X_k, Y_\sigma),
\]
and $W_N^{\psi_0}, W_N^{\psi_2}$ and $W_N^{\psi_3}$, similarly. Consequently, $W_N = W_N^\phi + W_N^{\psi_0} + W_N^{\psi_1} + W_N^{\psi_2} + W_N^{\psi_3}$. It then suffices to show $\mathbb{E}[W_N^2] = O(N^{-4})$ and $\mathbb{E}[(W_N^\psi)^2] = O(N^{-4})$ for $i \in \{0, 1, 2, 3\}$. The strategy here is the same as Proposition 28.

Corollary 32. Suppose the same assumptions in Lemma 31 hold. Then
\[
\mathbb{E}[(W_N^\phi)^2] \leq \frac{1}{N^2(N - 1)^2} \sum_{r=2}^{N} \frac{r^2(r - 1)^2}{r!} \sum_{\sigma \in S_r} 2^2r^{-r-2}\rho^2 C_S
\]
\[
\mathbb{E}[(W_N^\psi)^2] \leq \frac{1}{N^2(N - 1)^2} \sum_{r=2}^{N} \frac{r^2(r - 1)^2}{r!} \sum_{\sigma \in S_r} 2^2r^{-r-2}\rho^2 C_S, \quad \text{for } i \in \{0, 1, 2, 3\}
\]
In particular, $\mathbb{E}[(W_N^\phi)^2] = O(N^{-4})$ and $\mathbb{E}[(W_N^\psi)^2] = O(N^{-4})$ for $i \in \{0, 1, 2, 3\}$.
Proof. We only prove the bound for $\mathbb{E}[(W_N^\phi)^2]$. Notice that, using Lemma 23 for $A = [N]\{i,j\}$, we have

$$W_N^\phi = \frac{1}{N(N-1)} \sum_{\sigma \in S_N} \sum_{i \neq j} \phi(X_i, X_j, Y_{\sigma_i}, Y_{\sigma_j}) \prod_{k \in [N]\{i,j\}} \left[ \xi(X_k, Y_{\sigma_k}) - 1 \right].$$

Because $\phi(X_i, X_j, Y_{\sigma_i}, Y_{\sigma_j})$ is completely degenerate, an argument similar to the one in Lemma 24 shows that the Hoeffding decomposition of $W_N^\phi$ is given by

$$W_N^\phi := \sum_{|A|=|B|=1} W_{AB}^\phi,$$

where

$$W_{AB}^\phi := \sum_{\sigma \in S_N: \sigma_A = B, \sigma_B = A} \sum_{i \neq j \in A} \phi(X_i, X_j, Y_{\sigma_i}, Y_{\sigma_j}) \left[ \xi(X_k, Y_{\sigma_k}) - 1 \right].$$

Consequently,

$$\mathbb{E}[(W_N^\phi)^2] = \frac{1}{N^2(N-1)^2} \sum_{r=2}^{N} \sum_{|A|=|B|=r} \mathbb{E}[(W_{AB}^\phi)^2] = \mathbb{E}[(W_{r|r})^2],$$

where the last equality follows from exchangeability. Using a derivation similar to the one for (46),

$$\mathbb{E}[(W_{r|r})^2] = ((N-r)!)^2 \mathbb{E} \left[ \sum_{\sigma \in S_r} \sum_{1 \leq i \neq j \leq r} \phi(X_i, X_j, Y_{\sigma_i}, Y_{\sigma_j}) \prod_{k \in [r]\{i,j\}} \left[ \xi(X_k, Y_{\sigma_k}) - 1 \right] \right]^2$$

$$= ((N-r)!)^2 r! r(r-1) \sum_{\sigma \in S_r} \sum_{1 \leq i \neq j \leq r} \mathbb{E} \left[ \phi(X_1, X_2, Y_1, Y_2) \prod_{k=3}^{r} \left[ \xi(X_k, Y_{k|1}) - 1 \right] \phi(X_i, X_j, Y_{\sigma_i}, Y_{\sigma_j}) \prod_{k \in [r]\{i,j\}} \left[ \xi(X_k, Y_{\sigma_k}) - 1 \right] \right]$$

$$\leq ((N-r)!)^2 r! r(r-1) \sum_{\sigma \in S_r} \sum_{1 \leq i \neq j \leq r} s_1^{2(r-\#\sigma-2)} C^\# \sigma,$$

by Lemma 31.

Now, putting (70) and (71) together, we get

$$\mathbb{E}[(W_N^\phi)^2] \leq \frac{1}{N^2(N-1)^2} \sum_{r=2}^{N} \binom{N}{r}^2 \left( (N-r)! \right)^2 r! r(r-1) \sum_{\sigma \in S_r} \sum_{1 \leq i \neq j \leq r} s_1^{2(r-\#\sigma-2)} C^\# \sigma$$

$$= \frac{1}{N^2(N-1)^2} \sum_{r=2}^{N} \frac{r^2(r-1)^2}{r!} \sum_{\sigma \in S_r} s_1^{2(r-\#\sigma-2)} C^\# \sigma.$$

Proposition 33. Under Assumption 2 and Assumption 3, the second order remainder $R_2 = o_\mu(N^{-1})$ under the measure $\mu_\epsilon^N$.

Proof. Let $f := C^{-1}(\tilde{\eta})$. Note that

$$\mathbb{E}[W_{2,0}^{2p/(p-2)}(X_1, X_2)] = \int \left[ (I_{\rho_0} \otimes A^*) f(x, x') \right]^{2p/(p-2)} \rho_0(x) \rho_0(x') dx dx'.$$

$$\leq \int \left[ \int_f f(x, y') \xi(x', y') \rho_1(y') dy' \right]^{2p/(p-2)} \rho_0(x) \rho_0(x') dx dx'.$$

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$$\leq \int f^{2p/(p-2)}(x, y') \xi(x', y') \rho_1(y') dy' \rho_0(x) \rho_0(x') dx dx'.$$. 

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Since $\int \xi(x', y')\rho_0(x')dx' \leq 1$, integrating with respect to $x'$ in the above upper bound gives
\[ \int f^{2p}(x, y')\rho_1(y')\rho_0(x')dy' dx = E[f^{2p}(X_1, Y_1)] < \infty. \]

As a result,
\[ \|K_{2,0}\|_\mathbb{L}^{2q}(\rho_0 \otimes \rho_0 \otimes \rho_1 \otimes \rho_1) = E\left[\kappa_{2,0}^2(X_1, X_2)\xi^{2q}(X_1, Y_1)\xi^{2q}(X_2, Y_2)\right] \]
\[ \leq E[\kappa_{2,0}^{2q(p-1)/(p-2)}(X_1, Y_1)]^{\frac{p}{p-2}} E[\xi^{2q(p-1)}(X_1, Y_1)]^{1/(p-1)} \]
\[ = E[\kappa_{2,0}^{2q/(p-2)}(X_1, Y_1)]^{\frac{p}{p-2}} E[\xi^{2p}(X_1, Y_1)]^{1/(p-1)} < \infty. \]

Analogously, we have $\|K_{0,2}\|_\mathbb{L}^{2q}(\rho_0 \otimes \rho_0 \otimes \rho_1 \otimes \rho_1) < \infty$ and $\|K_{1,1}\|_\mathbb{L}^{2q}(\rho_0 \otimes \rho_0 \otimes \rho_1 \otimes \rho_1) < \infty$. As discussed before Corollary 32, we can then decompose $(K_{2,0} + \tilde{K}_{0,2} + \tilde{K}_{1,1})$ into third and fourth order terms using Hoeffding decomposition and invoke Corollary 32 to show $E[W_N^2] = O(N^{-4})$. Recall from (56) that $E[(\mathcal{L}_2D_N - W_N - V_N)^2] = O(N^{-4})$. Hence, by Corollary 30,
\[ E[(U_N - \mathcal{L}_2D_N)^2] \leq 3 \{ E[(U_N - V_N)^2] + E[W_N^2] + E[(\mathcal{L}_2D_N - V_N - W_N)^2]\} = O(N^{-4}). \]
It then follows from the discussion above (41) that $R_2 = o_p(N^{-1})$ under the measure $\mu^N$. \(\square\)

5. PROOF OF MAIN THEOREMS

In this section, we prove the main results under the original measure $(\rho_0 \otimes \rho_1)^N$. As before, we will write $\mathbb{P}$ and $\mathbb{E}$ as the probability and expectation under this measure. Recall that Theorem 1 has been proved in Section 2.

Proof of Theorem 2. Recall from Proposition 14 and Proposition 28 that
\[ R_1 := T_N - \theta - L_1 = o_p(N^{-1/2}), \] under the measure $\mu^N$. By the contiguity in Theorem 7, we know $R_1 = o_p(N^{-1/2})$ under the measure $(\rho_0 \otimes \rho_1)^N$. Hence,
\[ T_N - \theta = \frac{1}{N} \sum_{i=1}^{N} [(I - \mathcal{A}^* \mathcal{A})^{-1}(\kappa_{1,0} - \mathcal{A}^*\kappa_{0,1})(X_i) + (I - \mathcal{A}\mathcal{A}^*)^{-1}(\kappa_{0,1} - \mathcal{A}\kappa_{1,0})(Y_i)] + o_p(N^{-1/2}). \]
Now, Corollary 3 follows from the standard Lindeberg CLT [Bil95, Section 27]. \(\square\)

Proof of Theorem 4. By the assumption that $\xi^2 = 0$, we know the first order chaos $L_1 = 0$ almost surely. According to Proposition 33, it holds that $T_N - \theta - L_2 = o_p(N^{-1})$ under the measure $\mu^N$. Since $T_N$ and $L_2$ are $\mathbb{G}_N$ measurable, it follows from the contiguity in Theorem 7 that $T_N - \theta - L_2 = o_p(N^{-1})$ under the measure $(\rho_0 \otimes \rho_1)^N$. Recall from (30) that
\[ \mathcal{L}_2 := \frac{1}{N(N-1)} \left\{ \sum_{i \neq j} [\kappa_{2,0}(X_i, X_j) + \kappa_{0,2}(Y_i, Y_j)] + \sum_{i, j=1}^{N} \kappa_{1,1}'(X_i, Y_j) - \sum_{i=1}^{N} \ell_{1,1}'(X_i, Y_i) \right\}, \]
where $\ell_{1,1}'$ is an affine function such that $\kappa_{1,1}' = \ell_{1,1}' \in \mathbb{L}^2_0(\mu^N)$. This implies $(\rho_0 \otimes \rho_1)[\ell_{1,1}'] = \mu^N[\ell_{1,1}'] = \theta_{1,1}'$. By LLN, we know $\frac{1}{N} \sum_{i=1}^{N} \ell_{1,1}'(X_i, Y_i) = \theta_{1,1}' + o_p(1)$. Therefore,
\[ T_N - \theta + \frac{\theta_{1,1}'}{N} = \frac{1}{N(N-1)} \left\{ \sum_{i \neq j} [\kappa_{2,0}(X_i, X_j) + \kappa_{0,2}(Y_i, Y_j)] + \sum_{i, j=1}^{N} \kappa_{1,1}'(X_i, Y_j) \right\} + o_p(N^{-1}). \]
\(\square\)

Proof of Corollary 5. Recall from (20) that $\kappa_{1,1}' \in \mathbb{L}^2_0(\rho_0 \otimes \rho_1)$, so it holds that $\frac{1}{N(N-1)} \sum_{i=1}^{N} \kappa_{1,1}'(X_i, Y_i) = o_p(N^{-1})$ by LLN. Hence, we will ignore this term in the following derivation.
To begin with, we show the limiting distribution is well-defined. Since $\xi^2 = 0$ in Corollary 3, we know
\[ (I - \mathcal{A}^* \mathcal{A})^{-1}(\kappa_{1,0} - \mathcal{A}^*\kappa_{0,1})(x) \overset{a.s.}{=} 0 \] and \[ (I - \mathcal{A}\mathcal{A}^*)^{-1}(\kappa_{0,1} - \mathcal{A}\kappa_{1,0})(y) \overset{a.s.}{=} 0, \]
which implies
\[ \eta(x, y) := \eta(x, y) - \theta - (I - A^*A)^{-1}(\kappa_{1,0} - A^*\kappa_{0,1})(x) - (I - AA^*)^{-1}(\kappa_{0,1} - A\kappa_{1,0})(y) \equiv \eta(x, y) - \theta. \]
Consequently, \((\eta - \theta)\xi \in L^2_0(\rho_0 \otimes \rho_1)\) and thus, by Lemma 16, it has expansion
\[ (\eta - \theta)\xi = \sum_{k,l \geq 1} \gamma_{kl}(\alpha_k \otimes \beta_l), \quad \text{in } L^2(\rho_0 \otimes \rho_1), \]
where \(\sum_{k,l \geq 1} \gamma_{kl}^2 < \infty\). Recall from Assumption 2 that \(0 \leq s_k \leq s_1 < 1\) for all \(k \geq 1\), we have
\[ \sum_{k,l \geq 1} \frac{\gamma_{kl}^2}{(1 - s_k^2)^2(1 - s_l^2)^2} \leq \sum_{k,l \geq 1} \frac{\gamma_{kl}^2}{(1 - s_k^2)^4} < \infty. \]
Let \(\{U_k\}, \{V_l\}\) be independent sequences of \(i.i.d.\) standard normal random variables. We define
\[ Z := \sum_{k,l \geq 1} \frac{\gamma_{kl}}{(1 - s_k^2)(1 - s_l^2)}(U_kV_l + s_k s_l U_k V_k - s_i(U_k U_l - 1\{k = l\}) - s_k(V_k V_l - 1\{k = l\})) \]
\[ = \sum_{k,l \geq 1} \frac{1}{(1 - s_k^2)(1 - s_l^2)}((\gamma_{kl} + s_k s_l \beta_k)U_k V_l - s_i \gamma_{kl} U_k U_l - 1\{k = l\}) - s_k \gamma_{kl} (V_k V_l - 1\{k = l\})) \]
where the sum converges in \(L^2\). We will show \(Z_N := NL_2 \rightarrow_d Z\) by using characteristic functions, \(i.e.,\) by showing that, for each \(t \in \mathbb{R}\),
\[ \mathbb{E}[\exp(itZ_N)] \rightarrow \mathbb{E}[\exp(itZ)], \quad \text{as } N \rightarrow \infty. \]
The following proof is inspired by [Ser80, Chapter 5.5.2].

**Step 1.** We expand \(Z_N\) on \(\{\alpha_k \otimes \beta_l\}_{k,l \geq 0}\). For \(k \geq 1\), we denote
\[ \bar{\alpha}_k := (I - A^*A)^{-1}\alpha_k = (1 - s_k^2)^{-1}\alpha_k \quad \text{and} \quad \bar{\beta}_k := (I - AA^*)^{-1}\beta_k = (1 - s_k^2)^{-1}\beta_k. \]
By Lemma 18 it holds that \(C^{-1}(\alpha_k \otimes \beta_l) = \bar{\alpha}_k \otimes \bar{\beta}_l\), and then we get
\[ C^{-1}[\eta - \theta] = \sum_{k,l \geq 1} \gamma_{kl}(\bar{\alpha}_k \otimes \bar{\beta}_l) = \sum_{k,l \geq 1} \frac{\gamma_{kl}}{(1 - s_k^2)(1 - s_l^2)}(\alpha_k \otimes \beta_l). \]
It follows that
\[ \kappa_{1,0}(X_i, Y_j) := (\eta - \theta)\xi \mathbb{E}[\gamma(X_i, Y_j)] = \sum_{k,l \geq 1} \frac{\gamma_{kl}}{(1 - s_k^2)(1 - s_l^2)}[\alpha_k(X_i)\beta_l(Y_j) + s_k s_l \alpha_k(X_i)\beta_l(Y_j)] \]
\[ \kappa_{2,0}(X_i, X_j) := (I_{p_1} \otimes A^*)C^{-1}(\eta)(X_i, X_j) \mathbb{E}[\gamma_{X_i, X_j}] = \sum_{k,l \geq 1} \frac{\gamma_{kl}}{(1 - s_k^2)(1 - s_l^2)}s_l \alpha_k(X_i)\alpha_l(X_j) \]
\[ \kappa_{0,2}(Y_i, Y_j) := (\alpha \otimes I_{p_1})C^{-1}(\eta)(Y_i, Y_j) \mathbb{E}[\gamma_{Y_i, Y_j}] = \sum_{k,l \geq 1} \frac{\gamma_{kl}}{(1 - s_k^2)(1 - s_l^2)}s_k \beta_k(Y_i)\beta_l(Y_j). \]
Hence, \(Z_N\) admits the following expansion:
\[ Z_N = \frac{1}{N - 1} \sum_{i \neq j} \sum_{k,l \geq 1} \frac{\gamma_{kl}[\alpha_k(X_i)\beta_l(Y_j) + s_k s_l \alpha_k(X_i)\beta_l(Y_j) - s_i \alpha_k(X_i)\alpha_l(X_j) - s_k \beta_k(Y_i)\beta_l(Y_j)]}{(1 - s_k^2)(1 - s_l^2)} \]
\[ = \frac{1}{N - 1} \sum_{i \neq j} \sum_{k,l \geq 1} \frac{[\gamma_{kl} + s_k s_l \gamma_{kl}]\alpha_k(X_i)\beta_l(Y_j) - s_i \gamma_{kl} \alpha_k(X_i)\alpha_l(X_j) - s_k \gamma_{kl} \beta_k(Y_i)\beta_l(Y_j)}{(1 - s_k^2)(1 - s_l^2)}. \]

**Step 2.** We truncate the inner infinite sum. Fix an arbitrary integer \(K > 0\). Let
\[ Z^K_N := \frac{1}{N - 1} \sum_{i \neq j} \sum_{k,l = 1}^K \frac{[\gamma_{kl} + s_k s_l \gamma_{kl}]U_k V_l - s_i \gamma_{kl} (U_k U_l - 1\{k = l\}) - s_k \gamma_{kl} (V_k V_l - 1\{k = l\})]}{(1 - s_k^2)(1 - s_l^2)} \]
\[ Z^K := \sum_{k,l = 1}^K \frac{[\gamma_{kl} + s_k s_l \gamma_{kl}]U_k V_l - s_i \gamma_{kl} (U_k U_l - 1\{k = l\}) - s_k \gamma_{kl} (V_k V_l - 1\{k = l\})]}{(1 - s_k^2)(1 - s_l^2)}. \]
By triangle inequality, we have
\[
\left|\mathbb{E}[e^{itZ_N}] - \mathbb{E}[e^{itZ}]ight| \leq \left|\mathbb{E}[e^{itZ_N}] - \mathbb{E}[e^{itZ_N}] + \mathbb{E}[e^{itZ_N}] - \mathbb{E}[e^{itZ_N}] + \mathbb{E}[e^{itZ_N}] - \mathbb{E}[e^{itZ}]ight| = A + B + C
\]
(74)

Fix arbitrary \( t \in \mathbb{R} \) and \( \epsilon > 0 \), it now suffices to show that \( A, B, C \leq \epsilon \) for all sufficiently large \( N \) with an appropriate choice of \( K \).

**Step 3.** We bound \( A \) and \( C \). Using the inequality \( |e^z - 1| \leq |z| \), we get
\[
A \leq \mathbb{E}\left|e^{itZ_N} - e^{itZ_N^K}\right| \leq |t| \mathbb{E}|Z_N - Z_N^K| \leq |t| \mathbb{E}(Z_N^2 - Z_N^K)^2)^{1/2}.
\]
(75)

We rewrite \( Z_N - Z_N^K \) as \( \frac{1}{N-1} \sum_{i \neq j} \eta_{K}^{\alpha \beta}(X_i, X_j) - g_{K}^{\alpha \alpha}(X_i, X_j) - g_{K}^{\beta \beta}(Y_i, Y_j) \), where
\[
g_{K}^{\alpha \beta}(x, y) := \sum_{k,l \geq K} \frac{\gamma_{kl} + s_k s_l \gamma_{lk}}{(1 - s_k^2)(1 - s_l^2)} \alpha_k(x) \beta_l(y),
\]
\[
g_{K}^{\alpha \alpha}(x, x') := \sum_{k,l \geq K} \frac{\gamma_{kl} s_l}{(1 - s_l^2)} \alpha_k(x) \alpha_l(x'),
\]
\[
g_{K}^{\beta \beta}(y, y') := \sum_{k,l \geq K} \frac{\gamma_{kl} s_k}{(1 - s_k^2)} \beta_k(y) \beta_l(y').
\]

By the orthogonality of \( \{\alpha_k\}_{k \geq 0} \) and \( \{\beta_k\}_{k \geq 0} \), we know \( \mathbb{E}[\alpha_k(X_i) \beta_l(Y_j) \alpha_k(X_i) \beta_l(Y_j)] = 0 \) for all \( k, l \geq 1 \) and \( i \neq j \). This implies \( g_{K}^{\alpha \beta}(X_i, Y_j) \) and \( g_{K}^{\alpha \alpha}(X_i, X_j) \) are uncorrelated. Analogously, we have \( g_{K}^{\alpha \beta}(X_i, Y_j) \) and \( g_{K}^{\beta \beta}(Y_i, Y_j) \) are mutually uncorrelated for all \( i \neq j \). As a result, \( \mathbb{E}((Z_N^2 - Z_N^K)^2) \) reads
\[
(76) \quad \mathbb{E}((Z_N^2 - Z_N^K)^2) = \frac{1}{(N-1)^2} \mathbb{E}\left\{ \sum_{i \neq j} g_{K}^{\alpha \beta}(X_i, Y_j) \right\}^2 + \sum_{i \neq j} \mathbb{E}g_{K}^{\alpha \alpha}(X_i, X_j) \left\{ \sum_{i \neq j} \mathbb{E}g_{K}^{\beta \beta}(Y_i, Y_j) \right\}^2.
\]

Notice that \( \mathbb{E}[\alpha_k(X_1) \beta_l(Y_2) \mid X_1] = \mathbb{E}[\alpha_k(X_1) \beta_l(Y_2) \mid Y_2] = 0 \) for all \( k, l \geq 1 \), then
\[
\mathbb{E}[g_{K}^{\alpha \beta}(X_1, Y_2) \mid X_1] = \mathbb{E}[g_{K}^{\alpha \beta}(X_1, Y_2) \mid Y_2] = 0.
\]

As a result,
\[
\mathbb{E}\left( \sum_{i \neq j} g_{K}^{\alpha \beta}(X_i, Y_j) \right)^2 = N(N-1) \mathbb{E}[g_{K}^{\alpha \beta}(X_1, Y_2)^2] = N(N-1) \sum_{k,l \geq K} \left( \frac{\gamma_{kl} + s_k s_l \gamma_{lk}}{(1 - s_k^2)(1 - s_l^2)} \right)^2.
\]

Let \( \delta > 0 \) be such that \( |t| \delta < \epsilon \). It then follows from (73) that, for all sufficiently large \( K \), we have
\[
\frac{1}{(N-1)^2} \mathbb{E}\left( \sum_{i \neq j} g_{K}^{\alpha \beta}(X_i, Y_j) \right)^2 \leq \frac{N}{N-1} \sum_{k,l \geq K} \left( \frac{\gamma_{kl} + s_k s_l \gamma_{lk}}{(1 - s_k^2)(1 - s_l^2)} \right)^2 \leq \frac{N}{6(N-1)} \delta^2.
\]

The same bound for the rest of the two terms in (76) can be shown using similar arguments. Therefore, by (75),
\[
A \leq |t| \mathbb{E}((Z_N^2 - Z_N^K)^2)^{1/2} \leq \sqrt{\frac{N}{2(N-1)}} |t| \delta < \epsilon, \quad \text{for all } N \geq 2.
\]

Repeating the above argument for \( Z_N^K \) and \( Z \) gives \( C < \epsilon \) for all \( N \geq 2 \).

**Step 4.** We bound \( B \) by proving \( Z_N^K \to_d Z^K \) as \( N \to \infty \). Consider \( W_N := (W_{\alpha}^T, W_{\beta}^T) \) with
\[
W_{\alpha} := \frac{1}{\sqrt{N}} \left( \sum_{i=1}^N \alpha_k(X_i) \right)_k \quad \text{and} \quad W_{\beta} := \frac{1}{\sqrt{N}} \left( \sum_{i=1}^N \beta_k(Y_i) \right)_k.
\]
According to the multivariate CLT [BL95, Section 29], it holds $W_N \to_d \mathcal{N}_{2K}(0, I_{2K})$, where the covariance matrix $I_{2K}$ follows from the orthonormality of $\{\alpha_k\}_{k \geq 1}$ and $\{\beta_k\}_{k \geq 1}$. We then rewrite $Z_N^K$ as a quadratic form of $W_N$. Notice that

\[
\frac{1}{N} \sum_{i \neq j} \sum_{k,l=1}^{K} \frac{1}{(1-s_k^2)(1-s_l^2)} (\gamma_{kl} + s_k s_l \gamma_{lk}) \alpha_k(X_i) \alpha_l(Y_j) = \frac{1}{N} \sum_{i \neq j} \sum_{k,l=1}^{K} \frac{(\gamma_{kl} + s_k s_l \gamma_{lk})}{(1-s_k^2)(1-s_l^2)} \left\{ \left[ \sum_{i=1}^{N} \alpha_k(X_i) \right] \left[ \sum_{l=1}^{N} \beta_l(Y_i) \right] - \sum_{i=1}^{N} \alpha_k(X_i) \beta_l(Y_i) \right\}
\]

\[
= 2 W_{\alpha}^T \Sigma_{\alpha} \beta W_{\beta} - \frac{1}{N} \sum_{k,l=1}^{K} (\gamma_{kl} + s_k s_l \gamma_{lk}) \frac{1}{(1-s_k^2)(1-s_l^2)} \sum_{i=1}^{N} \alpha_k(X_i) \beta_l(Y_i),
\]

where $\Sigma_{\alpha} = \frac{(\gamma_{kl} + s_k s_l \gamma_{lk})}{(1-s_k^2)(1-s_l^2)}$ is the $(k,l)$-element in the matrix $\Sigma$. Similarly, it holds that

\[
\frac{1}{N} \sum_{i \neq j} \sum_{k,l=1}^{K} \frac{(\gamma_{kl})}{(1-s_k^2)(1-s_l^2)} s_l \alpha_k(X_i) \alpha_l(Y_j) = W_{\alpha}^T \Sigma_{\alpha} \alpha W_{\alpha} - \frac{1}{N} \sum_{k,l=1}^{K} \frac{(\gamma_{kl})}{(1-s_k^2)(1-s_l^2)} \sum_{i=1}^{N} \alpha_k(X_i) \alpha_l(X_i)
\]

\[
= W_{\alpha}^T \Sigma_{\alpha} \beta W_{\beta} - \frac{1}{N} \sum_{k,l=1}^{K} (\gamma_{kl}) \frac{1}{(1-s_k^2)(1-s_l^2)} \sum_{i=1}^{N} \beta_k(Y_i) \beta_l(Y_i),
\]

where $\Sigma_{\alpha} = \frac{(\gamma_{kl})}{(1-s_k^2)(1-s_l^2)}$ and $\Sigma_{\beta} = \frac{(\gamma_{kl})}{(1-s_k^2)(1-s_l^2)}$. Hence,

\[
Z_{N}^{K} := \frac{N}{N-1} W_{\alpha}^T \left( -\Sigma_{\alpha} \Sigma_{\alpha}^T \right)^{-1} W_{\beta} \left( -\Sigma_{\beta} \Sigma_{\beta}^T \right)^{-1} W_{\beta} - \frac{N}{N-1} \sum_{k,l=1}^{K} \frac{(\gamma_{kl} + s_k s_l \gamma_{lk}) \alpha_k(X_i) \beta_l(Y_i) - s_l \alpha_k(X_i) \alpha_l(X_i) - s_k \beta_k(Y_i) \beta_l(Y_i)}{\left(1-s_k^2\right)\left(1-s_l^2\right)} N \sum_{i=1}^{N} \left[ (\gamma_{kl} + s_k s_l \gamma_{lk}) \alpha_k(X_i) \beta_l(Y_i) - s_l \alpha_k(X_i) \alpha_l(X_i) - s_k \beta_k(Y_i) \beta_l(Y_i) \right] \to_p s_l 1 \{k = l\} - s_k 1 \{k = l\}.
\]

Since $\mathbb{E}[\alpha_k(X_i) \beta_l(Y_j)] = 0$ and $\mathbb{E}[\alpha_k(X_i) \alpha_l(X_i)] = \mathbb{E}[\beta_k(Y_i) \beta_l(Y_i)] = 1$ for all $k, l \geq 1$ and $i \in [N]$, we know from LLN that

\[
\frac{1}{N} \sum_{i=1}^{N} \left[ (\gamma_{kl} + s_k s_l \gamma_{lk}) \alpha_k(X_i) \beta_l(Y_i) - s_l \alpha_k(X_i) \alpha_l(X_i) - s_k \beta_k(Y_i) \beta_l(Y_i) \right] \to_p s_l 1 \{k = l\} - s_k 1 \{k = l\}.
\]

By Slutsky’s lemma, it holds $Z_{N}^{K} \to_d Z^{K}$, and thus we have $B < \epsilon$ for all sufficiently large $N$. Now, by (74), we get $|\mathbb{E}[e^{itZ_N}] - \mathbb{E}[e^{itZ}]| \leq 3\epsilon$ for all sufficiently large $N$. Since $\epsilon$ is arbitrary, this completes the proof. □

**APPENDIX A.**

*Proof of Lemma 16.* It is clear that $\{\alpha_i^{(0)} \otimes \alpha_j^{(1)}\}_{i, j \geq 0}$ is an orthonormal set in $L^2(\nu_0 \otimes \nu_1)$. It suffices to show that the linear subspace $\mathcal{H}_0 := \text{Span}\{\alpha_i^{(0)} \otimes \alpha_j^{(1)} : i, j \geq 0\}$ is dense in $L^2(\nu_0 \otimes \nu_1)$. Note that the linear subspace $\mathcal{H} := \text{Span}\{1_{B_0} \otimes B_1 : B_0, B_1 \subset \mathbb{R}^d \text{ have finite measure under } \nu_0, \nu_1\}$ is dense in $L^2(\nu_0 \otimes \nu_1)$. We only need to prove that $\mathcal{H}_0$ is dense in $\mathcal{H}$. In fact, for any $1_{B_0} \otimes B_1 \in \mathcal{H}$, we know $1_{B_0} \otimes B_1 = 1_{B_0} \otimes 1_{B_1}$. Since $\{\alpha_i^{(0)}\}_{i \geq 0}$ is an orthonormal basis of $L^2(\nu_0)$ and $1_{B_0} \in L^2(\nu_0)$, there exists a sequence $\{f_n\} \subset \text{Span}\{\alpha_i^{(0)} : i \geq 0\}$ such that $\|f_n - 1_{B_0}\|_{L^2(\nu_0)} \to 0$. Analogously, there exists a sequence $\{g_n\} \subset \text{Span}\{\alpha_i^{(1)} : i \geq 0\}$ such that $\|g_n - 1_{B_1}\|_{L^2(\nu_1)} \to 0$. On the one hand, we know by construction that $f_n \otimes g_n \in \mathcal{H}_0$. On the other hand, we have

\[
\|f_n \otimes g_n - 1_{B_0} \otimes 1_{B_1}\|_{L^2(\nu_0 \otimes \nu_1)} \leq \|f_n \otimes (g_n - 1_{B_0})\|_{L^2(\nu_0 \otimes \nu_1)} + \|(f_n - 1_{B_0}) \otimes 1_{B_1}\|_{L^2(\nu_0 \otimes \nu_1)}
\]

\[
= \|f_n\|_{L^2(\nu_0)} \|g_n - 1_{B_0}\|_{L^2(\nu_1)} + \|f_n - 1_{B_0}\|_{L^2(\nu_0)} \|1_{B_1}\|_{L^2(\nu_1)} .
\]

It follows from $\|f_n\|_{L^2(\nu_0)} \to \|1_{B_0}\|_{L^2(\nu_0)}$ that $\|f_n \otimes g_n - 1_{B_0} \otimes 1_{B_1}\|_{L^2(\nu_0 \otimes \nu_1)} \to 0$, and the claim holds. □
Let $\nu$ be a probability measure. Given a subspace (not necessarily closed) $H \subset L^2(\nu)$ and a statistic $T \in L^2(\nu)$, the $L^2$ projection of $T$ onto $H$ is defined as, if exists,

$$\text{Proj}_H(T) := \arg\min_{U \in H} \|T - U\|^2_{L^2(\nu)}.$$ 

The next lemma gives an equivalent definition using orthogonality. The proof is omitted.

**Lemma 34.** Let $U \in H$, then $U = \text{Proj}_H(T)$ iff $T - U \in H^\perp$.

In the following, we assume $(X_1, Y_1), \ldots, (X_N, Y_N)$ i.i.d. $\mu_\epsilon$, with $E$ denoting the expectation under this model, as before.

**A.1. A subspace decomposition of $H_1$ and $H_2$.** Recall the two subspaces $H_1, H_2 \subset L^2(\mu_\epsilon^N)$ defined in Section 3. We will give an alternative expression for both of them.

**Lemma 35.** The subspace $H_1 \subset L^2(\mu_\epsilon^N)$ admits the following alternative expression:

$$(77) \quad H_1 = \text{Span}\left\{ \sum_{i=1}^N (f_{1,0}(X_i) + f_{0,1}(Y_i)) : f_{1,0} \in L^2(\rho_0), f_{0,1} \in L^2(\rho_1) \right\}.$$ 

**Proof of Lemma 35.** For any $\sum_{i=1}^N (f_{1,0}(X_i) + f_{0,1}(Y_i)) \in H_1$, we get $E[f_{1,0}(X_1) + f_{0,1}(Y_1)] = 0$ since $H_0 \perp H_1$. Let $\theta_{1,0} := E[f_{1,0}(X_1)]$ and $\theta_{0,1} := E[f_{0,1}(Y_1)]$, then it holds that $\theta_{1,0} + \theta_{0,1} = 0$. Hence,

$$\sum_{i=1}^N f_{1,0}(X_i) + f_{0,1}(Y_i) = \sum_{i=1}^N \tilde{f}_{1,0}(X_i) + \tilde{f}_{0,1}(Y_i),$$

where $\tilde{f}_{1,0} := f_{1,0} - \theta_{1,0} \in L^2(\rho_0)$ and $\tilde{f}_{0,1} := f_{0,1} - \theta_{0,1} \in L^2(\rho_1)$, and the claim follows. \hfill $\Box$

**Lemma 36.** The subspace $H_2 \subset L^2(\mu_\epsilon^N)$ is spanned by functions of the form

$$(78) \quad \sum_{i<j} [f_{2,0}(X_i, X_j) + f_{2,1}(Y_i, Y_j)] + \sum_{i=1}^N f_{1,1}(X_i, Y_i) + \sum_{i \neq j} f_{1,1'}(X_i, Y_j),$$

where $f_{2,0} \in L^2(\rho_0 \otimes \rho_0), f_{0,2} \in L^2(\rho_1 \otimes \rho_1)$ are symmetric and $f_{1,1} \in L^2(\mu_\epsilon^2), f_{1,1'} \in L^2(\mu_\epsilon^2)$ are the same up to an affine term, that is, $f_{1,1}(x, y) = f_{1,1'}(x, y) + g_1(x) + g_2(y) + a$.

**Proof of Lemma 36.** Take any

$$T := \sum_{i,j} [f(X_i, X_j) + g(Y_i, Y_j)] + \sum_{i=1}^N h(X_i, Y_j) \in H_2.$$ 

Define $\bar{f}(x, x') := f(x, x') - f_0(x) - f_0(x') - \theta_f$ and $\bar{g}(y, y')$ analogously, where $\theta_f := E[f(X_1, X_2)]$ and $f_0(x) := E[f(X_1, X_2) - \theta_f \mid X_1](x) = E[f(X_1, X_2) - \theta_f \mid X_2](x)$. By definition, we know $\bar{f} \in L^2(\rho_0 \otimes \rho_0)$ and $\bar{g} \in L^2(\rho_1 \otimes \rho_1)$ are symmetric. Also, let

$$\bar{h}(x, y) := h(x, y) - (I + \mathcal{B})^{-1}(h_{1,0} \otimes h_{0,1})(x, y) - \theta_h,$n

$$\bar{h}'(x, y) := h(x, y) - h_{1,0}'(x) - h_{0,1}'(y) - \theta_h',$$

where

$$\begin{align*}
\theta_h &:= E[h(X_1, Y_1)], \quad h_{1,0}(x) := E[h(X_1, Y_1) - \theta_h \mid X_1](x), \quad h_{0,1}(y) := E[h(X_1, Y_1) - \theta_h \mid Y_1](y), \\
\theta_h' &:= E[h(X_1, Y_2)], \quad h_{1,0}'(x) := E[h(X_1, Y_2) - \theta_h' \mid X_1](x), \quad h_{0,1}'(y) := E[h(X_1, Y_2) - \theta_h' \mid Y_2](y).
\end{align*}$$

By construction, $\bar{h}$ and $\bar{h}'$ are the same up to an affine term. Furthermore, it follows from (23) and (26) that $\bar{h} \in L^2(\mu_\epsilon)$. Hence, to prove (78), we just need to show that $T$ is equal to

$$(79) \quad \bar{T} := \sum_{i<j} [\bar{f}(X_i, X_j) + \bar{g}(Y_i, Y_j)] + \sum_{i=1}^N \bar{h}(X_i, Y_i) + \sum_{i \neq j} \bar{h}'(X_i, Y_j).$$
Note that \( T \in H_0^+ \cap H_1^+ \), it holds that \( \mathbb{E}[T] = \frac{N(N-1)}{2}(\theta_f + \theta_g) + N\theta_h + N(N-1)\theta_h^* = 0 \) and
\[
\mathbb{E}[T - \mathbb{E}[T] \mid X_i] = (N-1)[f_0(X_i) + A^*g_0(X_i) + h_{1,0}(X_i) + A^*h_{0,1}(X_i)] + h_{1,0}(X_i) = 0
\]
\[
\mathbb{E}[T - \mathbb{E}[T] \mid Y_i] = (N-1)[A^*f_0(Y_i) + g_0(Y_i) + Ah_{1,0}(Y_i) + h_{0,1}(X_i)] + h_{0,1}(Y_i) = 0.
\]
This yields
\[
(N-1)(I - A^*A)(f_0 + h_{1,0})(X_i) + (h_{1,0} - A^*h_{0,1})(X_i) = 0
\]
and thus, using (26),
\[
0 = (N-1)[f_0(X_i) + g_0(Y_i) + h_{1,0}(X_i) + h_{0,1}(Y_i)] + (I - A^*A)^{-1}(h_{1,0} - A^*h_{0,1})(X_i) + (I + \mathcal{B})^{-1}(h_{1,0} \oplus h_{0,1})(X_i, Y_i).
\]
Putting all together, we obtain
\[
\hat{T} = T - \sum_{i < j}[f_0(X_i) + f_0(X_j) + g_0(Y_i) + g_0(Y_j) + \theta_f + \theta_g] - \sum_{i=1}^N[(I + \mathcal{B})^{-1}(h_{1,0} \oplus h_{0,1})(X_i, Y_i) + \theta_h]
\]
\[
- \sum_{i \neq j}[h_{1,0}(X_i) + h_{0,1}(Y_j) + \theta_h]
\]
\[
= T - (N-1)\sum_{i=1}^N[f_0(X_i) + g_0(Y_i) + h_{1,0}(X_i) + h_{0,1}(Y_i)] - \sum_{i=1}^N(I + \mathcal{B})^{-1}(h_{1,0} \oplus h_{0,1})(X_i, Y_i) - \mathbb{E}[T],
\]
which is exactly equal to \( T \) by (80) and the claim follows.

A.2. Closeness of \( H_1 \) and \( H_2 \). Let \( T^n := T^n(X_{[N]}, Y_{[N]}) \in \mathbb{L}^2(\mu^N) \) be permutation symmetric for each \( n \geq 1 \). Assume \( T^n \) converges in \( \mathbb{L}^2(\mu^N) \) to some \( T \). We show that \( T \) is also permutation symmetric, even though the underlying measure is not.

**Lemma 37.** Under Assumption 2, \( T \) is also permutation symmetric.

**Proof of Lemma 37.** Since \( T^n \rightarrow \mathbb{L}^2(\mu^N) \) as \( n \rightarrow \infty \), there exits a sub-sequence \( T^{n_k} \rightarrow_{a.s.} T \) as \( k \rightarrow \infty \). In other words, there exists a subset \( A \subset (\mathbb{R}^d \times \mathbb{R}^d)^N \) such that \( \mu^N(A) = 0 \) and \( T^{n_k} \rightarrow T \) on \( A^c \) as \( k \rightarrow \infty \). For all permutations \( \sigma, \tau \in \mathcal{S}_N \), define
\[ A_{\sigma, \tau} := \{(x_{\sigma([N])}, y_{\tau([N])}) : (x_{[N]}, y_{[N]}) \in A\}. \]

Since \( \mu^N \) is a probability density, we get \( \mu^N(A_{\sigma, \tau}) = 0 \), and thus \( \mu^N(A_{\sigma, \tau}) = 0 \) where \( A_{\mathcal{S}_N} := \bigcup_{\sigma, \tau \in \mathcal{S}_N} A_{\sigma, \tau} \).

Now, take any \( (x_{[N]}, y_{[N]}) \in A_{\mathcal{S}_N} \), it holds that \( T^{n_k}(x_{[N]}, y_{[N]}) \rightarrow T(x_{[N]}, y_{[N]}) \) as \( k \rightarrow \infty \). For any \( \sigma \in \mathcal{S}_N \), we know, by construction, that \( (x_{\sigma([N])}, y_{\sigma([N])}) \in A_{\mathcal{S}_N} \). Consequently, \( T^{n_k}(x_{[N]}, y_{\sigma([N])}) \rightarrow T(x_{[N]}, y_{\sigma([N])}) \) as \( k \rightarrow \infty \). It then follows from the permutation symmetry of \( T^n \) that \( T(x_{[N]}, y_{[N]}) = T(x_{[N]}, y_{\sigma([N])}) \). This implies, almost surely, \( T \) is permutation symmetric. Since every element in \( \mathbb{L}^2(\mu^N) \) is only defined up to a zero-measure set, we can conclude that \( T \) is permutation symmetric.

Recall from Proposition 14 that the projection \( \text{Proj}_{H_1}(T_N) \) exists and is given exactly by \( L_1 \) under Assumption 2. Let \( T := T(X_{[N]}, Y_{[N]}) \in \mathbb{L}^2(\mu^N) \) be an arbitrary statistic that is permutation symmetric. Repeating the argument for \( T \) shows that \( \text{Proj}_{H_1}(T) \) exists. With this at hand, we can show that the subspace \( H_1 \) is closed.

**Proposition 38.** Under Assumption 2, the subspace \( H_1 \subset \mathbb{L}^2(\mu^N) \) is closed.

**Proof of Proposition 38.** Take an arbitrary Cauchy sequence \( \{\sum_{i=1}^N f^n_{i,0}(X_i) + f^n_{0,1}(Y_i)\} \subset H_1 \) and assume \( T \) is its limit in \( \mathbb{L}^2(\mu^N) \). By linearity, each \( T^n := \sum_{i=1}^N f^n_{i,0}(X_i) + f^n_{0,1}(Y_i) \) is permutation symmetric. According
to Lemma 37, its limit $T$ is also permutation symmetric. Consequently, we can repeat the argument in Proposition 14 for $T$ and show that $\text{Proj}_{H_1}(T)$ exists. Hence,

$$\|T^n - \text{Proj}_{H_1}(T)\|_{L^2(\mu^N)}^2 + \|T - \text{Proj}_{H_1}(T)\|_{L^2(\mu^N)}^2 = \|T^n - T\|_{L^2(\mu^N)}^2 \to 0, \quad \text{as } n \to \infty.$$  

It then follows that $T^n \to_{L^2(\mu^N)} \text{Proj}_{H_1}(T) \in H_1$, and thus $H_1$ is closed. $\square$

Before we prove the closeness of $H_2$, let us consider the subspace $H_2^{i,j}$ spanned by functions of the type

$$g(X_i, X_j, Y_i, Y_j) := f_{2,0}(X_i, X_j) + f_{0,2}(Y_i, Y_j) + f_{1,1}^r(X_j, Y_i) + f_{1,1}^l(X_j, Y_i) + f_{1,1}(X_j, Y_j),$$  

where $f_{2,0} \in L^2_{0,0}(\rho_0 \otimes \rho_0)$, $f_{0,2} \in L^2_{0,0}(\rho_1 \otimes \rho_1)$ are symmetric, and $f_{1,1}^r \in L^2_{0,0}(\rho_0 \otimes \rho_1)$, $f_{1,1}^l \in L^2_{0,0}(\mu_*)$ are the same up to an affine term. We will show that $H_2^{i,j}$ is closed. The next lemma shows that every elements in this subspace is permutation symmetric.

**Lemma 39.** Let $f_{2,0} \in L^2_{0,0}(\rho_0 \otimes \rho_0)$, $f_{0,2} \in L^2_{0,0}(\rho_1 \otimes \rho_1)$, $f_{1,1}^r \in L^2_{0,0}(\rho_0 \otimes \rho_1)$ and $f_{1,1}^l \in L^2_{0,0}(\mu_*)$. Then $g(X_i, X_j, Y_i, Y_j)$ defined in (81) is permutation symmetric iff $f_{2,0}, f_{0,2}$ are symmetric and $f_{1,1}^r, f_{1,1}^l$ are the same up to an affine term.

**Proof of Lemma 39.** Define $T_{i,j}$ to be the operator that swaps $X_i$ and $X_j$. If $g(X_i, X_j, Y_i, Y_j)$ is permutation symmetric, then $T_{i,j}g(X_i, X_j, Y_i, Y_j) = g(X_i, X_j, Y_i, Y_j)$, that is,

$$f_{2,0}(X_i, X_j) + f_{1,1}^r(X_j, Y_i) + f_{1,1}^l(X_j, Y_i) + f_{1,1}(X_j, Y_j) = f_{2,0}(X_j, X_i) + f_{1,1}^r(X_j, Y_i) + f_{1,1}^l(X_j, Y_i) + f_{1,1}(X_j, Y_j).$$  

Taking the conditional expectation given $X_i, Y_i$ yields

$$f_{1,1}(X_i, Y_i) = f_{1,1}(X_i, Y_i) + g_1(X_i) + g_2(Y_i) + a,$$

where $a = E[f_{1,1}^r(X_j, Y_j)]$,

$$g_1(X_i) = E[f_{1,1}(X_j, Y_j) | X_i] \quad \text{and} \quad g_2(Y_i) = E[f_{1,1}(X_j, Y_j) | Y_i].$$

Now, plugging (83) into (82) gives

$$f_{2,0}(X_i, X_j) + \sum_{k,l \in \{i,j\}} f_{1,1}^r(X_k, Y_l) + g_1(X_i) + g_2(Y_i) + g_1(X_j) + g_2(Y_j) + 2a$$

and thus $f_{2,0}$ is symmetric. The symmetry of $f_{0,2}$ can be derived similarly. Conversely, when $f_{2,0}, f_{0,2}$ are symmetric and $f_{1,1}^r, f_{1,1}^l$ are the same up to an affine term, the identity (84) is true. As a result, $g(X_i, X_j, Y_i, Y_j)$ is permutation symmetric. $\square$

To prove the closeness of $H_2^{i,j}$, we introduce two operators using again the notation of tensor product: $C_{2,0} := (I - A^*A) \otimes (I - A^*A)$ and $C_{0,2} := (I - AA^*) \otimes (I - AA^*)$. Following an argument similar to the one for Lemma 18, we have the following lemma.

**Lemma 40.** Under Assumption 2, the inverse operators $C_{2,0}^{-1} : L^2_{0,0}(\rho_0 \otimes \rho_0) \to L^2_{0,0}(\rho_0 \otimes \rho_0)$ and $C_{0,2}^{-1} : L^2_{0,0}(\rho_1 \otimes \rho_1) \to L^2_{0,0}(\rho_1 \otimes \rho_1)$ are well-defined. Moreover, it holds $C_{2,0}^{-1} = (I - A^*A)^{-1} \otimes (I - A^*A)^{-1}$ and $C_{0,2}^{-1} = (I - AA^*)^{-1} \otimes (I - AA^*)^{-1}$.

**Proposition 41.** Suppose Assumption 2 holds true. Let $T \in H^+_1 \cap H^+_1$ be permutation symmetric in $X_{i,j}$ and in $Y_{i,j}$ for $i \neq j$. Define $k_{2,0}^{i,j}(x, x') := E[T | X_i, X_j](x, x')$, $k_{0,2}^{i,j}(y, y') := E[T | Y_i, Y_j](y, y')$, $k_{1,1}^{i,j}(x, y) := E[T | X_i, Y_j](x, y)$ and $k_{1,1}^{i,j} := E[T | X_i, Y_j]$, then the projection $\text{Proj}_{H_2^{i,j}}(T)$ is given by

$$U := g_{2,0}(X_i, X_j) + g_{0,2}(Y_i, Y_j) + g_{1,1}^r(X_i, Y_j) + g_{1,1}^l(X_i, Y_j) + k_{1,1}^{i,j}(X_i, Y_i) + k_{1,1}^{i,j}(X_j, Y_j).$$

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where
\[ g_{2,0} := C_{0,2}^{-1}[k_{i,j}^2 + (A^* \otimes A^*)k_{i,j}^2 - (I + T)(I_{\rho_0} \otimes A^*)k_{i,j}^2] \]
\[ g_{0,2} := C_{0,2}^{-1}[k_{i,j}^2 + (A \otimes A)k_{i,j}^2 - (I + T)(A \otimes I_{\rho_1})k_{i,j}^2] \]
\[ g_{1,1'} := C^{-1}[(I + B)|k_{i,j}^2| - (I_{\rho_0} \otimes A)|k_{i,j}^2| - (A^* \otimes I_{\rho_1})k_{i,j}^2]. \]

Moreover, the subspace $H_{2}^{i,j}$ is closed.

**Proof of Proposition 4.1.** We consider $(i,j) = (1,2)$ and omit the dependency on $(i,j)$ in $k$ for simplicity. By the permutation symmetry of $T$, we know $k_{1,1}(x,y) = E[T \mid X_1, Y_2](x,y) = E[T \mid X_2, Y_1](x,y)$ and $k_{1,1}(x,y) := E[T \mid X_2, Y_1](x,y) = E[T \mid X_2, Y_2](x,y)$. According to Lemma 34, it suffices to show $T - U \in (H_{2}^{i,j})^\perp$, or

\[ (86) \quad E[T - U \mid X_1, X_2] = E[T - U \mid Y_1, Y_2] = E[T - U \mid X_1, Y_1] = E[T - U \mid X_1, Y_2] = 0. \]

**Step 1.** We show $E[T - U \mid X_1, Y_1] = 0$. We start by showing the statistic $U$ is well-defined. Since $T \in H_0^\perp \cap H_1^\perp$, we know $k_{2,0} \in L_{0,0}^2(\rho_0 \otimes \rho_0)$, $k_{0,2} \in L_{0,0}^2(\rho_1 \otimes \rho_1)$, $k_{1,1'} \in L_{0,0}^2(\rho_0 \otimes \rho_1)$ and $k_{1,1} \in L_{0,0}^2(\mu_{\epsilon})$. According to Lemma 19, it holds that $(A^* \otimes A^*)k_{2,0} \in L_{0,0}^2(\rho_0 \otimes \rho_0)$ and $(I_{\rho_0} \otimes A^*)k_{1,1'} \in L_{0,0}^2(\rho_0 \otimes \rho_1)$. This implies

\[ k_{2,0} + (A^* \otimes A^*)k_{2,0} = (I + T)(I_{\rho_0} \otimes A^*)k_{2,0} \in L_{0,0}^2(\rho_0 \otimes \rho_0). \]

Hence, by Lemma 40, $g_{2,0} \in L_{0,0}^2(\rho_0 \otimes \rho_0)$ is well-defined. Similarly, $g_{0,2} \in L_{0,0}^2(\rho_1 \otimes \rho_1)$ and $g_{1,1'} \in L_{0,0}^2(\rho_0 \otimes \rho_1)$ are well-defined. Moreover,

\[ E[g_{2,0} \mid X_1, X_2] = E[g_{0,2} \mid X_1, Y_1] = E[g_{1,1'} \mid X_1, Y_1] = E[g_{1,1'} \mid X_1, Y_1] = 0. \]

Thus,

\[ (88) \quad E[U \mid X_1, Y_1] = k_{1,1}(X_1, Y_1) + E[k_{1,1}(X_2, Y_2)] \quad \text{(i)} \quad E[k_{1,1}(X_2, Y_2)] = E[T \mid X_1, Y_1], \]

where (i) follows from $k_{1,1} \in L_{0,0}^2(\mu_{\epsilon})$. Then the claim follows.

**Step 2.** We prove that $E[T - U \mid X_1, X_2] = 0$, that is,

\[ (89) \quad E[U \mid X_1, X_2] = E[T \mid X_1, X_2] = k_{2,0}(X_1, X_2). \]

Recall that $k_{1,1} \in L_{0,0}^2(\mu_{\epsilon})$, we then have

\[ E[k_{1,1}(X_1, Y_1) \mid X_1, X_2] = E[k_{1,1}(X_2, Y_2) \mid X_1, X_2] = 0. \]

Furthermore, according to Lemma 40, it holds that

\[ (A^* \otimes A^*)C_{0,2}^{-1} = A^*(I - A^*)^{-1} \otimes A^*(I - A^*)^{-1} = (I - A^*A)^{-1} \otimes (I - A^*A)^{-1}A^* = C_{0,2}^{-1}(A^* \otimes A^*), \]

where we have used Lemma 13 in (ii). This implies that $E[g_{0,2} \mid X_1, X_2]$ is equal to

\[ (89) \quad (A^* \otimes A^*)g_{0,2}(X_1, X_2) = C_{0,2}^{-1}|(A^* \otimes A^*)k_{0,2} + (A^* A \otimes A^*)k_{2,0} - (I + T)(A^* A \otimes A^*)k_{1,1'}| \]

Similarly, it follows from Lemma 18 that

\[ (I_{\rho_0} \otimes A^*)C_{0,2}^{-1} = (I - A^*A)^{-1} \otimes A^*(I - A^*)^{-1} = (I - A^*A)^{-1} \otimes (I - A^*A)^{-1}A^* = C_{0,2}^{-1}(I_{\rho_0} \otimes A^*), \]

and thus $E[g_{1,1'}(X_1, Y_2) + g_{1,1'}(X_2, Y_1) \mid X_1, X_2] = (I + T)(I_{\rho_0} \otimes A^*)g_{1,1'}(X_1, X_2)$ reads

\[ (I + T)C_{0,2}^{-1}[I_{\rho_0} \otimes A^*](I + B)k_{1,1'} - (I_{\rho_0} \otimes A^*)k_{2,0} - (A^* \otimes A^*)k_{0,2} = C_{2,0}^{-1}(I_{\rho_0} \otimes A^*), \]

where the equality follows from $(I_{\rho_0} \otimes A^*)B = (I_{\rho_0} \otimes A^*)T(A \otimes A^*) = T(A^* A \otimes A^*)$. Putting (90), (91) and (92) together, we have

\[ E[U \mid X_1, X_2] = C_{0,2}^{-1}[D_{2,0}k_{0,2} + D_{0,2}k_{0,2} + D_{1,1'}k_{1,1'}] \]

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where
\[
D_{2,0} = I + (A^* \mathcal{A} \otimes A^* \mathcal{A}) - (I + T)(I_{p_0} \otimes A^* \mathcal{A}) = I + (A^* \mathcal{A} \otimes A^* \mathcal{A}) - (A^* \mathcal{A} \otimes I_{p_0})T
\]
\[
D_{0,2} = 2(A^* \otimes A^*) - (I + T)(A^* \otimes A^*) = (A^* \otimes A^*) - (A^* \otimes A^*)T
\]
\[
D_{1,1'} = -(I + T)(I_{p_0} \otimes A^*) - (I + T)(A^* \mathcal{A} \otimes A^*) + (I + T)(I_{p_0} \otimes A^*) + (T + TT)(A^* \mathcal{A} \otimes A^*) = 0.
\]
Moreover, since \( T \) is permutation symmetric in \( X_{1,2} \), we know \( k_{2,0} \) is symmetric. As a result, \( T k_{2,0} = k_{2,0} \), which implies
\[
D_{2,0} k_{2,0} = [I + (A^* \mathcal{A} \otimes A^* \mathcal{A}) - (I_{p_0} \otimes A^* \mathcal{A}) - (A^* \mathcal{A} \otimes I_{p_0})]k_{2,0} = [(I - A^* \mathcal{A}) \otimes (I - A^* \mathcal{A})]k_{2,0} = C_{2,0} k_{2,0}
\]
\[
D_{0,2} k_{2,0} = [(A^* \otimes A^*) - (A^* \otimes A^*)]k_{2,0} = 0.
\]
Hence, the claim (98) follows. A similar argument yields \( E[U \mid Y_1, Y_2] = E[T \mid Y_1, Y_2] = k_{2,0}(Y_1, Y_2) \).

**Step 3.** We verify
\[
E[U \mid X_1, Y_2] = E[T \mid X_1, Y_2] = k_{1,1}(X_1, Y_2).
\]
Again, we prove it by direct computations. Analogous to (99), it holds that
\[
E[k_{1,1}(X_1, Y_1) \mid X_1, Y_2] = E[k_{1,1}(X_2, Y_2) \mid X_1, Y_2] = 0.
\]
Note that
\[
(I_{p_0} \otimes A)C_{2,0}^{-1} = (I - A^* \mathcal{A})^{-1} \otimes A(I - A^* \mathcal{A})^{-1} = (I - A^* \mathcal{A})^{-1} \otimes (I - AA^*)^{-1} A = C^{-1}(I_{p_0} \otimes A),
\]
\[
C^{-1}[(I_{p_0} \otimes A)k_{2,0} + (A^* \otimes AA^*)k_{0,2} - (I_{p_0} \otimes AA^*)k_{1,1'} - T(A^* \otimes A^*)k_{1,1'}](X_1, Y_2)
\]
\[
= C^{-1}[(I_{p_0} \otimes A)k_{2,0} + (A^* \otimes AA^*)k_{0,2} - (I_{p_0} \otimes AA^*)k_{1,1'} - T(A^* \otimes AA^*)k_{1,1'} - B k_{1,1'}](X_1, Y_2),
\]
and, analogously,
\[
E[g_{0,2}(Y_1, Y_2) \mid X_1, Y_2] = C^{-1}[(A^* \otimes I_{p_1})k_{0,2} + (A^* \otimes AA^*)k_{2,0} - (A^* \otimes I_{p_1})k_{1,1'} - B k_{1,1'}](X_1, Y_2).
\]
Since \( E[g_{1,1'}(X_2, Y_1) \mid X_1, Y_2] = E[g_{1,1'}(X_1, Y_2)] \), we get
\[
E[U \mid X_1, Y_2] = C^{-1} [D_{2,0} k_{2,0} + D_{0,2} k_{0,2} + D_{1,1'} k_{1,1'}](X_1, Y_2),
\]
where
\[
D_{2,0}' = (I_{p_0} \otimes A) + (A^* \mathcal{A} \otimes A) - (I + B)(I_{p_0} \otimes A) = (A^* \mathcal{A} \otimes A) - (A^* \mathcal{A} \otimes A)T
\]
\[
D_{0,2}' = (A^* \otimes I_{p_1}) + (A^* \otimes AA^*) - (I + B)(A^* \otimes I_{p_1}) = (A^* \otimes AA^*) - (A^* \otimes AA^*)T
\]
and
\[
D_{1,1'} = -(I_{p_0} \otimes AA^*) - B - (A^* \mathcal{A} \otimes I_{p_1}) - B + (I + B)(I + B)
\]
\[
= I + (A^* \mathcal{A} \otimes AA^*) - (I_{p_0} \otimes AA^*) - (A^* \mathcal{A} \otimes I_{p_1})
\]
\[
= (I_{p_0} - A^* \mathcal{A}) \otimes (I_{p_1} - AA^*) = C.
\]
Therefore, \( E[U \mid X_1, Y_2] = E[T \mid X_1, Y_2] = k_{1,1}(X_1, Y_2) \).

**Step 4.** We prove \( H_2^{1,2} \) is closed. Recall that \( H_2^{1,2} \) is spanned by \( g(X_1, X_2, Y_1, Y_2) \) given in (81). Take any Cauchy sequence \( \{g^n(X_1, X_2, Y_1, Y_2) \} \subset H_2^{1,2} \subset L^2(\mu^2) \), there exists \( g(X_1, X_2, Y_1, Y_2) \in L^2(\mu^2) \) such that \( g^n(X_1, X_2, Y_1, Y_2) \rightarrow g(X_1, X_2, Y_1, Y_2) \) in \( L^2(\mu^2) \). In the following, we will write \( g^n \) and \( g \) for short. Since \( g^n \) is permutation symmetric for each \( n \geq 1 \), we know, by Lemma 37, \( g \) is also permutation symmetric. As a result, the projection \( \text{Proj}_{H_2^{1,2}}(g) \) exists, and thus
\[
\|g^n - g\|^2_{L^2(\mu^2)} = \|g^n - \text{Proj}_{H_2^{1,2}}(g)\|^2_{L^2(\mu^2)} + \|g - \text{Proj}_{H_2^{1,2}}(g)\|^2_{L^2(\mu^2)} \rightarrow 0, \quad \text{as } n \rightarrow \infty.
\]
It then follows that \( g^n \rightarrow g \) in \( L^2(\mu^2) \) \( \text{Proj}_{H_2^{1,2}}(g) \), so \( H_2^{1,2} \) is closed. □

Now we are ready to show the closeness of \( H_2 \).

**Proposition 42.** Under Assumption 2, the subspace \( H_2 \subset L^2(\mu^N_\tau) \) is closed.
Proof of Proposition 42. We use the representation of $H_2$ given in Lemma 36. Take any Cauchy sequence

$$T^n := \sum_{i<j} [f_{2,0}^n(X_i, X_j) + f_{0,2}^n(Y_i, Y_j)] + \sum_{i=1}^N f_{1,1}^n(X_i, Y_i) + \sum_{i \neq j} f_{1,1}^n(X_i, Y_j),$$

we must have $E[(T^n - T^m)^2] \to 0$ as $m, n \to \infty$. Let $g^n(x, x', y, y') := f_{2,0}^n(x, x') + f_{0,2}^n(y, y') + f_{1,1}^n(x, y') + f_{1,1}^n(x', y)$. Observe that

$$g^n = E[X^n] + \sum_{i=1}^N f_{1,1}^n(X_i, Y_i).$$

Then, it suffices to show the limit lives in $H_2$. Let $g^n(x, x', y, y') := f_{2,0}^n(x, x') + f_{0,2}^n(y, y') + f_{1,1}^n(x, y') + f_{1,1}^n(x', y)$. Observe that

$$E[(T^n - T^m)^2] = \sum_{i<j} (g^n - g^m)(X_i, X_j, Y_i, Y_j)^2 + \sum_{i=1}^N (f_{1,1}^n - f_{1,1}^m)(X_i, Y_i)^2 + \sum_{i \neq j} (f_{1,1}^n - f_{1,1}^m)(X_i, Y_j)^2.$$

so we get, as $n, m \to \infty$,

$$E[(g^n - g^m)(X_1, X_2, Y_1, Y_2)^2] \to 0$$

and

$$E[((f_{1,1}^n - f_{1,1}^m)(X_1, Y_1)^2) \to 0.$$

Furthermore, since $g^n(X_1, X_2, Y_1, Y_2), f_{1,1}^n(X_1, Y_1) \in H_2 \cap H_2^\perp$ and $E[g^n(X_1, X_2, Y_1, Y_2) | X_1, Y_1] = 0$, there exist $g(X_1, X_2, Y_1, Y_2), f_{1,1}(X_1, Y_1) \in H_2 \cap H_2^\perp$ such that $E[g(X_1, X_2, Y_1, Y_2) | X_1, Y_1] = 0$.

It then suffices to show the limit lives in $H_2$.

According to (98), it holds that

$$g^n(X_1, X_2, Y_1, Y_2) + f_{1,1}^n(X_1, Y_1) \to \text{L}_2(\mu^N) g(X_1, X_2, Y_1, Y_2) + f_{1,1}(X_1, Y_1) + f_{1,1}(X_2, Y_2).$$

Since $g^n(X_1, X_2, Y_1, Y_2) + f_{1,1}^n(X_1, Y_1) + f_{1,1}^n(X_2, Y_2) \in H_2^\perp$ and $H_2^\perp$ is closed as shown in Proposition 41, we get that

$$g(X_1, X_2, Y_1, Y_2) + f_{1,1}(X_1, Y_1) + f_{1,1}(X_2, Y_2) \in H_2^\perp$$

and thus has the form

$$\sum_{i=1}^N g(X_i, X_j, Y_i, Y_j) + \sum_{i=1}^N f_{1,1}(X_i, Y_i) \in H_2,$$
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Sets and Functions

$[N]$  set of integers from 1 to $N$.
$S_N$  set of permutations of $[N]$.
$\#\sigma$  number of cycles in the permutation $\sigma$.
$1$  constant function with value 1.
$f \oplus g$  direct sum of $f$ and $g$, i.e., $(f \oplus g)(x, y) = f(x) + g(y)$.
$c$  cost function.
$\eta$  general test function.
$f(X, Y)$  summation $\sum_{i=1}^{N} f(X_i, Y_{i \sigma})$.
$f^\otimes(X, Y_\sigma)$  product $\prod_{i=1}^{N} f(X_i, Y_{i \sigma})$.

Probability and Statistics

$\rho_0, \rho_1$  probability densities on $\mathbb{R}^d$.
$\rho_0^N, \rho_1^N$  empirical measures of samples $\{X_i\}_{i=1}^{N}$ and $\{Y_i\}_{i=1}^{N}$ from $\rho_0$ and $\rho_1$, respectively.
$\rho_0 \otimes \rho_1$  product measure of $\rho_0$ and $\rho_1$.
$\mathbb{E}$  expectation under the product measure $(\rho_0 \otimes \rho_1)^N$.
$\mathbb{E}$  expectation under the measure $\mu_N^\epsilon$, the Schrödinger bridge.
$L^p(\mu)$  space of functions whose $p$th power is integrable with respect to the measure $\mu$.
$\text{Proj}^L$  $L^2$ projection.
$H_k$  subspace of $L^2(\mu_N^\epsilon)$ consists of symmetric statistics involving exactly $k$ variables and is orthogonal to $\oplus_{i=1}^{k-1} H_i$.
$L_1$  first order chaos, also the projection of $T_N$ on $H_1$.
$L_2$  second order chaos, also the projection of $T_N$ on $H_2$.

Operators

$I_\mu$  identity operator on $L^2(\mu)$.
$T$  swap operator, i.e., $T f(x, y) = f(y, x)$.
$\mathcal{A}$  integral operator mapping from $L^2(\rho_0)$ to $L^2(\rho_1)$ with kernel $\xi(x, y)\rho_0(x)$.
$\mathcal{A}^*$  integral operator mapping from $L^2(\rho_1)$ to $L^2(\rho_0)$ with kernel $\xi(x, y)\rho_1(y)$.
$\{s_k\}_{k \geq 0}$  singular values of $\mathcal{A}$.
$\{\alpha_k\}_{k \geq 0}$  singular functions of $\mathcal{A}$ and $\mathcal{A}^*$.
$\{\beta_k\}_{k \geq 0}$  singular functions of $\mathcal{A}$ and $\mathcal{A}^*$.
$\mathcal{A}_1 \otimes \mathcal{A}_2$  tensor product of operators $\mathcal{A}_1$ and $\mathcal{A}_2$.
$\mathcal{B}$  operator $T(\mathcal{A} \otimes \mathcal{A}^*)$ defined on $L^2(\rho_0 \otimes \rho_1)$.
$\mathcal{C}$  operator $(I_{\rho_0} - \mathcal{A} \mathcal{A}^*) \otimes (I_{\rho_1} - \mathcal{A}^* \mathcal{A})$ defined on $L^2(\rho_0 \otimes \rho_1)$.

Optimal transport

$\mathcal{C}(\rho_0, \rho_1)$  optimal cost of transporting $\rho_0$ to $\rho_1$ with cost function $c$.
$\Pi(\rho_0, \rho_1)$  space of probabilities defined on $\mathbb{R}^d \times \mathbb{R}^d$ with marginals $\rho_0$ and $\rho_1$.
$\mu_\epsilon$  (static) Schrödinger bridge connecting $\rho_0$ and $\rho_1$ at temperature $\epsilon$.
$\hat{\mu}_N^\epsilon$  (static) Schrödinger bridge connecting $\hat{\rho}_0^N$ and $\hat{\rho}_1^N$ at temperature $\epsilon$.
$T_N$  see (11).
$\xi$  nonnegative function on $\mathbb{R}^d \times \mathbb{R}^d$ such that $\mu_\epsilon(x, y) := \xi(x, y)\rho_0(x)\rho_1(y) \in \Pi(\rho_0, \rho_1)$.
$\theta$  mean of $\eta(X, Y)$ under the measure $\mu_\epsilon$, i.e., $\int \eta(x, y)\mu_\epsilon(x, y)dxdy$.
$\kappa_{1,0}, \kappa_{0,1}$  see (13).