Asymptotics for Strassen’s Optimal Transport Problem

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Abstract. In this paper, we consider Strassen’s version of optimal transport (OT) problem, which concerns minimizing the excess-cost probability (i.e., the probability that the cost is larger than a given value) over all couplings of two given distributions. We derive large deviation, moderate deviation, and central limit theorems for this problem. Our proof is based on Strassen’s dual formulation of the OT problem, Sanov’s theorem on the large deviation principle (LDP) of empirical measures, as well as the moderate deviation principle (MDP) and central limit theorems (CLT) of empirical measures. In order to apply the LDP, MDP, and CLT to Strassen’s OT problem, nested formulas for Strassen’s OT problem are derived. Based on these nested formulas and using a splitting technique, we construct asymptotically optimal solutions to Strassen’s OT problem and its dual formulation.

Abstract. Dans cet article, nous considérons la version de Strassen du problème de transport optimal (OT), qui concerne la minimisation de la probabilité de surcoût (c’est-à-dire la probabilité que le coût soit supérieur à une valeur donnée) sur tous les couplages de deux distributions données. Nous obtenons des théorèmes de grande déviation, de déviation modérée et de limite centrale pour ce problème. Notre preuve est basée sur la formulation duale de Strassen du problème OT, le théorème de Sanov sur le principe de grande déviation (LDP) des mesures empiriques, ainsi que le principe de déviation modérée (MDP) et les théorèmes centraux limites (CLT) des mesures empiriques. Afin d’appliquer les LDP, MDP et CLT au problème OT de Strassen, des formules imbriquées pour le problème OT de Strassen sont établies. Sur la base de ces formules imbriquées et en utilisant une technique de division, nous construisons des solutions asymptotiquement optimales au problème OT de Strassen et à sa formulation duale.

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1. Introduction

The theory of optimal transport (OT) has been studied for a long history due to its importance to related problems in physics, mathematics, economics, and other areas; see e.g. [1–5]. Recently, OT theory has been applied increasingly in computer science, mathematical imaging, machine learning, and information theory [6–11]. The OT problem was introduced by Monge [1] and Kantorovich [2], who defined it as the problem of minimizing the expectation of a cost function over all couplings of two given distributions. Let \((\mathcal{X}, \tau_1)\) and \((\mathcal{Y}, \tau_2)\) be Polish spaces. Let \(\Sigma(\mathcal{X})\) and \(\Sigma(\mathcal{Y})\) be respectively the Borel \(\sigma\)-algebras on \(\mathcal{X}\) and \(\mathcal{Y}\) that are generated by the topologies \(\tau_1\) and \(\tau_2\). Let \(\mathcal{P}(\mathcal{X})\) and \(\mathcal{P}(\mathcal{Y})\) denote the sets of probability measures (or distributions) on \(\mathcal{X}\) and \(\mathcal{Y}\) respectively. Let \(P_X \in \mathcal{P}(\mathcal{X})\) and \(P_Y \in \mathcal{P}(\mathcal{Y})\) be two distributions where the subscripts \(X\) and \(Y\) indicate which spaces the distributions are defined on. The coupling set of \((P_X, P_Y)\) is defined as

\[
\Pi(P_X, P_Y) := \left\{ P_{XY} \in \mathcal{P}(\mathcal{X} \times \mathcal{Y}) : P_{XY}(A \times \mathcal{Y}) = P_X(A), \forall A \in \Sigma(\mathcal{X}),
\right. \\
\left. P_{XY}(\mathcal{X} \times B) = P_Y(B), \forall B \in \Sigma(\mathcal{Y}) \right\}.
\]

Distributions in \(\Pi(P_X, P_Y)\) are termed couplings of \((P_X, P_Y)\). Let \(c : \mathcal{X} \times \mathcal{Y} \rightarrow [0, +\infty]\) be lower semi-continuous, which is called cost function.

**Definition 1.** The OT cost between \(P_X\) and \(P_Y\) is defined as

\[
\mathcal{E}(P_X, P_Y) := \min_{P_{XY} \in \Pi(P_X, P_Y)} \mathbb{E}_{(X,Y) \sim P_{XY}}[c(X,Y)].
\]

Any \(P_{XY} \in \Pi(P_X, P_Y)\) attaining \(\mathcal{E}(P_X, P_Y)\) is called an OT plan.

The minimization problem in (1) is called Monge–Kantorovich’s OT problem [4]. The functional \((P_X, P_Y) \in \mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{Y}) \mapsto \mathcal{E}(P_X, P_Y) \in [0, +\infty]\) is called the OT (cost) functional. If \((\mathcal{X}, \tau_1) = (\mathcal{Y}, \tau_2)\) and \(c = d^p\) where \(p \geq 1\) and \(d\) is a metric on the Polish space \((\mathcal{X}, \tau_1)\), then \(W_p(P_X, P_Y) := (\mathcal{E}(P_X, P_Y))^{1/p}\) is the so-called \(p\)-th Wasserstein distance between \(P_X\) and \(P_Y\). In [2], Kantorovich provided a dual formulation for Monge–Kantorovich’s OT problem, which is known as the Kantorovich duality theorem in the literature. Define the \(c\)-transform of a function \(\phi : \mathcal{X} \rightarrow \mathbb{R}\) as \(\phi^c(y) = \inf_{x \in \mathcal{X}} \phi(x) + c(x, y)\) for all \(y \in \mathcal{Y}\).

**Theorem 1** (Kantorovich Duality). [5, Theorem 5.10] It holds that

\[
\mathcal{E}(P_X, P_Y) = \sup_{(\phi, \psi) \in C_b(\mathcal{X}) \times C_b(\mathcal{Y}) : \phi + \psi \leq c} \int_{\mathcal{X}} \phi \ dP_X + \int_{\mathcal{Y}} \psi \ dP_Y
\]

\[
= \sup_{\phi \in L^1(P_X)} \int_{\mathcal{Y}} \phi^c \ dP_Y - \int_{\mathcal{X}} \phi \ dP_X
\]

where \(C_b(\mathcal{X})\) denotes the collection of bounded continuous functions \(\phi : \mathcal{X} \rightarrow \mathbb{R}\), and \(L^1(P_X)\) denotes the collection of integrable functions \(\phi : \mathcal{X} \rightarrow \mathbb{R}\) with respect to the distribution \(P_X\).

---

\[1\] The existence of the minimizers are well-known; see, e.g., [4, Theorem 1.3]. Furthermore, when the (joint) distribution of the random variables involved in an expectation is clear from context, we will omit the subscript \(\sim P_{XY}\).
In 1965, Strassen [12] considered an excess-cost probability version of the OT problem, in which the excess-cost probability, instead of the expectation, is to be minimized, as shown in the following definition. Here the excess-cost probability refers to the probability that the cost function is larger than a given value.

Definition 2. For \( \alpha \geq 0 \), the optimal excess-cost probability (ECP) between \( P_X \) and \( P_Y \) with respect to the cost function \( c \) is defined as:

\[
G_\alpha(P_X, P_Y) := \min_{P_{XY} \in \Pi(P_X, P_Y)} \mathbb{P}(X,Y) \sim P_{XY} \{c(X,Y) > \alpha\}.
\]  

(4)

Any \( P_{XY} \) attaining \( G_\alpha(P_X, P_Y) \) is called an optimal ECP plan.

We term the minimization problem in (4) as Strassen’s OT problem. In fact, Strassen’s OT problem is a \{0,1\}-valued cost version of Monge–Kantorovich’s OT problem in which the cost function is set to the indicator function \( 1_{c(x,y) > \alpha} \) (rather than \( c \) itself). Moreover, \( (x,y) \mapsto 1_{c(x,y) > \alpha} \) is lower semi-continuous since \( c \) is lower semi-continuous. Hence, we write “minimization”, instead of “infimization”, in (4). Furthermore, in Strassen’s OT problem, the optimal ECP reduces to the total variation (TV) distance if we set \( (X, \tau_1) = (Y, \tau_2) \), \( \alpha = 0 \), and set the cost function \( c \) to the discrete metric \( (x,y) \mapsto 1_{x \neq y} \) [4]. That is, for this case,

\[
G_0(P_X, P_Y) = \min_{P_{XY} \in \Pi(P_X, P_Y)} \mathbb{P}(X \neq Y) = \|P_X - P_Y\|_{TV}.
\]  

(5)

Here \( \|P - Q\|_{TV} := \sup_A P(A) - Q(A) \) denotes the TV distance between two distributions \( P \) and \( Q \) defined on the same measurable space, where the supremum is taken with respect to all possible measurable sets \( A \). Similarly to Monge–Kantorovich’s OT problem, Strassen’s OT problem also admits a dual representation, which was first given by Strassen [12]. Such a dual representation can be seen as a particular form (i.e., the \{0,1\}-valued cost version) of the Kantorovich duality theorem. If \( \{(x,y) : c(x,y) > \alpha\} = \emptyset \) for given \( c \) and \( \alpha \), then, obviously \( G_\alpha(P_X, P_Y) = 0 \). To exclude this trivial case, we make the following assumption.

Assumption 1 (Nonempty). We assume that \( \alpha \) is a number such that \( \{(x,y) : c(x,y) > \alpha\} \) is nonempty.

Theorem 2 (Strassen Duality). [3, Theorem 5.4.1] [4, Corollary 1.28] Under Assumption 1, it holds that

\[
G_\alpha(P_X, P_Y) = \sup_{\text{closed } E, F, c(x,y) > \alpha, \forall x \in E, y \in F} P_X(E) + P_Y(F) - 1
\]  

(6)

\[
= \sup_{\text{compact } E} P_X(E) - P_Y(\Gamma_{c \leq \alpha}(E)),
\]  

(7)

where for any set \( A \subseteq X \), denote the \( \alpha \)-enlargement of \( A \) under the cost function \( c \) as

\[
\Gamma_{c \leq \alpha}(A) := \bigcup_{x \in A} \{y \in Y : c(x,y) \leq \alpha\}.
\]  

(8)

In (6), “closed \( E, F \)” can be replaced by “measurable \( E, F \),” “compact \( E, F \)” (by inner regularity of probability measures on Polish spaces), or “open \( E, F \)” (by the tube lemma [13, Lemma 26.8]: if \( X \) is any topological space and \( Y \) a compact space, then the projection map \( X \times Y \to X \) is closed). By the tube lemma, \( \Gamma_{c \leq \alpha}(E) \) is closed in \( Y \) for any compact \( E \subseteq X \). From (7), given \( (P_X, P_Y) \), \( G_\alpha(P_X, P_Y) \) is right-continuous (and obviously non-increasing) in \( \alpha \). Furthermore, by symmetry, it also holds that \( G_\alpha(P_X, P_Y) = \sup_{\text{compact } F} P_Y(F) - P_X(\Gamma_{c \leq \alpha}(F)) \).

1.1. Main Result 1: Large Deviations Principle

Studying the asymptotic behavior of a sequence of random variables or probability distributions are central topics in probability theory. Although the OT theory has been widely studied in the literature, the asymptotic behaviors of OT problems have been rarely investigated. This is the major motivation for us to write this paper. In this paper, we investigate the asymptotic behavior of Strassen’s OT problem. To this end, we need first define the \( n \)-dimensional Strassen’s OT problem. Denote \( X^n \) as the \( n \)-fold product space of \( X \). For the product space \( X^n \times Y^n \), we consider an additive cost function \( c_n \) on \( X^n \times Y^n \), which is given by

\[
c_n(x^n, y^n) := \frac{1}{n} \sum_{i=1}^{n} c(x_i, y_i) \quad \text{for } (x^n, y^n) \in X^n \times Y^n,
\]
where $c$ is the cost function given above which is independent of $n$. Obviously, $c_n$ is lower semi-continuous since $c$ is lower semi-continuous. For $\alpha \geq 0$, the optimal ECP between the $n$-fold products of $P_X$ and $P_Y$ with respect to the cost function $c_n$ is

$$G_\alpha^{(n)}(P_X, P_Y) := \min_{P_{X_nY_n} \in \Pi(P_{X_n}^{\otimes n}, P_{Y_n}^{\otimes n})} P(X^n, Y^n) \sim P_{X_nY_n} \{c_n(X^n, Y^n) > \alpha\} \quad (9)$$

where $P_{X_n}^{\otimes n}$ and $P_{Y_n}^{\otimes n}$ denote the $n$-fold products of $P_X$ and $P_Y$ respectively. The minimization problem in (9) is termed the $n$-dimensional Strassen’s OT problem. It is easily verified that when $n = 1$, $G_\alpha^{(1)}(P_X, P_Y)$ reduces to the one-dimensional version $G_\alpha(P_X, P_Y)$ in (4). In this paper, we aim at characterizing the convergence rate of $G_\alpha^{(n)}(P_X, P_Y)$ as the dimension $n \to \infty$ for given $P_X, P_Y, c, n, \alpha$. To analyze the asymptotic behavior of Strassen’s OT problem, we plan to leverage existing limit theorems in probability theory. However, obviously an optimization is involved in Strassen’s OT problem and solving this optimization is very difficult in general [4]. Hence, it seems unfeasible to apply limit theorems directly to Strassen’s OT problem. To overcome this obstacle, we establish a formula, termed the nested formula, which forms a bridge between Strassen’s OT problem and existing limit theorems. Specifically, we observe that the minimization problem in (9) can be decoupled into two nested subproblems: an outer subproblem and an inner subproblem.

Given $n \geq 1$, the empirical measure (also known as type for the finite alphabet case) for a sequence $x^n \in X^n$ is

$$T_{x^n} := \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$$

where $\delta_x$ is Dirac mass at the point $x \in X$. The empirical joint measure, denoted by $T_{x^n,y^n}$, for a pair of sequences $(x^n, y^n) \in X^n \times Y^n$ is defined similarly. Obviously, empirical measures (or empirical joint measures) for $n$-length sequences are discrete distributions whose probability values are multiples of $1/n$. Denote $\mu_n, \nu_n$ as the laws of the empirical measures of $X^n \sim P_{X_n}^{\otimes n}$ and $Y^n \sim P_{Y_n}^{\otimes n}$ respectively. Denote $\Pi(\mu_n, \nu_n)$ as the set of couplings of $\mu_n, \nu_n$. Here $\mu_n, \nu_n$ and their couplings are respectively defined on Borel measurable spaces $\mathcal{P}(X), \mathcal{P}(Y), \mathcal{P}(X \times Y)$ induced by the weak topologies.

**Theorem 3 (Nested Formula for Strassen’s OT).** Given $P_X, P_Y, c, \text{ and } \alpha$, under Assumption 1, we have

$$G_\alpha^{(n)}(P_X, P_Y) = \min_{\pi \in \Pi(\mu_n, \nu_n)} \pi\{(Q_X, Q_Y) \in \mathcal{P}(X) \times \mathcal{P}(Y) : E(Q_X, Q_Y) > \alpha\} \quad (10)$$

$$= \sup_{\text{closed } A \subseteq \mathcal{P}(X), B \subseteq \mathcal{P}(Y): E(Q_X, Q_Y) > \alpha, \forall Q_X \in A, Q_Y \in B} \mu_n(A) + \nu_n(B) - 1 \quad (11)$$

$$= \sup_{\text{compact } A \subseteq \mathcal{P}(X)} \mu_n(A) - \nu_n(\Gamma_{E \leq \alpha}(A)), \quad (12)$$

where $(Q_X, Q_Y) \mapsto E(Q_X, Q_Y)$ is the OT functional given in (1) and

$$\Gamma_{E \leq \alpha}(A) := \bigcup_{Q_X \in A} \{Q_Y \in \mathcal{P}(Y) : E(Q_X, Q_Y) \leq \alpha\}.$$

The inner subproblem in (10) (i.e., the optimization in the definition of $E(Q_X, Q_Y)$) is nothing but (one-dimensional) Monge–Kantorovich’s OT problem defined in (1), while the outer subproblem corresponds to a new Strassen’s OT problem in which the marginal distributions $\mu_n, \nu_n$ (respectively defined on Borel measurable spaces $\mathcal{P}(X), \mathcal{P}(Y)$ induced by the weak topologies) are the laws of the empirical measures and the cost function is the OT functional $(Q_X, Q_Y) \mapsto \mathcal{P}(X) \times \mathcal{P}(Y) \mapsto E(Q_X, Q_Y)$.

Since $\mu_n, \nu_n$ in the nested formula in (10) are the laws of the empirical measures, given the dimension $n$, they are concentrated on the set of the empirical measures of $n$-length sequences. This in turn implies that the cost function in the nested formula, i.e., the OT functional $(Q_X, Q_Y) \mapsto E(Q_X, Q_Y)$, can be restricted to the set of the empirical joint distributions of pairs of $n$-length sequences. The set of empirical measures of sequences in $X^n$ is denoted as $\mathcal{P}_n(X^n) := \{T_{x^n} : x^n \in X^n\}$ and the set of empirical joint measures of pairs of sequences in $X^n \times Y^n$ is denoted as $\mathcal{P}_n(X \times Y^n) := \{T_{x^n,y^n} : (x^n, y^n) \in X^n \times Y^n\}$. We denote $\ell_1 : x^n \in X^n \mapsto T_{x^n}$ and $\ell_2 : y^n \in Y^n \mapsto T_{y^n}$ as the empirical measure functions, and denote $\ell : (x^n, y^n) \in X^n \times Y^n \mapsto T_{x^n,y^n}$ as the joint empirical measure function. By definition, it is easily verified that $\ell_1, \ell$ are continuous with respect to weak topologies, and hence measurable functions with respect to

---

1Note that $\mu_n, \nu_n$ are the laws of empirical measures, rather than empirical measures themselves.
the Borel $\sigma$-algebras (induced by weak topologies). Throughout this paper, we use $T_X, T_Y, T_{XY}$ to respectively denote elements in $P_n(\mathcal{X}), P_n(\mathcal{X}), P_n(\mathcal{X} \times \mathcal{Y})$, i.e., empirical measures on $\mathcal{X}, \mathcal{Y}, \mathcal{X} \times \mathcal{Y}$ of $n$-length sequences. Based on the notations above, the nested formula in (10) can be rewritten as

$$G^{(n)}_{\alpha}(P_X, P_Y) = \min_{\pi \in \Pi(\mu_n, \nu_n)} \pi \{ (T_X, T_Y) \in P_n(\mathcal{X}) \times P_n(\mathcal{Y}) : \mathcal{E}(T_X, T_Y) > \alpha \}. \quad (13)$$

The intuition behind Theorem 3 is as follows. Here we assume $c_n$ to be continuous. (Any lower semi-continuous function can be approximated by a nondecreasing sequence of continuous functions.) On one hand, the cost function $c_n(x^n, y^n)$ is permutation-invariant in the sense that it remains the same if the coordinate pairs of $(x^n, y^n)$ are arbitrarily rearranged. In other words, $c_n(x^n, y^n)$ depends on $(x^n, y^n)$ via their empirical joint measure $T_{x^n, y^n}$. On the other hand, any product distribution $P^{\otimes n}_X$ can be also rewritten as a mixture in the following form:

$$P^{\otimes n}_X = \int \text{Unif}(\ell^{-1}_1(T_X))d\mu_n(T_X),$$

where $\text{Unif}(\ell^{-1}_1(T_X))$ denotes the discrete uniform distribution on $\ell^{-1}_1(T_X)$, the set of sequences $x^n$ having empirical measure $T_X$. These two properties imply that the minimization in (9) can be decomposed into two sub-minimizations:

- The inner one is over the couplings (empirical joint measures) of two marginal empirical measures $T_{X^n}, T_{Y^n},$ and the outer one is over the couplings of the laws $\mu_n, \nu_n$. The optimal coupling attaining the minimum in (9) can be expressed as

$$P_{X^n, Y^n} = \int \text{Unif}(\ell^{-1}(T_{X^n,Y^n}(T_X, T_Y)))d\pi^*(T_X, T_Y),$$

where $T_{X^n,Y^n}(T_X, T_Y)$ is an optimal empirical joint measure attaining $\mathcal{E}(T_X, T_Y)$ such that\(^5\) $(T_X, T_Y) \mapsto T_{X^n,Y^n}(T_X, T_Y)$ is measurable under the $\sigma$-algebra induced by the weak topology, and $\pi^*$ is an optimal coupling attaining the minimum in (10) or (13). In fact, $\text{Unif}(\ell^{-1}(T_{X^n,Y^n}))$ automatically forms a coupling of $\text{Unif}(\ell^{-1}_1(T_X))$ and $\text{Unif}(\ell^{-1}_1(T_Y))$ if the empirical joint measure $T_{X^n,Y^n}$ is a coupling of $T_X, T_Y$.

Combining the nested formulas above with the large deviations principle (LDP) on empirical distributions (specifically, Sanov’s theorem [14, Theorem 6.2.10]), we show that $\alpha = \mathcal{E}(P_X, P_Y)$ is a phase transition point: For $\alpha < \mathcal{E}(P_X, P_Y)$, we have that $G^{(n)}_{\alpha}(P_X, P_Y)$ converges to one exponentially fast as $n \to \infty$, and for $\alpha > \mathcal{E}(P_X, P_Y)$, $G^{(n)}_{\alpha}(P_X, P_Y)$ converges to zero exponentially fast. The exponents of these convergences, called large deviations (LD) exponents, are characterized by us in terms of variational formulas (similarly to the large deviations theory for the empirical mean of i.i.d. random variables [14]). In order to derive our results, we require an assumption stronger than Assumption 1.

Assumption 2 (Interior-Point). We assume that $c$ is non-constant and $\alpha$ satisfies that $c_{\inf} < \alpha < c_{\sup}$, where $c_{\inf} := \inf_{x, y} c(x, y)$ and $c_{\sup} := \sup_{x, y} c(x, y)$.

Besides Assumption 2, we also need another mild assumption on the uniform continuity of the OT functional. Since $\mathcal{X}$ is a Polish space, $\mathcal{P}(\mathcal{X})$ equipped with the weak topology is also Polish [15, Theorem 6.2 and Theorem 6.5]. Let $L_1$ be the Lévy–Prokhorov metric on $\mathcal{P}(\mathcal{X})$ given by $L_1(Q_X, Q_X) = \inf \{ \delta : Q_X(A) \leq Q_X(A_\delta) + \delta, \forall \text{ closed } A \subseteq \mathcal{X} \}$, where given a metric $d$ on $\mathcal{X}$,

$${A}_\delta := \bigcup_{x \in A} \{ x' \in \mathcal{X} : d(x, x') < \delta \}$$

denotes the $\delta$-enlargement of $A$ under the metric $d$. Here $A_\delta$ corresponds to a variant of $\Gamma_{c \leq \delta}(A)$ defined in (8), in which the inequality sign “$\leq$” is replaced by the strict one “$<$” and the cost function $c$ is set to the metric $d$. It is well known that the Lévy–Prokhorov metric is compatible with the weak topology. Similarly, let $L_2$ be the Lévy–Prokhorov metric on $\mathcal{P}(\mathcal{Y})$. We additionally assume that the OT functional is uniformly continuous.

Assumption 3 (Uniform Continuity of OT Functional (UCOTF)). We assume that the optimal transport functional $(Q_X, Q_Y) \in \mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{Y}) \to \mathcal{E}(Q_X, Q_Y) \in [0, +\infty]$ is uniformly continuous, i.e.,

$$\lim_{\epsilon \downarrow 0} \sup_{Q_X', Q_Y', Q_X, Q_Y, L_1(Q_X', Q_X), L_2(Q_Y', Q_Y) \leq \epsilon} |\mathcal{E}(Q_X', Q_Y') - \mathcal{E}(Q_X, Q_Y)| = 0.$$ 

\(^4\)It can be shown that for any measurable $B$ in $\mathcal{X}^n$, $T_X \in P_n(\mathcal{X}) \to \text{Unif}(\ell^{-1}_1(T_X))(B) \in [0, 1]$ is measurable, which implies that $(T_X, B) \to \text{Unif}(\ell^{-1}_1(T_X))(B)$ is a Markov kernel (or transition probability). This Markov kernel is a regular conditional distribution of $P_X^{\otimes n}$ since $P_X^{\otimes n}$ is exchangeable (or permutation-invariant) and if the regular conditional distribution is not this Markov kernel then taking average of the permutation versions of this regular conditional distribution, we will get this Markov kernel (they are not equal up to a $\mu_n$-null set).

\(^5\)The existence of such a map for a continuous cost function follows from the measurable selection of optimal plans [5, Corollary 5.22].
Given \( \mathcal{X} \) and \( \mathcal{Y} \), the uniform continuity of \( \mathcal{E} \) is only determined by \( c \). The UCOTF is not necessarily satisfied in general, however, it indeed is satisfied for the following two cases.\(^6\)

1. (Countable Alphabet and Bounded Cost) \( \mathcal{X} \) and \( \mathcal{Y} \) are countable sets and \( c \) is bounded (i.e., \( \sup_{x,y} c(x, y) < \infty \)).
2. (Wasserstein Distance Induced by a Bounded Metric) \( \mathcal{X} = \mathcal{Y} \) is a Polish space equipped with a bounded metric \( d \), i.e., \( \sup_{x,y} d(x, y) < \infty \). The cost function \( c = d^p \) for \( p \geq 1 \). For this case, \( \mathcal{E} = W_p \).

For two distributions \( P,Q \) defined on the same space, we denote\(^7\) \( D(Q||P) := \int \log(\frac{dQ}{dP})dQ \) as the Kullback-Leibler (KL) divergence or relative entropy of \( Q \) from \( P \). We now state one of our main results in this paper, namely a LDP for Strassen’s OT problem.

**Theorem 4 (LDP for Strassen’s OT).** Under Assumptions 2 and 3, the following hold.

1. For \( \alpha < \mathcal{E}(P_X, P_Y) \), we have
   \[
   \lim_{n \to \infty} -\frac{1}{n} \log(1 - G^{(n)}_{\alpha}(P_X, P_Y)) = f(\alpha),
   \]
   where
   \[
   f(\alpha) := \inf_{Q_X \in \mathcal{P}(\mathcal{X}), Q_Y \in \mathcal{P}(\mathcal{Y}) : \mathcal{E}(Q_X, Q_Y) \leq \alpha} \max \{D(Q_X||P_X), D(Q_Y||P_Y)\}.
   \]

2. For \( \alpha > \mathcal{E}(P_X, P_Y) \), we have
   \[
   \lim_{\alpha \uparrow \mathcal{E}(P_X, P_Y)} g(\alpha') \leq \lim_{n \to \infty} -\frac{1}{n} \log G^{(n)}_{\alpha}(P_X, P_Y) \leq \lim_{n \to \infty} -\frac{1}{n} \log G^{(n)}_{\alpha}(P_X, P_Y) \leq g(\alpha),
   \]
   where
   \[
   g(\alpha) := \min \{g_{P_X, P_Y}(\alpha), g_{P_Y, P_X}(\alpha)\} \text{ with } g_{P_X, P_Y}(\alpha) \text{ defined as the infimum of } D(Q_X||P_X) \text{ over all } Q_X \in \mathcal{P}(\mathcal{X}) \text{ such that}
   \]
   \[
   \inf_{Q_Y \in \mathcal{P}(\mathcal{Y}) : D(Q_Y||P_Y) \leq D(Q_X||P_X)} \mathcal{E}(Q_X, Q_Y) > \alpha,
   \]
   and \( g_{P_Y, P_X}(\alpha) \) defined similarly.

It is easily verified that the function \( g \) in Theorem 4 is right-continuous. Furthermore, it is well known that the set of discontinuous points for a right-continuous function has Lebesgue measure zero. Hence \( g \) is continuous almost everywhere, which means that
\[
\lim_{n \to \infty} -\frac{1}{n} \log G^{(n)}_{\alpha}(P_X, P_Y) = g(\alpha) \text{ for almost every } \alpha \in (\mathcal{E}(P_X, P_Y), c_{\sup}).
\]

Theorem 4 bears a semblance to the classic LDP for the empirical mean of i.i.d. random variables; for the latter, see [14]. This is the reason why we call Theorem 4 as a theorem on the LDP for Strassen’s OT. Nevertheless, the exponents in our setting are different from, and more complicated than, those for the empirical mean of i.i.d. random variables, which is due to the additional minimization in (9) or the one in (10). Our proof is based on the nested formula in Theorem 3, Strassen’s dual formulation, and Sanov’s theorem. Besides these, some other specific techniques are also needed in our proof, for example, the splitting technique [16, 17]. Furthermore, the relative entropy \( D(\cdot||P) \) is the rate function for the LDP on the empirical measure, as stated in Sanov’s theorem [14, Theorem 6.2.10], which leads to the fact that relative entropies are involved in the expressions in Theorem 4.

Theorem 4 generalizes a result in [8]. In [8], the present author together with Tan only considered the finite alphabet case. For this case, by using the method of types, they derived the same expression for the LD exponent for the case of \( \alpha < \mathcal{E}(P_X, P_Y) \), but they only provided a bound for the case of \( \alpha > \mathcal{E}(P_X, P_Y) \).

---

\(^6\)By Lemma 10 in Appendix A, it is easy to show that UCOTF is satisfied for the first case. By [5, Corollary 6.13], UCOTF is satisfied for the second case. A special instance of Case 2 is \( (\mathbb{R}_+, d) \) with \( d(x, y) = \min\{\|x - y\|_q, C\} \) for \( q \geq 1 \) and a constant \( C > 0 \).

\(^7\)Throughout this paper, the base of log is \( e \).
1.2. Intuition of Main Result 1

In the following, we reveal some insights into the expressions in Theorem 4, from the perspective of the primal problem for the case of \( \alpha < \mathcal{E}(P_X, P_Y) \) and from the perspective of the dual problem for the case of \( \alpha > \mathcal{E}(P_X, P_Y) \). For brevity, we focus on the case of finite alphabets.

We first explain Theorem 4 for the case of \( \alpha < \mathcal{E}(P_X, P_Y) \). For a finite alphabet \( \mathcal{X} \), the number of possible empirical measures of sequences in \( \mathcal{X}^n \) is polynomial in \( n \) (more precisely, which is no larger than \( (n+1)^{|\mathcal{X}|} \)) [18]. This implies that every set \( A \subseteq \mathcal{P}(\mathcal{X}) \) which contains at least one empirical measure, has a dominant empirical measure \( T_X \in A \) for sufficiently large \( n \) in the sense that

\[
(n + 1)^{-|\mathcal{X}|} \mu_n(A) \leq \mu_n(T_X) \leq \mu_n(A). \tag{17}
\]

Furthermore, by Sanov’s theorem [14, Theorem 6.2.10], the law \( \mu_n \) of the empirical measure \( T_X^n \) of the i.i.d. sequence \( X^n \sim P_X^\otimes n \) (or \( Y^n \sim P_Y^\otimes n \)) satisfies a LDP with the relative entropy \( D(\cdot || P_X) \) as the rate function. Hence for a fixed set \( A \) not containing \( P_X \), the polynomial term \( (n + 1)^{-|\mathcal{X}|} \) in the left-hand side of (17) is dominated by the term \( \mu_n(A) \), since \( \mu_n(A) \) vanishes exponentially fast.

Observe that

\[
1 - \mathcal{G}_n^{(n)}(P_X, P_Y) = \sup_{\pi \in \Pi(\mu_n, \nu_n)} \pi\{(T_X, T_Y) : \mathcal{E}(T_X, T_Y) \leq \alpha\}
\]

and for any \( \pi \in \Pi(\mu_n, \nu_n) \),

\[
\pi\{(T_X, T_Y) : \mathcal{E}(T_X, T_Y) \leq \alpha\} = \sum_{T_X, T_Y : \mathcal{E}(T_X, T_Y) \leq \alpha} \pi\{(T_X, T_Y)\}
\]

\[
\leq \sum_{T_X, T_Y : \mathcal{E}(T_X, T_Y) \leq \alpha} \min\{\mu_n(T_X), \nu_n(T_Y)\}
\]

\[
= e^{n\alpha(1)} \max_{T_X, T_Y : \mathcal{E}(T_X, T_Y) \leq \alpha} \min\{\mu_n(T_X), \nu_n(T_Y)\}, \tag{18}
\]

where (18) follows since \( \mu_n(T_X) = \sum_{T_Y} \pi\{(T_X, T_Y)\} \) and \( \nu_n(T_Y) = \sum_{T_X} \pi\{(T_X, T_Y)\} \). Finally, expressing the exponents of \( \mu_n(T_X) \) and \( \nu_n(T_Y) \) by relative entropies \( D(\cdot || P_X) \) and \( D(\cdot || P_Y) \), we obtain \( f(\alpha) \). Hence the exponent in (14) is lower bounded by \( f(\alpha) \). Moreover, the exponent of the upper bound (19) is attained by some coupling \( \pi \in \Pi(\mu_n, \nu_n) \). Let \( (T_X^*, T_Y^*) \) be an optimal pair that attains the maximum in (19). We construct \( \pi \in \Pi(\mu_n, \nu_n) \) such that

\[
\pi\{(T_X^*, T_Y^*)\} = \min\{\mu_n(T_X^*), \nu_n(T_Y^*)\},
\]

which ensures that the exponent of the upper bound in (19) is asymptotically attained by such a coupling \( \pi \). Hence, the exponent in (14) is also upper bounded by \( f(\alpha) \). See the illustration for this case in Fig. 1a.

For the case of \( \alpha > \mathcal{E}(P_X, P_Y) \), the intuition behind the expression in (15) is less obvious, because it is difficult to construct an explicit coupling to asymptotically attain \( \mathcal{G}_n^{(n)}(P_X, P_Y) \). However, since \( \mathcal{G}_n^{(n)}(P_X, P_Y) \) can be rewritten in the form of Strassen’s duality (given in (12)), it suffices to construct an explicit (asymptotically) optimal solution to Strassen’s dual problem. As mentioned in the above case, the exponent of a set \( A \subseteq \mathcal{P}_n(\mathcal{X}) \) is asymptotically dominated by only one empirical measure \( T_X \) in it. Hence, it suffices to consider a singleton \( A = \{T_X\} \) for the optimization problem in (12). For such a singleton, the exponent of \( \mu_n(A) \) is \( D(T_X || P_X) \), and the exponent of \( \nu_n(\Gamma_{\mathcal{E} \leq \alpha}(A)) = \nu_n(T_Y : \mathcal{E}(T_X, T_Y) \leq \alpha) \) is \( \min_{T_Y : \mathcal{E}(T_X, T_Y) \leq \alpha} D(T_Y || P_Y) \). To maximize \( \mu_n(A) - \nu_n(\Gamma_{\mathcal{E} \leq \alpha}(A)) \), it suffices to consider \( A \) such that

\[
\min_{T_Y : \mathcal{E}(T_X, T_Y) \leq \alpha} D(T_Y || P_Y) > D(T_X || P_X), \tag{20}
\]

On the other hand, \( \mu_n(A) \) will be exponentially larger than \( \nu_n(\Gamma_{\mathcal{E} \leq \alpha}(A)) \), if the left-hand side in (20) is upper bounded away from the right-hand side in (20). Hence, roughly speaking, in this case the exponent of \( \mathcal{G}_n^{(n)}(P_X, P_Y) \) is the minimum of \( D(T_X || P_X) \) over all \( T_X \) satisfying (20). Observe that the condition in (20) is equivalent to the condition in (16), which implies that the exponent of \( \mathcal{G}_n^{(n)}(P_X, P_Y) \) is sandwiched between \( \lim_{\alpha \to \alpha} g_{P_X, P_Y}(\alpha') \) and \( g_{P_X, P_Y}(\alpha) \). However, in some cases, \( \mu_n(A) - \nu_n(\Gamma_{\mathcal{E} \leq \alpha}(A)) \) is maximized by a set \( A \) such that both \( \mu_n(A) \) and \( \nu_n(\Gamma_{\mathcal{E} \leq \alpha}(A)) \) approach one. For this case, the quantities \( \lim_{\alpha \to \alpha} g_{P_X, P_Y}(\alpha') \) and \( g_{P_X, P_Y}(\alpha) \) do not correspond to the exponent of the
difference $\mu_n(A) - \nu_n(\Gamma_{\leq \alpha}(A))$ any more. In fact, the exponent for this case is sandwiched between the counterparts $\lim_{\alpha' \uparrow \alpha} g_{P_Y, P_X}(\alpha')$ and $g_{P_Y, P_X}(\alpha)$. Hence, in a word, the exponent of $G^{(n)}(P_X, P_Y)$ is indeed sandwiched between $\lim_{\alpha' \uparrow \alpha} g(\alpha')$ and $g(\alpha)$. See the illustration for this case in Fig. 1b.

To further illustrate our results, the binary example is given in Section 2.

1.3. Main Result 2: Moderate Deviations Principle

In addition to the large deviations regime, we also consider the moderate deviations regime and central limit regime in the Strassen’s OT problem, in both of which the parameter $\alpha$ is allowed to vary with $n$ as $n$ going to infinity. For simplicity, in these two regimes, we only consider the case in which $\mathcal{X}$ and $\mathcal{Y}$ are finite sets. Without loss of generality, we assume $\mathcal{X} = \{1, 2, ..., M\}$ and $\mathcal{Y} = \{1, 2, ..., N\}$ for some positive integers $M, N$, and also assume that $\mathcal{X}$ and $\mathcal{Y}$ are respectively the supports of $P_X$ and $P_Y$. We now introduce a moderate deviations principle (MDP) for Strassen’s OT problem, in which we set $\alpha$ to $\alpha_n = \mathcal{E}(P_X, P_Y) + \Delta/\sqrt{na_n}$ for a positive sequence $\{a_n\}$ satisfying $a_n \to 0$ and $na_n \to \infty$ as $n \to \infty$. We characterize the limit of $-a_n \log(1 - G^{(n)}_{\alpha_n}(P_X, P_Y))$ for $\Delta < 0$, and the limit of $-a_n \log G^{(n)}_{\alpha_n}(P_X, P_Y)$ for $\Delta > 0$. These two limits are called moderate deviations (MD) exponents.
Assume $c$ is finite on the finite set $\mathcal{X} \times \mathcal{Y}$, i.e., $\max_{x,y} c(x,y) < \infty$. For this case, $\mathcal{P}(\mathcal{X})$ and $\mathcal{P}(\mathcal{Y})$ are probability simplices. Let $P_{X,Y}$ be an optimal coupling that attain $\mathcal{E}(P_X, P_Y)$. Denote $\mathcal{S}$ as the support of $P_{X,Y}$. Define the hyperplane

$$S_X := \left\{ \beta_X \in \mathbb{R}^{[X]} : \sum_x \beta_X(x) = 0 \right\},$$

(21)

which corresponds to the set of signed measures $\beta_X$ on $\mathcal{X}$ with total measure zero, i.e., $\beta_X(\mathcal{X}) = 0$. For $\mathcal{Y}$, define $S_Y$ similarly. For signed measures $\beta_X \in S_X$, $\beta_Y \in S_Y$, we define a functional

$$\theta(\beta_X, \beta_Y) := \min_{\beta_{XY} \in \Pi(\beta_X, \beta_Y)} \sum_{x,y} \beta_{XY}(x,y)c(x,y),$$

(22)

where $\Pi(\beta_X, \beta_Y)$ is the set of all signed (joint) measures on $\mathcal{X} \times \mathcal{Y}$ such that its $X$- and $Y$-marginals equal to $\beta_X$ and $\beta_Y$ respectively. By the strong duality in linear programming,

$$\theta(\beta_X, \beta_Y) = \max_{(\phi, \psi) \in D} \sum_x \phi(x)\beta_X(x) + \sum_y \psi(y)\beta_Y(y),$$

(23)

where

$$D := \{(\phi, \psi) \in \mathbb{R}^{[X]} \times \mathbb{R}^{[Y]} : \phi(x) + \psi(y) = c(x,y), \forall (x,y) \in \mathcal{S}, \phi(x) + \psi(y) \leq c(x,y), \forall (x,y) \in \mathcal{S}^c\}$$

is the set of optimal solutions to (2). In fact, $D$ is independent of the choice of $\mathcal{S}$, as long as $\mathcal{S}$ is the support of an optimal solution to the primal problem (1). This observation follows from the fact that if the strong duality holds (as in our case), then any pair of primal optimal solution and dual optimal solution forms a saddle point of the Lagrangian of the primal problem (1). Conversely, any saddle point of the Lagrangian must consist of primal optimal solution and dual optimal solution. In other words, the set of saddle points is the Cartesian product of the set of primal optimal solutions and the set of dual optimal solutions. See details on the page 239 of [19]. The formula in (23) coincides with the directional derivative given on the page 2771 of [20].

**Theorem 5 (MDP for Strassen’s OT).** Assume $\mathcal{X}$ and $\mathcal{Y}$ are finite, and $c$ is finite. Assume $c_0 := E(P_X, P_Y) \in (c_{\inf}, c_{\sup})$, where $c_{\inf}, c_{\sup}$ are defined in Assumption 2. Let $\{a_n\}$ be a positive sequence such that $a_n \to 0$ and $na_n \to \infty$ as $n \to \infty$. Then, the following hold.

1. If $\Delta < 0$, we have

$$\lim_{n \to \infty} -a_n \log(1 - G_{\beta_X + \Delta/\sqrt{n}}^{(n)}(P_X, P_Y)) = \hat{f}(\Delta),$$

where

$$\hat{f}(\Delta) := \min_{\beta_X \in S_X, \beta_Y \in S_Y : \theta(\beta_X, \beta_Y) \leq \Delta} \max\left\{ \frac{1}{2} \sum_x \beta_X(x)^2 P_X(x)^2, \frac{1}{2} \sum_y \beta_Y(y)^2 P_Y(y)^2 \right\}.$$

2. If $\Delta > 0$, we have

$$\lim_{\Delta \uparrow \Delta} \tilde{g}(\Delta') \leq \liminf_{n \to \infty} -a_n \log G_{\alpha_0 + \Delta/\sqrt{n}}^{(n)}(P_X, P_Y) \leq \limsup_{n \to \infty} -a_n \log G_{\alpha_0 + \Delta/\sqrt{n}}^{(n)}(P_X, P_Y) \leq \tilde{g}(\Delta),$$

where $\tilde{g}(\Delta) := \min\{\tilde{g}_{P_X, P_Y}(\Delta), \tilde{g}_{P_Y, P_X}(\Delta)\}$ with $\tilde{g}_{P_X, P_Y}(\Delta)$ defined as the minimum of $\frac{1}{2} \sum_x \beta_X(x)^2 P_X(x)$ over all $\beta_X \in S_X$ such that

$$\min_{\beta_Y \in S_Y : \sum_x \frac{\beta_X(x)^2}{P_X(x)} \leq \sum_y \frac{\beta_Y(y)^2}{P_Y(y)}} \theta(\beta_X, \beta_Y) > \Delta,$$

and $\tilde{g}_{P_Y, P_X}(\Delta)$ defined similarly.

---

Here we do not distinguish the signed measure $\beta_X$ and the function $x \mapsto \beta_X(\{x\})$, since $\beta_X$ is uniquely determined by the restriction $x \mapsto \beta_X(\{x\})$. We also denote $\beta_X(\{x\})$ as $\beta_X(x)$ for brevity.
Our proof relies on the MDP for the empirical measure, in which the rate function is $\beta \mapsto \frac{1}{2} \sum_x \frac{\beta(x)^2}{P(x)}$ (for the finite alphabet case). The characterizations of the MD exponents for Strassen’s OT problem are similar to the ones of the LD exponents, except that the relative entropies $D(Q_X \| P_X)$ and $D(Q_Y \| P_Y)$ are respectively replaced by $\frac{1}{2} \sum_x \frac{\beta_X(x)^2}{P_X(x)}$ and $\frac{1}{2} \sum_y \frac{\beta_Y(y)^2}{P_Y(y)}$, and the OT functional $\mathcal{E}(Q_X, Q_Y)$ is replaced by the functional $\theta(\beta_X, \beta_Y)$.

1.4. Main Result 3: Central Limit Theorem

For the central limit regime, we set $\alpha = \alpha_0 + \Delta/\sqrt{n}$ with $\alpha_0 = \mathcal{E}(P_X, P_Y)$, and study the asymptotic behavior of $G_{\alpha_0 + \Delta/\sqrt{n}}^{(n)}(P_X, P_Y)$. Similarly to the moderate deviations regime, $X$ and $Y$ are assumed to be finite (i.e., $X = \{1, 2, \ldots, M\}$ and $Y = \{1, 2, \ldots, N\}$) and also assumed to be respectively the supports of $P_X$ and $P_Y$. Assume $c$ is finite. Denote random variables $U_x = \mathbb{1}_{X=x}, x \in X$ with $X \sim P_X$. Denote $U = (U_x, x \in X)$ as a random vector. The mean and covariance of $U$ are respectively

$$\mathbb{E}[U] = (P_X(x))_{x \in X} \quad \text{and} \quad \text{Cov}(U) = \mathbb{E}[P_X(x)\mathbb{1}_{x=x'} - P_X(x)P_X(x')]_{(x,x') \in X^2}.$$

Define $\Phi_{P_X}$ as the Gaussian measure on $\mathbb{R}^{|X|}$ with zero mean and covariance $\text{Cov}(U)$. For $P_Y$, define $\Phi_{P_Y}$ similarly. Define a new Strassen’s OT problem as follows:

$$\Lambda_\Delta(P_X, P_Y) := \min_{\Psi \in \Pi(0,1)} \mathbb{E}\{\theta(\beta_X, \beta_Y) : \theta(\beta_X, \beta_Y) > \Delta\}$$

$$= \sup_{\text{closed } A \subseteq S_X, B \subseteq S_Y: \theta(\beta_X, \beta_Y) > \Delta} \Phi_{P_X}(A) + \Phi_{P_Y}(B) - 1$$

$$= \sup_{\text{compact } A \subseteq S_X} \Phi_{P_X}(A) - \Phi_{P_Y}(\Gamma_{\theta \leq \Delta}(A)).$$

where for $A \subseteq S_X$,

$$\Gamma_{\theta \leq \Delta}(A) := \bigcup_{\beta_Y \in A} \{\beta_Y \in S_Y : \theta(\beta_X, \beta_Y) \leq \Delta\}.$$

In Strassen’s OT problem in (24), the marginals are two Gaussian distributions and the cost function is the functional $(\beta_X, \beta_Y) \mapsto \theta(\beta_X, \beta_Y)$. Equations (25) and (26) follow by Strassen’s duality in Theorem 2. Recall the definition of $S_X$ in (21). In (25) and (26), “closed $A$, $B$” means that $A$ is closed in the space $S_X$ (i.e., under the weak topology, or equivalently, the relative topology) and $B$ is closed in $S_Y$. We bound the asymptotics of $G_{\alpha_0 + \Delta/\sqrt{n}}^{(n)}(P_X, P_Y)$ in the following theorem which is called the central limit theorem (CLT) for Strassen’s OT problem.

**Theorem 6** (CLT for Strassen’s OT). Assume $X$ and $Y$ are finite, and $c$ is finite. Assume $\alpha_0 := \mathcal{E}(P_X, P_Y) \in (\alpha_{\inf}, \alpha_{\sup})$. Then, we have

$$\Lambda_\Delta(P_X, P_Y) \leq \liminf_{n \to \infty} G_{\alpha_0 + \Delta/\sqrt{n}}^{(n)}(P_X, P_Y) \leq \limsup_{n \to \infty} G_{\alpha_0 + \Delta/\sqrt{n}}^{(n)}(P_X, P_Y) \leq \lim_{\Delta \uparrow \Delta} \Lambda_\Delta(P_X, P_Y).$$

Given $(P_X, P_Y)$, $\Lambda_\Delta(P_X, P_Y)$ is right-continuous in $\Delta$, which means that

$$\lim_{n \to \infty} G_{\alpha_0 + \Delta/\sqrt{n}}^{(n)}(P_X, P_Y) = \Lambda_\Delta(P_X, P_Y) \text{ for almost every } \Delta \in \mathbb{R}.$$

Furthermore, different from the CLT for empirical measures [21, Theorem 14.3], the CLT for Strassen’s OT here involves additional OT optimizations in every term in (27). These optimizations are taken over couplings of two empirical measures in the definition of $G_{\alpha_0 + \Delta/\sqrt{n}}^{(n)}(P_X, P_Y)$, and over couplings of two Gaussian measures in the definition of $\Lambda_\Delta(P_X, P_Y)$.

1.5. Connection to Empirical Optimal Transport

It is well known that for a pair of empirical measures $(T_X, T_Y)$, $\mathcal{E}(T_X, T_Y)$ is always attained by an empirical joint measure. In other words, if we define the empirical coupling set for a pair of empirical measures $(T_X, T_Y) \in \mathcal{P}_n(X) \times
\(\mathcal{P}_n(Y)\) as

\[
\Pi_n(T_X, T_Y) := \mathcal{P}_n(\mathcal{X} \times \mathcal{Y}) \cap \Pi(T_X, T_Y)
\]

(i.e., the set of couplings of \((T_X, T_Y)\) which is discrete and whose probability mass at each atom is a multiple of \(1/n\)), and define the empirical OT cost for \((T_X, T_Y) \in \mathcal{P}_n(\mathcal{X}) \times \mathcal{P}_n(\mathcal{Y})\) as

\[
\mathcal{E}_n(T_X, T_Y) := \min_{\mathcal{T}_{X,Y} \in \Pi_n(T_X, T_Y)} \mathcal{E}(X, Y) = \mathcal{E}(\mathcal{X}, \mathcal{Y}),
\]

then \(\mathcal{E}_n(T_X, T_Y)\) remains the same as \(\mathcal{E}(T_X, T_Y)\).

**Lemma 1 (Empirical OT).** [4, Page 5] For a pair of empirical measures \((T_X, T_Y) \in \mathcal{P}_n(\mathcal{X}) \times \mathcal{P}_n(\mathcal{Y})\) and for all \(n \geq 1\), we have

\[
\mathcal{E}_n(T_X, T_Y) = \mathcal{E}(T_X, T_Y).
\]

Such a result is a consequence of Birkhoff’s theorem [4, Page 5]. Combining this lemma and (13) yields the fact that characterizing the asymptotics of \(G^\omega_n(P_X, P_Y)\), as done in Sections 1.1-1.4, is equivalent to characterizing the asymptotic behavior of the (random) empirical OT cost \(\mathcal{E}_n(T_{X^n}, T_{Y^n})\) where \(T_{X^n}, T_{Y^n}\) are respectively the empirical measures of a pair of random vectors \((X^n, Y^n)\) that follows the optimal coupling of \((P_X^{\otimes n}, P_Y^{\otimes n})\) attaining the minimum in (9).

By definition, \(c_n(x^n, y^n) = \mathbb{E}(X, Y) = \min_{\mathcal{T}_{X,Y} \in \Pi_n(T_X, T_Y)} [e(X, Y)]\) for all \((x^n, y^n) \in \mathcal{X} \times \mathcal{Y}\). Hence, the empirical OT cost can be rewritten in the form of optimization over sequences, i.e., for two given sequences \(x^n\) and \(y^n\) whose empirical measures are respectively \(T_X\) and \(T_Y\), we have

\[
\mathcal{E}_n(T_X, T_Y) = \min_{\sigma} c_n(x^n, y^n), \quad (28)
\]

where the minimization is taken over all permutations \(\sigma\) on \(\{1, 2, ..., n\}\), and \(x^n_\sigma\) is the resultant sequence by permuting \(x^n\) according to \(\sigma\).

The minimization problem at the right-hand side of (28) is known as the optimal matching problem [22–23], the optimal value of which, as shown in (28), coincides with the empirical OT cost. If \(T_X, T_Y\) are set to the empirical measures of two independent random vectors \(X^n, Y^n\), each of which consists of i.i.d. components with a given distribution, i.e., \((X^n, Y^n) \sim P_X^{\otimes n} \otimes P_Y^{\otimes n}\) for some \(P_X\) and \(P_Y\), then the induced empirical OT cost \(\mathcal{E}_n(T_{X^n}, T_{Y^n})\) (or \(\min_{\sigma} c_n(X^n, Y^n)\)) is random as well. The asymptotic behavior of such \(\mathcal{E}_n(T_{X^n}, T_{Y^n})\) was widely studied in the literature; see for example [7, 10, 20, 22–32]. In contrast, in our setting, specifically in (9) or (13), the random vectors \(X^n, Y^n\) are not necessarily independent. More precisely, their joint distribution is implicitly specified by the minimization in (9) or (13) which is rather difficult to solve. Hence, our setting is more complicated.

The LDP and MDP of the empirical OT cost were investigated in [33]. In [33, Theorem 3.1], Ganesh and O’Connell showed that in the large deviation regime, the rate function of the empirical Wasserstein distance \(W_1(T_{X^n}, T_{Y^n})\) with \((X^n, Y^n) \sim P_X^{\otimes n} \otimes P_Y^{\otimes n}\) is \(I : t \in \mathbb{R} \mapsto \inf_{Q \in \mathcal{M}(\mathcal{X}, \mathcal{Y})} D(Q_X \| P_X^n) + D(Q_Y \| P_Y^n)\). This result is intuitive from Sanov’s theorem, since \((X^n, Y^n) \sim P_X^{\otimes n} \otimes P_Y^{\otimes n}\) and hence the rate function of the empirical joint measure is the sum of the one of the empirical measure induced by \(P_X^{\otimes n}\) and the one induced by \(P_Y^{\otimes n}\). A similar rate function for the MDP was also derived in [33], but with the relative entropy replaced by the half of the \(\chi^2\)-divergence. As for the central limit regime, Tameling, Sommerfeld, and Munk [7, 20] derived the limit law for the \(\sqrt{n}\)-scaled version of the empirical Wasserstein distance for \(P_X, P_Y\) defined on the same countable metric space \((\mathcal{X}, d)\). They showed that the limit law is not Gaussian in general, but it indeed is if the optimal solution (also known as the Kantorovich potential) to the Kantorovich dual problem in (3) (or (2)) is unique. del Barrio and Loubes [28] derived a similar central limit theorem for the quadratic empirical Wasserstein distance which shows that the limit law is Gaussian as well, if the distributions \(P_X, P_Y\) are distinct, absolutely continuous (with respect to the Lebesgue measure in the Euclidean space), and have moments of order \(4 + \delta\) for some \(\delta > 0\) and positive densities on their convex supports. These assumptions ensure that the optimal solution to the dual problem in (3) is unique, which in turn implies that del Barrio and Loubes’s results are consistent with Tameling, Sommerfeld, and Munk’s. The case when \(P_X = P_Y\) is the uniform distribution on the unit hypercube was investigated widely in the literature; see [22–25, 27]. The case of \(P_X = P_Y\) was extended to other atomless measures on Euclidean spaces in [29–32]. For these cases, the order of the empirical Wasserstein distance is strictly larger than \(\sqrt{n}\), which is hence different from the countable case in [7, 20] and the \(P_X \neq P_Y\) case in [28]. In other words, the asymptotic behavior of the empirical Wasserstein distance in the central limit regime is sensitive to the factors whether \(P_X\) and \(P_Y\) are identical and whether \(P_X\) and \(P_Y\) are countably supported. See relevant discussions in the introduction parts of [20, 28].
All the LDP, MDP, and CLT results mentioned above for the empirical Wasserstein distance are different from our results, since in these results, the (random) empirical measures are independent, while in our results, they are not. Even so, the convergence orders in our results remain the same as the ones in these results under the same settings. It is worth noting that in all of the related works mentioned above, the Kantorovich duality plays a crucial role. In addition, instead of studying the asymptotic behavior of the OT cost, Gozlan and Léonard [34] regarded the theory of large deviation as a tool, and applied it to derive new transportation cost inequalities.

Under the product distribution $P_X^n \otimes P_Y^n$, the (random) empirical measures $T_{X^n}$ of $X^n$ and $T_{Y^n}$ of $Y^n$ are independent, which means that the joint law of $(T_{X^n}, T_{Y^n})$ for this case is $\mu_n \otimes \nu_n$. Obviously, $\mu_n \otimes \nu_n$ is a coupling of $\mu_n$ and $\nu_n$. On the other hand, in the nested formula in (10), we minimize the probability of the event $\{(Q_X, Q_Y) : \mathcal{E}(Q_X, Q_Y) > \alpha\}$ over all couplings of $\mu_n$ and $\nu_n$. Hence,

$$G^{(n)}_\alpha(P_X, P_Y) \leq (\mu_n \otimes \nu_n)\{(Q_X, Q_Y) \in \mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{Y}) : \mathcal{E}(Q_X, Q_Y) > \alpha\}$$

$$= \mathbb{P}(X^n, Y^n) \sim P_X^n \otimes P_Y^n \{\mathcal{E}(T_{X^n}, T_{Y^n}) > \alpha\}. \quad (29)$$

Determining the asymptotics of the probability in (29) is just the empirical OT problem mentioned above, which involves only one OT problem in Monge–Kantorovich’s sense. In contrast, besides Monge–Kantorovich’s OT problem which acts as the inner subproblem, our nested formula also involves Strassen’s OT problem which acts the outer subproblem. By (29), our results in this paper form lower bounds for the empirical OT problem.

1.6. Applications

Beyond the theoretical interest of the problem, we would like to emphasize the potential impact on information-theoretic applications of our results. Here we provide an application to the covert reconstruction problem in information-theoretic security [8, 35–38]. Consider two terminals: a (legitimate) user and an eavesdropper. The user observes a stationary memoryless stochastic process (also known as a source) $\{X_i\}$ with each $X_i \sim P_X$, and he/she wants to produce a reconstruction process $\{\tilde{X}_i\}$, i.e., a distorted version of the source. However, the reconstruction device is being overheard by an eavesdropper all the time, no matter whether the source is being reconstructed or not. When nothing is being reconstructed, the process overhead by the eavesdropper is assumed to be another stationary memoryless stochastic process (white noise or a meaningless signal used to confuse the eavesdropper) $\{Y_i\}$ with each $Y_i \sim P_Y$. The eavesdropper aims at detecting whether there is a source being reconstructed at the current time according to the distribution of the process he/she is observing. Specifically, if the process that he/she is observing follows a distribution distinct from the one of $\{Y_i\}$, then he/she will claim that the source is being reconstructed; otherwise, he/she will claim that the source is not being reconstructed. To avoid the eavesdropper to detect the reconstruction successfully, the reconstruction of $\{X_i\}$ produced by the user must follow the distribution same as $\{Y_i\}$. If we consider the cost function $c$ as a measure of distortion, then the excess-cost probability is a measure of distortion as well. In fact, the excess-cost probability is also known as the excess-distortion probability, which is an important measure of distortion in information theory. For the covert reconstruction problem above, what is the minimum excess-distortion probability? It is easily checked that the minimum excess-distortion probability for the first $n$ random variables of the source is $g_{\alpha}^{(n)}(P_X, P_Y)$. Hence, our results characterize the asymptotic behavior of the excess-distortion probability for this problem. Furthermore, other applications of the optimization problems over couplings to information theory can be found in [8].

1.7. Notations and Organization

As mentioned at the beginning of the introduction, $(\mathcal{X}, \tau_1)$ and $(\mathcal{Y}, \tau_2)$ are Polish spaces, and $P_X$ and $P_Y$ are two probability measures (or distributions) defined respectively on $\mathcal{X}$ and $\mathcal{Y}$. Here $P_X$ and $P_Y$ can be thought of as the distributions of two random variables respectively taking values in $\mathcal{X}$ and $\mathcal{Y}$. We use $P_X \otimes P_Y$ to denote the product of $P_X$ and $P_Y$, and $P_X^n$ (resp. $P_Y^n$) to denote the $n$-fold product of $P_X$ (resp. $P_Y$). Throughout this paper, for a topological space $(Z, \tau)$, we use $\Sigma(Z, \tau)$ or simply $\Sigma(Z)$ to denote the Borel $\sigma$-algebra on $Z$ generated by the topology $\tau$. Hence $(Z, \Sigma(Z))$ forms a measurable space. For this measurable space, we denote the set of probability measures on $(Z, \Sigma(Z))$ as $\mathcal{P}(Z, \Sigma(Z))$ or simply $\mathcal{P}(Z)$. If we equip $\mathcal{P}(Z)$ with the weak topology, then the resultant space is a Polish space as well. For brevity, we also denote it as $\mathcal{P}(Z, \Sigma(\mathcal{P}(Z)))$.

We denote $x^n = (x_1, x_2, \ldots, x_n) \in \mathcal{X}^n$ as a sequence in $\mathcal{X}^n$. We use $T_X$ and $T_Y$ to respectively denote empirical measures of sequences in $\mathcal{X}^n$ and $\mathcal{Y}^n$, and $T_{XY}$ to denote an empirical joint measure of a pair of sequences in $\mathcal{X}^n \times \mathcal{Y}^n$. We denote $\ell_1 : x^n \in \mathcal{X}^n \mapsto T_{X^n}$ and $\ell_2 : y^n \in \mathcal{Y}^n \mapsto T_{Y^n}$ as the empirical measure functions, and denote $\ell : (x^n, y^n) \in \mathcal{X}^n \times \mathcal{Y}^n \mapsto T_{x^n, y^n}$ as the joint empirical measure function. For $P_X \in \mathcal{P}(\mathcal{X})$, denote $\mu_n$ as the law of the empirical
measure $\ell_1(X^n)$ of $X^n \sim P^n$, which means that $\mu_n$ is the push-forward measure $\mu_n = P_X^{\otimes n} \circ \ell_1^{-1}$. Obviously, $\mu_n$ is concentrated on $P_n(X)$. Similarly, for $P_Y \in \mathcal{P}(Y)$, denote $\nu_n$ as the law of the empirical measure of $Y^n \sim P_Y^{\otimes n}$.

We use $B_\delta(z) := \{ z' \in Z : d(z, z') < \delta \}$ and $B_{\leq \delta}(z) := \{ z' \in Z : d(z, z') \leq \delta \}$ to respectively denote an open ball and a closed ball. We use $A$, $A^c$; and $A^c := Z \setminus A$ to respectively denote the closure, interior, and complement of the set $A$. Denote the sublevel set of the relative entropy (or the divergence “ball”) as $D_{\leq \epsilon}(P_X) := \{ Q_X : D(Q_X \| P_X) \leq \epsilon \}$ for $\epsilon \geq 0$. As defined above, the Lévy–Prokhorov metric on $\mathcal{P}(X)$ is $L_1(Q_X, Q_Y) = \inf\{ \delta : Q_X(A) \leq Q_Y(A_{\leq \delta}) + \delta, \forall$ closed $A \subseteq X\}$, which is compatible with the weak topology. This metric, the TV distance, and the relative entropy admit the following relation: For any $Q_X, P_X$,

$$\sqrt{2D(Q_X \| P_X)} \geq \| Q_X - P_X \| \geq L_1(Q_X, P_X),$$

which implies for $\epsilon \geq 0$,

$$D_{\leq \sqrt{\epsilon}}(P_X) \subseteq B_{\leq \epsilon}(P_X).$$

The first inequality in (30) is known as Pinsker’s inequality, and the second inequality follows by definition.

We use $f(n, x) = a_n |x|$ (1) to denote that given each $x$, $f(n, x) \to 0$ pointwise as $n \to +\infty$. We denote $\inf \emptyset := +\infty$, $\sup \emptyset := -\infty$, and $[k] := \{1, 2, \ldots, k\}$. We denote $\| \cdot \|_q$ as the $\ell_q$-norm.

This paper is organized as follows. In Section 2, we first provide the binary example to further illustrate our main results. In Section 3-6, we provide the proofs for the nested formula and the LDP, MDP, and CLT results, respectively. Besides, some basic lemmas are provided in Appendix A, and the proofs of some other useful lemmas are provided in Appendices B and C.

2. Binary Example

To further illustrate our main results, we now focus on the binary alphabet case, i.e., $X = Y = \{0, 1\}$. We assume $P_X = \text{Bern}(a)$ and $P_Y = \text{Bern}(b)$, where $0 \leq a \leq b \leq 1$. Consider the Hamming distance as the cost function, i.e., $c(x, y) = \mathbb{1}_{x \neq y}$. For this case, by (5), $E(Q_X, Q_Y)$ coincides with the TV distance between $Q_X, Q_Y$. For the case $a = b$, $G_\alpha^n(P_X, P_Y)$ is attained by the identity coupling $P_X^{\otimes n}(x^n) \mathbb{1}_{y^n = x^n}$, and for this case, $G_\alpha^n(P_X, P_Y) = \mathbb{1}_{a < \alpha}$ holds for all $n \geq 1$. In the following, we focus on the case $0 \leq a < b \leq 1$, and apply Theorems 4, 5, and 6 to this case. We obtain explicit expressions or bounds for the asymptotics of $G_\alpha^n(P_X, P_Y)$ in large deviations, moderate deviations, and central limit regimes.

2.1. Large Deviations Principle

For distributions $Q_X = \text{Bern}(a')$ and $Q_Y = \text{Bern}(b')$, we have

$$E(Q_X, Q_Y) = \min_{P_{XY} \in \Pi(Q_X, Q_Y)} \mathbb{E}[c(X, Y)] = \|b' - a'\|.$$

The minimum in $E(Q_X, Q_Y)$ is uniquely attained by

$$Q_{XY} = \begin{cases} \begin{bmatrix} b' & -a' \\ 0 & a' \end{bmatrix}, & a' \leq b', \\ \begin{bmatrix} a' & 0 \\ a' - b' & 0 \end{bmatrix}, & a' > b'. \end{cases}$$

Here for a number $t \in [0, 1]$, we define $\overline{t} := 1 - t$.

Setting $a' \leftarrow a, b' \leftarrow b$ in (32), we obtain $E(P_X, P_Y) = b - a$ and the minimum in $E(P_X, P_Y)$ is uniquely attained by $P_{XY} = \begin{bmatrix} b - a \\ a \end{bmatrix}$. For $a', a \in [0, 1]$, denote $D(a' \| a) := D(\text{Bern}(a') \| \text{Bern}(a))$. We have the following corollary to Theorem 4.

**Corollary 1** (LDP for Binary OT). Given two Bernoulli distributions $P_X = \text{Bern}(a)$ and $P_Y = \text{Bern}(b)$ with $0 \leq a < b \leq 1$, we have:
1. If $0 < \alpha < b - a$, then
\[
\lim_{n \to \infty} -\frac{1}{n} \log(1 - G_{\alpha}^{(n)}(P_X, P_Y)) = D(a^*\|a),
\]
where $a^*$ denotes the unique solution to the equation $D(a' + \alpha\|b) = D(a'\|a)$ in $[a, b - \alpha]$ with $a'$ unknown.

2. If $b - a < \alpha < 1$, then (15) with $g(\alpha) = \min\{D(a^*\|a), D(b^*\|b)\}$ holds, where $a^*$ denotes the maximum of the two solutions to the equation $D(a' + \alpha\|b) = D(a'\|a)$ (with $a'$ unknown) such that $0 < a' \leq b - \alpha$ (if there is only one or no such solution, then $D(a^*\|a) := +\infty$), and $b^*$ denotes the minimum of the two solutions to the equation $D(b'\|b) = D(b' - \alpha\|a)$ (with $b'$ unknown) such that $a + \alpha \leq b' < 1$ (if there is only one or no such solution, then $D(b^*\|b) := +\infty$).

**Proof.** The first statement of this corollary follows by observing that
\[
f(\alpha) = \min_{a', b':|b' - a'| \leq \alpha} \max\{D(b'\|b), D(a'\|a)\}
= \min_{a' \in [a, b - \alpha]} \max\{D(a' + \alpha\|b), D(a'\|a)\}
= D(a^*\|a).
\]

We next prove the second statement. Observe that
\[
g_{P_X, P_Y}(\alpha) = \inf_{a'} D(a'\|a)\tag{33}
\]
where the infimum is taken over all $a'$ such that $\min_{b':D(b'\|b) \leq D(a'\|a)} |b' - a'| > \alpha$, or equivalently, $\min_{b':|b' - a'| \leq \alpha} D(b'\|b) > D(a'\|a)$. It is easily seen that the optimal $a'$ attaining the infimum in (33) is no greater than $b - \alpha$, and for this case, $\min_{b':|b' - a'| \leq \alpha} D(b'\|b) = D(a' + \alpha\|b)$. Hence,
\[
g_{P_X, P_Y}(\alpha) = \inf_{a' \leq b - \alpha; D(a' + \alpha\|b) > D(a'\|a)} D(a'\|a).
\]

However, if $\alpha > b$, then $g_{P_X, P_Y}(\alpha) = +\infty$. If there are two solutions to the equation $D(a' + \alpha\|b) = D(a'\|a)$ (with $a'$ unknown) such that $0 < a' \leq b - \alpha$, then $g_{P_X, P_Y}(\alpha) = D(a^*\|a)$ where $a^*$ is the maximum among the two solutions. If there is only one or no solution, then $g_{P_X, P_Y}(\alpha) = +\infty$.

Similarly,
\[
g_{P_Y, P_X}(\alpha) = \inf_{b' \geq a + \alpha; D(b' - \alpha\|a) > D(b'\|b)} D(b'\|b).
\]

For the case $\alpha > 1 - a$, then $g_{P_Y, P_X}(\alpha) = +\infty$. If there are two solutions to the equation $D(b'\|b) = D(b' - \alpha\|a)$ (with $b'$ unknown) such that $b - \alpha \leq b' < 1$, then $g_{P_Y, P_X}(\alpha) = D(b^*\|b)$ where $b^*$ is the minimum among the two solutions. If there is only one or no solution, then $g_{P_Y, P_X}(\alpha) = +\infty$.

Corollary 1 is illustrated in Fig. 2a.

### 2.2. Moderate Deviations Principle

We now focus on the moderate deviation regime. Let $P_X = \text{Bern}(a)$ and $P_Y = \text{Bern}(b)$ with $0 < a < b < 1$, and $\beta_X = (-a', a')$ and $\beta_Y = (-b', b')$. For this case, $\frac{1}{2} \sum_x \frac{\beta_X(x)^2}{P_X(x)} = \frac{a^2}{2(a - a')}$, $S = \{(0, 0), (1, 1), (0, 1)\}$, and
\[
\theta(\beta_X, \beta_Y) = \min_{\beta_{XY} \in \Pi(\beta_X, \beta_Y), \sum_{x,y} \beta_{XY}(x, y)c(x, y) = b' - a'} \sum_{x,y} \beta_{XY}(x, y)c(x, y) = b' - a'.
\]

We have the following corollary to Theorem 5. The proof is similar to that of Corollary 1, and hence omitted here.

**Corollary 2 (MDP for Binary OT).** Let $P_X = \text{Bern}(a)$ and $P_Y = \text{Bern}(b)$ with $0 < a < b < 1$. Let $\alpha_0 = b - a$. Let $\{a_n\}$ be a positive sequence such that $a_n \to 0$ and $na_n \to \infty$ as $n \to \infty$. The following hold.
1. If $\Delta < 0$, then
\[
\lim_{n \to \infty} -a_n \log(1 - G^{(n)}_{\alpha_0 + \Delta / \sqrt{n} a_n}(P_X, P_Y)) = \frac{1}{2} \left( \frac{\Delta}{\sqrt{a - a^2 + \sqrt{b - b^2}}} \right)^2.
\]
2. If $\Delta > 0$, then
\[
\lim_{n \to \infty} -a_n \log G^{(n)}_{\alpha_0 + \Delta / \sqrt{n} a_n}(P_X, P_Y) = \frac{1}{2} \left( \frac{\Delta}{\sqrt{b - b^2 - \sqrt{a - a^2}}} \right)^2.
\]
Corollary 2 is illustrated in Fig. 2b.

2.3. Central Limit Theorem

Recall the definition of $U$ in Subsection 1.4. For the binary case, $\mathbb{E}[U] = (1 - a, a)$ and $\text{Cov}(U) = (a - a^2) \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$.

Denote $\sigma^2_X := \text{Var}(U_0) = a - a^2$. The probability density function of $U_0 \sim \Phi_{U_0} := \mathcal{N}(0, \sigma^2_X)$ is
\[
\phi_X(a') = \frac{1}{\sqrt{2\pi}\sigma_X^2} e^{-\frac{a'^2}{2\sigma_X^2}},
\]
and the cumulative distribution function is
\[ F_X(a') = \int_{-\infty}^{a'} \phi_X(t)dt. \]

For \( P_Y \), define \( \sigma_Y^2 \), \( \Phi_{V_0} \), \( \phi_Y \), and \( F_Y \) similarly. Observe that \( U_0 + U_1 = 1 \). Hence \( \Phi_{P_X} \) is determined by \( F_X \). Similarly, \( \Phi_{P_Y} \) is determined by \( F_Y \). Hence by (26), we have
\[
A_\Delta(P_X, P_Y) = \sup_{\text{closed } A' \subseteq \mathbb{R}} \Phi_{U_0}(A') - \Phi_{V_0}(\bigcup_{a' \in A'} (-\infty, a' + \Delta])
\]
\[
= \sup_{a'} F_X(a') - F_Y(a' + \Delta),
\]
where (34) follows since the difference \( \Phi_{U_0}(A') - \Phi_{V_0}(\bigcup_{a' \in A'} (-\infty, a' + \Delta]) \) is maximized only when \( A' = (-\infty, a'] \) for some \( a' \in \mathbb{R} \).

To compute the optimal value of \( a' \) in (34), we need the following lemma, which is derived by simple algebraic manipulations and hence whose proof is omitted.

**Lemma 2.** If \( \sigma_X^2 = \sigma_Y^2 \), then \( a' = -\Delta/2 \) is the unique solution to the equation
\[
\phi_X(a') = \phi_Y(a' + \Delta). \tag{35}
\]

If \( \sigma_X^2 \neq \sigma_Y^2 \), then the equation (35) has two solutions:
\[
a' = \frac{-\sigma_X \Delta \pm \sigma_X \sigma_Y \sqrt{\Delta^2 + 2(\sigma_X^2 - \sigma_Y^2) \log \frac{\sigma_X}{\sigma_Y}}}{\sigma_X^2 - \sigma_Y^2}.
\]

If \( a = b \) or \( a + b = 1 \), then \( \sigma_X^2 = \sigma_Y^2 \). By the lemma above, for this case, \( a' = -\Delta/2 \) is the unique solution of (35). Hence for this case,
\[
A_\Delta(P_X, P_Y) = \begin{cases} F_X(-\Delta/2) - F_Y(\Delta/2) & \Delta \leq 0 \\ 0 & \Delta > 0 \end{cases}.
\]

If \( a \neq b \) and \( a + b \neq 1 \), then the equation (35) has two solutions. Denote them respectively as \( a'_1(\Delta) \) and \( a'_2(\Delta) \) such that \( a'_1(\Delta) \leq a'_2(\Delta) \). If additionally \( a(1 - a) \leq b(1 - b) \), then \( a'_2(\Delta) \) is the maximizer for the supremum in (34), which implies that \( A_\Delta(P_X, P_Y) = F_X(a'_2(\Delta)) - F_Y(a'_2(\Delta) + \Delta) \). Similarly, if \( a(1 - a) > b(1 - b) \), then \( A_\Delta(P_X, P_Y) = F_X(a'_1(\Delta)) - F_Y(a'_1(\Delta) + \Delta) \). Hence, we have the following corollary to Theorem 6.

**Corollary 3 (CLT for Binary OT).** Let \( P_X = \text{Bern}(a) \) and \( P_Y = \text{Bern}(b) \) with \( 0 < a < b < 1 \). Let \( \alpha_0 = b - a \). Then, we have
\[
\lim_{n \to \infty} G^{(n)}_{\alpha_0 + \Delta/\sqrt{n}}(P_X, P_Y) = \begin{cases} (F_X(-\Delta/2) - F_Y(\Delta/2))1_{\Delta \leq 0} & a = 1 - b \\ F_X(a'_2(\Delta)) - F_Y(a'_2(\Delta) + \Delta) & a < 1 - b \\ F_X(a'_1(\Delta)) - F_Y(a'_1(\Delta) + \Delta) & a > 1 - b \end{cases}.
\]

Corollary 3 is illustrated in Fig. 2c.

### 3. Proof of Theorem 3

In this section, we prove Theorem 3. It suffices to prove that \( G^{(n)}(P_X, P_Y) \) is equal to the expression in (11) since the other two expressions follow by Strassen’s duality in Theorem 2. More specifically, note that since \( \mathcal{X} \) is Polish, the space \( \mathcal{P}(\mathcal{X}) \) with the weak topology is also Polish [15, Theorem 6.2 and Theorem 6.5]. Similarly, \( \mathcal{P}(\mathcal{Y}) \) with the weak topology is Polish as well. On the other hand, by Lemma 7 in Appendix A, \( (Q_X, Q_Y) \to \mathcal{E}(Q_X, Q_Y) \) is lower semi-continuous. Assumption 1 implies that \( \{(Q_X, Q_Y) : \mathcal{E}(Q_X, Q_Y) > \alpha \} \) is nonempty. Applying Strassen’s duality in Theorem 2, we obtain (10) and (12).
We next that $\mathcal{G}^{(\alpha)}_n(P_X, P_Y)$ is equal to the expression in (11). By the Kantorovich duality in Theorem 1 and the fact that Strassen’s OT problem is a special case of Monge–Kantorovich’s OT problem, it is not difficult to show that Strassen’s OT problem also admits the following duality; see [4, Proof of Theorem 1.27].

$$
\mathcal{G}^{(\alpha)}_n(P_X, P_Y) = \sup_{(\phi, \psi) \in \Psi} \int_{\mathcal{X}^n} \phi \, dP_X^\otimes \mathcal{X} + \int_{\mathcal{Y}^n} \psi \, dP_Y^\otimes \mathcal{Y}
$$  

(36)

where $\Psi$ is the set of all pairs $(\phi, \psi) \in L^1_\alpha(\mathcal{X}^n) \times L^1_\alpha(\mathcal{Y}^n)$ such that

\[
\begin{aligned}
\phi(x^n) + \psi(y^n) &\leq 1_{c_\alpha > 0}(x^n, y^n), \forall (x^n, y^n), \\
0 &\leq \phi \leq 1, \quad -1 \leq \psi \leq 0, \\
\phi &\text{ is upper semi-continuous.}
\end{aligned}
\]

Note that $\Psi$ is convex.

Observe that $P_X^\otimes n$, $P_Y^\otimes n$, and $c_n$ are permutation-invariant (or $n$-symmetric) in the sense that for any permutation $\sigma$ of $[n]$, it holds that $P_X^\otimes n = P_X^\otimes n \circ \sigma^{-1}$, $P_Y^\otimes n = P_Y^\otimes n \circ \sigma^{-1}$, and $c_n = c_n \circ (\sigma^{-1}, \sigma^{-1})$. Hence, we can additionally assume $(\phi, \psi)$ is also permutation-invariant, since otherwise, we can take average of $(\phi, \psi)$ over all permutation $\sigma$ of $[n]$. We denote $\overline{\Psi}$ as the set of $(\phi, \psi) \in \Psi$ such that $(\phi, \psi)$ is permutation-invariant (i.e., $(\phi, \psi) = (\phi, \psi) \circ (\sigma^{-1}, \sigma^{-1})$ for any $\sigma$). Note that $\overline{\Psi}$ is still convex. Moreover, $\overline{\Psi}$ can be represented as a convex combination of pairs of indicators of measurable subsets. Here a set $A$ is said to be permutation-invariant if $x^n \in A$ if and only if its arbitrary permutations belong to $A$ as well.

**Lemma 3.** [4, Proof of Theorem 1.27] $\overline{\Psi}$ can be represented as a convex combination of pairs of the form $(1_A, -1_B)$ for permutation-invariant and measurable $A \subseteq \mathcal{X}^n$, $B \subseteq \mathcal{Y}^n$ such that $A$ is closed and $1_A(x^n) + 1_B(y^n) \leq 1_{c_\alpha > 0}(x^n, y^n)$, $\forall (x^n, y^n)$.

An original version of this lemma without the “permutation-invariant” condition was proven in [4, Proof of Theorem 1.27] by using the “layer cake representation”. It is easy to check that the proof still works when we impose the “permutation-invariant” condition.

By the lemma above and observing that the objective function in (36) is linear in $(\phi, \psi)$, we can rewrite (36) as

$$
\mathcal{G}^{(\alpha)}_n(P_X, P_Y) = \sup_{A, B} P_X^\otimes n(A) + P_Y^\otimes n(B),
$$

where the supremaization is taken over all pairs of permutation-invariant $A \in \Sigma(\mathcal{X}^n)$, $B \in \Sigma(\mathcal{Y}^n)$ such that

\[
\begin{aligned}
1_A(x^n) + 1_B(y^n) &\leq 1_{c_\alpha > 0}(x^n, y^n), \forall (x^n, y^n) \\
A &\text{ is closed.}
\end{aligned}
\]

Recall that $\ell_1 : x^n \in \mathcal{X}^n \rightarrow T_{\mathcal{X}^n}$ and $\ell_2 : y^n \in \mathcal{Y}^n \rightarrow T_{\mathcal{Y}^n}$ denote the empirical measure functions. Then, any permutation-invariant sets $A, B$ can be written as $A = \ell_1^{-1}(E)$, $B = \ell_2^{-1}(F)$ for some $E \subseteq \mathcal{P}(\mathcal{X})$, $F \subseteq \mathcal{P}(\mathcal{Y})$. Note that $E, F$ are not necessarily measurable with respect to the $\sigma$-algebras induced by weak topologies. We can rewrite (36) as

$$
\mathcal{G}^{(\alpha)}_n(P_X, P_Y) = \sup_{E, F} P_X^\otimes n(\ell_1^{-1}(E)) + P_Y^\otimes n(\ell_2^{-1}(F)),
$$

where the supremaization is taken over all pairs of $E \subseteq \mathcal{P}(\mathcal{X})$, $F \subseteq \mathcal{P}(\mathcal{Y})$ such that

\[
\begin{aligned}
1_E(T_X) + 1_F(T_Y) &\leq 1_{c_\alpha > 0}(T_X, T_Y), \forall (T_X, T_Y) \\
\ell_1^{-1}(E) &\text{ is closed, } \ell_2^{-1}(F) \in \Sigma(\mathcal{Y}^n).
\end{aligned}
\]

The function $\ell_1, \ell_2$ are continuous. For any $E, F$ such that $\ell_1^{-1}(E), \ell_2^{-1}(F)$ are Borel subsets of Polish spaces $\mathcal{X}^n, \mathcal{Y}^n$, we have that $E = \ell_1(\ell_1^{-1}(E))$, $F = \ell_2(\ell_2^{-1}(F))$ are analytic subsets of $\mathcal{P}(\mathcal{X}), \mathcal{P}(\mathcal{Y})$ respectively. Since given a probability measure, analytic sets are universally measurable and every measurable set in the completion of this probability measure space is the union of a Borel set and a subset of a null set (of this probability measure), there exists a Borel set $E' \subseteq E$ such that $\mu_n(E') = P_X^\otimes n(\ell_1^{-1}(E))$. Similarly, there exists a Borel set $F' \subseteq F$ such that $\nu_n(F') = P_Y^\otimes n(\ell_2^{-1}(F))$.

We claim that $E$ is closed in $P(\mathcal{X})$ if and only if $\ell_1^{-1}(E)$ is closed in $\mathcal{X}^n$. We now prove it. On one hand, since $\ell_1$ is continuous, for any closed $E$ in $P(\mathcal{X})$, $\ell_1^{-1}(E)$ is closed in $\mathcal{X}^n$. On the other hand, we next show that for any closed $A$ in
$A^n$, $\ell_1(A)$ is closed in $\mathcal{P}(X)$. Let $\{ T^{(k)}_X \}_{k \in \mathbb{N}}$ be a sequence of empirical measures that belongs to $\ell_1(A)$ and converges to some $T_X$ (under the weak topology). Any empirical measure $T_X$ can be written as $T_X = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$ for some sequence $x^n$. So does $T^{(k)}_X$, i.e., for each $k$, $T^{(k)}_X = \frac{1}{n} \sum_{i=1}^n \delta_{x_i^{(k)}}$ for some sequence $x^{n,(k)}$. Let $f : X \to \mathbb{R}$ be a continuous bounded function given by $f(x) = \sum_{i \in [n]} (\delta - d(x_i, x))^+$ where $\delta > 0$, $[t]^+ := \max\{t, 0\}$, and $d$ is the metric on $X$. By definition of the weak topology, $T^{(k)}_X \to T_X$ implies $\int f dT^{(k)}_X \to \int f dT_X$, i.e., $\sum_{i=1}^n f(x_i^{(k)}) \to n\delta$. This further implies that there exists a sequence of permutations $\{\sigma_k\}$ of $[n]$ such that $x_i^{(k)} \to x_i$ as $k \to \infty$ uniformly for all $i \in [n]$, where $x^{n,(k)} := x^{n,(k)}_{\sigma_k}$ denotes the rearrangement of $x^{n,(k)}$ via $\sigma_k$.

Equivalently, in the product space, $x^{n,(k)} \to x^n$ as $k \to \infty$ under the product topology. Since $A$ is closed, we know that $x^n \in A$. Hence, $T_X = \ell_1(x^n) \in \ell_1(A)$. That is, $\ell_1(A)$ is closed.

By the claim above,

$$G^{(n)}_{\alpha}(P_X, P_Y) = \sup_{E,F} \mu_n(E) + \nu_n(F),$$

where the supremization is taken over all pairs of measurable $E \subseteq \mathcal{P}(X)$, $F \subseteq \mathcal{P}(Y)$ such that

$$\begin{cases}
\mathbbm{1}_E(T_X) + \mathbbm{1}_F(T_Y) \leq \mathbbm{1}_{E \cup \{T_X, T_Y\}}, & \forall (T_X, T_Y) \\
E \text{ is closed}.
\end{cases}$$

By the inner regularity of the probability measures, without changing the value of the supremization above, we can require both $E, F$ to be closed. Moreover, the first condition in (37) is equivalent to $E(Q_X, Q_Y) > \alpha$, $\forall Q_X \subseteq E$, $Q_Y \subseteq F$. Hence, we have (11).

Remark 1. Theorem 3 can be also proven from the primal formulation in (10). See the intuition given below Theorem 3.

### 4. Proof of Theorem 4

In this section, we prove Theorem 4.

#### 4.1. Case of $\alpha < \mathcal{E}(P_X, P_Y)$

In this subsection, we prove (14). To this end, it suffices to prove the following result. Without the assumption of UCOTF, it holds that for $\alpha < \mathcal{E}(P_X, P_Y)$,

$$f^{-}(\alpha) := \lim_{n \to \infty} \inf_{n} \frac{1}{n} \log(1 - G^{(n)}_{\alpha}(P_X, P_Y)) \leq \lim_{n \to \infty} \sup_{n} \frac{1}{n} \log(1 - G^{(n)}_{\alpha}(P_X, P_Y)) \leq f^{+}(\alpha),$$

where

$$f^{+}(\alpha) := \lim_{\epsilon \downarrow 0} \inf_{Q_X, Q_Y : \mathcal{E}(Q_X, Q_Y) \leq \alpha} \max_{\forall Q_X' \subseteq B_\epsilon(Q_X), Q_Y' \subseteq B_\epsilon(Q_Y)} \{D(Q_Y || P_Y), D(Q_X' || P_X)\}$$

and

$$f^{-}(\alpha) := \lim_{\epsilon \downarrow 0} \inf_{Q_X, Q_Y : \mathcal{E}(Q_X, Q_Y) \leq \alpha} \max_{\exists Q_X' \subseteq B_\epsilon(Q_X), Q_Y' \subseteq B_\epsilon(Q_Y)} \{D(Q_Y || P_Y), D(Q_X' || P_X)\}$$

with $B_\epsilon(\cdot)$ denoting a ball of radius $\epsilon$ under the Lévy–Prokhorov metric.

Equation (14) is a consequence of (38) and (39) as shown in the following. By the UCOTF assumption, $f^{-}(\alpha) \geq \lim_{\alpha' \downarrow \alpha} f(\alpha')$ and $f^{+}(\alpha) \leq \lim_{\alpha' \uparrow \alpha} f(\alpha')$. On the other hand, by the convexity of the relative entropy and Lemmas 7 and 9 in Appendix A, $f$ is continuous on $(\epsilon_{\min}, +\infty)$. Hence, (14) holds.

#### 4.1.1. Lower Bound

By Lemma 3,

$$1 - G^{(n)}_{\alpha}(P_X, P_Y) = \inf_{\text{closed } A : \mathcal{E}(Q_X, Q_Y) > \alpha, \forall Q_X \subseteq A, Q_Y \subseteq B} \mu_n(A^c) + \nu_n(B^c).$$
Let $E = D_{≥ r}(P_X)$ and $F = D_{≥ r}(P_Y)$ be two sublevel sets of the relative entropies for $r > 0$. Then by [39, Theorem 20], $E$ and $F$ are compact. By the definition of compactness, for any $\epsilon > 0$, there exists a cover $\{B_r(Q_{X,i})\}_{i=1}^{k_1}$ with a finite size $k_1$ for $E$. That is, there exists a positive integer $k_1$ and a collection $\{B_r(Q_{X,i})\}_{i=1}^{k_1}$ of $k_1$ open balls in $\mathcal{P}(\mathcal{X})$ such that $E \subseteq E_\epsilon := \bigcup_{i=1}^{k_1} B_r(Q_{X,i})$. Similarly, there also exists another cover $\{B_r(Q_{Y,i})\}_{i=1}^{k_2}$ with a finite size $k_2$ for $F$. Define $F_\epsilon := \bigcup_{i=1}^{k_2} B_r(Q_{Y,i})$. Define $E_{< \epsilon} := \bigcup_{i=1}^{k_1} B_{< \epsilon}(Q_{X,i})$ and $F_{< \epsilon} := \bigcup_{i=1}^{k_2} B_{< \epsilon}(Q_{Y,i})$, which are closed.

We choose $r, \epsilon > 0$ such that $\mathcal{E}(Q_X, Q_Y) > \alpha, \forall Q_X \in E_{< \epsilon}, Q_Y \in F_{< \epsilon}$. Then, the set pair $(E_{< \epsilon}, F_{< \epsilon})$ constructed here satisfy the constraints in the optimization at the right-hand side of (41). Hence, the right-hand side of (41) is upper bounded by $\mu_n(E_{< \epsilon}) + \nu_n(F_{< \epsilon})$. By Sanov’s theorem [14, Theorem 6.2.10], for fixed $r, \epsilon > 0$, we have

$$\liminf_{n \to \infty} \frac{1}{n} \log \mu_n(E_{< \epsilon}) \geq \inf_{Q_X \in E_{< \epsilon}} D(Q_X \| P_X) \geq r,$$

$$\liminf_{n \to \infty} \frac{1}{n} \log \nu_n(F_{< \epsilon}) \geq \inf_{Q_Y \in F_{< \epsilon}} D(Q_Y \| P_Y) \geq r.$$

Therefore,

$$\liminf_{n \to \infty} \frac{1}{n} \log (1 - G_\alpha^{(n)}(P_X, P_Y)) \geq \liminf_{n \to \infty} \frac{1}{n} \log \left[ \mu_n(E_{< \epsilon}) + \nu_n(F_{< \epsilon}) \right] \geq r.$$

We can take infimum over all feasible $r, \epsilon > 0$, and then obtain that $\liminf_{n \to \infty} \frac{1}{n} \log (1 - G_\alpha^{(n)}(P_X, P_Y))$ is lower bounded by

$$\sup_{r, \epsilon > 0: \mathcal{E}(Q_X, Q_Y) > \alpha, \forall Q_X \in E_{< \epsilon}, Q_Y \in F_{< \epsilon}} r \geq \sup_{r, \epsilon > 0: \mathcal{E}(Q_X, Q_Y) > \alpha, \forall Q_X \in E_{< \epsilon}, Q_Y \in F_{< \epsilon}} \inf_{r, \epsilon > 0: \mathcal{E}(Q_X, Q_Y) \leq \alpha, \exists Q_X \in E_{< \epsilon}, Q_Y \in F_{< \epsilon}} r$$

(42)

where $E_{< \epsilon} := \bigcup_{Q_X \in E} B_{< \epsilon}(Q_X)$ and $F_{< \epsilon} := \bigcup_{Q_Y \in F} B_{< \epsilon}(Q_Y)$, and the equality above follows by the monotonicity of the sublevel sets $E, F$ and the continuity of real numbers. Note that for each $Q_X \in E_{< \epsilon}$, there is $Q_X' \in E$ such that $Q_X = B_{< \epsilon}(Q_X')$, and for each $Q_Y \in F_{< \epsilon}$, there is $Q_Y' \in F$ such that $Q_Y = B_{< \epsilon}(Q_Y')$. By the definition of $E, F$, we have $r \geq \max \{ D(Q_X' \| P_X), D(Q_Y' \| P_Y) \}$. Hence, (42) is further lower bounded by $f^-(\alpha)$ given in (40). (Note that the notations $Q_X', Q_Y'$ and $Q_X, Q_Y$ are exchanged in the definition of $f^-(\alpha)$.)

4.1.2 Upper Bound

In the following, we use a splitting technique to design a desired coupling $\pi$ of $\mu_n$ and $\nu_n$. Let $(Q_X, Q_Y)$ be a pair of distributions such that

$$B_r(Q_X) \times B_r(Q_Y) \subseteq \{(Q_X, Q_Y) : \mathcal{E}(Q_X, Q_Y) \leq \alpha\}$$

(43)

for sufficiently small $\epsilon > 0$. If there is no such pair, then $f^+(\alpha) = +\infty$, and hence, the upper bound $f^+(\alpha)$ in (39) holds trivially. Denote

$$p := \min \{ \mu_n(B_r(Q_X)), \nu_n(B_r(Q_Y)) \}.$$

By large deviations theory, it is not difficult to see that $p > 0$ for sufficiently large $n$; this point will be confirmed later. Denote $\mu_n|_{B_r(Q_X)}$ as the conditional distribution induced by $\mu_n$ given the event $B_r(Q_X)$. The conditional distribution $\nu_n|_{B_r(Q_Y)}$ is defined similarly. Define two new distributions

$$\mu_n' := \frac{\mu_n - p \cdot \mu_n|_{B_r(Q_X)}}{1 - p}, \quad \nu_n' := \frac{\nu_n - p \cdot \nu_n|_{B_r(Q_Y)}}{1 - p}.$$

Then $\mu_n$ and $\nu_n$ can be written as the following mixtures:

$$\mu_n = (1 - p)\mu_n' + p \cdot \mu_n|_{B_r(Q_X)}, \quad \nu_n = (1 - p)\nu_n' + p \cdot \nu_n|_{B_r(Q_Y)}.$$

This is the so-called splitting technique, which was previously used to study limit theorems of recurrent Markov processes [16, 17], used to construct a coupling of the original Markov chain and the target Markov chain in the study of the mixing
rate of Markov Chain Monte Carlo (MCMC) [40], and also used to prove the noncompact version of the Kantorovich duality given in Theorem 1 [4].

We now define a new mixture distribution
\[
\pi := (1 - p) \cdot \mu_n^o \otimes \nu_n^o + p \cdot \mu_n|_{B_n(Q_X)} \otimes \nu_n|_{B_n(Q_Y)}.
\] (44)

Obviously, \(\pi \in \Pi(\mu_n, \nu_n)\). Moreover, by (43) and (44), we have
\[
\pi\{(Q_X, Q_Y) : \mathcal{E}(Q_X, Q_Y) \leq \alpha\} \geq \pi(B_n(Q_X) \times B_n(Q_Y)) \geq p.
\]

Combining this with the nested formula in Theorem 3 yields that
\[
\lim_{n \to \infty} \sup \frac{1}{n} \log(1 - G_{\alpha}^{(n)}(P_X, P_Y)) \leq \lim_{n \to \infty} \frac{1}{n} \log p
\leq \max \left\{ \inf_{Q_X \in B_n(Q_X)} D(Q_X' \| P_X), \inf_{Q_Y \in B_n(Q_Y)} D(Q_Y' \| P_Y) \right\}
\leq \max\{D(Q_X \| P_X), D(Q_Y \| P_Y)\},
\]
where the second inequality follows by Sanov’s theorem. Since \((Q_X, Q_Y)\) is an arbitrary pair of distributions satisfying (43) and \(\epsilon > 0\) in (43) is also arbitrary, we have
\[
\lim_{n \to \infty} \frac{1}{n} \log(1 - G_{\alpha}^{(n)}(P_X, P_Y)) \leq f^+(\alpha).
\]

4.2. Case of \(\alpha > \mathcal{E}(P_X, P_Y)\)

4.2.1. Lower Bound

We now prove the direction of “\(\geq\)” in (15), i.e., \(g(\alpha)\) is a lower bound on the left side of (15). Compared to the case of \(\alpha < \mathcal{E}(P_X, P_Y)\), our proof for the case \(\alpha > \mathcal{E}(P_X, P_Y)\) is more complicated, especially for the lower bound case. This is because for this case, it seems difficult to construct an explicit coupling that asymptotically attains the lower bound on the exponent. So, instead, we utilize Strassen’s dual formula given in (11) to derive the lower bound.

We first provide a heuristic proof idea for the lower bound case. For the supremum in (11), it does not change if we restrict \(\nu_n(B^c) \leq \mu_n(A)\). That is,
\[
G_{\alpha}^{(n)}(P_X, P_Y) = \sup_{\text{closed } A, B : \nu_n(B^c) \leq \mu_n(A), \mathcal{E}(Q_X, Q_Y) > \alpha, \forall Q_X \in A, \forall Q_Y \in B} \mu_n(A) - \nu_n(B^c),
\]
which yields the following simpler upper bound by omitting the negative term \(-\nu_n(B^c)\).
\[
G_{\alpha}^{(n)}(P_X, P_Y) \leq \sup_{\text{closed } A, B : \nu_n(B^c) \leq \mu_n(A), \mathcal{E}(Q_X, Q_Y) > \alpha, \forall Q_X \in A, \forall Q_Y \in B} \mu_n(A).
\] (45)

By Sanov’s theorem [14, Theorem 6.2.10], roughly speaking, \(-\frac{1}{n} \log \mu_n(A) = D(Q_X \| P_X) + o_n(A)\) for some \(Q_X\) and \(-\frac{1}{n} \log \nu_n(B^c) = D(Q_Y \| P_Y) + o_n(B)\) for some \(Q_Y\). The latter means \(B^c \subseteq \{Q_Y' : D(Q_Y' \| P_Y) \geq D(Q_Y \| P_Y) + o_n(B)\}\). Furthermore, to approach the exponent of the supremum in the right-hand side of (45), the sets \(A\) and \(B\) should be chosen as small as possible under the conditions that \(\nu_n(B^c) \leq \mu_n(A)\) and that the exponent of \(\mu_n(A)\) remains unchanged. Hence we should choose \(A = \{Q_X\}\) and \(B = \{Q_Y' : D(Q_Y' \| P_Y) \leq D(Q_Y \| P_Y)\}\). Substituting these into (45), we obtain
\[
\liminf_{n \to \infty} \frac{1}{n} \log G_{\alpha}^{(n)}(P_X, P_Y)
\geq \inf_{Q_X, Q_Y : \mathcal{E}(Q_X, Q_Y) \geq \mathcal{E}(Q_X, Q_Y), \forall Q_Y' \text{ s.t. } D(Q_Y' \| P_Y) \leq D(Q_Y \| P_Y)} D(Q_X \| P_X).
\] (46)

\[
= \inf_{Q_X, Q_Y : \mathcal{E}(Q_X, Q_Y) \geq \mathcal{E}(Q_X, Q_Y), \forall Q_Y' \text{ s.t. } D(Q_Y' \| P_Y) \leq D(Q_X \| P_X)} D(Q_X \| P_X)
\]
\[
= g(\alpha),
\] (48)
where (48) follows since, roughly speaking, given \( Q_X \), the optimal \( Q_Y \) in (46) satisfies \( D(Q_Y \| P_Y) = D(Q_X \| P_X) \). We should note that there are two obstacles in this heuristic proof.

1. Although we claim that the optimal \( B \) should be \( \{ Q'_Y : D(Q'_Y \| P_Y) \leq D(Q_Y \| P_Y) \} \) in the proof idea above, this is not necessarily true since we only know that \( B \supseteq \{ Q'_Y : D(Q'_Y \| P_Y) < D(Q_Y \| P_Y) \} \). This implies that to obtain a lower bound, we only can relax \( B \) to \( \{ Q'_Y : D(Q'_Y \| P_Y) < D(Q_Y \| P_Y) \} \). This difference is subtle but crucial, since if we replace “\( \leq \)” in (47) with “\( \leq \)”, then (47) becomes zero (by observing that \( Q_X = P_X \) is feasible in the infimization of (47)). However, \( g(\alpha) \) is bounded away from zero. Hence, (48) is “discontinuous” in the feasible region in the sense that whether excluding the point \( Q_X = P_X \) from the feasible region in (48) will result in different values. In the following, we provide a formal proof, in which we clear away this obstacle by excluding \( P_X \) from \( A \). That is, we add the constraint \( Q_X \neq P_X \) into the infimum in (47), which makes the value of (47) do not change, and more precisely, remain to be equal to \( g(\alpha) \) no matter whether we replace “\( \leq \)” in (47) with “\( \leq \)”.

2. Another obstacle is that in order to show the inequality in (46), we need to swap \( \lim \inf_{n \to \infty} \) and the infimization operation in (46). However, this is not feasible in general. In the formal proof, we use a covering technique (or compactness technique) to address this obstacle.

We next provide a formal proof for the lower bound \( g(\alpha) \).

We denote \( P_{XY} \in \Pi(P_X, P_Y) \) as a coupling such that \( E_{P_{XY}}[c(X, Y)] < \alpha \). This is feasible since \( \mathcal{E}(P_X, P_Y) < \alpha \). Denote \( P_{XY}^{\otimes n} \) as the \( n \)-fold product of \( P_{XY} \). Then by the definition of \( \mathcal{G}_\alpha^{(n)}(P_X, P_Y) \) and by weak law of large number,

\[
\mathcal{G}_\alpha^{(n)}(P_X, P_Y) \leq P_{XY}^{\otimes n}\left\{ (x^n, y^n) : \frac{1}{n} \sum_{i=1}^{n} c(x_i, y_i) > \alpha \right\} \to 0 \text{ as } n \to \infty.
\]

Hence in Strassen’s dual formula in (11), \( \mu_n(A) + \nu_n(B) - 1 \) converges to zero. That is, given any \( \delta > 0 \) and for sufficiently large \( n \), it suffices to restrict \( A, B \) in the constraints in (11) to satisfy that \( \mu_n(A) \leq \frac{1}{2} + \delta \) or \( \nu_n(B) \leq \frac{1}{2} + \delta \).

Therefore, for any \( \delta \in (0, \frac{1}{2}) \), we have

\[
\mathcal{G}_\alpha^{(n)}(P_X, P_Y) = \max \{ \Upsilon_1, \Upsilon_2 \},
\]

where

\[
\Upsilon_1 := \sup_{\text{closed } A, B, \mu_n(A) \leq \frac{1}{2} + \delta, \mathcal{E}(Q_X, Q_Y) > \alpha, \forall Q_X \in A, Q_Y \in B} \mu_n(A) - \nu_n(B^c),
\]

\[
\Upsilon_2 := \sup_{\text{closed } A, B, \nu_n(B) \leq \frac{1}{2} + \delta, \mathcal{E}(Q_X, Q_Y) > \alpha, \forall Q_X \in A, Q_Y \in B} \nu_n(B) - \mu_n(A^c).
\]

First consider the term (50). For the optimization problem in (50), it suffices to consider \( A, B \) such that

\[
\nu_n(B^c) \leq \mu_n(A) \leq \frac{1}{2} + \delta.
\]

Now we exclude a neighborhood of \( P_X \) from \( A \). We show that the condition “\( \mu_n(A) \leq \frac{1}{2} + \delta \)” in the constraints under the supremum in (50) can be replaced by “\( A \subseteq B_\epsilon(P_X)^c \)” for sufficiently small \( \epsilon \).

**Lemma 4.** Assume UCOTF. Then for \( \delta \in (0, \frac{1}{2}) \) and for \( \epsilon > 0 \) such that

\[
\epsilon + \sup_{Q_X \in B_\epsilon(P_X)} \mathcal{E}(Q_X, P_Y) < \alpha,
\]

there exists an \( N_{\delta, \epsilon} \in \mathbb{N} \) such that for all \( n \geq N_{\delta, \epsilon} \),

\[
\sup_{\text{closed } A, B, \mu_n(B^c) \leq \mu_n(A) \leq \frac{1}{2} + \delta, \mathcal{E}(Q_X, Q_Y) > \alpha, \forall Q_X \in A, Q_Y \in B} \mu_n(A) - \nu_n(B^c) \leq \sup_{\text{closed } A, B : A \subseteq B_\epsilon(P_X)^c, \mathcal{E}(Q_X, Q_Y) > \alpha, \forall Q_X \in A, Q_Y \in B} \mu_n(A) - \nu_n(B^c).
\]

**Proof of Lemma 4.** Define \( A_n := \{ Q_X : \mathcal{E}(Q_X, P_Y) \geq \alpha - \epsilon \} \). Denote \( (A_n, B_n) \) as any pair of closed sets satisfying the constraints in the left side of (53), i.e., they satisfy that

\[
\nu_n(B_n^c) \leq \mu_n(A) \leq \frac{1}{2} + \delta,
\]

\[
\mathcal{E}(Q_X, Q_Y) > \alpha, \forall Q_X \in A_n, Q_Y \in B_n.
\]
In order to show \( A_n \subseteq B_{\epsilon}(P_X)^\epsilon \) for sufficiently large \( n \), we first prove that for any \( \epsilon > 0 \), \( A_n \subseteq A_{\epsilon} \) holds for sufficiently large \( n \), and then prove that \( A_{\epsilon} \subseteq B_{\epsilon}(P_X)^\epsilon \) holds for all \( \epsilon > 0 \) satisfying (52).

We now prove \( A_n \subseteq A_{\epsilon} \) by contradiction. Suppose that for infinitely many \( n \), there is \( Q_X(n) \in A_n \) such that
\[
E(Q_X(n), P_Y) < \alpha - \epsilon.
\]
(56)

By the assumption of UCOTF, for \( \epsilon' > 0 \),
\[
\sup_{Q_Y \in B_{\epsilon'}(P_Y)} E(Q_X(n), Q_Y) \leq E(Q_X(n), P_Y) + o_{\epsilon'}(1).
\]
(57)

Let \( \epsilon' \) be small enough such that \( o_{\epsilon'}(1) < \epsilon \). Then combining (56) and (57), we have
\[
\sup_{Q_Y \in B_{\epsilon'}(P_Y)} E(Q_X(n), Q_Y) \leq \alpha.
\]
(58)

Combining (55) and (58) yields that \( B_{\epsilon'}(P_Y) \subseteq B^{\epsilon'}_\alpha \). On the other hand, by Sanov’s theorem [14, Theorem 6.2.10], for fixed \( \epsilon' > 0 \), \( \nu_n(D_{\epsilon', \alpha}/P_Y) \to 1 \) as \( n \to \infty \), which, combined with (31), implies that \( \nu_n(B_{\epsilon'}(P_Y)) \to 1 \) as \( n \to \infty \). This contradicts with the condition \( \nu_n(B^{\epsilon'}_\alpha) \leq \frac{1}{2} + \delta \) (see (54)). Hence for sufficiently large \( n \), \( A_n \subseteq A_{\epsilon} \).

By the condition in (52) and the definition of \( A_\epsilon \), we have \( B_{\epsilon}(P_X) \subseteq A_\epsilon \), i.e., \( A_n \subseteq B_{\epsilon}(P_X)^\epsilon \). This completes the proof of Lemma 4.

By the assumption of UCOTF, \( \epsilon + \sup_{Q_X \in B_{\epsilon}(P_X)} E(Q_X, P_Y) \to E(P_X, P_Y) \) as \( \epsilon \downarrow 0 \). On the other hand, \( E(P_X, P_Y) < \alpha \). Hence (52) holds for all sufficiently small \( \epsilon > 0 \). Hence, given a sufficiently small \( \epsilon > 0 \), for all sufficiently large \( n \), it suffices to consider \( A \) such that \( A \subseteq \tilde{B}_\epsilon(P_X)^\epsilon \) in (50).

In fact, Obstacle 1 has been addressed now since we have already added the condition \( A \subseteq B_{\epsilon}(P_X)^\epsilon \) into the constraints. Such a condition will exclude the distribution \( P_X \) from the feasible region in the final expression \( g(\alpha) \). We will discuss this near the end of the proof. We next address Obstacle 2 by using a covering technique.

Denote \( F_1 := D_{\leq s}(P_X) \) and \( F_2 := D_{\leq s}(P_Y) \). Then by [39, Theorem 20], \( F_1 \) and \( F_2 \) are compact. By compactness, for any \( \delta > 0 \), there exists a cover \( \{B_\delta(Q_x,i)\}_{i=1}^{k_1} \) (consisting of \( k_1 \) equal balls) for \( F_1 \). Similarly, there also exists another cover \( \{B_\delta(Q_y,i)\}_{i=1}^{k_2} \) with a finite size \( k_2 \) for \( F_2 \). Define \( G_1 := \bigcup_{i=1}^{k_1} B_{\delta}(Q_X,i) \) and \( G_2 := \bigcup_{i=1}^{k_2} B_{\delta}(Q_Y,i) \).

Obviously, \( G_1 \) and \( G_2 \) are closed.

Now we continue (53): The right-hand side of (53) is further upper bounded by
\[
\sup_{\epsilon} \mu_n(A \cap G_1) + \nu_n(B \cap G_2) - 1 + \mu_n(G_1^\epsilon) + \nu_n(G_2^\epsilon) = \mu_n(G_1^\epsilon) + \nu_n(G_2^\epsilon) + \sup_{\epsilon} \mu_n(A) + \nu_n(B) - 1.
\]
(59)

By Sanov’s theorem [14, Theorem 6.2.10], for \( i = 1, 2 \), \( \lim_{n \to \infty} -\frac{1}{n} \log \mu_n(G_i^\epsilon) \geq \inf_{Q_X \in G_1} D(Q_X \| P_X) \geq s \).

Hence if we choose \( s > g(\alpha) \), then the exponent of \( \mu_n(G_1^\epsilon) + \nu_n(G_2^\epsilon) \) would be larger than \( g(\alpha) \). Hence, for this case, to show the lower bound \( g(\alpha) \) on the exponent of the optimal ECP, we only need to prove the exponent of the supremum term in (59) is also larger than or equal to \( g(\alpha) \).

Let \( A \subseteq G_1, B \subseteq G_2 \) be two sets satisfying the constraints under the supremum in (59), i.e., they are closed and satisfy that \( A \subseteq B_{\epsilon}(P_X)^\epsilon \) and \( E(Q_X, Q_Y) > \alpha, \forall Q_X \in A, Q_Y \in B \). We denote \( L_1 := \{ i \in [k_1] : B_{\delta}(Q_X,i) \cap A \neq \emptyset \} \) and \( L_2 := \{ i \in [k_2] : B_{\delta}(Q_Y,i) \cap B \neq \emptyset \} \). By definition, obviously the following property holds.

**Property 1.** For every \( i \in L_1 \), \( j \in L_2 \), there exist \( Q_X \in B_{\leq s}(Q_X,i), Q_Y \in B_{\leq s}(Q_Y,j) \) such that \( Q_X \in B_{\epsilon}(P_X)^\epsilon, E(Q_X, Q_Y) > \alpha \).

Now we set \( \delta = \epsilon/4 \) by the triangle inequality of the assumption of UCOTF, Property 1 implies Property 2.

**Property 2.** For every \( i \in L_1, j \in L_2, \) all \( Q_X \in B_{\leq s/4}(Q_X,i), Q_Y \in B_{\leq s/4}(Q_Y,j) \) satisfy \( Q_X \in B_{\epsilon/2}(P_X)^\epsilon, E(Q_X, Q_Y) > \alpha - \kappa(\epsilon), \) where \( \kappa : (0, +\infty) \to (0, +\infty) \) is some positive and increasing function such that \( \lim_{\epsilon \to 0} \kappa(\epsilon) = 0 \).

We now upper bound the supremum term in (59) as follows. First, observe that the objective function \( \mu_n(A) + \nu_n(B) - 1 \) is upper bounded by \( \mu_n \left( \bigcup_{i \in L_1} B_{\leq s/4}(Q_X,i) \right) + \nu_n \left( \bigcup_{j \in L_2} B_{\leq s/4}(Q_Y,j) \right) \) - 1. By Sanov’s theorem [14, Theorem 6.2.10], it is further upper bounded by \( e^{-n(E_1 + o_{\alpha}(1))} - e^{-n(b_{2} + o_{\alpha}(1))} \), where
\[
E_1 := \inf_{Q_X \in \bigcup_{i \in L_1} B_{\leq s/4}(Q_X,i)} D(Q_X \| P_X), \quad E_2 := \inf_{Q_Y \in \bigcup_{j \in L_2} B_{\leq s/4}(Q_Y,j)} D(Q_Y \| P_Y),
\]
Rigorously speaking, the terms $o_{n|\epsilon}(1)$ in the exponents above depend on the union sets, or equivalently, depend on the sets $L_1, L_2$. However, such dependence can be removed, since $k_1$ and $k_2$ are finite and fixed. That is, given $\epsilon$, the terms $o_{n|\epsilon}(1)$ in the exponents above can be made to converge to zero uniformly for all $L_1 \subseteq [k_1], L_2 \subseteq [k_2]$, and hence $o_{n|\epsilon}(1)$ can be assumed to be independent of $L_1, L_2$. Combining all above, the supremum term in (59) can be upper bounded by

$$e^{-n o_{n|\epsilon}(1)} \sup_{L_1 \subseteq [k_1], L_2 \subseteq [k_2]} e^{-n (E_1 + o_{n|\epsilon}(1))} - e^{-n E_2}.$$  

(60)

If we relax the union sets $\bigcup_{i \in L_1} B_{\epsilon/4}(Q_{X,i}), \bigcup_{i \in L_2} B_{\epsilon/4}(Q_{Y,i})$ to any closed sets $A, B$ such that all $Q_{X} \in A, Q_{Y} \in B$ satisfy $Q_{X} \in B_{\epsilon/2}(P_{X})$, $E(Q_{X}, Q_{Y}) > \alpha - \kappa(\epsilon)$, then the supremum term in (60) is further upper bounded by

$$e^{-n \inf_{Q_{X} \in A} D(Q_{X} \| P_{X}) + o_{n|\epsilon}(1))} - e^{-n \inf_{Q_{Y} \in B} D(Q_{Y} \| P_{Y}).}$$

(61)

Note that the term $o_{n|\epsilon}(1)$ is independent of $A, B$. Until now, Obstacle 2 has been addressed. Furthermore, (61) can be rewritten as

$$e^{-n \inf_{Q_{X} \in A} D(Q_{X} \| P_{X}) + o_{n|\epsilon}(1))} - e^{-n \inf_{Q_{Y} \in B} D(Q_{Y} \| P_{Y}).}$$

(62)

(Observed, to approach the supremum in (62), the set $A$ should be as small as possible. Hence without loss of optimality, we can restrict that $A = \{Q_{X}\}$. That is, (62) can be further rewritten as

$$e^{-n \inf_{Q_{X} \in A} D(Q_{X} \| P_{X}) + o_{n|\epsilon}(1))} - e^{-n \inf_{Q_{Y} \in B} D(Q_{Y} \| P_{Y})}.$$}

(63)

For set $B$, define $r := \inf_{Q_{Y} \in B} D(Q_{Y} \| P_{Y}).$ Then $B^{c} \subseteq \{Q_{Y} : D(Q_{Y} \| P_{Y}) \geq r\},$ i.e.,

$$B \supseteq \{Q_{Y} : D(Q_{Y} \| P_{Y}) \leq r\}.$$}  

(64)

Given any sufficiently small $\epsilon > 0$ and any $\epsilon' > 0$, for all sufficiently large $n$, (63) is upper bounded by

$$\sup_{r, Q_{X} \in B_{\epsilon/2}(P_{X}), } e^{-n (D(Q_{X} \| P_{X})-\epsilon')} - e^{-nr},$$

(65)

which follows since $o_{n|\epsilon}(1) \geq -\epsilon'$ for sufficiently large $n$ given $\epsilon$, and moreover, by (64), the closed set $B$ is relaxed to

$$\{Q_{Y} : D(Q_{Y} \| P_{Y}) \leq r\}.$$  

(66)

By the equivalence of a statement and its contrapositive, we have

$$E(Q_{X}, Q_{Y}) > \alpha - \kappa(\epsilon) \text{ for all } Q_{Y} \text{ s.t. } D(Q_{Y} \| P_{Y}) < r$$

$$\iff D(Q_{Y} \| P_{Y}) \geq r \text{ for all } Q_{Y} \text{ s.t. } E(Q_{X}, Q_{Y}) \leq \alpha - \kappa(\epsilon).$$

Hence, (65) is further upper bounded by

$$\sup_{r, Q_{X} \in B_{\epsilon/2}(P_{X}), } e^{-n (D(Q_{X} \| P_{X})-\epsilon')} - e^{-nr} \sup_{Q_{X} \in B_{\epsilon/2}(P_{X})} e^{-n \phi_{Q_{X}}(\alpha - \kappa(\epsilon))},$$

(67)

where $\phi_{Q_{X}}(t) := \inf_{Q_{Y} : E(Q_{X}, Q_{Y}) \leq t} D(Q_{Y} \| P_{Y})$ for $t \geq 0$. Since (67) is an upper bound on a nonnegative quantity, it is nonnegative as well. Hence, without loss of optimality, one can add the condition $\phi_{Q_{X}}(\alpha - \kappa(\epsilon)) \geq D(Q_{X} \| P_{X}) - \epsilon'$ into the constraints under the supremization in the right side of (67). Moreover, the second term (i.e., the negative one) can be removed, in order to obtain a further upper bound.

Combining all points above (from (51) to the current point) and taking $\liminf_{n \to \infty} -\frac{1}{n} \log$, we have that for all sufficiently small $\epsilon, \epsilon' > 0$,

$$E_{X}(\alpha) := \liminf_{n \to \infty} -\frac{1}{n} \log Y_{1} \geq \inf_{Q_{X} \in E_{\epsilon, \epsilon'}} D(Q_{X} \| P_{X}) - \epsilon'.$$

(68)
where $\Upsilon_1$ is defined in (50), and

$$Q_{\epsilon, \epsilon'} := \{Q_X \in B_{k/2}(P_X)^c : \phi_{Q_X}(\alpha - \kappa(\epsilon)) \geq D(Q_X \| P_X) - \epsilon' \}.$$  

From (68), we obtain that

$$E_X(\alpha) \geq \lim_{\epsilon \downarrow 0} \inf_{\epsilon' > 0} \inf_{Q_X \in Q_{\epsilon, \epsilon'}} D(Q_X \| P_X).$$

(69)

We next remove the limits in the lower bound above.

Define $\phi_{Q_X}(t) := \lim_{s \uparrow 0} \phi_{Q_X}(s).$ Obviously, $\phi_{Q_X}(t) \geq \varphi_{Q_X}(t),$ and $\phi_{Q_X}$ is nonincreasing (since $\phi_{Q_X}$ is nonincreasing) and left-continuous. Hence,

$$Q_{\epsilon, \epsilon'} \subseteq Q^-_{\epsilon, \epsilon'} := \{Q_X \in B_{k/2}(P_X)^c : \phi_{Q_X}(\alpha - \kappa(\epsilon)) \geq D(Q_X \| P_X) - \epsilon' \}.$$  

We now claim that given $\epsilon, \epsilon' \epsilon'^{2}$, $Q^-_{\epsilon, \epsilon'}$ is closed. To show this, it suffices to show that given $t > 0$, $Q_X \ni \varphi_{Q_X}(t)$ is upper semi-continuous (under the weak topology). This follows since, on one hand, for any sequence $\{Q_X^k\}$ such that $Q_X^k \rightarrow Q_X$ as $k \rightarrow \infty$, by the assumption of UCOTF, we have

$$\lim_{k \rightarrow \infty} \sup_{\epsilon > 0} \phi^-_{Q_X}(t) \leq \lim_{s \uparrow 0} \phi^-_{Q_X}(s) = \phi^-_{Q_X}(t).$$

Hence, $Q^-_{\epsilon, \epsilon'}$ is closed.

Note that $Q^-_{\epsilon, \epsilon'}$ is non-increasing in $\epsilon'$, and hence, the operation $\lim_{\epsilon' \downarrow 0}$ in (69) can be replaced by $\sup_{\epsilon' > 0}$. Applying Lemma 8, we obtain that

$$\sup_{\epsilon' > 0} \inf_{Q_X \in Q^-_{\epsilon, \epsilon'}} D(Q_X \| P_X) = \inf_{Q_X \in Q^-} D(Q_X \| P_X),$$

where $Q^- := \bigcap_{\epsilon > 0} Q^-_{\epsilon, \epsilon'}.$ It is easily seen that

$$Q^- = \{Q_X \in B_{k/2}(P_X)^c : \phi_{Q_X}(\alpha - \kappa(\epsilon)) \geq D(Q_X \| P_X) \} \subseteq \tilde{Q}_{\epsilon} \setminus \{P_X\},$$

where $\tilde{Q}_{\epsilon} := \{Q_X : \phi_{Q_X}(\alpha - \kappa(\epsilon)) \geq D(Q_X \| P_X)\}$ is closed and non-decreasing in $\epsilon > 0.$ By Lemma 8 and (69),

$$E_X(\alpha) \geq \sup_{\epsilon > 0} \inf_{Q_X \in \tilde{Q}_{\epsilon} \setminus \{P_X\}} D(Q_X \| P_X) = \inf_{Q_X \in Q^-} D(Q_X \| P_X),$$

(70)

where $Q^- := \bigcap_{\epsilon > 0} Q^-_{\epsilon, \epsilon'}.$

Let $\epsilon$ be small enough such that $\mathcal{E}(P_X, P_Y) < \alpha - \kappa(\epsilon).$ We now claim that for such $\epsilon$, $\tilde{Q}_{\epsilon} \setminus \{P_X\}$ is closed. We next prove this claim.

First observe that for any sequence $\{Q_X^k\} \subseteq \tilde{Q}_{\epsilon} \setminus \{P_X\}$ such that $Q_X^k \rightarrow Q_X$ as $k \rightarrow \infty$, we have $Q_X \in \tilde{Q}_{\epsilon}$ since $\tilde{Q}_{\epsilon}$ is closed. Hence, it suffices to prove $Q_X \neq P_X$, which will be proven by contradiction in the following. Suppose $Q_X = P_X$. Then, by the assumption of UCOTF, $\mathcal{E}(Q_X^k, P_Y) \rightarrow \mathcal{E}(P_X, P_Y) < \alpha - \kappa(\epsilon).$ Hence, for all sufficiently large $k$, it always holds that $\phi_{Q_X^k}(\alpha - \kappa(\epsilon)) = 0$, i.e., for this case, $Q_Y = P_Y$ is a feasible (and also optimal) solution to the infimization in the definition of $\phi_{Q_X^k}(\alpha - \kappa(\epsilon))$. However, since $Q_X^k \neq P_X$, we have $D(Q_X^k \| P_X) > 0$ for all $k$. Hence, for sufficiently large $k$, $Q_X^k \notin \tilde{Q}_{\epsilon}$. This contradict with the choice of the sequence $\{Q_X^k\}$. Hence, $Q_X \neq P_X$, which in turn implies that $Q_X \in \tilde{Q}_{\epsilon} \setminus \{P_X\}$. Since the convergent sequence $\{Q_X^k\}$ is arbitrarily chosen, we have that $\tilde{Q}_{\epsilon} \setminus \{P_X\}$ is closed, completing the proof of the claim.

In fact, the set $\tilde{Q}_{\epsilon}$ consists of two disjoint closed subsets $\tilde{Q}_{\epsilon} \setminus \{P_X\}$ and $\{P_X\}$. The subset $\tilde{Q}_{\epsilon} \setminus \{P_X\}$ is the "reasonable" feasible region for the infimization in (70); see Obstacle 1. Here we address Obstacle 1 by excluding $P_X$ from $\tilde{Q}_{\epsilon}$. In the following, we show that by doing this, the resultant lower bound turns into $g(\alpha)$.

By the claim above, we can write $Q^- = \bigcap_{\epsilon > 0} (\tilde{Q}_{\epsilon} \setminus \{P_X\})$. It is easily seen that

$$\tilde{Q}_{\epsilon} \subseteq \{Q_X : \phi_{Q_X}(\alpha - 2\kappa(\epsilon)) \geq D(Q_X \| P_X)\},$$

which follows since $\phi_{Q_X}(t) \leq \varphi_{Q_X}(t - \delta)$ for any $\delta > 0$, and here we set $\delta = \kappa(\epsilon)$.
Define \( \psi_{Q_X}(t) := \inf_{Q_Y : D(Q_Y \| P_Y) \leq D(Q_Y \| P_X)} \mathcal{E}(Q_X, Q_Y) \) for \( t \geq 0 \). Define \( \psi_{Q_X}^+(t) := \lim_{s \uparrow t} \psi_{Q_X}(s) \) for \( t > 0 \). Then, \( \hat{Q}_\alpha^+ \setminus \{P_X\} \subseteq \{Q_X : \psi_{Q_X}(D(Q_X \| P_X)) \geq \alpha - 2\kappa(\epsilon)\} \), which implies that \( Q_\alpha^+ \subseteq \{Q_X : \psi_{Q_X}(D(Q_X \| P_X)) \geq \alpha\} \).

Therefore, by (49),

\[
\mathcal{E}(\alpha) \geq \inf_{Q_X : \psi_{Q_X}(D(Q_X \| P_X)) \geq \alpha} D(Q_X \| P_X).
\]

By symmetry, we obtain

\[
\mathcal{E}_Y(\alpha) := \lim_{n \to \infty} -\frac{1}{n} \log \mathcal{T}_2 \geq \lim_{\alpha' \uparrow \alpha} g_{P_Y}(\alpha').
\]

Therefore, by (49),

\[
\lim_{n \to \infty} -\frac{1}{n} \log G_{\alpha}^{(n)}(P_X, P_Y) \geq \lim_{\alpha' \uparrow \alpha} g(\alpha').
\]

### 4.2.2. Upper Bound

We next prove the direction of "\( \leq \)" in (15), i.e., \( g(\alpha) \) is an upper bound on the left side of (15). For this case, (49) still holds. Setting \( A = B_{\leq \epsilon}(Q_X) := \{Q'_X : |Q'_X - Q_X| \leq \epsilon\} \) for some fixed \( Q_X \) and some \( \epsilon > 0 \) and then applying Sanov’s theorem [14, Theorem 6.2.10] to \( \mu_n(A) \) and \( \nu_n(\Gamma_{\leq \alpha}(A)) \), we obtain that

\[
\mathcal{T}_1 = \sup_{\text{compact } A \subseteq \mathcal{P}(X)} \mu_n(A) - \nu_n(\Gamma_{\leq \alpha}(A)) \geq e^{-n(\inf_{Q'_X \in B_{\leq \epsilon}(Q_X) \cap \mathcal{E}(Q'_X, Q_Y)) \mathcal{E}(Q_X, Q_Y) \leq \alpha})} - e^{-n(\inf_{Q_Y \in B_{\leq \alpha}(Q_X) \cap \mathcal{E}(Q_X, Q_Y) \leq \alpha})}.
\]

Since \( Q_X \in B_{\leq \epsilon}(Q_X)^\circ \), we have

\[
\inf_{Q'_X \in B_{\leq \epsilon}(Q_X)^\circ} D(Q'_X \| P_X) \leq D(Q_X \| P_X).
\]

On the other hand, by the assumption of UCOTF,

\[
\Gamma_{\leq \alpha}(B_{\leq \epsilon}(Q_X)) = \{Q_Y : \exists Q'_X \in B_{\leq \epsilon}(Q_X), \mathcal{E}(Q'_X, Q_Y) \leq \alpha\} \subseteq \{Q_Y : \mathcal{E}(Q_X, Q_Y) \leq \alpha + \kappa(\epsilon)\},
\]

where \( \kappa : (0, +\infty) \to (0, +\infty) \) is some positive and increasing function such that \( \lim_{\alpha \to 0} \kappa(\epsilon) = 0 \). By Lemma 7 (or the assumption of UCOTF), the set at the most right-hand side above is closed. Therefore,

\[
\overline{\Gamma}_{\leq \alpha}(B_{\leq \epsilon}(Q_X)) \subseteq \{Q_Y : \mathcal{E}(Q_X, Q_Y) \leq \alpha + \kappa(\epsilon)\}.
\]

Substituting (72) and (73) into (71) yields that

\[
\mathcal{T}_1 \geq e^{-n[D(Q_X \| P_X) + o_n(Q_X, \epsilon)]} - e^{-n[D(Q_X \| P_X) + o_n(Q_X, \epsilon)]}.
\]

where \( \phi_{Q_X}(t) := \inf_{Q_Y : \mathcal{E}(Q_X, Q_Y) \leq t} D(Q_Y \| P_Y) \) for \( t \geq 0 \).

Now we choose

\[
Q_X \in \hat{Q} := \{Q_X : \phi_{Q_X}(\alpha) > D(Q_X \| P_X)\},
\]
which means that $D(Q_X \parallel P_X)$ is finite for all $Q_X \in \hat{Q}$. Then given each $Q_X \in \hat{Q}$, for all sufficiently small $\epsilon > 0$,

$$\phi_{Q_X}(\alpha + \kappa(\epsilon)) \geq D(Q_X \parallel P_X) + \epsilon,$$

which follows by the right-continuity of $\phi_{Q_X}$; see Lemma 9. Fixing a pair $(Q_X, \epsilon)$ satisfying (75) and (76), and letting $n \to \infty$ in (74), we obtain

$$\mathbb{E}_X(\alpha) := \limsup_{n \to \infty} -\frac{1}{n} \log \Upsilon_1 \leq D(Q_X \parallel P_X).$$

Since $Q_X \in \mathcal{Q}$ is arbitrary, we take infimum over all $Q_X \in \hat{Q}$. Then we obtain

$$\mathbb{E}_X(\alpha) \leq \inf_{Q_X \in \hat{Q}} D(Q_X \parallel P_X).$$

(77)

We now bound $\hat{Q}$. By an equivalence similar to (66), we have

$$\hat{Q} \supseteq \hat{Q}_1 := \bigcup_{\epsilon > 0} \{Q_X : \psi_{Q_X}(D(Q_X \parallel P_X) + \epsilon) > \alpha \},$$

(78)

where $\psi_{Q_X}(t) := \inf_{Q_Y : D(Q_Y \parallel P_Y) \leq t} \mathcal{E}(Q_X, Q_Y)$ for $t \geq 0$. Indeed the union operation in (78) can be replaced by $\lim_{\epsilon \downarrow 0}$, since the set inside the union operation is nonincreasing in $\epsilon > 0$. We now remove the union operation in (78). We claim that

$$\hat{Q}_1 = \hat{Q}_2 := \{Q_X : \psi_{Q_X}(D(Q_X \parallel P_X)) > \alpha \}. $$

(79)

We next prove this claim.

By the monotonicity of $\psi_{Q_X}$, $\hat{Q}_1 \subseteq \hat{Q}_2$. We next prove the other direction. By Lemma 9, given $Q_X$, $\psi_{Q_X}$ is right-continuous. Hence, for $Q_X \in \hat{Q}_2$,

$$\lim_{\epsilon \downarrow 0} \psi_{Q_X}(D(Q_X \parallel P_X) + \epsilon) = \psi_{Q_X}(D(Q_X \parallel P_X)) > \alpha.$$

Hence, given $Q_X \in \hat{Q}_2$, for all sufficiently small $\epsilon > 0$,

$$\psi_{Q_X}(D(Q_X \parallel P_X) + \epsilon) > \alpha.$$

That is, $Q_X \in \hat{Q}_1$, which implies (79), i.e., the claim above.

Combining (78) and (79) yields $\hat{Q}_2 \subseteq \hat{Q}$. Then, combining this with (77), we have $\mathbb{E}_X(\alpha) \leq g_{P_X, P_Y}(\alpha)$. By symmetry, we obtain $\mathbb{E}_Y(\alpha) := \limsup_{n \to \infty} -\frac{1}{n} \log \Upsilon_2 \leq g_{P_Y, P_X}(\alpha)$. Therefore, by (49),

$$\limsup_{n \to \infty} -\frac{1}{n} \log G^{(n)}_{\alpha}(P_X, P_Y) \leq g(\alpha).$$

5. Proof of Theorem 5

Before proving Theorem 5, we need introduce two lemmas on properties of $\theta(\beta_X, \beta_Y)$. The first lemma is the following which shows that $\theta(\beta_X, \beta_Y)$ is Lipschitz continuous on $\mathbb{S}_X \times \mathbb{S}_Y$. The proof of this lemma is provided in Appendix B.

Lemma 5. The function $\theta(\beta_X, \beta_Y)$ is uniformly continuous on $\mathbb{S}_X \times \mathbb{S}_Y$. More precisely,

$$|\theta(\beta_X, \beta_Y) - \theta(\beta'_X, \beta'_Y)| \leq C \max \{\|\beta_X - \beta'_X\|_\infty, \|\beta_Y - \beta'_Y\|_\infty\},$$

(80)

where $C > 0$ is a constant only depending on $P_X, P_Y$, and $c$.

Based on Lemma 5, in the following lemma, we show that the functional $(\beta_X, \beta_Y) \mapsto \theta(\beta_X, \beta_Y)$ corresponds to the directional derivative of $(Q_X, Q_Y) \mapsto \mathcal{E}(Q_X, Q_Y)$. The proof is provided in Appendix C.

Lemma 6. Denote $\alpha_0 = \mathcal{E}(P_X, P_Y)$. Then the following hold.
1. For a pair of distributions \((Q_X, Q_Y)\) and a number \(t > 0\), we have

\[
\frac{\mathcal{E}(Q_X, Q_Y) - \alpha_0}{t} \geq \theta(\beta_X, \beta_Y),
\]

where \(\beta_X := \frac{Q_X - P_X}{t}\) and \(\beta_Y := \frac{Q_Y - P_Y}{t}\).

2. For any \((\beta_X, \beta_Y)\), we have

\[
\limsup_{t \to 0} \frac{\mathcal{E}(P_X + t\beta_X, P_Y + t\beta_Y) - \alpha_0}{t} \leq \theta(\beta_X, \beta_Y).
\]

Moreover, for a pair of bounded subsets \(A \subseteq S_X, B \subseteq S_Y\) (under the relative topologies), we have

\[
\limsup_{t \to 0} \sup_{\beta_X \in A, \beta_Y \in B} \left( \frac{\mathcal{E}(P_X + t\beta_X, P_Y + t\beta_Y) - \alpha_0}{t} - \theta(\beta_X, \beta_Y) \right) \leq 0.
\]

Note that the differentiability of \(t \mapsto \mathcal{E}(P_X + t\beta_X, P_Y + t\beta_Y)\) at \(t = 0\) can be also proven by the theorems on Hadamard directional differentiability in [41], as done in [20]. However, here we require a stronger condition, the “uniform differentiability” given in (81) and (83). This restricts our attention on finite alphabets. However, it is interesting to investigate how to extend our proof to infinite alphabets, which remains to be done in the future.

The proof of Theorem 5 is in fact almost the same as the proof of Theorem 4, except that the quantities \(\mathcal{E}(P_X, P_Y)\) and \(D(Q_X \| P_X)\) are respectively replaced by \(\theta(\beta_X, \beta_Y)\) and \(\frac{1}{2} \sum_x \frac{\beta_X(x)^2}{P_X(x)}\). The feasibility of the first replacement follows by Lemma 6 and the feasibility of the second one follows by the moderate deviation theorem in [42] or [14, Theorem 3.7.1]. We omit the detailed proof here.

### 6. Proof of Theorem 6

For a discrete distribution, it is uniquely determined by its probability mass function (pmf). Moreover, a pmf can be thought of as a vector \((P_X(i))_{i \in [M]}\) where \(X = [M]\). Hence, the empirical measure \(T_X^n = X^n \sim P_X^n\) corresponds a random vector \((T_X^n(i))_{i \in [M]}\). Denote \(\hat{\mu}_n\) as the law of \(\sqrt{n} \cdot (T_X^n(i) - P_X(i))_{i \in [M]}\). We extend the law \(\hat{\mu}_n\) to the space \(\mathcal{M}_1(\mathcal{X})\) of signed measures with total measure 1 by taking \(\hat{\mu}_n(A) = \hat{\mu}_n(A \cap \mathcal{M}_1(\mathcal{X}))\) for measurable \(A \subseteq \mathcal{M}_1(\mathcal{X})\). By the multivariate central limit theorem, the distribution \(\hat{\mu}_n\) converges weakly to the Gaussian distribution \(\Phi_{P_X}\) given in Section 1.4. Similarly, denote \(\hat{\nu}_n\) as the law of \(\sqrt{n} \cdot (T_Y^n(i) - P_Y(i))_{i \in [N]}\) with \(Y^n \sim P_Y^n\), and extend the law \(\hat{\nu}_n\) to the space \(\mathcal{M}_1(\mathcal{Y})\). Then, \(\hat{\nu}_n\) converges weakly to the Gaussian distribution \(\Phi_{P_Y}\).

### 6.1. Lower bound

Choose \(A' \subseteq S_X\) and \(B' \subseteq S_Y\) as closed sets such that \(\theta(\beta_X, \beta_Y) > \Delta\) for all \(\beta_X \in A', \beta_Y \in B'\), and

\[
\Phi_{P_X}(A') + \Phi_{P_Y}(B') - 1 \geq \Lambda_\Delta(P_X, P_Y) - \epsilon.
\]

We obtain that

\[
\liminf_{n \to \infty} \mathcal{E}_{\alpha_0 + \Delta/\sqrt{n}}(P_X, P_Y) = \liminf_{n \to \infty} \sup_{\psi \in \mathcal{P}(X, Y)} \mu_n(A) + \nu_n(B) - 1
\]

\[
\geq \liminf_{n \to \infty} \sup_{A, B: \theta(\sqrt{n}(Q_X - P_X), \sqrt{n}(Q_Y - P_Y)) > \Delta, \psi \in \mathcal{P}(X, Y)} \mu_n(A) + \nu_n(B) - 1
\]

\[
\geq \liminf_{n \to \infty} \hat{\mu}_n(A') + \hat{\nu}_n(B') - 1
\]

\[
\geq \Phi_{P_X}(A') + \Phi_{P_Y}(B') - 1
\]

\[
\geq \Lambda_\Delta(P_X, P_Y) - \epsilon,
\]

where (84) follows by Strassen’s duality, (85) follows by Lemma 6, in (86) we choose \(A = P_X + A'/\sqrt{n}\) and \(B = P_Y + B'/\sqrt{n}\), and (87) follows by the multivariate central limit theorem. Since (88) holds for any \(\epsilon > 0\), we have

\[
\liminf_{n \to \infty} \mathcal{E}_{\alpha_0 + \Delta/\sqrt{n}}(P_X, P_Y) \geq \Lambda_\Delta(P_X, P_Y).
\]
6.2. Upper bound

The proof of the upper bound follows steps similar to those from (59)-(61). Note that both $\hat{\mu}_n$ and $\Phi_{P_X}$ are concentrated on the hyperplane $\mathbb{S}_X$. Obviously, $\Phi_{P_X}$ is tight on $\mathbb{S}_X$ equipped with relative topology, i.e., for any $\epsilon > 0$, there is a compact $K_X \subseteq \mathbb{S}_X$ such that $\Phi_{P_X}(K_X) \leq \epsilon$. Since $K_X$ is compact, for any $\delta > 0$, it has a finite cover which consists of finitely many $\delta$-radius balls $\{B_\delta(\beta_X,i)\}_{i=1}^k$. Similarly, for $\hat{\nu}_n$, there is a compact $K_Y \subseteq \mathbb{S}_Y$ such that $\Phi_{P_Y}(K_Y) \leq \epsilon$, which has a finite cover consisting of finitely many $\delta$-radius balls $\{B_\delta(\beta_Y,i)\}_{i=1}^k$.

For any measurable $A \subseteq \mathbb{S}_X, B \subseteq \mathbb{S}_Y$, \[
\hat{\mu}_n(A) \leq \hat{\mu}_n(A \cap K_X) + \hat{\mu}_n(K_X^c) \leq \hat{\mu}_n\left(A \cup \bigcup_{i \in [k_1]} B_\leq \delta(\beta_X,i)\right) + \hat{\mu}_n(K_X^c).
\]

For the second term in the last line, $\hat{\mu}_n(K_X^c) \rightarrow \Phi_{P_X}(K_X^c) \leq \epsilon$ as $n \rightarrow \infty$. Define $\theta_n(\beta_X, \beta_Y) := \sqrt{n}\left(E(P_X + \beta_X / \sqrt{n}, P_Y + \beta_Y / \sqrt{n}) - \alpha_0\right)$.

Then, by Strassen’s duality in (11),
\[
G^{(n)}_{\alpha_0 + \Delta/\sqrt{n}}(P_X, P_Y) + 1 = \sup_{\text{closed } A \subseteq P(X), B \subseteq P(Y): E(Q_X, Q_Y) > \alpha_0 + \Delta/\sqrt{n}} \mu_n(A) + \nu_n(B) 
= \sup_{\text{closed } A \subseteq \mathbb{S}_X, B \subseteq \mathbb{S}_Y: \theta_n(\beta_X, \beta_Y) > \Delta, \forall \beta_X \in A, \beta_Y \in B} \hat{\mu}_n(A) + \hat{\nu}_n(B)
\leq \sup_{\text{closed } A \subseteq \mathbb{S}_X, B \subseteq \mathbb{S}_Y: \theta_n(\beta_X, \beta_Y) > \Delta, \forall \beta_X \in A, \beta_Y \in B} \hat{\mu}_n\left(A \cup \bigcup_{i \in [k_1]} B_\leq \delta(\beta_X,i)\right) + \hat{\nu}_n\left(B \cap \bigcup_{i \in [k_2]} B_\leq \delta(\beta_Y,i)\right) + \hat{\mu}_n(K_X^c) + \hat{\nu}_n(K_Y^c) = \hat{\mu}_n(K_X^c) + \hat{\nu}_n(K_Y^c) + \sup_{\text{closed } A \subseteq \bigcup_{i \in [k_1]} B_\leq \delta(\beta_X,i), B \subseteq \bigcup_{i \in [k_2]} B_\leq \delta(\beta_Y,i): \theta_n(\beta_X, \beta_Y) > \Delta, \forall \beta_X \in A, \beta_Y \in B} \hat{\mu}_n(A) + \hat{\nu}_n(B). (89)
\]

By Lemma 6, for bounded subsets $A \subseteq \mathbb{S}_X, B \subseteq \mathbb{S}_Y, \theta_n(\beta_X, \beta_Y) \rightarrow \theta(\beta_X, \beta_Y)$ as $n \rightarrow \infty$ uniformly for all $\beta_X \in A, \beta_Y \in B$. Hence, given $\epsilon' > 0$, for any sufficiently large $n$, the supremum term in (89) is upper bounded by a variant of this supremum term in which “$\theta_n(\beta_X, \beta_Y) > \Delta$” is replaced by “$\theta(\beta_X, \beta_Y) > \Delta - \epsilon'$.”

For sets $A, B$, we denote $L_1 := \{i \in [k_1] : B_\leq \delta(\beta_X,i) \cap A \neq \emptyset\}$ and $L_2 := \{i \in [k_2] : B_\leq \delta(\beta_Y,i) \cap B \neq \emptyset\}$. Then, $A \subseteq \bigcup_{\in L_1} B_\leq \delta(\beta_X,i)$ and $B \subseteq \bigcup_{\in L_2} B_\leq \delta(\beta_Y,i)$. Moreover, by the uniform continuity of $\theta$ (Lemma 5), $|\theta(\beta_X, \beta_Y) - \theta(\beta_X', \beta_Y')| < \alpha(1), \forall \beta_X \in B_\leq \delta(\beta_X), \beta_Y' \in B_\leq \delta(\beta_Y)$. Hence, given $\epsilon', \delta > 0$, the supremum term in (89) is further upper bounded by
\[
\max_{\text{closed } A \subseteq \mathbb{S}_X, B \subseteq \mathbb{S}_Y: \theta(\beta_X, \beta_Y) > \Delta - \epsilon' - \alpha(1), \forall \beta_X \in A, \beta_Y \in B} \hat{\mu}_n\left(\bigcup_{i \in L_1} B_\leq \delta(\beta_X,i)\right) + \hat{\nu}_n\left(\bigcup_{i \in L_2} B_\leq \delta(\beta_Y,i)\right)
\leq \sup_{\text{closed } A \subseteq \mathbb{S}_X, B \subseteq \mathbb{S}_Y: \theta_n(\beta_X, \beta_Y) > \Delta - \epsilon' - \alpha(1), \forall \beta_X \in A, \beta_Y \in B} \hat{\mu}_n(A) + \hat{\nu}_n(B). (90)
\]

Therefore, substituting the upper bound in (90) into (89), and taking limits, we have that given $\epsilon, \epsilon', \delta > 0$,
\[
\limsup_{n \rightarrow \infty} G^{(n)}_{\alpha_0 + \Delta/\sqrt{n}}(P_X, P_Y) + 1 \leq 2\epsilon + \sup_{\text{closed } A \subseteq \mathbb{S}_X, B \subseteq \mathbb{S}_Y: \theta_n(\beta_X, \beta_Y) > \Delta - \epsilon' - \alpha(1), \forall \beta_X \in A, \beta_Y \in B} \Phi_{P_X}(A) + \Phi_{P_Y}(B).
\]

Letting $\epsilon, \epsilon', \delta \downarrow 0$, we obtain
\[
\limsup_{n \rightarrow \infty} G^{(n)}_{\alpha_0 + \Delta/\sqrt{n}}(P_X, P_Y) \leq \Lambda_{\Delta'}(P_X, P_Y).
\]
Appendix A: Basic Lemmas

In this section, we prove several basic lemmas for the OT problem. These lemmas will be used to prove our main results in Sections 3-6.

**Lemma 7.** Let $X$ and $Y$ be Polish spaces. Assume that the cost function $c$ satisfies the lower semi-continuity assumption. Then for $(P_X, P_Y) \in \mathcal{P}(X) \times \mathcal{P}(Y)$, we have that $\mathcal{E}(P_X, P_Y)$ is convex in $(P_X, P_Y)$ and lower semi-continuous in $(P_X, P_Y)$ in the weak topology.

**Proof.** By definition, it is easy to verify that $\mathcal{E}(P_X, P_Y)$ is convex in $(P_X, P_Y)$; see [5, Theorem 4.8]. We next prove the lower semi-continuity. For any sequence of $\{(P_X^{(n)}, P_Y^{(n)})\}$ such that $(P_X^{(n)}, P_Y^{(n)}) \to (P_X, P_Y)$ in the weak topology, we have

$$
\liminf_{n \to \infty} \mathcal{E}(P_X^{(n)}, P_Y^{(n)}) = \liminf_{n \to \infty} \sup_{(\phi, \psi) \in \mathcal{C}_b(X) \times \mathcal{C}_b(Y) : \phi + \psi \leq c} \int_X \phi \, dP_X^{(n)} + \int_Y \psi \, dP_Y^{(n)} \\
\geq \sup_{(\phi, \psi) \in \mathcal{C}_b(X) \times \mathcal{C}_b(Y) : \phi + \psi \leq c} \liminf_{n \to \infty} \int_X \phi \, dP_X^{(n)} + \int_Y \psi \, dP_Y^{(n)} \\
= \sup_{(\phi, \psi) \in \mathcal{C}_b(X) \times \mathcal{C}_b(Y) : \phi + \psi \leq c} \int_X \phi \, dP_X + \int_Y \psi \, dP_Y \\
= \mathcal{E}(P_X, P_Y).
$$

**Lemma 8.** Let $Z$ be a compact set in a topological space. Let $\epsilon \in (0, +\infty) \to A_\epsilon \subseteq Z$ be a set-valued function. Assume $A_\epsilon$ is closed for every $\epsilon > 0$, and non-decreasing in $\epsilon$ (i.e., $A_\epsilon \subseteq A_{\epsilon'}$ for all $\epsilon < \epsilon'$). Let $f : Z \to [0, +\infty]$ be a lower semi-continuous function. Then

$$
\sup_{\epsilon > 0} \inf_{z \in A_\epsilon} f(z) = \inf_{z \in \bigcap_{\epsilon > 0} A_\epsilon} f(z).
$$

**Proof.** Obviously,

$$
\sup_{\epsilon > 0} \inf_{z \in A_\epsilon} f(z) \leq \inf_{z \in \bigcap_{\epsilon > 0} A_\epsilon} f(z).
$$

Hence we only need to prove

$$
\sup_{\epsilon > 0} \inf_{z \in A_\epsilon} f(z) \geq \inf_{z \in \bigcap_{\epsilon > 0} A_\epsilon} f(z).
$$

By definition, both the operations “$\sup_{\epsilon > 0}$” and “$\bigcap_{\epsilon > 0}$” in (91) can be replaced by “$\lim_{\epsilon \downarrow 0}$”. In particular,

$$
\sup_{\epsilon > 0} \inf_{z \in A_\epsilon} f(z) = \lim_{\epsilon \downarrow 0} \inf_{z \in A_\epsilon} f(z),
$$

since $A_\epsilon$ is non-decreasing in $\epsilon$. Let $\{\epsilon_n\}$ be a decreasing positive sequence such that $\lim_{n \to \infty} \epsilon_n = 0$ and

$$
\lim_{n \to \infty} \inf_{z \in A_{\epsilon_n}} f(z) = \lim_{\epsilon \downarrow 0} \inf_{z \in A_\epsilon} f(z).
$$

Let $\delta > 0$ be a positive number. We denote $\{z_n \in A_{\epsilon_n} : n \in \mathbb{N}\}$ as a sequence such that for each $n$,

$$
f(z_n) \leq \inf_{z \in A_{\epsilon_n}} f(z) + \delta.
$$

Since $Z$ is compact, we can pass the sequence $\{z_n : n \in \mathbb{N}\}$ into a convergent subsequence, and assume the limit of this subsequence is $\hat{z} \in Z$. By the monotonicity and closedness of $A_\epsilon$ in $\epsilon$, we have $\hat{z} \in A_\epsilon$ for any $\epsilon > 0$, which further implies

$$
\hat{z} \in \bigcap_{\epsilon > 0} A_\epsilon.
$$
Therefore,
\[
\sup_{\epsilon > 0} \inf_{z \in A_\epsilon} f(z) = \lim_{n \to \infty} \inf_{z \in A_n} f(z) \geq \liminf_{n \to \infty} f(z_n) - \delta \geq f(\hat{z}) - \delta \geq \inf_{z \in \bigcap_{n > 0} A_n} f(z) - \delta,
\]
where the equality follows from (93) and (94), the first inequality follows from (95), the second inequality follows by the lower semi-continuity of \( f \), and the last inequality follows from (96). Since \( \delta > 0 \) is arbitrary, we obtain (92).

Lemma 9. Let \( Z \) be a convex set. Let \( f, g : Z \to [0, +\infty] \) be convex functions. Define
\[
F : t \in [0, +\infty) \mapsto \inf_{z \in \{ z \in Z : g(z) \leq t \}} f(z).
\]
Denote \( t_{\inf} := \inf \{ t \in [0, +\infty) : F(t) < +\infty \} \). Then, the following three statements hold.

1. \( F \) is non-increasing and convex on \([0, +\infty)\), and continuous on \((t_{\inf}, +\infty)\).
2. If additionally, \( Z \) is a compact topological space and \( f, g \) are lower semi-continuous, then \( F \) is continuous on \([t_{\inf}, +\infty)\).
3. If additionally, \( Z \) is a topological space, \( f, g \) are lower semi-continuous, and any sublevel set of \( f \) or \( g \) is a compact subset of \( Z \), then \( F \) is continuous on \([t_{\inf}, +\infty)\).

Remark 2. In the second and third statements, \( F \) is in fact right-continuous on \([0, +\infty)\).

Proof. We first prove the first statement. By definition, it is easy to verify that \( F \) is nonincreasing and convex on \([0, +\infty)\). Furthermore, any convex function is continuous on any open interval on which it is finite. Hence \( F \) is continuous on \((t_{\inf}, +\infty)\).

We next prove the second statement. To this end, we only need to show that \( F \) is right-continuous at \( t = t_{\inf} \). For a sequence \( \{ t_k \} \) such that \( t_k \downarrow t_{\inf} \) as \( k \to \infty \) and for any given \( \delta > 0 \), one can find a sequence \( \{ z_k \} \) such that \( g(z_k) \leq t_k \) and \( f(z_k) \leq F(t_k) + \delta \). If additionally, \( Z \) is a compact set, then we can pass \( \{ z_k \} \) to its convergent subsequence with the limit denoted by \( \hat{z} \). For this limit \( \hat{z} \), by the lower semi-continuity of \( f, g \), we have \( g(\hat{z}) \leq \liminf_{k \to \infty} g(z_k) \leq t_{\inf} \) and \( f(\hat{z}) \leq \liminf_{t \downarrow t_{\inf}} F(t) + \delta \), which imply that \( \hat{z} \) is a feasible solution for the case \( t = t_{\inf} \). Hence, \( F(t_{\inf}) \leq \liminf_{t \downarrow t_{\inf}} F(t) + \delta \). Since \( \delta > 0 \) is arbitrary, we have \( F(t_{\inf}) \leq \liminf_{t \downarrow t_{\inf}} F(t) \).

We now prove the last statement. We first assume that any sublevel set of \( f \) is a compact subset of \( Z \). If \( \lim_{t \downarrow t_{\inf}} F(t) = +\infty \), then by monotonicity of \( F \), \( F(t_{\inf}) = +\infty \) and hence, \( F \) is right-continuous at \( t = t_{\inf} \). If \( \lim_{t \downarrow t_{\inf}} F(t) < +\infty \), then without loss of optimality, one can replace the constraint \( z \in Z \) with \( z \in A_r := \{ z : f(z) \leq r \} \) for \( r > \lim_{t \downarrow t_{\inf}} F(t) \) in the constraints in the infimization in (97). In other words, for any \( t > t_{\inf} \),
\[
F(t) = \inf_{z \in A_r : g(z) \leq t} f(z).
\]
Since \( A_r \) is compact, applying the second statement, we have that \( F \) is right-continuous at \( t = t_{\inf} \).

We next assume that any sublevel set of \( g \) is a compact subset of \( Z \). Similarly to the above, we only need to consider the case \( \lim_{t \downarrow t_{\inf}} F(t) < +\infty \). For this case, without loss of optimality, for any \( t \leq r \) with some \( r > t_{\inf} \), one can replace the constraint \( z \in Z \) with \( z \in B_r := \{ z : g(z) \leq r \} \) in the constraints in the infimization in (97). In other words, for any \( t \leq r \),
\[
F(t) = \inf_{z \in B_r : g(z) \leq t} f(z).
\]
Since \( B_r \) is compact, applying the second statement, we have that \( F \) is right-continuous at \( t = t_{\inf} \).

Lemma 10. For Polish spaces \( X \) and \( Y \), let \( P_X, Q_X \) be two distributions on \( X \), and \( P_Y, Q_Y \) two distributions on \( Y \). Then for any \( Q_{XY} \in \Pi(Q_X, Q_Y) \), there exists \( P_{XY} \in \Pi(P_X, P_Y) \) such that
\[
\| P_{XY} - Q_{XY} \|_{TV} \leq \| P_X - Q_X \|_{TV} + \| P_Y - Q_Y \|_{TV}.
\]

Proof. Let \( Q_{X,Y} \in \Pi(P_X, Q_X) \) and \( Q_{Y,Y'} \in \Pi(P_Y, Q_Y) \) be two couplings. Define \( Q_{X',X} \cap Q_{Y,Y'} = Q_{X',X} Q_{XY} Q_{Y,Y'} \). (Such a joint distribution is well-defined, since for Polish \( X \) and \( Y \), the regular conditional distributions \( Q_{X'|X} \) and \( Q_{Y'|Y} \) exist.) Hence \( Q_{X,Y} \in \Pi(P_X, P_Y) \).
On the other hand, the joint distribution \( Q_{X'Y'} \) constructed above satisfies
\[
Q_{X'Y'} \{ (x', x, y, y') : (x, y) \neq (x', y') \} \\
\leq Q_{XX'} \{ (x, x') : x \neq x' \} + Q_{YY'} \{ (y, y') : y \neq y' \}.
\] (98)

Taking infimum over all \( Q_{X', Y} \in \Pi(P_X, Q_X), Q_{Y', Y} \in \Pi(P_Y, Q_Y) \) for both sides of (98), we have
\[
\| Q_{X'Y'} - Q_{XY} \|_{TV} \\
= \inf_{P_{X'Y'} \in \Pi(Q_{X'Y'}, Q_{X})} P_{X'Y'Y'} \{ (x', x, y, y') : (x, y) \neq (x', y') \} \\
\leq \inf_{Q_{X'} \in \Pi(P_X, Q_X)} Q_{X'Y'} \{ (x', x, y, y') : (x, y) \neq (x', y') \} \\
\leq \inf_{Q_{X'} \in \Pi(P_X, Q_X)} Q_{X'} \{ (x, x') : x \neq x' \} + \inf_{Q_{Y', Y} \in \Pi(P_Y, Q_Y)} Q_{Y'} \{ (y, y') : y \neq y' \} \\
= \| P_X - Q_X \|_{TV} + \| P_Y - Q_Y \|_{TV},
\]
where the two equalities above follow by the maximal coupling equality given in (5). Hence \( Q_{X'Y'} \) is a desired distribution.

\( \square \)

Appendix B: Proof of Lemma 5

Obviously, for \( (\beta_X, \beta_Y), (\beta_X', \beta_Y') \in S_X \times S_Y \), we have
\[
\min_{\beta_{XY} \in \Pi(\beta_X, \beta_Y), \{(x,y) : \beta_{XY}(x,y) < 0 \} \subseteq S} \sum_{x,y} \beta_{XY}(x,y)c(x,y) \\
\leq \min_{\beta_{XY} \in \Pi(\beta_X - \beta_X', \beta_Y - \beta_Y'), \{(x,y) : \beta_{XY}(x,y) < 0 \} \subseteq S} \sum_{x,y} \beta_{XY}(x,y)c(x,y).
\] (99)

Observe that
\[
C := \sup_{\| \beta_X \|_\infty, \| \beta_Y \|_\infty \leq 1} \min_{\beta_{XY} \in \Pi(\beta_X, \beta_Y), \{(x,y) : \beta_{XY}(x,y) < 0 \} \subseteq S} \sum_{x,y} \beta_{XY}(x,y)c(x,y)
\]
satisfies that \( C < +\infty \). Otherwise, \( E(P_X + \epsilon \hat{\beta}_X, P_Y + \epsilon \hat{\beta}_Y) = +\infty \) holds for any \( \epsilon > 0 \), which is impossible since \( E(P_X, P_Y) \leq c_{\sup} = \max_{x,y} c(x,y) < +\infty \) for any \( (P_X, P_Y) \). By the upper boundness of \( C \), we have
\[
\min_{\beta_{XY} \in \Pi(\beta_X - \beta_X', \beta_Y - \beta_Y'), \{(x,y) : \beta_{XY}(x,y) < 0 \} \subseteq S} \sum_{x,y} \beta_{XY}(x,y)c(x,y) \leq C \max\{\| \beta_X - \beta_X' \|_\infty, \| \beta_Y - \beta_Y' \|_\infty \}.
\] (100)

Combining (99) with (100) yields
\[
\theta(\beta_X, \beta_Y) \leq \theta(\beta_X', \beta_Y') + C \max\{\| \beta_X - \beta_X' \|_\infty, \| \beta_Y - \beta_Y' \|_\infty \}.
\]

By symmetry, we can obtain
\[
\theta(\beta'_X, \beta'_Y) \leq \theta(\beta_X, \beta_Y) + C \max\{\| \beta_X - \beta_X' \|_\infty, \| \beta_Y - \beta_Y' \|_\infty \}.
\]
Therefore, (80) holds.

Appendix C: Proof of Lemma 6

We first prove (81). Denote \( Q_{XY}^* \) as an optimal distribution attaining \( E(Q_X, Q_Y) \). Recall that \( P_{XY}^* \) is an optimal distribution attaining \( E(P_X, P_Y) \) with support \( S \). For such \( P_{XY}^* \) and \( Q_{XY}^* \), we can write \( Q_{XY}^* = P_{XY}^* + t \beta_{XY}^* \), where
\[ \beta_{XY} := \frac{Q_{xy} - P_{xy}}{t}. \]
Obviously, \( \beta_{XY} \in \overline{P}(\beta_X, \beta_Y) \) and \( \{(x, y) : \beta^*_{XY}(x, y) < 0\} \subseteq S \). Therefore,
\[
\mathcal{E}(Q_X, Q_Y) = \sum_{x,y} (P^*_{xy}(x, y) + t\beta^*_{XY}(x, y))c(x, y) = \alpha_0 + t \sum_{x,y} \beta^*_{XY}(x, y)c(x, y) \geq \alpha_0 + t\theta(\beta_X, \beta_Y),
\]
where the inequality above follows by the definition of the function \( \theta \) in (22).

Next we prove (82). Since \( \mathcal{X} \) and \( \mathcal{Y} \) are respectively the supports of \( P_X \) and \( P_Y \), given \( \beta_X, \beta_Y \) and for sufficiently small \( t \), the measures \( P_X + t\beta_X, P_Y + t\beta_Y \) are two distributions. Hence, for sufficiently small \( t \), by definition,
\[
\mathcal{E}(P_X + t\beta_X, P_Y + t\beta_Y) = \min_{P_{xy} \in \Pi(P_X + t\beta_X, P_Y + t\beta_Y)} \mathbb{E}[c(X, Y)].
\]
For \( \epsilon > 0 \), denote \( \beta_{XY}^\epsilon \in \overline{P}(\beta_X, \beta_Y) \) as a bivariate function which \( \epsilon \)-approximately attains \( \theta(\beta_X, \beta_Y) \) in the sense that \( \{(x, y) : \beta^*_{XY}(x, y) < 0\} \subseteq S \) and \( \sum_{x,y} \beta^*_{XY}(x, y)c(x, y) \leq \theta(\beta_X, \beta_Y) + \epsilon \). Now we set \( P_{XY}^{(t)} = P_{XY} + t\beta_{XY}^\epsilon \). Then, for sufficiently small \( t \), \( P_{XY}^{(t)} \) is a distribution, and moreover, \( P_{XY}^{(t)} \in \Pi(P_X + t\beta_X, P_Y + t\beta_Y) \). Hence for sufficiently large \( n \),
\[
\mathcal{E}(P_X + t\beta_X, P_Y + t\beta_Y) \leq \mathbb{E}[P_{XY}^{(t)} c(X, Y)] = \alpha_0 + t \sum_{x,y} \beta_{XY}^\epsilon(x, y)c(x, y) \leq \alpha_0 + t(\theta(\beta_X, \beta_Y) + \epsilon).
\]
(101)

Since \( \epsilon > 0 \) is arbitrary, we obtain (82).

Furthermore, the sets \( A, B \) in (83) are assumed to be bounded, which means that \( \|\beta_X\|_\infty, \|\beta_Y\|_\infty \) are bounded on \( A, B \). Let \( t \) be small enough and choose \( \epsilon \) fixed for all \( \beta_X \in A, \beta_Y \in B \), then the proof for (82) still works, i.e., (101) holds for all \( \beta_X \in A, \beta_Y \in B \). Letting \( \epsilon \downarrow 0 \), we obtain (83).

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