Exact Exponents for Concentration and Isoperimetry in Product Polish Spaces

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Abstract—In this paper, we derive variational formulas for the asymptotic exponents (i.e., convergence rates) of the concentration and isoperimetric functions in the product Polish probability space under certain mild assumptions. These formulas are expressed in terms of relative entropies (which are from information theory) and optimal transport cost functionals (which are from optimal transport theory). Hence, our results verify an intimate connection among information theory, optimal transport, and concentration of measure or isoperimetric inequalities. In the concentration regime, the corresponding variational formula is in fact a dimension-free bound in the sense that this bound is valid for any dimension. A cardinality bound for the alphabet of the auxiliary random variable in the expression of the asymptotic isoperimetric exponent is provided, which makes the expression computable by a finite-dimensional program for the finite alphabet case. We lastly apply our results to obtain an isoperimetric inequality in the classic isoperimetric setting, which is asymptotically sharp under certain conditions. The proofs in this paper are based on information-theoretic and optimal transport techniques.

Index Terms—Concentration of measure, isoperimetric inequality, optimal transport, information-theoretic method.

I. INTRODUCTION

C

ONCENTRATION of measure in a probability metric space refers to a phenomenon that a slight enlargement of any measurable set of not small probability will always have large probability. In the language of functional analysis, it is equivalent to the phenomenon that the value of any Lipschitz function is concentrated around its median. The concentration of measure phenomenon was pushed forward in the early 1970s by V. Milman in the study of the asymptotic geometry of Banach spaces. It was then studied in depth by Milman and many other authors including Gromov, Maurey, Pisier, Schechtman, Talagrand, Ledoux, etc. In particular, Talagrand [32] studied the concentration of measure in product spaces equipped with product probability measures, and derived a variety of concentration of measure inequalities for these spaces. In information theory, concentration of measure is known as the blowing-up lemma [1], [25], which was employed by Gács, Ahlswede, and Körner to prove the strong converses of two coding problems in information theory.

It is worth mentioning that Marton is the first to introduce information-theoretic techniques, especially transport-entropy inequalities, in the study of the concentration of measure [25], which yields an elegant and short proof for this phenomenon. By developing a new transport-entropy inequality, Talagrand extended her idea to the case of Gaussian measure and Euclidean metric [33]. Since then, such a textbook beautiful argument became popular and emerged in many books, e.g., [23], [30], and [36]. By replacing the “linear” transport-entropy inequality in Marton’s argument with a “nonlinear” version, Gozlan and Léonard obtained the sharp dimension-free bound on the concentration function [18]. In other words, their bound is exponentially tight in the sense that the exponent of their bound asymptotically coincides with that of the concentration function. Furthermore, Gozlan [17] also used Marton’s argument to prove the equivalence between the Gaussian bound of the concentration function and Talagrand’s transport-entropy inequality. Dembo [13] provided a new kind of transport-entropy inequalities, and used them to recover several results of Talagrand [32].

Ahlswede et al. [2], [3] focused on the isoperimetric regime of the concentration problem, in which they assumed the set to be small enough such that its enlargement is small as well. In this regime, the problem turns into an isoperimetric problem where the difference between the enlargement and the original set is regarded as the “boundary” of the set. They characterized the asymptotic exponents for this problem by using information-theoretic methods. Their results was used as a key tool to study the identification problem [2].

In this paper, we investigated the concentration (or isoperimetric) problem in the product Polish space. Specifically, we minimize the probability of the $t$-enlargement (or $t$-neighborhood) $A^t$ of a set $A$ under the condition that the probability of $A$ is given. Here, different from the common setting in concentration of measure, the probability of $A$ is not necessarily restricted to be around $1/2$. The probability of $A$ could be small or large. We now introduce the mathematical formulation.

Let $\mathcal{X}$ and $\mathcal{Y}$ be Polish spaces (i.e., separable completely metrizable spaces, including Euclidean spaces and countable metric spaces as special cases). Let $\Sigma(\mathcal{X})$ and $\Sigma(\mathcal{Y})$ be
respectively the Borel σ-algebras on \( \mathcal{X} \) and \( \mathcal{Y} \) that are generated by the topologies on \( \mathcal{X} \) and \( \mathcal{Y} \). 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 \( P_Y \in \mathcal{P}(\mathcal{Y}) \). In other words, \( P_X \) and \( P_Y \) are respectively the distributions of two random variables \( X \) and \( Y \). Let \( c : \mathcal{X} \times \mathcal{Y} \to [0, +\infty) \) be lower semi-continuous, which is called a cost function. Denote \( \mathcal{X}^n \) as the \( n \)-fold product space of \( \mathcal{X} \). For the product space \( \mathcal{X}^n \times \mathcal{Y}^n \) and given \( c \), we consider an additive cost function \( c_n \) on \( \mathcal{X}^n \times \mathcal{Y}^n \) given by

\[
c_n(x^n, y^n) := \sum_{i=1}^{n} c(x_i, y_i) \quad \text{for} \quad (x^n, y^n) \in \mathcal{X}^n \times \mathcal{Y}^n,
\]

where \( c \) given above is independent of \( n \). Obviously, \( c_n \) is lower semi-continuous since \( c \) is lower semi-continuous.

For a set \( A \subseteq \mathcal{X}^n \), denote its \( t \)-enlargement under \( c \) as

\[
A^t := \bigcup_{x^n \in A} \{ y^n \in \mathcal{Y}^n : c_n(x^n, y^n) \leq t \}.
\]

To address the measurability of \( A^t \), we assume that either of the following two conditions holds throughout this paper.

1) For lower semi-continuous \( c \), we restrict \( A \) to be a closed set.

2) If \( \mathcal{X} \) and \( \mathcal{Y} \) are the same Polish space and \( c = d^p \), where \( p > 0 \) and \( d \) is a complete metric that induces the topology on this Polish space, then \( A \) can be any Borel set.

For the first case, since \( \mathcal{X}^n \) and \( \mathcal{Y}^n \) are Polish and a projection map is continuous, by definition, the projection of a closed (or open) subset of \( \mathcal{X}^n \times \mathcal{Y}^n \) to \( \mathcal{X}^n \) is analytic (or Souslin) [7]. Note that for closed \( A \), \( A^t \) is the projection of the closed set \( c_n^{-1}((-\infty, t]) \cap (A \times \mathcal{Y}^n) \) to \( \mathcal{X}^n \). So, the set \( A^t \) is analytic and hence, universally measurable. If we extend \( P^\otimes n \) to the collection of analytic sets, then \( P^\otimes n \otimes n = (A^{(1)} \otimes n) \) is well defined. Hence, for this case, we by default adopt this extension to avoid the measurability problem. For the second case, for any Borel set \( A \), \( A^t \) is always Borel (since it is countable intersections of Borel sets \( \bigcup_{x^n \in A} \{ y^n \in \mathcal{Y}^n : c_n(x^n, y^n) < t + \frac{1}{k} \}, k = 1, 2, \ldots \).

Define the isoperimetric function (or isoperimetric profile) as for \( a \in [0, 1], t \geq 0 \),

\[
\Gamma^{(n)}(a, t) := \inf_{A : P^\otimes n \otimes n (A) \geq a} P^\otimes n (A^t),
\]

where the set \( A \) is assumed to satisfy either of the above two conditions. We call \((a, t) \mapsto 1 - \Gamma^{(n)}(a, t)\) as the concentration function, which reduces to the usual concentration function \( t \mapsto 1 - \Gamma^{(n)}(\frac{t}{2}, t) \) in the theory of concentration of measure when \( a \) is set to 1/2. Throughout this paper, we set

\[
a = e^{-n\alpha}, t = n\tau.
\]

Define the isoperimetric and concentration exponents respectively as

\[
E^{(n)}(\alpha, \tau) := -\frac{1}{n} \log \Gamma^{(n)}(e^{-n\alpha}, n\tau)
\]

In fact,

\[
\Gamma^{(n)}(e^{-n\alpha}, n\tau) = e^{-nE^{(n)}(\alpha, \tau)} = 1 - e^{-nE^{(n)}(\alpha, \tau)}.
\]

In the classic setting, \( \mathcal{X} = \mathcal{Y} \) equipped with a metric \( d \) is a Polish metric space, and moreover, \( P_X = P_Y =: P \) and \( c = d^p \) with \( p \geq 1 \). For a set \( A \), its boundary measure is defined by

\[
(P^\otimes n)^+(A) := \liminf_{r \to 0} \frac{P^\otimes n (A^r) - P^\otimes n (A)}{r}.
\]

In the classic isoperimetric problem, the objective is to minimize \((P^\otimes n)^+(A)\) over all sets \( A \) with a given probability.

In this paper, we aim at characterizing the asymptotics of the concentration and isoperimetric exponents in (3) and (4), as well as applying these results to obtain an asymptotically sharp inequality on the classic isoperimetric problem (under certain conditions).

A. Our Contributions

Our contributions in this paper are as follows.

1) We characterize the asymptotic concentration exponent \( \lim_{n \to \infty} E^{(n)}(\alpha, \tau) \) (under certain mild assumptions) in terms of two fundamental quantities from other fields—“relative entropy” which comes from information theory (or large deviations theory) and “optimal transport cost” which comes from the theory of optimal transport. The (conditional) empirically typical sets are shown to be optimal in attaining the asymptotic concentration exponent. Hence, this result further verifies an intimate connection among concentration of measure, information theory, and optimal transport. The obtained expression for \( \lim_{n \to \infty} E^{(n)}(\alpha, \tau) \) is shown to be a dimension-free bound on \( E^{(n)}(\alpha, \tau) \). This bound is tighter than Marton’s bound [25], [26] and an improved version by Gozlan and Léonard [16], [18], especially when the probability of the set is small. It also sharpens Talagrand’s concentration inequality in [32]. The improvement is due to that the single-letterization part in our proof relies on the subadditivity of optimal transport (OT) costs (or equivalently, relies on a new and more general transport-entropy inequality), and bypasses the traditional transport-entropy inequality in Marton’s proof and the nonlinear transport-entropy inequality in Gozlan and Léonard’s proof. As applications, we also consider the case that \( c = d^p \) with \( p \geq 1 \) and \( d \) denoting a metric and the case that \( c \) is the Hamming metric. We obtain cleaner expressions for the asymptotic concentration exponents for these two cases, and also recover existing results for the setting of \( a = \frac{1}{2} \), including Gozlan and Léonard’s [16], [18] and Alon, Boppana, and Spencer’s in [4].

\[1\] Throughout this paper, the base of \( \log \) is \( e \). Our results are still true if the bases are chosen to other values, as long as the bases of the logarithm and exponent are the same.

\[2\] For the discrete metric, this definition does not make sense, since \( (P^\otimes n)^+(A) = 0 \) for any set \( A \). So, in this case, \( (P^\otimes n)^+(A) \) can be defined by \( (P^\otimes n)^+(A) := P^\otimes n (A^1) - P^\otimes n (A) \).
2) We also provide upper and lower bounds for the asymptotic isoperimetric exponent \( \lim_{n \to \infty} E_0^n(\alpha, \tau) \) (under certain mild assumptions) for Polish spaces. These bounds are also expressed in terms of the relative entropy and the optimal transport cost. Under a continuity assumption, the bounds coincide, which yields an exact characterization of the asymptotic isoperimetric exponent. This result is a generalization of Ahlswede and Zhang’s [3] from finite spaces to Polish spaces. In fact, similar to Ahlswede and Zhang’s proof, our proof also relies on the inherently typical subset lemma, but requires new techniques since the spaces are much more general.

3) Our another contribution is deriving dual formulas for the bounds or expressions mentioned above for the asymptotic concentration or isoperimetric exponents. By our dual formulas, on one hand, we verify the equivalence between our formula and Alon, Boppana, and Spencer’s in [4] for the asymptotic concentration exponent; on the other hand, we provide a bound on the alphabet size of the auxiliary random variable in the expression of the asymptotic isoperimetric exponent. These two observations are not obvious from the perspective of primal formulas. Previously, there was no bound on the alphabet size of the auxiliary random variable, even for the finite alphabet case considered by Ahlswede and Zhang [3]. As explicitly mentioned in [2, Remark 1 on p. 50], deriving cardinality bounds for the auxiliary random variable is not easy. Deriving cardinality bounds is also important, since it makes the expression “computable” for the finite alphabet case. That is, it enables us to evaluate the expression by a finite-dimensional program when the alphabets are finite.

4) The isoperimetric problem mentioned above concerns thick boundaries. In contrast, in the classic isoperimetric problem, the boundary is extremely thin, as shown in (5). We apply our results to obtain the following isoperimetric inequality:

\[
(P^\otimes n)^+ (A) \geq n^{1-1/p} e^{-\alpha n} (\xi(\alpha) + o_n(1)),
\]

where \( \xi(\alpha) \) is a certain function defined in (33). This inequality is asymptotically sharp under certain conditions.

C. Notations

1) Probability Theory: Throughout this paper, for a topological space \( Z \), we use \( \Sigma(\mathcal{Z}) \) to denote the Borel \( \sigma \)-algebra on \( Z \) generated by the topology of \( Z \). Hence \( (Z, \Sigma(\mathcal{Z})) \) forms a measurable space. For this measurable space, we denote the set of probability measures on \( (Z, \Sigma(\mathcal{Z})) \) as \( \mathcal{P}(\mathcal{Z}) \). For a Polish space \( Z \), if \( d \) is a complete metric that induces the topology on this space, then \( (Z, d) \) is called a Polish metric space. For a Polish space \( Z \), if we equip \( \mathcal{P}(\mathcal{Z}) \) with the weak topology, then the resultant space is Polish as well. For brevity, we denote it as \( (\mathcal{P}(\mathcal{Z}), \Sigma(\mathcal{P}(\mathcal{Z}))) \).

As mentioned at the beginning of the introduction, \( X \) and \( Y \) are Polish spaces, and \( P_X \) and \( P_Y \) are two probability measures defined respectively on \( X \) and \( Y \). We also use \( Q_X, R_X \) to denote another two probability measures on \( X \). The probability measures \( P_X, Q_X, R_X \) can be thought as the push-forward measures (or the distributions) induced jointly by the same measurable function \( X \) (random variable) from an underlying measurable space to \( X \) and by different probability measures \( P, Q, R \) defined on the underlying measurable space. Without loss of generality, we assume that \( X \) is the identity map, and \( P, Q, R \) are the same as \( P_X, Q_X, R_X \). So, \( P_X, Q_X, R_X \) could be independently specified to arbitrary probability measures. We say that all probability measures induced by the underlying measure \( P \), together with the corresponding measurable spaces, constitute the \( P \)-system. So, \( P_X \) is in fact the distribution of the random variable \( X \) in the \( P \)-system, where the letter “\( P \)” in the notation \( P_X \) refers to the system and the subscript “\( X \)” refers to the random variable. When emphasizing the random variables, we write \( X \sim P_X \) to indicate that \( X \) follows the distribution \( P_X \) in the \( P \)-system.

For a random variable (a measurable function) \( f \) from \( X \) to another measurable space \( Z \), the distribution \( P_{Y|X}(f) \) of \( f \) in different systems is clearly different, e.g., it is \( P_X \circ f^{-1} \) in the \( P \)-system, but it is \( Q_X \circ f^{-1} \) in the \( Q \)-system.

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. \( P_Y \)). For a probability measure \( P_X \) and a transition probability measure (or Markov kernel) \( P_{Y|X} \) from \( X \) to \( Y \), we denote \( P_X P_{Y|X} \) as the joint probability measure induced by \( P_X \) and \( P_{Y|X} \). Here \( P_{Y|X} \) is called the regular conditional distribution of \( P_X P_{Y|X} \). We denote \( P_Y \) or \( P_Y \circ P_{Y|X} \) as the marginal distribution on \( Y \) of the joint distribution \( P_X P_{Y|X} \) on \( Y \). Moreover, we can pick up probability measures or transition probabilities from different probability systems to constitute a joint probability measure, e.g., \( P_X Q_{Y|X} \). For a distribution \( P_X \) on \( X \) and a measurable subset \( A \subseteq X \), \( P_X(\cdot | A) \) denotes the conditional probability measure given \( A \). For brevity, we write \( P_X(x) := P_X(\{x\}) \), \( x \in X \). In particular, if \( X \sim P_X \) is discrete, the restriction of \( P_X \) to the set of singletons corresponds to the probability mass function of \( X \) in the \( P \)-system.

We denote \( x^n := (x_1, x_2, \ldots, x_n) \in \mathbb{X}^n \) as a sequence in \( \mathbb{X}^n \). Given \( x^n \), denote \( x^k_i := (x_i, x_{i+1}, \ldots, x_k) \) as a subsequence of \( x^n \) for \( 1 \leq i \leq k \leq n \), and \( x^k := x^n_{[1:k]} \). For a probability measure \( P_{X^n} \) on \( \mathbb{X}^n \), we use \( P_{X^k|X^{k-1}} \) to denote the regular conditional distribution of \( X_k \) given \( X^{k-1} \) induced by \( P_{X^n} \). For a measurable function \( f : X \to \mathbb{R} \), sometimes we adopt the notation \( P_X(f) = \int_X f \ dP_X \).
Given \( n \geq 1 \), the empirical measure (also known as type for the finite alphabet case in information theory [12, 14]) for a sequence \( x^n \in \mathcal{X}^n \) is

\[
L_{x^n} := \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}
\]

where \( \delta_{x} \) is Dirac mass at the point \( x \in \mathcal{X} \). Let \( L_n : x^n \in \mathcal{X}^n \mapsto L_{x^n} \in \mathcal{P}(\mathcal{X}) \) be the empirical measure map. For a pair of sequences \( (x^n, y^n) \in \mathcal{X}^n \times 3^m \), the empirical joint measure \( L_{x^n, y^n} \) and empirical conditional measure \( L_{y^n|x^n} \) are defined similarly. Obviously, empirical measures (or empirical joint measures) for \( n \)-length sequences are discrete distributions whose probability masses are multiples of \( 1/n \).

2) Information Theory: For two distributions \( P, Q \) defined on the same space, the relative entropy [Kullback-Leibler (KL) divergence] of \( P \) with respect to \( Q \), denoted as \( D(P \| Q) \), is defined as

\[
D(P \| Q) := \begin{cases} \int \log \left( \frac{dP}{dQ} \right) dQ, & P \ll Q \\ \infty, & \text{otherwise.} \end{cases}
\]

For brevity, we denote binary relative entropy function \( D(p \| q) := D(\text{Bern}(p) \| \text{Bern}(q)) \) where \( p, q \in [0, 1] \). Define the conditional version as

\[
D(Q \| P) := D(Q \| P) := D(Q \| P) := D(Q \| P).
\]

We use \( B_{\delta}(x) := \{ x' \in \mathcal{X} : d(x, x') < \delta \} \) and \( B_{\delta}(x) := \{ x' \in \mathcal{X} : d(x, x') \leq \delta \} \) to respectively denote an open ball and a closed ball. We use \( \mathcal{A}, \mathcal{A}', \) and \( \mathcal{A} := \mathcal{X} \setminus \mathcal{A} \) to respectively denote the closure, interior, and complement of the set \( \mathcal{A} \subseteq \mathcal{X} \). Denote the Lévy–Prokhorov metric on \( \mathcal{P}(\mathcal{X}) \) as

\[
d_{\mathcal{L}}(Q', Q) = \inf \{ \delta > 0 : Q'(A) \leq Q(A) + \delta, \forall A \subseteq \mathcal{X} \}
\]

where \( A := \bigcup_{\gamma \in \mathcal{A}} \{ x' \in \mathcal{X} : d(x, x') < \delta \} \), which is compatible with the weak topology for the Polish metric space \( (\mathcal{X}, d) \). Denote the total variation (TV) distance as

\[
||Q' - Q||_{TV} := \sup_A \{ Q'(A) - Q(A) \},
\]

where the supremum is taken over all measurable \( A \) in \( \mathcal{P}(\mathcal{X}) \). The supremum here is in fact a maximum. Denote the sublevel set of the relative entropy (or the divergence “ball”) as \( D_{\varepsilon}(P) := \{ Q : D(Q \| P) \leq \varepsilon \} \) for \( \varepsilon \geq 0 \). The Lévy–Prokhorov metric, the TV distance, and the relative entropy admit the following relation.

For any \( Q, P \in \mathcal{P}(\mathcal{X}) \),

\[
d_{\mathcal{L}}(P, Q) \leq ||Q - P||_{TV} \leq \sqrt{\frac{1}{2} D(P \| Q)}, \tag{6}
\]

which implies for \( \varepsilon \geq 0, \)

\[
B_{\varepsilon}(P) \supseteq D_{\varepsilon + \varepsilon}(P).
\]

The first inequality in (6) follows by definition [15], and the second inequality is known as Pinsker’s inequality.

For a Polish space \( \mathcal{X} \) and an empirical measure \( T \) of \( n \)-length sequence in \( \mathcal{X}^n \), \( L_n^{-1}(T) \) is called the empirical class of \( T \). When \( \mathcal{X} \) is finite, an empirical class is also called a type class [11]. For a Polish space \( \mathcal{X} \) and \( \varepsilon > 0 \), the empirically \( \varepsilon \)-typical set of \( P \) [28] is defined as

\[
T_{\varepsilon}^{(n)}(P) := \{ x^n \in \mathcal{X}^n : \sum_{a \in \mathcal{X}} |L_n(a) - P(a)| = 2 \varepsilon \}.
\]

For a transition probability measure \( P_{X|W} \) from a finite set \( \mathcal{Y} \) to a Polish space \( \mathcal{X} \) and for \( \varepsilon > 0 \), denote \( B_{\varepsilon}(P_{X|W}) := \{ x^n \in \mathcal{X}^n : ||x^n - x^n||_W = \varepsilon \} \) which is a closed ball of radius \( \varepsilon \) in \( \mathcal{P}(\mathcal{X} \times \mathcal{Y}) \) equipped with the metric \( \max_{\mathcal{X}, \mathcal{Y}} d_{\varepsilon}(R_{X|W}, P_{X|W}) \to \max_{\mathcal{X}} d_{\varepsilon}(R_{X|W}, P_{X|W}) \). Given a sequence \( w^n \), define the conditional empirically \( \varepsilon \)-typical set of \( P_{X|W} \) w.r.t. \( w^n \) as

\[
T_{\varepsilon}^{(n)}(P_{X|W}|w^n) := \{ x^n \in \mathcal{X}^n : ||x^n - x^n||_W = \varepsilon \}.
\]

For discrete random variables \( (X, Y) \sim Q_{XY} \), the (Shannon) entropy

\[
H_Q(X) = - \sum_x Q_X(x) \log Q_X(x),
\]

and the conditional (Shannon) entropy

\[
H_Q(X|Y) = - \sum_{x,y} Q_{XY}(x,y) \log Q_{XY}(x,y).
\]

For brevity, we denote the binary entropy function \( H(p) := H_{\text{Bern}(p)}(X) = -p \log p - (1 - p) \log (1 - p) \) where \( p \in [0, 1] \). In fact, for discrete random variables, \( I_Q(X; Y) = H_Q(X) - H_Q(X|Y) \).

3) Optimal Transport: In this paper, our results involve the OT cost functional, which is introduced now. The coupling set of \( (P_X, P_Y) \) is defined as

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

Distributions in \( C(P_X, P_Y) \) are termed couplings of \( (P_X, P_Y) \). The OT cost between \( P_X \) and \( P_Y \) is defined as

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

The existence of the minimizers are well-known; see, e.g., [36, 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 \( (X, Y) \sim P_{XY} \).
Any $P_{XY} \in C(P_X, P_Y)$ attaining $C(P_X, P_Y)$ is called an OT plan. The minimization problem in (8) is called the Monge–Kantorovich’s OT problem [36]. The functional $(P_X, P_Y) \in \mathcal{P}(X) \times \mathcal{P}(Y) \mapsto C(P_X, P_Y) \in [0, +\infty]$ is called the OT (cost) functional. If $X = Y$, $d$ is a complete metric that induces the topology on this space [i.e., $(X, d)$ is a Polish metric space], and $c = d^p$ with $p \geq 1$, then $W_p(P_X, P_Y) := (C(P_X, P_Y))^{1/p}$ is the so-called $p$-th Wasserstein metric between $P_X$ and $P_Y$. For the $n$-dimensional case, $W_p(P_{X^n}, P_{Y^n}) := (C(P_{X^n}, P_{Y^n}))^{1/p}$ with $c_n(x^n, y^n) = \sum_{i=1}^n d^p(x_i, y_i)$ is the $p$-th Wasserstein metric between $P_{X^n}$ and $P_{Y^n}$ for the product metric $d_n(x^n, y^n) = c_n(x^n, y^n)^{1/p}$ where $p \geq 1$.

Furthermore, for another distribution $P_W$ on a Polish space $\mathcal{W}$, the conditional coupling set of transition probability measures $P_{X|\mathcal{W}}$ and $P_{Y|\mathcal{W}}$ is defined as

$$C(P_{X|\mathcal{W}}, P_{Y|\mathcal{W}}) := \mathcal{P}(X \times \mathcal{Y}|\mathcal{W}) : \begin{cases} P_{XY|\mathcal{W}} \in \mathcal{P}(X \times \mathcal{Y}|\mathcal{W}) : & P_{XY|\mathcal{W}} \in C(P_{X|\mathcal{W}=\mathcal{W}}, P_{Y|\mathcal{W}=\mathcal{W}}), \forall \mathcal{W} \in \mathcal{W}, \end{cases}$$

where $\mathcal{P}(X \times \mathcal{Y}|\mathcal{W})$ denotes the set of transition probability measures from $\mathcal{W}$ to $X \times \mathcal{Y}$. The conditional OT cost between transition probability measures $P_{X|\mathcal{W}}$ and $P_{Y|\mathcal{W}}$ given $P_W$ is defined as

$$C(P_{X|\mathcal{W}}, P_{Y|\mathcal{W}}|P_W) := \min_{P_{XY|\mathcal{W}} \in C(P_{X|\mathcal{W}}, P_{Y|\mathcal{W}})} \mathbb{E}_{(W, X, Y) \sim P_W} P_{XY|\mathcal{W}}[c(X, Y)],$$

(9)

where $P_{XY|\mathcal{W}}$ denotes the joint probability measure induced by $P_{X|\mathcal{W}}$ and $P_{Y|\mathcal{W}}$. The conditional OT cost can be alternatively expressed as

$$C(P_{X|\mathcal{W}}, P_{Y|\mathcal{W}}|P_W) = \mathbb{E}_{P_{XY|\mathcal{W}}} C(P_{X|\mathcal{W}}, P_{Y|\mathcal{W}}).$$

4) Others: We use $f(n) = o_n(1)$ to denote that $f(n) \to 0$ pointwise as $n \to +\infty$. When there is no specification, by default, we denote $\inf \emptyset := +\infty, \sup \emptyset := -\infty$, and $[k] := \{1, 2, \ldots, k\}$. Denote $\hat{g}$ as the lower concave envelope of a function $g$, and $\tilde{g}$ as the upper concave envelope of $g$.

II. Main Results

A. Asymptotic Concentration Exponent

1) General Cost: We now characterize the asymptotic concentration exponent $\lim_{n \to \infty} E_1^{(n)}(\alpha, \tau)$. To this end, given $P_X, P_Y$, and $c$, we define

$$\phi(\alpha, \tau) := \inf_{D \in \mathbb{R}^+} D_Q |\{ Q_X \in \mathbb{P}(X), Q_Y \in \mathbb{P}(Y) : D(Q_X|P_X) \leq \alpha, C(Q_X, Q_Y) > \tau \}}$$

(10)

Denote $\tilde{\phi}(\alpha, \tau)$ as the lower convex envelope of $\phi(\alpha, \tau)$, which can be also expressed as

$$\tilde{\phi}(\alpha, \tau) = \inf_{Q_X, Q_Y, W : D(Q_X|P_X) \leq \alpha, C(Q_X, Q_Y) > \tau} \mathbb{E}_{Q_Y} D(Q_Y|P_Y),$$

(11)

where $W$ is an auxiliary random variable defined on a Polish space. However, by Carathéodory’s theorem, the alphabet size of $Q_W$ can be restricted to be no larger than 4. In fact, the alphabet size can be further restricted to be no larger than 3, since it suffices to consider the boundary points of the convex hull of

$$\{ (D(Q_X|P_X), D(Q_Y|P_Y), C(Q_X, Q_Y)) \}_{w \in \mathcal{W}}.$$

To characterize the asymptotic concentration exponent, we need the following assumption. Define the $(X', \epsilon)$-smooth OT functional as

$$C_{X',\epsilon}(Q_X, Q_Y) := \inf_{Q_X'^{|\mathcal{W}}} C(Q_X', Q_Y),$$

by definition, $C_{X',\epsilon}(Q_X, Q_Y) \leq C_{X,\epsilon}(Q_X, Q_Y)$ and by the lower semicontinuity of the OT functional, $\lim_{\epsilon \downarrow 0} C_{X,\epsilon}(Q_X, Q_Y) \geq C(Q_X, Q_Y)$. So, $\lim_{\epsilon \downarrow 0} C_{X,\epsilon}(Q_X, Q_Y) = C(Q_X, Q_Y)$ pointwise.

Assumption 1: (Uniform Convergence of $(X', \epsilon)$-Smooth OT Functional): We assume that there is a function $\delta(\epsilon) : (0, \infty) \to (0, \infty)$ vanishing as $\epsilon \to 0$ such that

$$C_{X,\epsilon}(Q_X, Q_Y) \geq C(Q_X, Q_Y) - \delta(\epsilon)$$

holds for all $(Q_X, Q_Y)$. In other words, $C_{X,\epsilon}(Q_X, Q_Y) \to C(Q_X, Q_Y)$ as $\epsilon \downarrow 0$ uniformly for all $(Q_X, Q_Y)$.

Obviously, if the optimal transport cost functional $(Q_X, Q_Y) \to C(Q_X, Q_Y)$ is uniformly continuous under the Lévy–Prokhorov metric (which was assumed by the author in [41] in studying the asymptotics of Strassen’s optimal transport problem), then Assumption 1 holds. The following two examples satisfying Assumption 1 were provided in [41].

Example 1 (Countable Alphabet and Bounded Cost): $X$ and $\mathcal{Y}$ are countable sets and $c$ is bounded (i.e., $\sup_{x, y} c(x, y) < \infty$).

Example 2 (Wasserstein Metric Induced by a Bounded Metric): $X = \mathcal{Y}$ equipped with a bounded metric $d$ is a Polish metric space, i.e., $\sup_{x, y} d(x, y) < \infty$. The cost function is set to $c = d^p$ for $p \geq 1$, and hence, $C = W_p^d$.

The following theorem characterizes the asymptotic concentration exponent. The proof is provided in Section III. For a function $f : [0, \infty]^k \to [0, \infty]$ with $k \geq 1$, denote the effective domain of $f$ as

$$\text{dom} f = \{ f(x) \in [0, \infty]^k : f(z) < \infty \}.$$

By definition, $\text{dom} \hat{f} = \text{dom} \tilde{f} = \text{dom} f$ if $f$ is monotonous in each parameter (given others).

Example 2 satisfying Assumption 1 follows by the fact that the Wasserstein metric induced by a bounded metric $d$ is equivalent to the Lévy–Prokhorov metric in the sense that $d_{\text{sup}}^{p+1} \leq W_p^d \leq d^p + d_{\text{sup}} d_P$ where $d_{\text{sup}} = \sup_{x, x' \in X} d(x, x')$ is the diameter of $X$ [15].
Theorem 3 (Asymptotics of $E_{1}^{(n)}$ and Dimension-Free Bound): For Polish $X$ and $Y$, the following hold.

1) For any $\alpha \geq 0, \tau \geq 0$ and any positive integer $n$,
$$E_{1}^{(n)}(\alpha, \tau) \geq \tilde{\phi}(\alpha, \tau). \tag{12}$$

2) Under Assumption 1, for any $(\alpha, \tau)$ in the interior of $\text{dom} \tilde{\phi}$, it holds that $\lim_{n \to \infty} E_{1}^{(n)}(\alpha, \tau) = \tilde{\phi}(\alpha, \tau)$.

3) Let $(a_{n})$ be a sequence such that $e^{-o(n)} \leq a_{n} \leq 1 - e^{-o(n)}$ (and hence $a_{n} = -\frac{1}{n} \log a_{n} \to 0$). Then, under Assumption 1, it holds that for any $\tau$ in the interior of $\text{dom} \tilde{\phi}$,
$$\lim_{\alpha \to 0} \tilde{\phi}(\alpha, \tau) \leq \liminf_{n \to \infty} E_{1}^{(n)}(\alpha, n, \tau) \leq \limsup_{n \to \infty} E_{1}^{(n)}(\alpha, n, \tau) \leq \tilde{\phi}(\tau),$$

where
$$\varphi(\tau) := \phi(0, \tau) = \inf_{Q_{Y}:\mathcal{C}(P_{X}, Q_{Y})>\tau} D(Q_{Y}||P_{Y}). \tag{13}$$

The condition $e^{-o(n)} \leq a_{n} \leq 1 - e^{-o(n)}$ implies that the sequence $(a_{n})$ does not approach 0 or 1 too fast, in the sense that the sequence $(a_{n})$ is sandwiched between a sequence that subexponentially approaches zero and a sequence that subexponentially approaches one.

The expression $\tilde{\phi}(\alpha, \tau)$ for the asymptotic concentration exponent is elegant in the sense that it is expressed in terms of two fundamental quantities from other fields—“relative entropy” which comes from information theory (or large deviations theory) and “optimal transport” cost—which comes from the theory of optimal transport. Hence, this verifies an intimate connection among concentration of measure, information theory, and optimal transport.

The first bound like the one in (12) was derived by Marton [25], [26], which was improved by Gozlan and Léonard in [16], [18]. Our proof relies on the subadditivity of OT costs, instead of traditional transport-entropy inequalities, leading to that our bound in (12) is strictly better than Gozlan and Léonard’s especially when the measure of the set is small. When $c = d^{p}$ and $\alpha$ is close to zero, e.g., $\alpha = \frac{1}{2} \log 2$ (i.e., $a = \frac{1}{2}$; recall the relation $a = e^{-n\alpha}$ in (2)), our bound and theirs do not differ too much, and as $n \to \infty$, they coincide asymptotically. However, if $\alpha$ is bounded away from zero, our bound is usually asymptotically tight but theirs are not.

The bound in (12) can be expressed as an exponentially sharp version of Talagrand’s concentration inequalities. Given $P_{X}, P_{Y}$, and $c$, we define for $\tau \geq 0, \lambda \in [0, 1]$,
$$\phi_{\lambda}(\tau) := \inf_{Q_{X}, Q_{Y}:\mathcal{C}(Q_{X}, Q_{Y})>\tau} (1 - \lambda) D(Q_{Y}||P_{Y}) + \lambda D(Q_{X}||P_{X}), \tag{14}$$

which is a nonlinear variant of the transport-entropy inequalities in [20, Definition 4.1]. Denote $\phi_{\lambda}(\tau)$ as the lower convex envelope of $\tilde{\phi}(\alpha, \tau)$.

Corollary 4 (Improved Talagrand’s Concentration Inequality): For Polish $X$ and $Y$, it holds that for any $\tau \geq 0, \lambda \in [0, 1]$, $t = n\tau$, and any $A$,
$$P_{Y}^{\otimes n}(A^{t}) \leq e^{-n\tilde{\phi}(\tau)}, \tag{15}$$

where $\tilde{\phi}_{\lambda}$ can be alternatively expressed as
$$\tilde{\phi}_{\lambda}(\tau) = \inf_{\alpha \geq 0} \lambda \alpha + (1 - \lambda) \tilde{\phi}(\alpha, \tau). \tag{16}$$

Moreover, under Assumption 1 and given any $\tau$ which together with the optimal $\alpha$ attaining the infimum in (16) is in the interior of $\text{dom} \tilde{\phi}$, the inequality in (15) is exponentially sharp in the sense that there is a sequence of sets $A_{n}$ such that the induced exponents of two sides asymptotically coincide.

Remark 5: The kind of inequalities like the one in (15) are the so-called Talagrand’s concentration inequalities; see a weaker version for Hamming metric in [32, p. 86]. An inequality weaker than the one in (15) was proven by Gozlan et al. [20] in which linear bounds on $\phi_{\lambda}(\tau)$, instead of $\tilde{\phi}(\alpha, \tau)$ itself, were applied in the proof.

Remark 6: The function $\tilde{\phi}_{\lambda}$ suggests a new and more general class of transport-entropy inequalities, which plays the same role in our proof of Theorem 3 as the traditional transport-entropy inequalities in Marton’s proof [25], [26].
where
\[ \varphi_X(\tau) := \inf_{Q_X \in \mathcal{C}(P_X, Q_X) > \tau} D(Q_X \| P_X). \] (18)
In particular, if the cost function is set to \( d^p \) with \( p \geq 1 \) and \( d \) denoting a metric, and define
\[ \varphi_{X, \geq}(\tau) := \inf_{Q_X \in \mathcal{C}(P_X, Q_X) \geq \tau} D(Q_X \| P_X), \] (19)
then the assumption is equivalent to saying that \( \varphi_{X, \geq}(\tau) \) is strictly increasing in \( \tau \geq 0 \) (since \( \varphi_{X, \geq}(0) = 0 \)).

An equivalent statement of Assumption 2 is that \( P_X, C(P_X, Q_X) \) is bounded away from zero, then so is \( D(Q_X \| P_X) \). In other words, given \( P_X \), convergence in information (i.e., \( D(Q_X \| P_X) \)) implies convergence in optimal transport (i.e., \( C(P_X, Q_X) \to 0 \)).

**Statement 3** is not new; see Proposition 4.6 and Theorem 4.7. Then, the following hold.

1. For any \( \alpha, \tau \geq 0 \) and any positive integer \( n \),
   \[ E^{(n)}_1(\alpha, \tau) = \phi(\alpha, \tau), \] (20a)
2. For any \( \alpha, \tau \) in the interior of \( \text{dom} \phi \), it holds that
   \[ \lim_{n \to \infty} E^{(n)}_1(\alpha, \tau) = \phi(\alpha, \tau). \] (20b)
3. Let \( (a_n) \) be a sequence such that \( e^{-a_n} \leq a_n \leq 1 - e^{-a(n)} \) (and hence \( a_n = -\frac{1}{p} \log\alpha_n \to 0 \)). Then, for any \( \tau \) in the interior of \( \text{dom} \phi \),
   \[ \lim_{n \to \infty} E^{(n)}_1(\alpha_n, \tau) \leq \varphi(\tau), \] (21)
and under Assumption 2,
\[ \lim_{n \to \infty} E^{(n)}_1(\alpha_n, \tau) = \varphi(\tau), \]
where \( \varphi_X \) is defined in (18). In particular, for the case of \( P_X = P_Y \), \( \lim_{n \to \infty} E^{(n)}_1(\alpha_n, \tau) > 0 \) holds for all sufficiently small (equivalently for all) \( \tau > 0 \) (i.e., exponential convergence) if and only if Assumption 2 holds.

**Theorem 7** is a consequence of **Theorem 3** and proven in Section IV. **Statement 1** in **Theorem 7** is a restatement of **Statement 1** in **Theorem 3** for the case of \( c = d^p \). **Statement 3** is not new; see Proposition 4.6 and **Theorem 5.4** in [19]. **Statements 2** and **3** in **Theorem 7** might be proven alternatively by the large deviation theorems on the Wasserstein metric in [37] and [38]. In fact, for this setting of \( a = \frac{1}{2} \), Alon et al. in [4] provided an alternative expression for \( \lim_{n \to \infty} E^{(n)}_1(\alpha_n, \tau) \) when \( X \) is finite (Assumption 2 automatically is satisfied for this case). The equivalence between theirs and ours is discussed in details in Section II-C.

By Talagrand’s transport inequality, the function \( \phi \) can be derived for the case of Gaussian distribution and Euclidean distance.

**Example 8** (GaussianDistribution and EuclideanDistance): For Gaussian distributions \( P_X = P_Y = \mathcal{N}(0, 1) \) and \( c(x, y) = (x - y)^2 \) (with \( p = 2 \)), the function \( \hat{\phi}(\alpha, \tau) = \phi(\alpha, \tau) = \begin{cases} \frac{1}{2} (\sqrt{\tau - 2 \alpha})^2, & \tau > 2 \alpha \\ 0, & \text{otherwise.} \end{cases} \)

**Remark 10:** This theorem implies that for the Hamming metric, the asymptotic concentration exponent for a pair of arbitrary distributions (\( P_X, P_Y \)) is the same as that of (Bern(p), Bern(q)), some quantized version of (\( P_X, P_Y \)).
In fact, given an arbitrary $P_X$, it can be obtained from (21) that
\[
\phi(\alpha, \tau) \geq \inf_{p \in [0,1]: \omega(p) < \infty} \theta(p, \omega(p)) \geq \inf_{p \in [0,1]} \theta(p, \tilde{\omega}(p)).
\]
(24)

Compared with determining the function $\omega$, itself, it is much easier to determine $\tilde{\omega}$, since by the Neyman–Pearson lemma, the graph of $\tilde{\omega}$ coincides with the lower convex envelope of the curve $\{ (P_X(A_r), P_Y(A_r)) : r \geq 0 \}$, where $A_r := \{ x : dP_X/dR(x) \leq rdP_Y/dR(x) \}$ with $R$ denoting an arbitrary probability measure such that $P_X, P_Y \ll R$. Moreover, $\omega$ coincides with $\tilde{\omega}$ if $P_X$ is atomless, and for this case, the lower bound in (24) is tight, as shown in (22).

For the case of $P_X = P_Y$,\[
\phi(\alpha, \tau) = \inf_A \theta(P_X(A)) \geq \phi(\alpha, \tau) := \inf_{p \in [0,1]} \theta(p),
\]
(25)
where
\[
\theta(p) := \theta(p, p) = \inf_{s, t \in [0,1]: D(s||p) \leq \alpha, s \leq t \geq \tau} D(t||p) = \begin{cases} 0 & p \leq s^{*}(p) - \tau \\ D(s^{*}(p) - \tau||p) & p > s^{*}(p) - \tau > 0 \\ \infty & s^{*}(p) - \tau \leq 0. \end{cases}
\]

By the convexity of the relative entropy, it is easy to see that $\phi$ is convex. Moreover, the equality in (25) holds when $P_X = P_Y$ is atomless. Hence, for this case, $\phi(\alpha, \tau) = \phi(\alpha, \tau)$. In other words, for any $\alpha > 0, \tau \in (0,1)$, all atomless distributions admit the same smallest asymptotic concentration exponent $\phi(\alpha, \tau)$. The graph of $\phi$ is shown in Fig. 1. In particular, for the case in Statement 3 of Theorem 9 with $P_X = P_Y$, it was shown in [34] that $\varphi(\tau) \geq \min_{\epsilon \in [\tau,1]} D(p - \tau||p)$, with equality if $P_X = P_Y$ is atomless [5].

B. Asymptotic Isoperimetric Exponent

We next derive the asymptotic expression of $E_0^{(n)}(\alpha, \tau)$. Define
\[
\psi(\alpha, \tau) := \sup_{Q_{XW} : D(Q_{XW}||P_X||P_W) \leq \alpha} \inf_{Q_{YW} : D(Q_{YW}||P_Y||P_W) \leq \tau} D(Q_{YW}||P_{YW}),
\]
(26)
with the supremum taken over all $W$ defined on finite alphabets.

**Theorem 11:** The alphabet size of $W$ in (26) can be restricted to be no larger than 2.

We will restate this theorem in Theorem 20 in Section II-C, and the proof of Theorem 20 is provided in Section VII. It is worth noting that bounding the alphabet size of $W$ is not obvious as that for the function $\phi$ in (11), since the auxiliary random variable $W$ here does no longer play the role of the convex combination in the lower convex envelope. So, Carathéodory’s theorem cannot be applied. Instead, our proof of Theorem 11 is based on the dual expression of $\psi$.

Based on $\psi$, the asymptotic expression of $E_0^{(n)}$ is characterized in the following theorem. Define the $(\mathcal{X}, \epsilon)$-smooth cost function w.r.t. $c$ as
\[
c_{\mathcal{X}, \epsilon}(x, y) := \inf_{x' : d(x, x') \leq \epsilon} c(x', y).
\]
By definition, $c_{\mathcal{X}, \epsilon}(x, y) \leq c_{\mathcal{X}, 0}(x, y) = c(x, y)$, and by the lower semicontinuity of $c$, $\lim_{\epsilon \downarrow 0} c_{\mathcal{X}, \epsilon}(x, y) \geq c(x, y)$. So, $\lim_{\epsilon \downarrow 0} c_{\mathcal{X}, \epsilon}(x, y) = c(x, y)$ pointwise.

**Assumption 3:** (Uniform Convergence of $(\mathcal{X}, \epsilon)$-Smooth Cost Function): We assume there is a function $\delta(\epsilon) : (0, \infty) \to (0, \infty)$ vanishing as $\epsilon \downarrow 0$ such that
\[
c_{\mathcal{X}, \epsilon}(x, y) \geq c(x, y) - \delta(\epsilon)
\]
(27)
holds for all $(x, y)$. In other words, $c_{\mathcal{X}, \epsilon}(x, y) \to c(x, y)$ as $\epsilon \downarrow 0$ uniformly for all $(x, y)$.

Assumption 3 is automatically satisfied if $\mathcal{X} = \mathcal{Y}$ and $c = d$. Moreover, Assumption 3 is implied by Assumption 1. By choosing $Q_X, Q'_X, Q_Y$ as Dirac measures $\delta_x, \delta_{x'}, \delta_y$ in Assumption 1 and by the fact that $d_P(\delta_x, \delta_{x'}) = d(x, x')$ when $d(x, x') \leq 1$, it is easy to verify that Assumption 3 holds for this case.

**Theorem 12** (Asymptotics of $E_0^{(n)}$): Assume that $\mathcal{X}$ and $\mathcal{Y}$ are Polish spaces. Then the following hold.
1) Assume that $c(x, y) \leq c_X(x) + c_Y(y)$ for some measurable functions $c_X : \mathcal{X} \to \mathbb{R}, c_Y : \mathcal{Y} \to \mathbb{R}$. Assume that $P_X$ concentrates on a compact set and $P_Y$ satisfies $\mathbb{E}[\exp(c_Y^2(Y))] < \infty$. Then, under Assumption 3, for any $\alpha \geq 0, \tau \geq 0$, it holds that
\[
\lim_{n \to \infty} \sup E_0^{(n)}(\alpha, \tau) \leq \lim_{\tau' \downarrow \tau} \psi(\alpha, \tau').
\]
(28)
2) If $c$ is bounded and satisfies Assumption 3, then for any $\alpha \geq 0, \tau \geq 0$, it holds that
\[
\lim_{n \to \infty} \sup E_0^{(n)}(\alpha, \tau) \leq \lim_{\alpha' \downarrow \alpha} \lim_{\tau' \downarrow \tau} \psi(\alpha', \tau').
\]
(29)
3) Under Assumption 1 (given in Section II-A1), for any $(\alpha, \tau)$ in the interior of $\text{dom}\psi$, it holds that

$$\lim_{n \to \infty} \inf E_0^{(n)}(\alpha, \tau) \geq \psi(\alpha, \tau).$$

4) Assume that $X = \mathcal{Y}$ equipped with a metric $d$ is a Polish metric space, and the cost function is set to $c = d^p$ for $p \geq 1$. Then, for any $(\alpha, \tau)$ in the interior of $\text{dom}\psi$, it holds that

$$\lim_{n \to \infty} \inf E_0^{(n)}(\alpha, \tau) \geq \psi(\alpha, \tau).$$

**Remark 13:** It is not straightforward to derive upper bound $\lim_{n \to \infty} E_0^{(n)}(\alpha, \tau)$ for the case in which the cost is unbounded and $P_X$ does not concentrate on a compact set. One may wonder if it is possible to generalize the result for the compact $X$ to the noncompact (Polish) $X$ by truncating the noncompact space into a compact one. In fact, this idea is adopted in the proof of Statement 2 in Theorem 12; see Section VI-B. As shown in this proof, the set $A \subseteq X^n$ is projected to a space of dimension $n'$ where $n' = (1 - \epsilon')n$ for small $\epsilon'$. Such an idea seems not to work for unbounded costs, since in this case, the remaining space of dimension $cn$ cannot be omitted by paying only a finite cost. Another possible way is to generalize the inherently typical subset lemma [2] to infinite (countably infinite or uncountable) spaces. The continuity of information quantities in the weak topology is the key point in the proof of the inherently typical subset lemma [2]. However, it is well known that in an infinite space, convergence in weak topology does not imply convergence in Shannon information quantities in general, i.e., Shannon information quantities are discontinuous [22]. So, certain assumptions must be posed in this method.

**Remark 14:** In fact, we can obtain the following “dimension-free” bound: For arbitrary Polish $X$ and $\mathcal{Y}$, it holds that for any $(\alpha, \tau)$,

$$E_0^{(n)}(\alpha, \tau) \leq \lim_{\alpha \to \alpha' \in A} \sup_{Q_{X|W|K}} \inf_{(\tau_k)_{k \in [n]}, Q_{Y|X|W|K}} D(Q_{X|W|K}||P_X|Q_{W|K}) \leq \alpha$$

where $K \sim \text{Unif}[n]$ and there is no restriction on the alphabet size of $W$. To prove this bound, we redefine $Q_{X^n}$ in Step 2 of Section VI-A1 as the uniform distribution on the set $A$ itself, instead of an inherently typical subset of $A$, and rechoose $Q_{Y^n|X^n}$ in Step 3 of Section VI-A1 as $Q_{Y^n|X^n} = \prod_{k=1}^n Q_{Y_k|X_k}$ where $Q_{Y_k|X_k}, k \in [n]$ are transition probability measures such that $c(x_k, y_k) \leq \tau_k$ a.s. under $Q_{Y_k|X_k} = x_k$ for any $x_k$. Then, following the proof steps in Section VI-A1, the “dimension-free” bound is obtained. Note that the inherently typical subset lemma is not involved here. However, by comparing this bound with the upper bound in (29) or (28), it is easy to see that this “dimension-free” bound is not asymptotically tight. It is not obvious to see whether our bound $\lim_{n \to \infty} \inf_{\alpha' \sim \tau', \psi(\alpha', \tau')} E_0^{(n)}(\alpha, \tau)$ is a dimension-free bound for $E_0^{(n)}(\alpha, \tau)$. If yes, finding a proof is an interesting but challenging task.

The following is an example that satisfies all the conditions in Statement 1 in Theorem 12.

**Example 15:** The space $X = \mathcal{Y}$ equipped with a metric $d$ is a Polish metric space, and the cost function is set to $c = d$. Moreover, $P_X$ concentrates on a compact set and $P_Y$ satisfies $\mathbb{E}[\exp(d^p(x, Y))] < \infty$ for some (and hence all) $x$. In this case, by the inequality $d(x, y) \leq d(x, x_0) + d(y, x_0)$, we can choose $c_Y(x) = d(x, x_0)$ and $c_Y(y) = d(y, x_0)$.

Statement 3 in Theorem 12 only requires Assumption 1. So, Statement 3 in Theorem 12 holds for Examples 1 and 2 given below Assumption 1.

Assumption 3 is satisfied by Example 2. So, Statement 2 in Theorem 12 holds for Example 2. We now verify this point. It suffices to consider small enough $\epsilon$ such that $d(x, x') \leq \epsilon < d(x, y)$.

$$d^p(x', y) \geq (d(x, y) - d(x', x))p \geq (d(x, y) - \epsilon)p.$$ So,

$$d^p(x, y) - d^p(x', y) \leq d^p(x, y) - (d(x, y) - \epsilon)p.$$ Since $t \in [0, d_{sup}] \to t^p$ is continuous and hence uniformly continuous, there is a function $\delta(\epsilon) : (0, \infty) \to (0, \infty)$ vanishing as $\epsilon \downarrow 0$ such that $t^p - (t - \epsilon)^p \leq \delta(\epsilon)$ for all $t \in [\epsilon, M].$

If $\psi$ is continuous at $(\alpha, \tau)$, then all the inequalities in (29) turn into equalities. Given $Q_{X|W}$, the infimization in (29), $g(\tau) := \inf_{Q_{Y|X|W} : \mathbb{E}[\phi(\tau)Y] \leq \tau} D(Q_{Y|W}||P_Y|Q_{W})$, is convex and nonincreasing in $\tau$, and hence, it is only possible to be discontinuous at the point $\tau_0 := \inf\{\tau : g(\tau) < \infty\}$. The proof of Theorem 12 is provided in Section VI. Furthermore, to make it consistent with the expression of $\phi$, the infimization in (26) can be written as the infimization over $Q_{Y|W}$ such that $C(Q_{X|W}, Q_{Y|W}|Q_{W}) \leq \tau$.

Theorem 12 generalizes Ahlswede and Zhang’s result [3] from finite spaces to Polish spaces. Similar to Ahlswede and Zhang’s, our proof is also based on the inherently typical subset lemma, but requires more technical treatments since the spaces are much more general. Furthermore, previously, there was no bound on the alphabet size of $W$ in the definition of $\psi$, even for the finite alphabet case. For the finite alphabet case, Ahlswede and Zhang [2], [3] showed that

$$\psi_N(\alpha, \tau) \leq \psi(\alpha, \tau) = \psi_N(\alpha, \tau) + O\left(\frac{\log^2 N}{N^{1/2}}\right),$$

where $\psi_N$ is defined similarly as $\psi$ but with $W$ restricted to concentrate on the alphabet $\mathcal{W}$ satisfying $|\mathcal{W}| = N$. Theorem 20 shows that $\psi(\alpha, \tau) = \psi_N(\alpha, \tau)$ for any $N \geq 2$, which does not only sharpen Ahlswede and Zhang’s result, but also makes $\psi(\alpha, \tau)$ “computable” for the finite alphabet case in the sense that $\psi(\alpha, \tau)$ can be evaluated by a finite-dimensional program.

**C. Dual Formulas**

We now provide dual formulas for $\psi$ in (26) and variants of $\phi$ in (10) and $\varphi$ in (13). Our motivations for this part are two-fold: One is to verify the equivalence between our formula $\varphi_X(\tau)$ and Alon, Boppana, and Spencer’s in [4] for
the asymptotic concentration exponent; the other is to prove the bound on the alphabet size of $W$ given in Theorem 11. The main tool used in deriving dual formulas is the Kantorovich duality for the optimal transport cost and the duality for the I-projection. In the following, for a measurable function $f : X \to \mathbb{R}$, we adopt the notation $P_X(f) = \int_X f \, dP_X$.

We define a variant of $\phi$ as for $\alpha \geq 0, \tau \geq 0$,

$$
\phi^\geq(\alpha, \tau) := \inf_{Q_Y \in \mathcal{P}(Y), \alpha > 0, \tau \geq 0} D(Q_Y \| P_Y).
$$

Then, $\phi^\geq(\alpha, \tau) \leq \phi(\alpha, \tau) \leq \lim_{\tau \to 1^+} \phi^\geq(\alpha, \tau')$. Hence, for all $(\alpha, \tau)$ in the interior of dom$\phi$, $\phi^\geq(\alpha, \tau) = \phi(\alpha, \tau)$. We next derive a dual formula for $\phi^\geq$.

**Theorem 16:** For all $\alpha \geq 0, \tau \geq 0$,

$$
\phi^\geq(\alpha, \tau) = \inf_{(f,g) \in C_b(X) \times C_b(Y)} \sup_{f + g \leq c} \lambda \tau - \log P_Y(e^{\lambda g}),
$$

$$
- \eta\alpha - \eta \log P_Y(e^{\frac{\alpha}{2} f}).
$$

Moreover, for all $(\alpha, \tau)$ in the interior of dom$\phi$, $\phi^\geq(\alpha, \tau) = \phi(\alpha, \tau)$.

Define a variant of $\psi$ as

$$
\psi^\geq(\alpha, \tau) := \inf_{Q_Y \in \mathcal{P}(Y), \alpha > 0, \tau \geq 0} D(Q_Y \| P_Y).
$$

As a consequence of Theorem 16, we have a dual formula for $\psi^\geq$.

**Corollary 17:** For all $\tau \geq 0$,

$$
\psi^\geq(\tau) = \inf_{(f,g) \in C_b(X) \times C_b(Y)} \sup_{f + g \leq c} \lambda \tau - \log P_Y(e^{\lambda g}).
$$

Moreover, for all $\tau$ in the interior of dom$\tilde{\psi}$, $\tilde{\psi}^\geq(\tau) = \tilde{\psi}(\tau)$.

When $P_X = P_Y$, the function $\psi^\geq$ reduces to the function $\psi_{X,\geq}$ defined in (19):

$$
\psi_{X,\geq}(\tau) = \inf_{Q_X \in \mathcal{P}(X), Q_X \geq \tau} D(Q_X \| P_X).
$$

For this case, we can write $\psi^\geq$ as follows.

**Proposition 18:** When $P_X = P_Y$ and $c = d$ with $d$ being a metric, we have for any $0 \leq \tau < \tau_{\text{max}}$.

$$
\psi_{X,\geq}(\tau) = \inf_{1\text{-Lip } f : P_X(f) = 0} \sup_{\lambda \geq 0} \lambda \tau - \log P_X(e^{\lambda f}).
$$

Moreover, for all $\tau$ in the interior of dom$\tilde{\psi}_X$, $\tilde{\psi}^\geq(\tau) = \tilde{\psi}_X(\tau)$.

Based on the dual formula in (30), we next show the equivalence between our formula $\tilde{\psi}_X(\tau)$ and Alon, Boppana, and Spencer’s in [4]. When $(X, P_X)$ and $(Y, P_Y)$ are the same finite metric probability space, the cost function $c$ is set to the metric $d$ on this space, and $a$ is set to $\frac{1}{2}$ (equivalently, $\alpha_n = \frac{1}{n} \log 2$), Alon et al. in [4] proved an alternative expression for $\lim_{n \to \infty} E_1(n) / (\alpha_n, \tau)$ which is

$$
r(\tau) := \sup_{\lambda \geq 0} \lambda \tau - L_G(\lambda).
$$

Here $G = (X, d, P_X)$ denotes the metric probability space we consider, and $L_G(\lambda)$ denotes the maximum of $\log P_X(e^{\lambda f})$ over all 1-Lipschitz functions $f : X \to \mathbb{R}$ with $P_X(f) = 0$.

**Theorem 19:** For a finite metric probability space $G = (X, d, P_X)$ and all $\tau > 0$, $\tilde{\psi}_X(\tau) = r(\tau)$.

Lastly, we provide a dual formula for $\psi$.

**Theorem 20:** For all $\alpha \geq 0, \tau \geq 0$,

$$
\psi(\alpha, \tau) = \sup_{f + g \leq c} \inf_{\lambda \geq 0} \sup_{\eta \geq 0} \max_{w \in \{0, 1\}} \left( \eta \alpha + \eta \log P_X(e^{\frac{\alpha}{2} f}) - \lambda \tau - \log P_Y(e^{-\lambda g}) \right),
$$

where $(f, g, w) \in C_b(X) \times C_b(Y), \forall w$. Moreover, the alphabet size of $W$ in the definition of $\psi$ in (26) can be restricted to be no larger than 2.

The second statement of Theorem 20 is exactly Theorem 11.

**Corollary 21:** For $\alpha > 0$, $\lim_{\alpha \to 0} \lim_{\tau \to 1^+} \psi(\alpha', \tau') = \psi(\alpha, \tau)$.

### D. Applications to Other Problems

1) *Strassen’s Optimal Transport:* We have characterized or bounded the concentration and isoperimetric exponents. Our results extend Alon, Boppana, and Spencer’s in [4], Gozlan and Léonard’s [18], and Ahlswede and Zhang’s in [3]. Furthermore, the concentration or isoperimetric function is closely related to Strassen’s optimal transport problem, for which we aim at characterizing

$$
S_t^{(n)}(P_X, P_Y) := \min_{P_{X^n}, P_{Y^n} \in \mathcal{C}(P_X, P_Y)} \{c_n(X^n, Y^n) > t\}
$$

for $t \geq 0$. By Strassen’s duality [41],

$$
S_t^{(n)}(P_X, P_Y) = \sup_{A \subseteq X} \{ P_X(\cap A^c) - P_Y(\cup A^c) \} \geq \sup_{a \in [0,1]} \{ a - \Gamma(n)(a, t) \}.
$$

Therefore, if $\Gamma(n)(a, t)$ is characterized, then so is $S_t^{(n)}(P_X, P_Y)$. In fact, the asymptotic exponents of $S_t^{(n)}(P_X, P_Y)$ were already characterized by the author in [41]. Moreover, it has been shown in [41] that it suffices to restrict $A$ in the supremum in (31) to be “exchangeable” (or “permutation-invariant”). In other words, $A$ could be specified by a set $A$ of empirical measures in the way $A = L_n^{-1}(A)$. Hence, the supremum in (31) can be written as an optimization over empirical measures. From this point, we observe that if $a \mapsto \Gamma(n)(a, t)$ is convex, then computing $\Gamma(n)(a, t)$ for $a \in [0, 1]$ is equivalent to computing $\inf_{a \in [0, 1]} \{ P_X(\cap A^c) - P_Y(\cup A^c) \}$ for $\lambda \geq 0$. Similarly, to the argument in [41], the set $A$ in the definition of $\Gamma(n)(a, t)$ (see (1)) can be also restricted to be “exchangeable”. In this case, central limit theorems can be applied to derive the limit of $\Gamma(n)(a, t_n)$ with a fixed and $t_n$ set to a sequence approaching $\mathcal{C}(P_X, P_Y)$ in the order of $1/\sqrt{n}$, just like central limit results in derived in [41].

2) *Classic Isoperimetric Problem:* The isoperimetric problem considered in Section II-B concerns thick boundaries. In contrast, in the classic isoperimetric problem, the boundary is extremely thin. We assume that $X = Y$ equipped with a metric $d$ is a Polish metric space, and moreover, $P_X = P_Y =: P$ and $c = dv$ with $p \geq 1$. Recall the boundary measure defined in (5). Obviously, the boundary measure do not change if the metric $d$ is replaced by $d_s := \min\{d, s\}$ for a number
s > 0. So, without loss of generality, we assume that d is bounded. The boundary measure can be alternatively expressed as

$$(P_{\otimes}^n)^+(A) = \lim_{r \downarrow 0} \frac{P_{\otimes}^n(A^r)}{\log P_{\otimes}^n(A^r) - \log P_{\otimes}^n(A)} \log P_{\otimes}^n(A^r) - \log P_{\otimes}^n(A)$$

$$= P_{\otimes}^n(A) \lim_{r \downarrow 0} \frac{\log[P_{\otimes}^n(A^r)/P_{\otimes}^n(A)]}{r} = n^{1-1/p} P_{\otimes}^n(A) \lim_{r \downarrow 0} F_{\epsilon}^{(n)}(A), \quad (32)$$

where

$$F_{\epsilon}^{(n)}(A) := \frac{1}{n} \log[P_{\otimes}^n(A^\epsilon^n)/P_{\otimes}^n(A)]$$

is the slope of the line through two points at s = 0 and s = r on the curve s → $\frac{1}{n} \log P_{\otimes}^n(A^s)$. Note that

$$\lim_{r \downarrow 0} F_{\epsilon}^{(n)}(A) = \text{lower right-hand derivative (i.e., the lower Dini derivative)} \text{ of } s \mapsto \frac{1}{n} \log P_{\otimes}^n(A^s).$$

Assumption 4: (Isoperimetric Stability): (a). Given $\alpha > 0$, there are a sequence of sets $B_n \subseteq X^n$ of probability $e^{-\alpha n}$ and a function $\delta : (0, \infty) \times \mathbb{N} \to [0, \infty)$ such that $B_n$ minimizes the boundary measure $(P_{\otimes}^n)^+(A)$ over all sets A of probability $e^{-\alpha n}$, $\lim_{n \to \infty} \sup_{n \to \infty} \delta(\epsilon, n) = 0$, and meanwhile

$$\lim_{r \downarrow 0} F_{\epsilon}^{(n)}(B_n) \geq F_{\epsilon}^{(n)}(B_n) - \delta(\epsilon, n), \quad \forall \epsilon > 0, n \in \mathbb{N}.$$ (b). Given $\alpha > 0$, there are a family of sets $A_{n,\epsilon} \subseteq X^n$ of probability $e^{-\alpha n}$ and a function $\delta : (0, \infty) \times \mathbb{N} \to [0, \infty)$ such that $A_{n,\epsilon}$ minimizes $P_{\otimes}^n(A^{\epsilon n})$ over all sets A of probability $e^{-\alpha n}$, $\lim_{n \to \infty} \sup_{n \to \infty} \delta(\epsilon, n) = 0$, and meanwhile

$$\lim_{r \downarrow 0} F_{\epsilon}^{(n)}(A_{n,\epsilon}) \leq F_{\epsilon}^{(n)}(A_{n,\epsilon}) + \delta(\epsilon, n), \quad \forall \epsilon > 0, n \in \mathbb{N}.$$ Part (a) of Assumption 4 is true if the probability of the $n^{1/p} e$-enlargement of $B_n$ under the product metric $c_n$ does not change dramatically as $\epsilon \downarrow 0$ for all sufficiently large n. Part (b) is true if $A_{n,\epsilon}$ has a similar property. Assumption 4 is satisfied by the tuple of the standard Gaussian measure, Euclidean distance, and $p = 2$. In this case, the Gaussian isoperimetric inequality states that half-spaces minimizes the Gaussian boundary measure [8], [31]. Moreover, for half-spaces $B_n$ of probability $e^{-\alpha n}$, $P_{\otimes}^n(B_n^{\epsilon n}) = \Phi(\Phi^{-1}(e^{-\alpha n}) + r \sqrt{n})$ which is log-concave in $r$. Hence, it can be seen that

$$\lim_{r \downarrow 0} F_{\epsilon}^{(n)}(B_n) \sim \sqrt{2n}, \quad \epsilon \downarrow 0.$$ So, Part (a) of Assumption 4 holds in this case. Note that the Gaussian isoperimetric inequality also implies that a half-space minimizes $P_{\otimes}^n(A^{\epsilon n})$ over all sets with the probability same as that of the half-space. So, Part (b) of Assumption 4 follows.

Define

$$\xi(\alpha) := \lim_{r \downarrow 0} \frac{\alpha - \log \psi(\alpha, r^p)}{r}, \quad (33)$$

where $\psi$ is defined in (26) but with both $P_X$ and $P_Y$ therein set to P.

Theorem 22 (Isoperimetric Inequality): Assume that $\mathcal{X} = \mathcal{Y}$ is a Polish space and the metric d is bounded. Let $\alpha > 0$. Then, under Part (a) of Assumption 4, it holds that for any set A of probability $e^{-\alpha n}$,

$$(P_{\otimes}^n)^+(A) \geq n^{1-1/p} e^{-\alpha n}(\xi(\alpha) + o_n(1)), \quad (34)$$

where $o_n(1)$ is a term vanishing as $n \to \infty$ which is independent of A, but depends on $(\alpha, p, P)$. Moreover, under Part (b) of Assumption 4, if $\alpha \mapsto \psi(\alpha, r^p)$ is continuous at $\alpha$ for all sufficiently small $r > 0$, then the inequality in (34) is asymptotically sharp in the sense that there is a sequence of sets $A_n \subseteq X^n$ of probability $e^{-\alpha n}$ such that

$$(P_{\otimes}^n)^+(A_n) \leq n^{1-1/p} e^{-\alpha n}(\xi(\alpha) + o_n(1)). \quad (35)$$

Remark 23: The “dimension-free” bound given in Remark 14 can be used to derive an isoperimetric inequality similar to the one in (34) but without the Assumption 4, which will not be given here, since this inequality is not expected to be asymptotically sharp.

The proof of this theorem is provided in Section VIII. Removing Assumption 4 for the inequality in (34) is left to be investigated in the future. Furthermore, the equivalence between the isoperimetric problem with thick boundaries and the one with thin boundaries under other certain conditions is investigated by Milman [27]. However, E. Milman only focuses on complete Riemannian manifolds, while our setting concerns general Polish spaces.

The inequality in (34) can be seen as a generalization of Gaussian isoperimetric inequality [8], [31]. In the setting of the standard Gaussian measure and the Euclidean distance,

$$(P_{\otimes}^n)^+(A) \geq \varphi(\Phi^{-1}(e^{-\alpha n})) \sim e^{-\alpha n} \sqrt{2n},$$

where $\varphi$ is the probability density function of the standard Gaussian, and the asymptotic equality follows by the fact that $\varphi(\Phi^{-1}(a)) \sim \sqrt{2 \log(1/a)}$ as $a \downarrow 0$. Half-spaces are exactly optimal in the Gaussian setting, and intuitively close to optimal in other product probability measures on Euclidean spaces if the volume is fixed, which follows by the functional central limit theorem. In contrast, when the volume is exponentially small, as indicated by Theorem 22, the empirically typical sets are conjectured to be asymptotically optimal.

III. PROOF OF THEOREM 3

A. Statement 1

The proof idea is essentially due to Marton [25], [26]. Our proof relies on the subadditivity of OT costs or the tensorization of a new kind of transport-entropy inequalities given in (14), instead of traditional transport-entropy inequalities.

Let $A \subseteq X$ be a measurable subset. Denote $t = nr$. Denote $Q_{X^n} = P_{X^n}^\otimes(\cdot|A)$ and $Q_{Y^n} = P_{X^n}^\otimes(\cdot|A^r \times Y^n)$. For two sets $A, B$, denote $c_n(A, B) = \inf_{x^n \in A, y^n \in B} c_n(x^n, y^n)$. We first claim that

$$C(Q_{X^n}, Q_{Y^n}) > t.$$
We now prove it. If \( c_n(A, (A^t)^c) \) is attained by some pair \((x^n, y^n)\), then
\[
C(Q_{X^n}, Q_{Y^n}) \geq c_n(A, (A^t)^c) = c_n(x^n, y^n) > t.
\]

We next consider the case that \( c_n(A, (A^t)^c) \) is not attained. Denote the optimal coupling that attains the infimum in the definition of \( C(Q_{X^n}, Q_{Y^n}) \) as \( Q_{X \leftrightarrow Y^n} \) (the existence of this coupling is well known). Therefore,
\[
C(Q_{X^n}, Q_{Y^n}) = \mathbb{E}_Q c_n(X^n, Y^n).
\]

By definition, \( c_n(x^n, y^n) > t \) for all \( x^n \in A, y^n \in B \). Since any probability measure on a Polish space is tight, we have that for any \( \epsilon > 0 \), there exists a compact set \( F \) such that \( Q_{X \leftrightarrow Y^n}(F) > 1 - \epsilon \). By the lower semi-continuity of \( c \) and compactness of \( F \), we have that \( \inf_{(x^n, y^n) \in F} c_n(x^n, y^n) \) is attained, and hence, \( \inf_{(x^n, y^n) \in F} c_n(x^n, y^n) > t \), i.e., there is some \( \delta > 0 \) such that \( c_n(x^n, y^n) \geq t + \delta \) for all \((x^n, y^n) \in F\). This further implies that \( C(Q_{X^n}, Q_{Y^n}) \geq (1 - \epsilon)(t + \delta) + \epsilon t > t \). Hence, the claim above is true.

Furthermore, by definition of \( Q_{X^n}, Q_{Y^n} \), we then have
\[
\begin{align*}
\frac{1}{n} D(Q_{X^n}||P_{X^n}) &= -\frac{1}{n} \log P_{X^n}(A) \\
\frac{1}{n} D(Q_{Y^n}||P_{Y^n}) &= -\frac{1}{n} \log P_{Y^n}((A^t)^c).
\end{align*}
\]

Therefore,
\[
E_1^{(n)}(\alpha, \tau) = -\frac{1}{n} \log \left( 1 - \inf_{A: P_{X^n}(A) \geq \epsilon^{-n} - n\tau} P_{Y^n}(A^t) \right)
\geq \inf_{Q_{X^n}, Q_{Y^n}} \frac{1}{n} D(Q_{Y^n}||P_{Y^n}).
\] (35)

Note that this lower bound depends on the dimension \( n \).

We next single-letterize this bound, i.e., make it independent of \( n \). To this end, we need the chain rule for relative entropies and the chain rule for OT costs. For relative entropies, we have the chain rule:
\[
D(Q_{X^n}||P_{X^n}) = \sum_{k=1}^{n} D(Q_{X_k||X_{k-1}}||P_{X_k||X_{k-1}})
\] (36)
\[
D(Q_{Y^n}||P_{Y^n}) = \sum_{k=1}^{n} D(Q_{Y_k||Y_{k-1}}||P_{Y_k||Y_{k-1}}).
\]

For OT costs, we have a similar “chain rule”.

**Lemma 24 (“Subadditivity” for OT Costs):**

For any transition probability measures \( Q_{X_i||X_{i-1}}, Q_{Y_i||Y_{i-1}}, i \in [n] \), it holds that
\[
C(Q_{X^n}, Q_{Y^n}) \leq \sum_{k=1}^{n} C(Q_{X_k||X_{k-1}}, Q_{Y_k||Y_{k-1}}(Q_{X_{k-1}}, Q_{Y_{k-1}}),
\]
where \( Q_{X_k} := \prod_{i=1}^{k} Q_{X_i||X_{i-1}}, Q_{Y_k} := \prod_{i=1}^{k} Q_{Y_i||Y_{i-1}}, \) and
\[
C(Q_{X_k||X_{k-1}}, Q_{Y_k||Y_{k-1}}|Q_{X_{k-1}}, Q_{Y_{k-1}}) := \sup_{Q_{X_{k-1}Y_{k-1}} \in C(Q_{X_{k-1}}, Q_{Y_{k-1}})} C(Q_{X_k||X_{k-1}}, Q_{Y_k||Y_{k-1}}|Q_{X_{k-1}Y_{k-1}}).
\]

For completeness, we provide the proof of Lemma 24 since it is very short.

**Proof of Lemma 24:** We need the following lemma on composition of couplings, which is well-known in OT theory; see the proof in, e.g., [42, Lemma 9].

**Lemma 25 (Composition of Couplings):** For any transition probability measures \( (P_{X_i||X_{i-1}}, P_{Y_i||Y_{i-1}}), i \in [n] \) and any \( Q_{X_i,Y_i||X_{i-1},Y_{i-1}}, i \in [n] \), we have
\[
\prod_{i=1}^{n} Q_{X_i,Y_i||X_{i-1},Y_{i-1}} \in C(P_{X_i||X_{i-1}}, P_{Y_i||Y_{i-1}}), i \in [n], \text{ and}
\]
\[
\prod_{i=1}^{n} P_{X_{i-1}X_i||Y_{i-1}Y_i} \in C(P_{X_{i-1}X_i}, P_{Y_{i-1}Y_i}, i \in [n], \text{ and}
\]
\[
\prod_{i=1}^{n} P_{Y_{i-1}Y_i} \in C(P_{Y_{i-1}Y_i}).
\]

By the lemma above, we have
\[
C(Q_{X^n}, Q_{Y^n}) \leq \inf_{Q_{X^n}, Q_{Y^n}} \frac{1}{n} \sum_{k=1}^{n} E_1^{(n)}(\alpha_k, \tau_k)
\]

\[
\leq \inf_{Q_{X^n}, Q_{Y^n}} \frac{1}{n} \sum_{k=1}^{n} E_1^{(n)}(\alpha_k, \tau_k)
\]

\[
= \inf_{Q_{X^n}, Q_{Y^n}} \frac{1}{n} \sum_{k=1}^{n} E_1^{(n)}(\alpha_k, \tau_k)
\]

\[
= \inf_{Q_{X^n}, Q_{Y^n}} \frac{1}{n} \sum_{k=1}^{n} E_1^{(n)}(\alpha_k, \tau_k)
\]

\[
\leq \sum_{k=1}^{n} C(Q_{X_k||X_{k-1}}, Q_{Y_k||Y_{k-1}}|Q_{X_{k-1}}, Q_{Y_{k-1}}),
\]

where in (37), Lemma 25 is applied.

We continue the proof of (12). From (36), we know that for any \( Q_{X^n} \) such that \( \frac{1}{n} D(Q_{X^n}||P_{X^n}) \leq \alpha \), there must exist nonnegative numbers \( \{\alpha_k\} \) such that
\[
D(Q_{X_k||X_{k-1}}||P_{X_k||X_{k-1}}) \leq \alpha_k
\]
and \( \frac{1}{n} \sum_{k=1}^{n} \alpha_k = \alpha \). Similarly, from Lemma 24, we know that for \( (Q_{X^n}, Q_{Y^n}) \) such that \( \frac{1}{n} C(Q_{X^n}, Q_{Y^n}) > \tau \), there must exist nonnegative numbers \( \{\tau_k\} \) such that
\[
C(Q_{X_k||X_{k-1}}, Q_{Y_k||Y_{k-1}}|Q_{X_{k-1}}, Q_{Y_{k-1}}) > \tau_k
\]
and \( \frac{1}{n} \sum_{k=1}^{n} \tau_k = \tau \). These lead to that for some sequence of nonnegative pairs \( \{(\alpha_k, \tau_k)\} \) such that \( \frac{1}{n} \sum_{k=1}^{n} \alpha_k = \alpha, \frac{1}{n} \sum_{k=1}^{n} \tau_k = \tau \), we have
\[
E_1^{(n)}(\alpha, \tau) \geq \frac{1}{n} \sum_{k=1}^{n} \phi_k(\alpha_k, \tau_k, Q_{X_k||X_{k-1}}, Q_{Y_k||Y_{k-1}}),
\]
where
\[
\phi_k(\alpha_k, \tau_k, Q_{X_k||X_{k-1}}, Q_{Y_k||Y_{k-1}})
\]
We now simplify the expression of \( \phi_k(\alpha_k, \tau_k, Q_{X^k}, Q_{Y^k}) \). Note that
\[
C(Q_{X^k}|X^k-1, Q_{Y^k}|Y^k-1) > \tau_k
\]
if and only if there exists a coupling \( Q_{X^k-1}Y^k-1 \) of \( (Q_{X^k-1}, Q_{Y^k}) \) such that
\[
C(Q_{X^k}|X^k-1, Q_{Y^k}|Y^k-1) > \tau_k
\]
and at the same time, we relax the coupling \( Q_{X^k-1}Y^k-1 \) of \( (Q_{X^k-1}, Q_{Y^k}) \) to any joint distribution.

B. Statement 2
From the dimension-free bound in (12),
\[
\lim\inf_{n \to \infty} E_1^{(n)}(\alpha, \tau) \geq \tilde{\phi}(\alpha, \tau)
\]
due to apply Sanov’s theorem and estimate their distance by definition.

We assume that \( \mathcal{W} \) is finite, and without loss of generality, we assume \( \supp(Q_{W^n}) = [m] = \{1, 2, \ldots, m\} \). Let \( \epsilon > 0 \). Let \( Q_{W^n} Q_{X^n} | W \) be an optimal pair attaining \( \tilde{\phi}(\alpha - \epsilon, \tau + \epsilon) \). That is,
\[
D(Q_{X^n} | W) \leq \alpha - \epsilon
\]
and
\[
C(Q_{X^n} | W, Q_{Y^n} | W) > \tau + \epsilon
\]
and
\[
D(Q_{Y^n} | W) \leq \tilde{\phi}(\alpha - \epsilon, \tau + \epsilon) + \epsilon.
\]
For each \( n \), let \( Q_{(n)} \) be an \( n \)-type (i.e., the empirical measure of an \( n \)-length sequence) such that \( \supp(Q_{W^n}) \subseteq [m] \) and \( Q_{W^n} \to Q_W \) as \( n \to \infty \). Let \( Q_{X_W} := Q_{W^n} Q_{X^n} | W, Q_{Y_W} := Q_{W^n} Q_{Y^n} | W \). Let \( u^n = (1, \ldots, 1, \ldots, 2, \ldots, 2, \ldots, m, \ldots, m) \) be an \( n \)-length sequence, where \( i \) appears \( n_i := nQ_{W_i} \) times. Hence, the empirical measure of \( u^n \) is \( Q_{W^n} \).

We now choose \( A \) and \( B \) as conditional empirically typical sets. Specifically, for \( \epsilon' > 0 \),
\[
A = T_{n}(Q_{X^n} | W) | u^n = L_{n}^{-1}(A)w^n = \prod_{u=1}^{m} L_{n}^{-1}(A_{w}),
\]
\[
B = T_{n}(Q_{Y^n} | W) | u^n = L_{n}^{-1}(B)w^n = \prod_{u=1}^{m} L_{n}^{-1}(B_{w}),
\]
where \( A_{w} := B_{\epsilon'}(Q_{X^n} | W = w), B_{w} := B_{\epsilon'}(Q_{Y^n} | W = w) \) for \( w \in [m], A = B_{\epsilon'}(Q_{X^n} | W), B_{\epsilon'}(Q_{Y^n} | W) \). For each \( w, A_{w} \) is closed. Since the empirical measure map \( L \) is continuous under the weak topology, \( L_{n}^{-1}(A_{w}) \) is closed in \( W_{n} \). Therefore, \( A \) is closed in \( W_{n} \). Similarly, \( B \) is closed in \( W_{n} \).

By Sanov’s theorem,
\[
\lim_{n \to \infty} \frac{1}{n} \log P_{X_{W}^{n}}(A) = \sum_{w} Q_{W}(w) \lim_{n \to \infty} \frac{1}{n} \log P_{X_{W}^{n}}(L_{n}^{-1}(A_{w})) \leq \sum_{w} Q_{W}(w) \inf_{R \in A_{w}} D(R_{X} \| P_{X}) \leq \sum_{w} Q_{W}(w) D(Q_{X|W} \| | P_{X}) \leq D(Q_{X} \| | P_{X}| W) \leq \alpha - \epsilon.
\]

Hence,
\[
-\frac{1}{n} \log P_{X_{W}^{n}}(A) \leq \alpha \text{ for all sufficiently large } n.
\]
Similarly,
\[
-\frac{1}{n} \log P_{Y_{W}^{n}}(B) \leq D(Q_{Y|W} \| | P_{Y}| Q_{W}) \leq \tilde{\phi}(\alpha - \epsilon, \tau + \epsilon) + 2\epsilon\]

for all sufficiently large \( n \).

We next estimate the distance between \( A \) and \( B \), and show that
\[
c_{n}(x^n, y^n) > n\tau, \quad \forall x^n \in A, y^n \in B.
\]
Observe that for $L_{x|w^n} \in A$, $L_{y|w^n} \in B$,

$$ \frac{1}{n} c_n(x^n, y^n) = \mathbb{E}_{L_{x|w^n}, L_{y|w^n}} C(X, Y) $$

$$ \geq C(L_{x|w^n}, L_{y|w^n}) $$

$$ \geq \inf_{R_{X|W} \in A, R_{Y|W} \in B} C(R_{X|W}, R_{Y|W}) $$

$$ = \mathbb{E}_{W \sim L_{w^n}} \inf_{R_{X|W} \in A, R_{Y|W} \in B} C(R_{X}, R_{Y}) $$

$$ = \mathbb{E}_{W \sim L_{w^n}} \inf_{R_{X|W} \in A, R_{Y|W} \in B} C(R_{X}, R_{Y}) $$

$$ = \inf_{R_{X|W} \in A, R_{Y|W} \in B} C(R_{X|W}, R_{Y|W}) $$

$$ =: \eta. $$

So, it remains to show that $\eta > \tau$.

By Assumption 1, we obtain that

$$ \eta \geq \inf_{R_{Y|W} \in B} C(Q_{X|W}, R_{Y|W}|Q_W) - \delta(\epsilon'), $$

where $\delta(\epsilon')$ is positive and vanishes as $\epsilon' \downarrow 0$.

Observe that

$$ B_0 := \{(R_{Y|W} = w)_{w \in m} \} \in \mathcal{P}(\mathcal{Y})^m : $$

$$ C(Q_{X|W}, R_{Y|W}|Q_W) > \tau + \epsilon $$

is open in $\mathcal{P}(\mathcal{Y})^m$ equipped with the product topology. Since $Q_{Y|W} \in B_0$, $B_0$ contains the product of $\mathcal{F}_w, w \in [m]$ for some open sets $\mathcal{F}_w \subseteq \mathcal{P}(\mathcal{Y})$ such that $Q_{Y|W = w} \in \mathcal{F}_w$. So $B_0 \subseteq \mathcal{F}_w \cup (\mathcal{F}_w \cup \cdots)$, for sufficiently small $\epsilon'$ (which was used in the definition of $B_0$), which means in this case, $B \subseteq B_0$. This implies that the RHS of (45) is further lower bounded by $\tau + \epsilon - \delta(\epsilon')$. So, if we let $\epsilon > 0$ be fixed and $\epsilon' > 0$ be sufficiently small such that $\epsilon > \delta(\epsilon')$, then for sufficiently large $n$, we have (44).

Lastly, combining (42), (43), and (44) yields that

$$ \limsup_{n \to \infty} E_1(n)(\alpha, \tau) \leq \tilde{\phi}(\alpha - \epsilon, \tau + \epsilon) + \epsilon. $$

Since $\tilde{\phi}$ is convex, it is continuous on the interior of $\text{dom} \tilde{\phi}$. We hence have that for all $\alpha, \tau > 0$, $\limsup_{n \to \infty} E_1(n)(\alpha, \tau) \leq \tilde{\phi}(\alpha, \tau)$.

**C. Statement 3**

The lower bound follows by the dimension-free bound in (12). We next prove the upper bound. For this case, we set $\alpha = 0$ in the proof above, and re-choose $(Q_W, Q_{Y|W})$ as an optimal pair containing $\tilde{\phi}(\tau + \epsilon)$. That is,

$$ C(P_X, Q_{Y|W}|Q_W) > \tau + \epsilon $$

$$ D(Q_{Y|W}||P_Y|Q_W) \leq \tilde{\phi}(\tau + \epsilon) + \epsilon. $$

On one hand, we choose $A := B_1(|P_X|)$ for $\epsilon' > 0$, and $A = L_1^{-1}(A(w^n))$. Then, we have

$$ \limsup_{n \to \infty} \frac{1}{n} \log(1 - P_X^\infty(A)) $$

$$ \geq \inf_{Q_X \in \mathcal{P}(\mathcal{X})} D(Q_X||P_X) $$

$$ \geq \epsilon^2/2, $$

where the last inequality follows since $D(Q_X||P_X) \geq 2d_P(Q_X, P_X)^2$ (see (6)). Hence, for fixed $\epsilon' > 0$, $P_X^\infty(A) \to 1$ as $n \to +\infty$ exponentially fast.

On the other hand, we retain the choices of $B_w$ and $B$. Similarly to (43), we obtain

$$ -\frac{1}{n} \log P_Y^\infty(B) \leq \tilde{\phi}(\epsilon + \epsilon) + 2\epsilon $$

for all sufficiently large $n$.

Similarly to the above, it can be shown that $\frac{1}{n} c_n(x^n, y^n) > \tau$ for sufficiently large $n$. We hence have that for all $\tau > 0$, $\limsup_{n \to \infty} E_1(n)(\alpha, \tau) \leq \tilde{\phi}(\tau)$.

**IV. PROOF OF THEOREM 7**

Statement 1 in Theorem 7 is a restatement of Statement 1 in Theorem 3 for the case of $c = d^p$. We next prove Statements 2 and 3.

**Statement 2 (Case $\alpha > 0$):** From the dimension-free bound in (12), $\liminf_{n \to \infty} E_1(n)(\alpha, \tau) \geq \tilde{\phi}(\alpha, \tau)$. We next prove $\limsup_{n \to \infty} E_1(n)(\alpha, \tau) \leq \tilde{\phi}(\alpha, \tau)$, where $E_1(n)(\alpha, \tau)$ is the quantity $E_1(n)(\alpha, \tau)$ given in (4) but defined for $c = d^p$, and similarly, $\tilde{\phi}(\alpha, \tau)$ is the $\tilde{\phi}(\alpha, \tau)$ defined for $c = d^p$. Explicitly,

$$ \tilde{\phi}(\alpha, \tau) := \inf_{Q_{X|W}, Q_{Y|W}, Q_W} D(Q_{X|W}||P_X|Q_W) $$

$$ \geq \frac{Q_{X|W}}{Q_{Y|W}}|Q_X|Q_{Y|W}|Q_W \leq \tilde{\phi}(\alpha, \tau) $$

where $C_{\alpha}(Q_{X|W}, Q_{Y|W}|Q_W)$ is the OT cost for $c = d^p$.

Observe that for the same $A$,

$$ A = \bigcup_{x^n \in A} \{ y^n \in \mathcal{Y}^m : \sum_{i=1}^{n} d^p(x_i, y_i) \leq t \} $$

$$ \subseteq \bigcup_{x^n \in A} \{ y^n \in \mathcal{Y}^m : \sum_{i=1}^{n} d^p(x_i, y_i) \leq t \} =: A' $$

So, $E_1(n)(\alpha, \tau) \leq E_1(n)(\alpha, \tau)$. Hence, $\limsup_{n \to \infty} E_1(n)(\alpha, \tau) \leq \tilde{\phi}(\alpha, \tau)$. Taking limit as $s \to \infty$, we obtain $\limsup_{n \to \infty} E_1(n)(\alpha, \tau) \leq \limsup_{n \to \infty} \tilde{\phi}(\alpha, \tau)$. To prove Statement 2, it suffices to show that $\limsup_{n \to \infty} \tilde{\phi}(\alpha, \tau) = \tilde{\phi}(\alpha, \tau)$. On the other hand, $\tilde{\phi}(\alpha, \tau) \geq \tilde{\phi}(\alpha, \tau)$ since $C_{\alpha}(Q_{X|W}, Q_{Y|W}|Q_W) \leq C_{\alpha}(Q_{X|W}, Q_{Y|W}|Q_W)$. So, it suffices to prove $\limsup_{n \to \infty} \tilde{\phi}(\alpha, \tau) \leq \tilde{\phi}(\alpha, \tau)$ for all $\alpha, \tau > 0$.

Let $\epsilon > 0$. Let $(Q_W, Q_{X|W}, Q_{Y|W})$ $\epsilon$-approximately attain $\tilde{\phi}(\alpha, \tau)$ in the sense that

$$ D(Q_{X|W}||P_X|Q_W) \leq \alpha $$

$$ C_{\alpha}(Q_{X|W}, Q_{Y|W}|Q_W) > \tau $$

$$ D(Q_{Y|W}||P_Y|Q_W) \leq \tilde{\phi}(\alpha, \tau) + \epsilon. $$



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9This is because $R_{Y|W} \leftrightarrow C(Q_{X|W}, R_{Y|W}|Q_W)$ is a convex combination of lower semi-continuous functions $R_{Y|W} \leftrightarrow C(Q_{X|W}, R_{Y|W}|Q_W)$. So, $C(Q_{X|W}, R_{Y|W}|Q_W)$ is lower semi-continuous as well in $\mathcal{P}(\mathcal{Y})^m$ equipped with the product topology. Hence, its strict superlevel sets are open.
Lemma 27: Given \((Q_X, Q_Y)\),
\[
\lim_{s \to \infty} C_s(Q_X, Q_Y) = C(Q_X, Q_Y).
\]

Proof: Obviously, \(C_s(Q_X, Q_Y) \leq C(Q_X, Q_Y)\). Hence,
\[
\lim_{s \to \infty} C_s(Q_X, Q_Y) \leq C(Q_X, Q_Y).
\]

By Kantorovich duality [37, Theorem 5.10] (also given in Lemma 32),
\[
C(Q_X, Q_Y) = \sup_{f+g \leq c} \int_X f \, dQ_X + \int_Y g \, dQ_Y
\]
where \(C_b(\mathcal{X})\) denotes the collection of bounded continuous functions \(f : \mathcal{X} \to \mathbb{R}\). Given \(c > 0\), let \((f^*, g^*) \in C_b(\mathcal{X}) \times C_b(\mathcal{Y})\) \(\epsilon\)-approximately attain the supremum above in the sense that
\[
\int_X f^* \, dQ_X + \int_Y g^* \, dQ_Y \geq C(Q_X, Q_Y) - \epsilon.
\]

Then, by the boundness, \(f^* + g^* \leq c\) for all sufficiently large \(s\). By Kantorovich duality again,
\[
C_s(Q_X, Q_Y) = \sup_{f+g \leq c} \int_X f \, dQ_X + \int_Y g \, dQ_Y.
\]

For sufficiently large \(s\), \((f^*, g^*)\) is a feasible solution to (47). Hence,
\[
C_s(Q_X, Q_Y) \geq \int_X f^* \, dQ_X + \int_Y g^* \, dQ_Y \geq C(Q_X, Q_Y) - \epsilon.
\]

Since \(\epsilon > 0\) is arbitrary, \(\lim_{s \to \infty} C_s(Q_X, Q_Y) \geq C(Q_X, Q_Y)\), completing the proof. \(\square\)

Since by definition, the conditional OT cost is the weighted sum of the unconditional version, given \((Q_W, Q_X|W, Q_Y|W)\), we immediately have
\[
\lim_{s \to \infty} C_s(Q_X|W, Q_Y|W) = C(Q_X|W, Q_Y|W) > \tau.
\]

So, for sufficiently large \(s\), \(C_s(Q_X|W, Q_Y|W) \geq \tau\) which means that \((Q_W, Q_X|W, Q_Y|W)\) is a feasible solution to the infimization in (46) with \(\alpha\) substituted by \(\alpha - \epsilon\). Therefore,
\[
\lim_{s \to \infty} \tilde{\phi}_s(\alpha, \tau) \leq D(Q_Y|W||P_Y|Q_W) \leq \tilde{\phi}(\alpha, \tau) + \epsilon.
\]

Letting \(\epsilon \downarrow 0\), we obtain \(\lim_{s \to \infty} \tilde{\phi}_s(\alpha, \tau) \leq \tilde{\phi}(\alpha, \tau)\). This completes the proof.

Statement 3 (Case \(\alpha_n \to 0\)): The proof for the upper bound is similar to the above for Statement 2, and hence is omitted here.

We next prove \(\liminf_{n \to \infty} E_1^{(n)}(\alpha_n, \tau) \geq \tilde{\phi}_X(\tau)\). The proof is essentially same as Marton’s in [25] or Gozlan’s in [16]. From the dimension-free bound in 3, we have for fixed \(\tau\), \(E_1^{(n)}(\alpha_n, \tau) \geq \tilde{\phi}(\alpha_n, \tau)\). Under the condition \(D(Q_X|W||P_X|Q_W) \leq \alpha_n\), we have
\[
C(Q_X|W||P_X|Q_W) \leq \tilde{\kappa}_X(\alpha_n),
\]
where \(\tilde{\kappa}_X(\alpha_n)\) is the upper concave envelope of
\[
\kappa_X(\alpha) := \sup_{Q_X: D(Q_X||P_X) < \alpha} C(P_X, Q_X).
\]

The generalized inverse of \(\tilde{\phi}_X(\tau)\) is for \(\alpha \geq 0\),
\[
\tilde{\phi}_X(\alpha) := \inf \{ \tau \geq 0 : \varphi_X(\tau) \geq \alpha \} = \tilde{\kappa}_X(\alpha).
\]

By Assumption 2, \(\tilde{\kappa}_X(\alpha) \to 0\) as \(\alpha \to 0\). By the triangle inequality (since for this case, \(C^{1/p}(\cdot, \cdot)\) is a Wasserstein metric), we then have that for \((Q_X|W, Q_Y|W, Q_W)\) satisfying the constraints in (11),
\[
C^{1/p}(P_X|Q_W, Q_Y|W|Q_W) \geq C^{1/p}(Q_X|W, Q_Y|W|Q_W) - C^{1/p}(Q_X|W, P_X|Q_W) > \tau^{1/p} - \tilde{\kappa}_X(\alpha_n)^{1/p}.
\]

We finally obtain
\[
\tilde{\phi}(\alpha, \tau) \geq \varphi((\tau^{1/p} - \tilde{\kappa}_X(\alpha_n)^{1/p})^p).
\]

Letting \(n \to \infty\), \(\liminf_{n \to \infty} \tilde{\phi}(\alpha, \tau) \geq \varphi(\tau)\). Therefore, \(\liminf_{n \to \infty} E_1^{(n)}(\alpha_n, \tau) \geq \varphi(\tau)\).

V. PROOF OF THEOREM 9

Statement 1: Observe that given any \(A\), by the DPI, it holds that \(D(Q_X|P_X) \geq D(Q_X(A)||P_X(A))\) and \(D(Q_Y|P_Y) \geq D(Q_Y(A)||P_Y(A))\). Therefore, for \(\alpha \geq 0, \tau \in [0, 1]\), it holds that
\[
\phi(\alpha, \tau) = \inf_A \inf_{Q_X(A), Q_Y(A) : D(Q_X(A)||P_X(A)) \leq \alpha} D(Q_Y(A)||P_Y(A)) = \inf_A \theta_{\alpha, \tau}(P_X(A), P_Y(A)).
\]

That is, for the Hamming metric, (21) holds. By (12), it holds that \(E_1^{(n)}(\alpha_n, \tau) \geq \phi(\alpha, \tau)\).

If \(P_X\) is finitely-supported or atomless, then the infimum in (23) is attained. This is because, for the finitely-supported case, \(A\) in (23) can be restricted to be a subset of the support of \(P_X\) (which is a finite set); for the atomless case, by the Neyman-Pearson lemma, the optimal set \(A\) in (23) is any set such that \(P_X(A) = p\) and
\[
\{ x : dP_X/dR(x) < rdP_X/dR(x) \} \subseteq A
\]
for some \(r \geq 0\), where \(R\) is an arbitrary probability measure such that \(P_X(P_Y < R)\). For finitely-supported or atomless \(P_X\),
\[
\phi(\alpha, \tau) = \inf_A \theta_{\alpha, \tau}(P_X(A), P_Y(A)) = \inf_{p \in [0, 1]} \inf_A \theta_{\alpha, \tau}(P_X(A), P_Y(A)) = \inf_{p \in [0, 1]} \inf_{\omega(p) \in (0, \infty)} \theta_{\alpha, \tau}(p, \omega(p)) = \inf_{p \in [0, 1]} \inf_{\omega(p) \in (0, \infty)} \theta_{\alpha, \tau}(p, \omega(p)) \quad (48)
\]
where (48) follows since on one hand, from (20), it is observed that given \(p, \theta_{\alpha, \tau}(p, q)\) is nondecreasing in \(q\), and on the other hand, the infimum in (23) is attained.

Statement 2: By Statement 1, if \(\phi(\alpha, \tau) = \infty\), then \(E_1^{(n)}(\alpha, \tau) = \infty\). So, it suffices to consider the
case \( \phi(\alpha, \tau) < \infty \). Moreover, if \( \tau = 1 \), then for any nonempty set \( A \subseteq X^n \), its \( n \)-enlargement is always \( X^n \). So, \( \Gamma(a, n) = 1 \) for any \( a > 0 \), and hence \( E_1^{(n)}(a, 1) = \infty \) for any finite \( \alpha \), which coincides with \( \phi(\alpha, 1) = 1 \). It remains to consider the case of \( \alpha > 0, \tau \in (0, 1) \) and \( \phi(\alpha, \tau) < \infty \).

Given \( (\alpha, \tau) \) and \( \epsilon > 0 \), let \( A \) be a set that \( \epsilon \)-approximately attains the infimum in (21). That is, \( A \) satisfies

\[
\theta_{a, \tau}(p, q) \leq \phi(\alpha, \tau) + \epsilon, \quad (49)
\]

where \( p := P_X(A) \), \( q := P_Y(A) \). We partition \( X \) into \( \{A, A^c\} \). Let \( X \sim P_X, Y \sim P_Y \). Denote \( I = 1 \) if \( X \in A \); \( I = 0 \) otherwise. Denote \( J = 1 \) if \( Y \in A \); \( J = 0 \) otherwise. So, \( I \) and \( J \) are random variables, whose distributions are given by \( P_I = \text{Bern}(p) \) and \( P_J = \text{Bern}(q) \). Define the isoperimetric function for \( P_I, P_J \), and Hamming metric as for \( a \in [0, 1], t \geq 0,
\[
\Gamma_b(a, t) := \inf_{B \subseteq X^n: |P^n(B)| \geq a} P^\otimes n_j(B^t),
\]

and concentration exponent as for \( a \geq 0, \epsilon > 0, \phi = E_{b, n}(\alpha, \tau) := -\frac{1}{n} \log(1 - \Gamma_b(a, t)) \).

Here the subscript “b” denotes “Bernoulli” or “binary”. By definition, \( \Gamma^{(n)}(a, t) \leq \Gamma_b(a, t) \), and hence, \( E_1^{(n)}(a, \tau) \leq E_{b, n}(a, \tau) \).

Since the space \( \{0, 1\} \) with the Hamming metric satisfies Example 1 given below Assumption 1, by Theorem 3, for distributions \( P_I, P_J \), and any \( (\alpha, \tau) \) in the interior of \( \text{dom} \bar{\phi}_b \), it holds that \( \lim_{n \to \infty} E_{b, n}(\alpha, \tau) = \bar{\phi}_b(\alpha, \tau) \).

Lastly, we verify that \((\alpha, \tau)\) is in the interior of \( \text{dom} \bar{\phi}_b \).

It is easy to see that

\[
\bar{\phi}_b(\alpha, \tau) = \inf_{s, t \in [0, 1]: |D(s||p) - \alpha, s - t > \tau} D(t||q).
\]

By definition, \( \phi_b(\alpha, \tau) \leq \theta_{a, \tau}(p, q) \). Combining it with \( \theta_{a, \tau}(p, q) \leq \phi(\alpha, \tau) + \epsilon \) and \( E_1^{(n)}(\alpha, \tau) \leq \bar{\phi}_b(\alpha, \tau) \), it yields \( \limsup_{n \to \infty} E_1^{(n)}(\alpha, \tau) \leq \phi_b(\alpha, \tau) + \epsilon \). Since \( \epsilon > 0 \) is arbitrary, it holds that \( \limsup_{n \to \infty} E_1^{(n)}(\alpha, \tau) \leq \phi_b(\alpha, \tau) \), which combined with \( E_1^{(n)}(\alpha, \tau) \geq \phi(\alpha, \tau) \), yields \( \lim_{n \to \infty} E_1^{(n)}(\alpha, \tau) = \phi(\alpha, \tau) \).

Combining all the cases above implies \((\alpha, \tau)\) is in the interior of \( \text{dom} \bar{\phi}_b \), completing the proof of Statement 2.

Statement 3: The proof of Statement 3 is similar to that of Statement 2. We first quantize the random variables \( X, Y \) into Bernoulli random variables \( I, J \), and then apply Statement 3 of Theorem 7 (or Statement 3 of Theorem 3) to \( P_I, P_J \), yielding the desired formula. We omit the proof details.

VI. PROOF OF THEOREM 12

A. Statement 1

We first prove the upper bound for the case of finite \( X \) (and Polish \( Y \)), and then generalize it to compact \( X \) and further to Polish \( X \).

1) Finite \( X \): We first consider that \( X \) is a finite metric space. For this case, we extend Ahlswede, Yang, and Zhang’s method [2], [3] to the case in which \( Y \) is an arbitrary Polish space (but \( X \) is still a finite metric space). We divide the proof into four steps.

For this case, we prove

\[
\limsup_{n \to \infty} E_0^{(n)}(\alpha, \tau) \leq \psi(\alpha, \tau).
\]

We assume \( \psi(\alpha, \tau) < \infty \), since otherwise, the inequality holds trivially.

Step 1 (Inherently Typical Subset Lemma): In our proof, we utilize the inherently typical subset lemma in [2] and [3]. We now introduce this lemma. Let \( A \) be any subset of \( X^n \).

For any \( 0 \leq i \leq n - 1 \), define

\[
A_i = \{x^i \in X^i: x^i \text{ is a prefix of some element of } A\},
\]

which is the projection of \( A \) to the space \( X^i \) of the first \( i \) components.

Definition 28: \( A \subseteq X^n \) is called \( m \)-inherently typical if there exist a set \( \mathcal{W}_m \) with \( |\mathcal{W}_m| \leq (m + 1)^{|X|} \) and \( n \) mappings \( \phi_i: A_i \to \mathcal{W}_m, i \in [0 : n - 1] \) such that the following hold:

(i) There exists a distribution (empirical measure) \( Q_{XW} \) such that for any \( x^n \in A \), \( L_{x^n w^n} = Q_{XW} \)

where \( w^n \) is a sequence defined by \( w_i = \phi_i(x^{i-1}) \) for all \( 1 \leq i \leq n \). Such a sequence is called a sequence associated with \( x^n \) through \( (\phi_i) \).

(ii) \( H_Q(X|W) - \frac{\log^2 m}{m} \leq -\frac{1}{n} \log |A| \leq H_Q(X|W) \).

For an \( m \)-inherently typical set \( A \), let \( Q_{X^n} \) be the uniform distribution on \( A \). We now give another interpretation of the \( m \)-inherently typical set in the language of sufficient statistics. Let \( W_i = \phi_i(X^{i-1}) \). First, observe that

\[
\frac{1}{n} \log |A| = H_{Q}(X^n) = \sum_{i=1}^{n} H_{Q}(X_i|X^{i-1}) = \sum_{i=1}^{n} H_{Q}(X_i|X^{i-1}, W_i) = H_{Q}(X_K|X^{K-1}, W_K, K).
\]
where $K$ is a random time index uniformly distributed over $[n]$ which is independent of $X^n$. Moreover,

$$Q_{X_K, W_K} = E_{(X^n, W^n) \sim Q_{X^n, W^n}}[Q_{X_K, W_K}|X^n, W^n] = E_{(X^n, W^n) \sim Q_{X^n, W^n}}[k|X^n, W^n] = Q_X, W.$$  

\[ (51) \]

Hence, the inequalities in (50) can be rewritten as

$$0 \leq I_Q(X_K; X^{K-1}, K|W_K) \leq \frac{\log^2 m}{m}. $$

The first inequality holds trivially since mutual information is nonnegative. For sufficiently large $m$, the bound $\frac{\log^2 m}{m}$ is sufficiently small. Hence, $I_Q(X_K; X^{K-1}, K|W_K)$ is close to zero. In this case, $X_K$ and $(X^{K-1}, K)$ are approximately conditionally independent given $W_K$. In other words, $W_K$ is an approximate sufficient statistic for “underlying parameter” $X_K$; we refer readers to [9, Section 2.9] for sufficient statistics and [21] for approximate versions.

As for $m$-inherent typical sets, one of the most important results is the inherently typical subset lemma, which concerns the existence of inherent typical sets. Such a lemma was proven by Ahlswede et al. [2, 3].

**Lemma 29 (Inherently Typical Subset Lemma):** For any $m \geq 2^{16}|X|^2$, $n$ satisfying \((m+1)^{5|X|+4} \log(n+1)/n \leq 1\), and any $A \subseteq X^n$, there exists an $m$-inherently typical subset $\tilde{A} \subseteq A$ such that

$$0 \leq -\frac{1}{n} \log \left| \frac{A}{|\tilde{A}|} \right| \leq |X|(m+1)^|X| \frac{\log(n+1)}{n}. $$

**Step 2 (Multi-Letter Bound):** For any $A \subseteq X^n$, denote $A_{Q_X} := A \cap \{x^n : L_{x^n} = Q_X\}$ for empirical measure $Q_X$. Since $A = \bigcup_{Q_X} A_{Q_X}$ and the number of distinct types is no more than $(n+1)^{|X|}$, by the pigeonhole principle, we have

$$P_{X^n}^\otimes(A_{Q_X}) \geq P_{X^n}^\otimes(A)(n+1)^{-|X|} $$

for some empirical measure $Q_X$. By the lemma above, given $m \geq 2^{16}|X|^2$, for all sufficiently large $n$, there exists an $m$-inherently typical subset $\tilde{A} \subseteq A_{Q_X}$ such that

$$|\tilde{A}| \geq |A_{Q_X}| \cdot (n+1)^{-b} $$

where $b = |X|(m+1)|X|.$ Observe that for any $B \subseteq \{x^n : L_{x^n} = Q_X\}$, we have $P_{X^n}^\otimes(B) = |B|e^n \sum_x Q_X(x) \log P_X(x)$.

Hence,

$$P_{X^n}^\otimes(\tilde{A}) \geq P_{X^n}^\otimes(A_{Q_X})(n+1)^{-b} \geq P_{X^n}^\otimes(A)(n+1)^{-b'} $$

where $b' = b + |X| = |X|(1 + (m+1)|X|).$

Let $Q_X$ be the uniform distribution on $\tilde{A}$. Then, (51) and (58) still hold, and moreover,

$$D(Q_X^n||P_X^n) = -\frac{1}{n} \log P_X^n(\tilde{A}) \leq -\frac{1}{n} \log P_X^n(\tilde{A}) + o_n(1).$$

If $P_X^n(A) \geq e^{-na}$, we have

$$D(Q_X^n||P_X^n) \leq \alpha + o_n(1). $$

Denote $t = nt$. Let $Q_{Y^n|x^n}$ be a conditional distribution such that given each $x^n$, $Q_{Y^n|x^n=x^n}$ is concentrated on the cost ball $B_t(x^n) := \{y^n : c_n(x^n, y^n) \leq t\}$. Then, we have that $Q_{Y^n|x^n} = Q_X^n \circ Q_{Y^n|X^n}$ is concentrated on $A'$, which implies that $-\frac{1}{n} \log P^n_Y(A') \leq -\frac{1}{n} D(Q_Y^n||P_X^n) \leq -\frac{1}{n} D(Q_Y^n||P_X^n)$.

Here $D_0(Q||P) := -\log P\{Q < P\} > 0$ is the Rényi divergence of order 0, which is no greater than the relative entropy $D(Q||P)$ [35]. Since $Q_{Y^n|x^n}$ is arbitrary, we have

$$-\frac{1}{n} \log P_X^n(A') \leq \inf_{Q_{Y^n|x^n} : c_n(x^n, Y^n) \leq t \text{ a.s.}} -\frac{1}{n} D(Q_Y^n||P_X^n). $$

Taking supremum of the RHS overall $Q_{X^n}$ satisfying (51), (58), and (52), we have

$$P_0(n)(\alpha, \tau) \leq \eta_n(\alpha, \tau) := \sup_{Q_X^{X^n} : Q_X^{X^n}, Q_{X^n}^{X^n} \leq \tau \text{ a.s.}} -\frac{1}{n} D(Q_X^n||P_X^n), $$

(53)

where $W_i = \tilde{\psi}_i(\{x^n, w^n\})$. The condition $Q_{X^n}^{X^n} \{x^n, W^n\} : L_{x^n, w^n} = Q_X^n \leq 1$ implies $Q_{X_K, W_K} = Q_{X^n}^{X^n}$.

**Step 3 (Single-Letterizing the Cost Constraint):** We next make a special choice of $Q_{Y^n|x^n}$. Let $\delta > 0$ be sufficiently small such that $\psi_m(\alpha + \delta, \tau - \delta) < \infty$, where $\psi_m$ is defined similarly as $\psi$ but with $W$ restricted to concentrate on the alphabet $W_m$ satisfying $|W_m| \leq (m+1)|X|$. Let $Q_{X,W}^{X,W}$ be the conditional distribution given in Lemma 30. By standard information-theoretic techniques, it holds that

$$\frac{1}{n} D(Q_X^n||P_X^n) \leq \frac{1}{n} \sum_{k=1}^n D(Q_{X_k|x_k-k-1}||P_X|Q_{X_k-k-1}) \leq I_Q(X_k; X^{K-1}K) + D(Q_{X^n}|X^n||P_X|Q_W) \geq D(Q_{X^n}|X^n||P_X|W) $$

So, the condition $\frac{1}{n} D(Q_X^n||P_X^n) \leq \alpha + o_n(1)$ in (53) implies that (55) is satisfied for all sufficiently large $n$. The conclusions in Lemma 30 hold for the $Q_{X,W}$ induced by $Q_X^n$ in the optimization in (53). However, the product distribution $Q_{Y^n|x^n}$ does not satisfy the constraint $c_n(x^n, Y^n) \leq t$ a.s. So, we cannot substitute it into (53) directly. We next construct a conditional version of $Q_{Y^n|x^n}$ and then substitute this conditional version into (53).
Denote

\[ \mu := \mathbb{E}_Q c(X, Y) \leq \tau - \delta. \]

Then, for all \((x^n, w^n)\) with type \(Q_{X|W}\) with \(w_i = \phi_i(x^{i-1})\) and for \(Y^n \sim Q_{Y^n|X^n,W^n}(\cdot|x^n, w^n)\), it holds that

\[ \mathbb{E} \epsilon_n(x^n, Y^n) = \frac{n}{\epsilon_n} \mathbb{E} c(x_k, Y_k) \geq \mathbb{E} \mu(x_k, w_k) = n \mathbb{E} Q_{X|W} \mu(X, W) = n \mu, \]

where \(\mu(x, w) := \mathbb{E} Q_{Y^n|X^n,W^n}(x, w) c(x, Y)\). By Chebyshev’s inequality, it holds that

\[ \epsilon_n := Q\{Y^n \notin \{x^n\}\} \leq \mathbb{E} Q\{\epsilon_n(x^n, Y^n) > n \tau\} \leq \mathbb{E} Q\{\epsilon_n(x^n, Y^n) - n \mu\}^2 \leq \frac{\sum_{k=1}^n \mathbb{E} Q\{c(x_k, Y_k) - \mu(x_k, w_k)\}^2}{n^2 (\tau - \mu)^2} = \frac{\mathbb{E} Q_{X|W} \text{Var}(c(X, Y)|X, W)}{n (\tau - \mu)^2} \leq \frac{\mathbb{E} Q\{c(X, Y)\}}{n (\tau - \mu)^2}. \]

(56)

Recall that \(Q\) denotes the underlying probability measure that induces \(Q_{Y^n|X^n,W^n}\). Combining (54) and (56) yields that \(\epsilon_n\) vanishes as \(n \to \infty\) uniformly for all \(Q_{X^n}\) induced by \(Q_X\) in the optimization in (53).

Denote \(\hat{Q}_{Y^n|X^n,W^n}\) as a distribution given by

\[ \hat{Q}_{Y^n|X^n,W^n} = Q_X^n \| \hat{Q}_{Y^n|X^n,W^n} = (x^n, w^n) = \left( \prod_{k=1}^n Q_{Y|X,W}(x_k,w_k) \right) (\cdot|\{x^n\}^c). \]

for all \(x^n\) and \(w_k = \phi_i(x^{i-1})\). Denote \(\hat{Q}_{Y^n|X^n,W^n} = Q_{Y^n|X^n,W^n}\) as a mixture:

\[ Q_{Y^n|X^n,W^n}(\cdot|x^n, w^n) = (1 - \epsilon_n) \hat{Q}_{Y^n|X^n,W^n} + \epsilon_n \hat{Q}_{Y^n|X^n,W^n}. \]

We can rewrite \(Q_{Y^n|X^n,W^n}\) as a mixture:

\[ Q_{Y^n|X^n,W^n}(\cdot|x^n, w^n) = (1 - \epsilon_n) \hat{Q}_{Y^n|X^n,W^n} + \epsilon_n \hat{Q}_{Y^n|X^n,W^n}. \]

(58)

For the same input distribution \(Q_X\), the output distributions of channels \(Q_{Y|X^n,W^n}\), \(Q_{Y^n|X^n,W^n}\), and \(\hat{Q}_{Y^n|X^n,W^n}\) are respectively denoted as \(Q_{Y^n}\), \(\hat{Q}_{Y^n}\), and \(\hat{Q}_{Y^n}\), which satisfy

\[ Q_{Y^n} = (1 - \epsilon_n) \hat{Q}_{Y^n} + \epsilon_n \hat{Q}_{Y^n}. \]

Denote \(J \sim Q_J := \text{Bern}(\epsilon_n)\), and \(Q_{Y^n}|J=1 = \hat{Q}_{Y^n}\), \(Q_{Y^n}|J=0 = \hat{Q}_{Y^n}\). Then,

\[ Q_{Y^n} = Q_J(1)Q_{Y^n}|J=1 + Q_J(0)Q_{Y^n}|J=0. \]

Observe that

\[ D(Q_{Y^n}|J||P_Y^\otimes n)(Q_J) = (1 - \epsilon_n) D(Q_{Y^n}||P_Y^\otimes n) + \epsilon_n D(Q_{Y^n}||P_Y^\otimes n) \geq (1 - \epsilon_n) D(Q_{Y^n}||P_Y^\otimes n). \]

On the other hand,

\[ D(Q_{Y^n}|J||P_Y^\otimes n)(Q_J) = D(Q_{Y^n}||P_Y^\otimes n) + D(Q_{J|Y^n}||Q_J|Q_{Y^n}), \]

and

\[ D(Q_{J|Y^n}||Q_J|Q_{Y^n}) = I_Q(J;Y^n) \leq H_Q(J) \leq \log 2. \]

Hence,

\[ D(Q_{Y^n}||P_Y^\otimes n) \leq \frac{D(Q_{Y^n}||P_Y^\otimes n) + \log 2}{1 - \epsilon_n}. \]

(57)

By choosing \(Q_{Y^n|X^n} = x^n\) in (53) as a feasible solution such that \(Q_{Y^n|X^n} = x^n = Q_{Y^n|X^n,W^n} = (x^n, w^n)\) for all \(x^n\) where \(w_i = \phi_i(x^{i-1})\), we then have that the objective function \(\frac{1}{n} D(Q_{Y^n}||P_Y^\otimes n)\) in (53) is upper bounded as shown in (57).

It means that for the fixed distribution \(Q_{Y^n|X^n}\) given in Lemma 30, it holds that

\[ \eta_n(\alpha, \tau) \leq \frac{D(Q_{Y^n}||P_Y^\otimes n)}{n(1 - \epsilon_n)} + o_n(1). \]

Step 4 (Single-Letterization): We next completely the single-letterization. By standard information-theoretic techniques, we obtain that

\[ \frac{1}{n} D(Q_{Y^n}||P_Y^\otimes n) \]

\[ = \frac{1}{n} \sum_{k=1}^n D(Q_{Y_k|Y^{k-1}}||P_Y|Q_{Y^{k-1}}) \]

\[ \leq \frac{1}{n} \sum_{k=1}^n D(Q_{Y_k|X^{k-1}Y^{k-1}}||P_Y|Q_{X^{k-1}Y^{k-1}}) + \frac{1}{n} \sum_{k=1}^n D(Q_{Y_k|X^{k-1}}||P_Y|Q_{X^{k-1}}) \]

\[ = \frac{1}{n} \sum_{k=1}^n D(Q_{Y_k|X^{k-1}}||P_Y|Q_{X^{k-1}}) \]

\[ + \frac{1}{n} \sum_{k=1}^n I_Q(Y_k; Y^{k-1}X^{k-1}) \]

\[ = \frac{1}{n} \sum_{k=1}^n D(Q_{Y_k|X^{k-1}}||P_Y|Q_{X^{k-1}}) \]

\[ = \frac{1}{n} \sum_{k=1}^n D(Q_{Y_k|X^{k-1}W_K}||P_Y|Q_{X^{k-1}W_K}) + D(Q_{Y_k|W_K}||P_Y|Q_{W_K}) \]

\[ = I_Q(Y_K; X^{K-1}W_K) + D(Q_{Y_K|W_K}||P_Y|Q_{W_K}) \]

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where

- (58) follows since under the distribution $Q_{X^n W^n} Q_{Y|XW}^\otimes$, $W^k$ is a function of $X^{k-1}$, and moreover, $Y_k$ and $Y^{k-1}$ are conditionally independent given $(X^{k-1}, W^k)$ for each $k$;
- (59) follows since under the distribution $Q = Q_{X^n W^n} Q_{Y|XW}^\otimes$, $W^k$ with $Q_k = \text{Unif}[n]$, $(K, X^{K-1})$ and $Y_K$ are conditionally independent given $(X_K, W_K)$, and hence,

$$I_Q(Y_K; X^{K-1}, K|W_K) \leq I_Q(X_K; X^{K-1}, K|W_K) = o(m(1));$$

- in (60), $Q_{Y|W}$ is induced by the distribution $Q_{X^n W^n} Q_{Y|XW}$, and (60) follows since $Q_{Y|W}$ is induced by the distribution $Q_{X^n W^n} Q_{Y|XW}$, and hence, $Q_{Y|W} = Q_{Y|W}$ (recall that $Q_{X^n W^n} = Q_{X^n W^n}$);
- the last line follows by Lemma 50.

Hence,

$$\eta_n(\alpha, \tau) \leq \frac{\psi_m(\alpha + \delta, \tau - \delta) + \delta + o_m(1)}{1 - \epsilon_n} + o_n(1).$$

Letting $n \to \infty$ first and $\delta \downarrow 0$ then, we obtain

$$\limsup_{n \to \infty} E_0^{(m)}(\alpha, \tau) \leq \limsup_{n \to \infty} \psi_m(\alpha', \tau') \quad (61).$$

Since $\mathcal{P}(X \times W_m)$ is a probability simplex, by the standard technique of passing to a convergent subsequence, one can prove that $n_0$ is upper semicontinuous, i.e.,

$$\limsup_{\alpha' \to \alpha, \tau' \to \tau} \psi_m(\alpha', \tau') = \psi(\alpha, \tau).$$

By (61) and the upper semicontinuity of $\psi_m$, and letting $m \to \infty$, we obtain

$$\limsup_{n \to \infty} E_0^{(m)}(\alpha, \tau) \leq \psi(\alpha, \tau).$$

2) Compact $X'$: We next generalize the result from finite $X$ to compact $X'$ by the standard quantization technique. Since $X'$ is compact, for any $r > 0$, it can be covered by a finite number of open balls $\{B_r(x_i)\}_{i=1}^k$. Denote $E_i := B_r(x_i) \cup \bigcup_{j=1}^{i-1} B_r(x_j)$, $i \in [k]$, which are measurable. Hence, $\{E_i\}_{i=1}^k$ forms a partition of $X'$, and $E_i$ is a subset of $B_r(x_i)$. For each $i$, we choose a point $z_i \in E_i$. Consider $Z := \{z_1, z_2, \ldots, z_k\}$ as a sample space, and define a probability mass function $P_Z$ on $Z$ given by $P_Z(z_i) = P_X(E_i), \forall i \in [k]$. In other words, $Z \sim P_Z$ is a quantized version of $X \sim P_X$ in the sense that $Z = z_i$ if $X \in E_i$ for some $i$.

For a vector $i^n := (i_1, i_2, \ldots, i_n) \in [k]^n$, denote $E_{i^n} := \prod_{i=1}^n E_{i^n}$. Consequently, $\{E_{i^n} : i^n \in [k]^n\}$ forms a partition of $X^n$. Similarly, for $X^n \sim P_X^{\otimes n}$, we denote $Z^n$ as a random vector where $Z^n$ is the quantized version of $X^n$, $i \in [n]$. Obviously, $Z^n \sim P_Z^{\otimes n}$.

For any measurable set $A \subseteq X^n$, denote $I := \{i^n \in [k]^n : E_{i^n} \cap A \neq \emptyset\}$. Denote $\hat{A} := \bigcup_{i^n \in I} E_{i^n}$ which is a superset of $A$, i.e., $A \subseteq \hat{A}$. On the other hand, for each $i^n \in I$ and any $\hat{\tau} > 0$, the $\hat{\tau}$-enlargement of $E_{i^n}$ with $\hat{\tau} := n \hat{\tau}$ satisfies that

$$\hat{E}_{i^n} = \{y^n : c_n(x^n, y^n) \leq \hat{\tau}, \exists x^n \in E_{i^n}\}.$$

$$\subseteq \{y^n : c_n(x^n, y^n) \leq \hat{\tau}, d(x_i, \hat{x}_i) \leq r, \forall i \in [n], \exists x^n \in A, x^n \in \hat{A}\}$$

$$= \{y^n : \inf_{x^n \in \hat{E}_{i^n}} c_n(x^n, y^n) \leq \hat{\tau}, \exists x^n \in A\}$$

$$= \{y^n : \sum_{i=1}^n \inf_{x_i : d(x_i, \hat{x}_i) \leq r} c(x_i, y_i) \leq \hat{\tau}, \exists x^n \in A\}$$

$$\leq \{y^n : \sum_{i=1}^n c(x_i, y_i) \leq n(\hat{\tau} + \delta(r)), \exists x^n \in A\}$$

$$= A^{n(\hat{\tau} + \delta(r))},$$

where

- (62) follows from the fact that $\exists x^n \in E_{i^n}$ implies $d(x_i, \hat{x}_i) \leq r, \forall i \in [n]$ for some $\hat{x}_n \in A, x^n \in A'$$;
- in (63) $(\hat{\tau}(r)$ is a positive function of $r$ which vanishes as $r \downarrow 0$, and (63) follows by Assumption 3 (i.e., (27)).

Hence,

$$\hat{A}^\hat{\tau} = \bigcup_{\hat{\tau} \in I} E_{i^n} \subseteq A^{n(\hat{\tau} + \delta(r))}.$$

If we choose $\hat{\tau} = \delta(r)$, then $\hat{A}^\hat{\tau} \subseteq A^{\tau}$. Combining this with $A \subseteq \hat{A}$ implies

$$P_Y^{\otimes n}(A^{\tau}) \geq P_Y^{\otimes n}(\hat{A}^\hat{\tau})$$

$$= P_X^{\otimes n}(A) \leq P_X^{\otimes n}(\hat{A}),$$

which further imply that

$$\inf_{A : P_X^{\otimes n}(A) \geq a} P_Y^{\otimes n}(A^{\tau})$$

$$\geq \inf_{A : P_X^{\otimes n}(A) \geq a} P_Y^{\otimes n}(\hat{A}^{\hat{\tau}})$$

$$= \inf_{I \subseteq [k]^n : P_X^{\otimes n}(\bigcup_{i^n \in I} E_{i^n}) \geq a} P_Y^{\otimes n}((\bigcup_{i^n \in I} E_{i^n})^{\hat{\tau}})$$

$$= \inf_{B \subseteq Z^n : P_Z^{\otimes n}(B) \geq a} P_Y^{\otimes n}(B^{\hat{\tau}}),$$

where $B^{\hat{\tau}} = \{y^n : c_n(z^n, y^n) \leq n \hat{\tau}, \exists z^n \in B\}$. Therefore,

$$E_0^{(n)}(\alpha, \tau|P_Z) \leq E_0^{(n)}(\alpha, \hat{\tau}|P_Z),$$

where $E_0^{(n)}(\cdot, \cdot|P_X)$ is the exponent $E_0^{(n)}$ defined for distribution pair $(P_X, P_Y)$, and $E_0^{(n)}(\cdot, \cdot|P_Z)$ is the exponent $E_0^{(n)}$ defined for $(P_Z, P_Y)$.

Denote $\psi(\cdot, \cdot|P_X)$ as the function $\psi$ defined for $(P_X, P_Y)$, and $\psi(\cdot, \cdot|P_Z)$ as the one defined for $(P_Z, P_Y)$. Since $Z$ is a finite metric space (with the discrete/Hamming metric), by the result proven in Section VI-A1, we have

$$\limsup_{n \to \infty} E_0^{(n)}(\alpha, \hat{\tau}|P_Z) \leq \psi(\alpha, \hat{\tau}|P_Z).$$

Therefore,

$$\limsup_{n \to \infty} E_0^{(n)}(\alpha, \tau|P_Z) \leq \psi(\alpha, \tau|P_Z)$$

$$= \psi(\alpha, \tau - \delta(r)|P_Z).$$

We next show that $\psi(\alpha', \tau' + \delta(r)|P_Z) \leq \psi(\alpha', \tau'|P_Z)$ for any $\alpha' \geq 0, \tau' > 0$. For any $Q_{X|W}$, we define a mixture distribution $Q_{X|W}$ such that for each $w$,

$$Q_{X|W = w} = \sum_{i=1}^k Q_{Z|W}(z_i|w)P_X(\cdot|E_i),$$

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which implies
\[
\frac{dQ_{X|W}(x|w)}{dP_X} = \sum_{i=1}^{k} Q_{Z|W}(z_i|w) \frac{1}{P_X(E_i)} = \sum_{i=1}^{k} Q_{Z|W}(z_i|w) \frac{1}{P_Z(z_i)}, \forall x.
\] (65)

For such \( Q_{X|W} \),
\[
D(Q_{X|W}||P_X|Q_W) = D(Q_{Z|W}||P_Z|Q_W). \tag{66}
\]

Note that for such a construction, \( Z \sim Q_Z \) can be seen as a quantized version of \( X \sim Q_X \).

By Assumption 3, we have that \( c(X, Y) \geq c(Z, Y) - \delta(r) \) a.s. where \( Z \) is the quantized version of (and also a function of) \( X \). We hence have that for \( Q_{X|W} \) constructed above,

\[
\mathcal{C}(Q_{X|W}, Q_{Y|W}|Q_W) = \min_{Q_{X|W} \in \mathcal{C}(Q_{X|W}, Q_{Y|W}|Q_W)} \mathbb{E}_{Q_W} Q_{X,Y|W}[c(X,Y)] \\
\geq \min_{Q_{X|W} \in \mathcal{C}(Q_{X|W}, Q_{Y|W}|Q_W)} \mathbb{E}_{Q_W} Q_{X,Y|W}[c(Z,Y)] - \delta(r) \\
\geq \min_{Q_{X|W} \in \mathcal{C}(Q_{X|W}, Q_{Y|W}|Q_W)} \mathbb{E}_{Q_W} Q_{X,Y|W}[c(Z,Y)] - \delta(r) \\
= \mathcal{C}(Q_{Z|W}, Q_{Y|W}|Q_W) - \delta(r).
\]

Therefore,
\[
\inf_{Q_{Y|W}: \mathcal{C}(Q_{X|W}, Q_{Y|W}|Q_W) \leq \tau'} D(Q_{Y|W}||P_Y|Q_W) \\
\geq \inf_{Q_{Y|W}: \mathcal{C}(Q_{X|W}, Q_{Y|W}|Q_W) \leq \tau' + \delta(r)} D(Q_{Y|W}||P_Y|Q_W).
\]

Taking supremum over \( Q_{Z|W} \) such that \( D(Q_{Z|W}||P_Z|Q_W) \leq \alpha' \), we obtain
\[
\sup_{Q_{Z|W}: D(Q_{Z|W}||P_Z|Q_W) \leq \alpha'} \inf_{Q_{Y|W}: \mathcal{C}(Q_{X|W}, Q_{Y|W}|Q_W) \leq \tau'} D(Q_{Y|W}||P_Y|Q_W) \\
\geq \psi(\alpha', \tau' + \delta(r)|P_Z).
\]

where \( Q_{X|W} \) at the LHS above is induced by \( Q_{Z|W} \) as shown in (65). By (66), the LHS above is in turn upper bounded by \( \psi(\alpha', \tau'|P_X) \) (by replacing the supremum above with the supremum over \( Q_{X|W} \) such that \( D(Q_{X|W}||P_X|Q_W) \leq \alpha' \)). Hence,
\[
\psi(\alpha', \tau' + \delta(r)|P_Z) \leq \psi(\alpha', \tau'|P_X).
\]

For \( \tau > 2\delta(r) \) (when \( \tau > 0 \) and \( r \) is sufficiently small), substituting \( \alpha' \leftarrow \alpha, \tau' \leftarrow \tau - 2\delta(r) \) into the above inequality, we have
\[
\psi(\alpha, \tau - \delta(r)|P_Z) \leq \psi(\alpha, \tau - 2\delta(r)|P_X). \tag{67}
\]

Combining (64) and (67) and letting \( r \downarrow 0 \), we have
\[
\limsup_{n \to \infty} E_0^{(n)}(\alpha, \tau|P_X) \leq \limsup_{\tau' \uparrow \tau} \psi(\alpha, \tau' |P_X).
\]

B. Statement 2

Since \( X \) is Polish, any probability measure on it is tight. So, for any \( \epsilon \in (0, 1) \), there is a compact set \( B \subseteq \mathcal{X} \) such that \( P_X(B^c) \leq \epsilon \). Let \( X_n \sim P_X^{(n)} \) and \( Z_i := 1_{B_n}(X_i), i \in [n] \). Then, \( Z_n \sim \text{Bern}(P_X(B^c))^{\otimes n} \). By Sanov’s theorem, for any \( \epsilon' \in (0,1) \),
\[
P\{\sum_{i=1}^{n} Z_i \geq n\epsilon'\} \leq e^{-nD(\epsilon'|P_X)} \leq e^{-nD(\epsilon'|\epsilon)},
\]

where the second inequality follows since \( \epsilon \mapsto D(\epsilon'|\epsilon) \) is decreasing for \( \epsilon < \epsilon' \). Since \( \epsilon \mapsto D(\epsilon'|\epsilon) \) goes to infinity as \( \epsilon \downarrow 0 \), given any \( \epsilon' > 0 \), we can choose \( \epsilon \) small enough so that \( D(\epsilon'|\epsilon) > \alpha \). For example, we can choose \( \epsilon = e^{\epsilon'-1/\epsilon^2} \) and choose \( \epsilon' \) small enough. For any measurable set \( A \) such that \( P_X^{(n)}(A) \geq e^{-n\alpha} \), it holds that
\[
P\{X^n \in A, \sum_{i=1}^{n} Z_i < n\epsilon'\} \\
\geq P\{X^n \in A\} - P\{\sum_{i=1}^{n} Z_i \geq n\epsilon'\} \\
\geq e^{-n\alpha} - e^{-nD(\epsilon'|\epsilon)}.
\]

Given any \( \delta > 0 \), for all sufficiently large \( n \),
\[
P\{X^n \in A, \sum_{i=1}^{n} Z_i < n\epsilon'\} \geq e^{-n(\alpha+\delta)}.
\tag{68}
\]

For a subset \( J \subseteq [n] \), denote \( C_J \) as the event that \( X_i \in B \) for \( i \in J \) and \( X_i \in B^c \) for \( i \in J^c \). Then, (68) can be rewritten as
\[
P\{X^n \in A \cap \bigcup_{|J| \geq n(1-\epsilon')} C_J\} \geq e^{-n(\alpha+\delta)}.
\tag{69}
\]

On the other hand, there are \( \binom{n}{\leq n'} := \sum_{i=1}^{n} \binom{n}{i} \) \( n' \)-sets \( J' \subseteq [n] \) such that \( |J'| \geq n(1-\epsilon') \). Note that by Sanov’s theorem, \( \binom{n}{\leq n'} \leq e^{nH(\epsilon')} \), where \( H(\epsilon') \) is the binary entropy function of \( \epsilon' \). Combining this with (69) yields that
\[
\max_{|J| \geq n(1-\epsilon')} P\{X^n \in A \cap C_J\} \geq e^{-n(\alpha+\delta+H(\epsilon'))}.
\tag{70}
\]

Let \( J^* \) be the optimal \( J \) attaining the maximum in the above equation. Without loss of generality, we assume \( J^* = [n^*] \) for some \( n^* \geq n' := n(1-\epsilon') \). Denote \( A' := \bigcup_{x \in A} \{x^n\} \subseteq \mathcal{X}^{n^*} \) as the projection of \( A \) to the first \( n^* \) coordinates. Then, the maximum in (70) is upper bounded by \( P\{X'^n \in A' \cap B'^n\} = P_X^{(n^*)}(A' \cap B'^n) \). Denote \( c_{sup} := \sup_{x,y} c(x,y) \), which by assumption is finite. Moreover,
\[
A^t \supseteq (A \cap C_{J^*})^t \\
= \bigcup_{x^n \in A \cap C_{J^*}} \{x^n\}^t \\
\supseteq \bigcup_{x^n \in A \cap C_{J^*}} \left(\{x^n\}^t(n-n') c_{sup} \times \prod_{i=n'+1}^{n} \{x_i\} c_{sup}\right).
\tag{71}
\]
\[ \sum_{i=1}^{n} c(x_i, y_i) \leq t \text{ is relaxed to } \sum_{i=1}^{n'} c(x_i, y_i) \leq t - (n - n')c_{\text{sup}} \text{ and } c(x_i, y_i) \leq c_{\text{sup}} \text{ for } i \in [n' + 1 : n]; \]

where

- (71) follows since in the enlargement operation, \( \sum_{i=1}^{n'} c(x_i, y_i) \leq t \) is relaxed to \( \sum_{i=1}^{n'} c(x_i, y_i) \leq t - (n - n')c_{\text{sup}} \) and \( c(x_i, y_i) \leq c_{\text{sup}} \) for \( i \in [n' + 1 : n] \);

- (72) follows since \( \{x\}c_{\text{sup}} = Y \) for any \( x \).

Denoting \( \tilde{A} := A' \cap B' \) and summarizing the above, it holds that

\[ P_X^{\otimes n}(\tilde{A}) \geq e^{-n(\alpha + \delta + H'(r))}, \]
\[ P_Y^{\otimes n}(A') \geq P_Y^{\otimes n}(A^t, (n-n')c_{\text{sup}}) \geq P_Y^{\otimes n}(\tilde{A}^t, n'c_{\text{sup}}). \]

Setting \( t = n\tau \), we then have that

\[ P_Y^{\otimes n}(A^n) \geq \inf_{\tilde{A} \subseteq B' : P_Y^{\otimes n}(\tilde{A}) > e^{-n\alpha - n'}c_{\text{sup}}} P_Y^{\otimes n}(\tilde{A}^t, \tau'), \]

where \( \tau' := \tau - n'c_{\text{sup}} \) and \( \alpha' := \frac{\alpha + \delta + H'(r)}{1 - e^{-\tau'}} \). That is,

\[ E_0^{(n)}(\alpha, \tau | P_X) \leq E_0^{(n)}(\alpha' + \log P_X(B), \tau' | P_X(\cdot | B)). \]

Since \( B \) is compact, applying the upper bound on the isoperimetric exponent for compact \( X \) (proven in Section VI-A2), we obtain that

\[ \limsup_{n \to \infty} E_0^{(n)}(\alpha, \tau | P_X) \leq \limsup_{n \to \infty} E_0^{(n)}(\alpha' + \log P_X(B), \tau' | P_X(\cdot | B)) \leq \liminf_{\tau' \to \tau} \psi(\alpha' + \log P_X(B), \tau' | P_X(\cdot | B)). \]

Observe that

\[ \psi(\alpha' + \log P_X(B), \tau' | P_X(\cdot | B)) = \sup_{Q_{XY} : D(Q_{XY} | P_X(\cdot | B) | P_Y)} \inf_{Q_{YX} : D(Q_{YX} | P_X)} D(Q_{XY} | P_Y | Q_W) \leq \sup_{Q_{XY} : D(Q_{XY} | P_X)} \inf_{Q_{YX} : D(Q_{YX} | P_X)} D(Q_{XY} | P_Y | Q_W) \leq \psi(\alpha', \tau' | P_X). \]

Therefore,

\[ \limsup_{n \to \infty} E_0^{(n)}(\alpha, \tau | P_X) \leq \lim_{\tau' \to \tau} \psi(\alpha', \tau' | P_X). \]

Letting \( \epsilon' \downarrow 0 \) first and \( \delta \downarrow 0 \) then, we obtain that

\[ \limsup_{n \to \infty} E_0^{(n)}(\alpha, \tau | P_X) \leq \lim_{\epsilon' \downarrow 0} \lim_{\delta \downarrow 0} \psi(\alpha', \tau' | P_X). \]

C. Statement 3

The proof of the lower bound is based on the large deviations theory, which is similar to that of Statement 2 of Theorem 3 given in Section III.

Let \( \epsilon > 0 \) and \( m \geq 2 \). Let \( Q_{WY} \) be such that \( |\text{supp}(Q_{WY})| \leq m \) and \( D(Q_{X|W} | P_X) | Q_W \) \( \leq \alpha - \epsilon \). Without loss of generality, we assume \( \text{supp}(Q_{WY}) = [m] \), under which the function \( \psi \) does not change by Theorem 11. For each \( n \), let \( Q_{WY}^{(n)} \) be an empirical measure of an \( n \)-length sequence (i.e., \( n \)-type) such that \( |\text{supp}(Q_{WY}^{(n)})| \leq m \) and \( Q_{WY}^{(n)} \to Q_{WY} \) as \( n \to \infty \). Let \( L = \{ Q_{WY}^{(n)} \} \). Let \( w^n = (1, \ldots, 1, 2, \ldots, 2, \ldots, m, \ldots, m) \) be an \( n \)-length sequence, where \( i \) appears \( n_i := nQ_{WY}^{(n)}(i) \) times. Hence, the empirical measure of \( w^n \) is \( Q_{WY}^{(n)} \).

Let \( \epsilon > 0 \). We now choose \( A \) as the conditional empirically \( \epsilon \)-typical sets. That is, \( A = A_{n-1}(A_{n-1}) = \prod_{w \in \{1, \ldots, m\}} L_{n-1}(A_{n-1}) \), where \( A_{n-1} = B_{n-1}(Q_{WY}^{(n)}) \) for \( w \in [m] \), and \( A = \{ R_{WY} : R_{WY} \in A_{n-1}, \forall w \in [m] \} \). As shown in Section III, \( A \) is closed in \( A_{n-1} \), and \( -\frac{1}{n} \log P_X^{\otimes n}(A) \leq \alpha \) for all sufficiently large \( n \).

Denote \( t = n\alpha \). Observe that

\[ A^{(n)} = \{ y^n : \exists x^n, L_{x^n | w^n} \in A, c_n(x^n, y^n) \leq t \} = \{ y^n : \exists x^n, L_{x^n | w^n} \in A, \exists x_{n-1} | w_{n-1} \in A_{n-1}(x, Y) \leq \tau \} \subseteq \{ y^n : \exists R_{WY} \in A, C(R_{WY}, | L_{x^n | w^n} | Q_{WY}^{(n)} \leq \tau) \} \leq \{ y^n : \exists R_{WY} \in A, C(R_{WY}, | Q_{WY}^{(n)} | Q_{WY}^{(n)} \leq \tau) \} \]

Hence, we have \( A^{(n)} \subseteq A_{n-1}(B | w^n) \), where

\[ B = \{ R_{WY} : C(R_{WY}, | R_{WY} | Q_{WY}^{(n)} \leq \tau, \exists R_{WY} \in A \}. \]

By a conditional version of Sanov’s theorem,

\[ E := \inf_{n \to \infty} \frac{1}{n} \log P_{X^{(n)}}(L_{n-1}(B | w^n)) \geq \inf_{R_{WY} \in B'} \left( D(D_{R_{WY}} | P_Y \otimes Q_W) \right) ; \]

where \( B' := \{ R_{WY} : R_{WY} \in B_{n-1}(Q_{WY}^{(n)}) \), \( R_{WY} \in B \}. \)

To simplify this lower bound, denoting

\[ B' := \{ R_{WY} : R_{WY} \in B_{n-1}(Q_{WY}^{(n)}) \}, \]

and \( B' \) is closed (in the weak topology).

Proof of Lemma 31: By Assumption 1, for any \( R_{WY} \), it holds that given \( \epsilon'' > 0 \), for sufficiently small \( \epsilon' \),

\[ \inf_{R_{WY} \in A} C(R_{WY}, | R_{WY} | Q_{WY}^{(n)}) \geq C(R_{WY}, R_{WY} | Q_{WY}^{(n)}) - \epsilon''. \]

Note that the minimization in the conditional optimal transport can be taken in a pointwise way for each condition \( W = w \). Combining this with the condition that \( c \) is bounded, we have that \( R_{WY} \mapsto C(R_{WY}, R_{WY} | R_{WY}) \) is continuous. So, given \( \epsilon'' > 0 \), for sufficiently large \( n \),

\[ C(Q_{WY}^{(n)}, R_{WY} | Q_{WY}^{(n)}) \geq C(Q_{WY}^{(n)}, R_{WY} | Q_{WY}) - \epsilon''. \]
This implies that given \( \epsilon'' \), for sufficiently small \( \epsilon' \), \( B' \subseteq B' \).

Hence, \( B' \subseteq B' \).

We next prove that for sufficiently small \( \epsilon \), \( B' \) is closed.

Let \((R_{WY})_k\) be an arbitrary sequence drawn from \( B' \), which converges to \( R_{WY} \) (under the weak topology). Obviously, \( R_{WY}^{(k)} \rightarrow R_{WY} = Q_W \) and \( R_{Y|W=w}^{(k)} \rightarrow R_{Y|W=w}^* \) for each \( w \). By the lower semi-continuity of \( R_Y \rightarrow C(R_X, R_Y) \), we have that

\[
\liminf_{k \to \infty} C(Q_{X|W=w}, R_{Y|W=w}^{(k)}) \geq C(Q_{X|W=w}, R_{Y|W=w}^*).
\]

Hence,

\[
\liminf_{k \to \infty} C(Q_{X|W}, R_{Y|W}^{(k)}) \geq C(Q_{X|W}, R_{Y|W}^*).
\]

On the other hand, by the choice of \((R_{WY})_k\),

\[
C(Q_{X|W}, R_{Y|W}^{(k)}) \leq \tau + 2\epsilon''.
\]

Hence, \( B' \) is closed. This completes the proof of Lemma 31.

By Lemma 31 and (73),

\[
E \geq \inf_{R_{WY} \in B'} D(R_{WY} || P_Y \otimes Q_W) = \inf_{R_{WY} \in B', R_{Y|W}: C(Q_{X|W}, R_{Y|W}^{(k)}) \leq \tau + 2\epsilon''} D(R_{WY} || P_Y || Q_W).
\]

Let \((R_{WY}, R_{Y|W})\) be such that

\[
R_{WY} \in \mathcal{B}_{\frac{\epsilon}{2}}(Q_W),
\]

\[
C(Q_{X|W}, R_{Y|W}^{(k)}) \leq \tau + 2\epsilon'',
\]

\[
D(R_{WY} || P_Y || Q_W) \leq \beta + \frac{1}{k}.
\]

Since \( R_{WY}^{(k)} \) is in the probability simplex, by passing to a subsequence, we assume \( R_{WY}^{(k)} \rightarrow Q_W \). Since sublevel sets of the relative entropy \( R_Y \rightarrow D(R_Y || P_Y) \) are compact, by the fact that for each \( w \), \( D(R_{Y|W=w} || P_Y) \) is finite, passing to a subsequence, we have \( R_{Y|W=w}^{(k)} \rightarrow R_{Y|W=w}^* \). By the lower semi-continuity of the relative entropy and the optimal transport cost functional, we have

\[
\liminf_{k \to \infty} D(R_{Y|W}^{(k)} || P_Y || Q_W) \geq D(R_{Y|W}^* || P_Y || Q_W),
\]

\[
\liminf_{k \to \infty} C(Q_{X|W}, R_{Y|W}^{(k)}) \geq C(Q_{X|W}, R_{Y|W}^* || Q_W).
\]

Hence, \( R_{Y|W}^* \) satisfies that

\[
C(Q_{X|W}, R_{Y|W}^* || Q_W) \leq \tau + 2\epsilon''
\]

\[
D(R_{Y|W}^* || P_Y) \leq \beta.
\]

Therefore, \( E \geq g(\tau + 2\epsilon'', Q_{XW}) \), where

\[
g(t, Q_{XW}) := \inf_{Q_{Y|XW}: C(Q_{X|XW}, Q_{Y|XW}) \leq t} D(Q_{Y|XW} || P_Y || Q_W)
\]

Since \( Q_{XW} \) is arbitrary distribution on \( X \times W \) satisfying \( D(Q_{X|W} || P_X || Q_W) \leq \alpha - \epsilon \), taking supremum over all such distributions, we obtain

\[
\limsup_{n \to \infty} E_n^{(n)}(\alpha, \tau) \geq \sup_{Q_{XW}: D(Q_{X|W} || P_X || Q_W) \leq \alpha - \epsilon} g(\tau + 2\epsilon'', Q_{XW}) = \psi(\alpha - \epsilon, \tau + 2\epsilon'').
\]

Letting \( \epsilon \downarrow 0 \) and \( \epsilon'' \downarrow 0 \), we obtain

\[
\limsup_{n \to \infty} E_n^{(n)}(\alpha, \tau) \geq \limsup_{\alpha \to \infty} \lim sup_{\alpha' \to \alpha + \epsilon''} \psi(\alpha', \tau') = \psi(\alpha, \tau),
\]

where the last line will be proven in Corollary 21.

VII. PROOFS OF DUAL FORMULAS

It is well known that the OT cost admits the following duality.

**Lemma 32 (Kantorovich Duality):** [37, Theorem 5.10] Let \( X \) and \( Y \) be Polish spaces. It holds that

\[
C(Q_X, Q_Y) = \sup_{f, g \in C_b(\mathcal{X}) \times C_b(\mathcal{Y})} Q_X(f) + Q_Y(g),
\]

where \( C_b(\mathcal{X}) \) denotes the collection of bounded continuous functions \( f : \mathcal{X} \rightarrow \mathbb{R} \).

We also need the following duality for the I-projection, which is well-known if the space is Polish since both sides in (74) correspond to the same large deviation exponent.

**Lemma 33 (Duality for the I-Projection):** Let \( f : \mathcal{X} \rightarrow \mathbb{R} \) be a measurable bounded above function. Then, it holds that for any real \( \tau \),

\[
\inf_{Q: D(Q||P) \leq \tau} D(Q||P) = \sup_{\lambda \geq 0} \lambda \tau - \log P(e^{\lambda f}),
\]

and for any real \( \alpha \geq 0 \),

\[
\sup_{Q: D(Q||P) \leq \alpha} Q(f) = \inf_{\eta > 0} \alpha \eta + e \log P(e^{(1/\eta) f}).
\]

The supremum in (74) can be replaced by \( \sup_{\lambda \geq 0} \)

This lemma is a direct consequence of the following lemma. The following lemma can be easily verified by definition.

**Lemma 34** [10]: For a measurable bounded above function \( f : \mathcal{X} \rightarrow \mathbb{R} \) and \( \lambda \geq 0 \), define a probability measure \( Q_\lambda \) with density

\[
\frac{dQ_\lambda}{dP} = e^{\lambda f},
\]

then

\[
D(Q||P) - D(Q_\lambda||P) = D(Q||Q_\lambda) + \lambda (Q(f) - Q_\lambda(f)) \geq \lambda (Q(f) - Q_\lambda(f)).
\]

The function \( f \) in Lemmas 33 and 34 can be assumed to be unbounded, but \( P(e^{\lambda f}) \) should be finite for Lemma 34, \( P(e^{\lambda f}) \) should be finite for \( \lambda \geq 0 \) such that \( Q_\lambda(f) = \tau \).
for (74), and \( P(e^{(1/n)f}) \) should be finite for \( \eta > 0 \) such that \( D(Q_{1/\eta}||P) = \alpha \) for (75).

The conditional version of Lemma 33 is as follows, which can be proven similarly to the unconditional version.

**Lemma 35:** Let \( \mathcal{W} \) be a finite set and \( f : \mathcal{X} \times \mathcal{W} \to \mathbb{R} \) be a measurable bounded above function. Let \( P_W \) be a probability measure on \( W \). Then, for any real \( \tau \), it holds that

\[
\inf_{Q_{X|W}:P_W Q_{X|W}(f) \geq \tau} D(Q_{X|W}||P_{X|W}P_W) = \sup_{\lambda > 0} \lambda \tau - P_W(\log P_{X|W}e^{\lambda f}),
\]

and for any real \( \alpha \geq 0 \), it holds that

\[
\sup_{Q_{X|W}:D(Q_{X|W}||P_{X|W}Q_W) \leq \alpha} P_W Q_{X|W}(f) = \inf_{\eta > 0} \eta \alpha + \eta P_W(\log P_{X|W}e^{(1/n)f}).
\]

Based on the duality lemmas above, we prove Theorem 16, Proposition 18, Theorem 19, and Theorem 20.

**Proof of Theorem 16:** By the definition of \( \phi \geq \) and by the Kantorovich duality,

\[
\phi(\alpha, \tau) = \inf_{Q_X, Q_Y, f : g \leq c} \inf_{D(Q_X || P_X) \leq \alpha} D(Q_Y || P_Y) = \inf_{Q_X, Q_Y, f : g \leq c} \inf_{D(Q_X || P_X) \leq \alpha} D(Q_Y || P_Y).
\]  

(76)

By Lemma 33,

\[
\phi(\alpha, \tau) = \inf_{f : g \leq c} \inf_{Q_X : D(Q_X || P_X) \leq \alpha} \sup_{\lambda > 0} \lambda (\tau - Q_X(f)) - \log P_Y(e^{\lambda g}).
\]  

(77)

The objective function in (77) is linear in \( \lambda \) and also linear in \( Q_X \), and moreover, \( \{Q_X : D(Q_X || P_X) \leq \alpha\} \) is compact. So, by the minimax theorem [43, Theorem 2.10.2], the second infminimization and the supremum can be swapped. Hence, the inf-sup part in (76) is equal to

\[
\sup_{\lambda > 0} \inf_{Q_X : D(Q_X || P_X) \leq \alpha} \lambda (\tau - Q_X(f)) - \log P_Y(e^{\lambda g}).
\]

which by Lemma 33, can be rewritten as

\[
\sup_{\lambda > 0} \inf_{\eta > 0} \lambda (\tau - \eta a + \eta \log P_X(e^{(1/n)f})) + \log P_Y(e^{\lambda g}).
\]

Substituting this into (77) completes the proof. 

**Proof of Proposition 18:** By the Kantorovich–Rubinstein formula [37, (5.11)],

\[
\varphi_{\geq X}(\tau) = \inf_{Q_X, 1-Lip f : P_X(f) = 0} D(Q_X || P_X) = \inf_{1-Lip f : P_X(f) = 0} \inf_{\lambda > 0} D(Q_X || P_X) + \lambda (\tau - Q_X(f)) = \inf_{1-Lip f : P_X(f) = 0} \inf_{\lambda > 0} \lambda \tau - \log P_X(e^{\lambda f}).
\]

**Proof of Theorem 19:** It is easy to see that \( \varphi_{\geq X}(\tau) = \varphi_X(\tau) \). If we swap the inf and sup in (30), then we will obtain \( r(\tau) \). However, this is infeasible in general.

Obviously, from (30), \( \varphi_{\geq X}(\tau) \geq r(\tau) \), and by definition, \( r(\tau) \) is convex. So, taking the lower convex envelope, we obtain \( \varphi_{\geq X}(\tau) \geq r(\tau) \). It remains to prove \( \varphi_{\geq X}(\tau) \leq r(\tau) \). We next do this.

By [4, Theorem 3.10], given any \( \tau \geq 0 \), there is a \( \lambda^* \) such that \( r(\tau) = \lambda^* \tau - L_G(\lambda^*) \). Because the function \( \lambda \mapsto \lambda \tau - L_G(\lambda) \) has a maximum at \( \lambda^* \), its right derivative at \( \lambda^* \) is at most 0, and its left derivative is at least 0. In other words, we have \( L_G(\lambda^*) \leq \tau \leq L_G(\lambda^*) \). Therefore, \( L_G(\lambda^*) \) must be a function \( g : \mathcal{X} \to \mathbb{R} \) such that \( L_G(\lambda^*) \) and \( L_G(\lambda^*) \geq \tau \). Because \( L_G(\lambda^*) \leq \tau \), there must be a function \( h : \mathcal{X} \to \mathbb{R} \) such that \( L_h(\lambda^*) = L_G(\lambda^*) \) and \( L_h(\lambda^*) \leq \tau \). Hence for any \( \epsilon > 0 \), there are positive integer \( n \) and nonnegative integer \( k \) such that \( t = \epsilon \), where

\[
\hat{\tau} := pL_G(\lambda^*) + (1 - p)L_h(\lambda^*)
\]

and \( p = \frac{k}{n} \).

Let \( X^n \sim P_X^\otimes n \). Denote \( f : \mathcal{X}^n \to \mathbb{R} \) by

\[
f(x^n) = \sum_{i=1}^{k} g(x_i) + \sum_{i=k+1}^{n} h(x_i).
\]

Since \( g,h \) are 1-Lipschitz, so is \( f \) (on the product space). Then, for any \( \lambda \geq 0 \),

\[
L_f(\lambda) = kL_g(\lambda) + (n - k)L_h(\lambda).
\]

Then,

\[
r(\tau) = \lambda^\ast \tau - L_G(\lambda^*) \leq \lambda^\ast \hat{\tau} - (pL_G(\lambda^*) + (1 - p)L_h(\lambda^*)) + \lambda^\ast \epsilon \\
= \sup_{\lambda \geq 0} \lambda \hat{\tau} - (pL_G(\lambda) + (1 - p)L_h(\lambda)) + \lambda^\ast \epsilon
\]

\[
\leq \lambda \hat{\tau} - \frac{1}{n} L_f(\lambda) + \lambda^\ast \epsilon
\]

\[
\geq \frac{1}{n} \sup_{1-Lip f : P_X^\otimes n(f) = 0} \lambda \hat{\tau} - \frac{1}{n} L_f(\lambda) + \lambda^\ast \epsilon
\]

\[
= \frac{1}{n} \varphi_n(t) + \lambda^\ast \epsilon
\]

\[
\geq \varphi_{\geq X}(\hat{\tau}) + \lambda^\ast \epsilon,
\]

(79)

(80)

whereform (78) follows since the objective function in it is strictly convex in \( \lambda \) and its derivative is zero at \( \lambda^\ast \); \( \varphi_n \) in (79) given by

\[
\varphi_n(t) = \inf_{Q_X \in P(X^n) : C(\mathcal{P}_X^\otimes n, Q_X) \geq t} D(Q_{X^n} || P_X^\otimes n)
\]

is the \( n \)-dimensional extension of \( \varphi_{\geq X}(\tau) \), and (79) follows by Proposition 18 for the \( n \)-dimensional version \( \varphi_n \); (80) follows the single-letterization argument same to that used for (35).

Lastly, letting \( \epsilon \to 0 \), we have \( \hat{\tau} \to \tau \). By the continuity of \( \varphi_{\geq X}(\tau) \) and (80), we have \( r(\tau) \geq \hat{\varphi}_{\geq X}(\tau) \).
Proof of Theorem 20: We first give a dual formula for
\[
\theta(\tau, Q_{XW}) := \inf_{Q_Y|W: C(Q_{XW}, Q_Y|W) \leq \tau} D(Q_Y|W\| P_Y|Q_W).
\]

Observe that
\[
\theta(\tau, Q_{XW}) = \inf_{Q_Y|W: C(Q_{XW}, Q_Y|W) \leq \tau} D(Q_Y|W\| P_Y|Q_W)
= \inf_{Q_Y|W \geq 0} D(Q_Y|W\| P_Y|Q_W)
+ \lambda(C(Q_{XW}, Q_Y|W) - \tau)
= \sup_{\lambda \geq 0} \inf_{Q_Y|W \geq 0} D(Q_Y|W\| P_Y|Q_W)
+ \lambda(C(Q_{XW}, Q_Y|W) - \tau)
= \sup_{\lambda \geq 0} \inf_{Q_Y|W \geq 0} D(Q_Y|W\| P_Y|Q_W)
+ \lambda(E_{Q_W}[C(Q_{XW}|W, Q_Y|W)]) - \tau
\]
(81)

where
\[
\begin{align*}
\text{the inf and sup are swapped in (81) which follows by the general minimax theorem [29, Theorem 5.2.2] together with the convexity of the relative entropy and optimal transport cost functional;}
\end{align*}
\]
(82)
\[
\text{follows by the Kantorovich duality with } f, g \text{ denoting bounded continuous functions;}
\]
(83)
\[
\text{in (83) inf}_{Q_Y|W} \text{ is taken in a pointwise way;}
\]
(84)
\[
\text{the inf and sup are swapped in (84) which follows by the general minimax theorem [29, Theorem 5.2.2] by identifying that 1) the optimal value of the sup-inf in (84) is finite (since upper bounded by } \lambda(C(Q_{XW}|W, P_Y) - \tau)), \text{ and 2) by choosing } f, g \text{ as zero functions, the objective function turns to be } Q_{Y|W = w} \rightarrow D(Q_{Y|W = w}|P_Y) - \lambda \tau \text{ whose sublevels are compact under the weak topology;}
\]
(85)
\[
\text{and (85) follows by Lemma 34 (and the supremum over } f, g \text{ is moved outside of the expectation).}
\]

Substituting the dual formula of } \theta \text{ to } \psi, \text{ we obtain
\[
\begin{align*}
\psi(\alpha, \tau) &= \sup_{Q_{XW}: D(Q_{XW}|P_X|Q_W) \leq \alpha} \theta(\tau, Q_{XW})
= \sup_{\lambda \geq 0} \sup_{f_w + g_w \leq c, \forall w \in \{0,1\}} \inf_{D(Q_{XW}|P_X|Q_w) \leq \alpha} \lambda(E_{Q_W}[C(Q_{XW}|W, Q_Y|W)]) - \tau
- \log P_Y(\tau)
\end{align*}
\]
(86)

where
\[
\text{in (86), by Carathéodory's theorem, the alphabet size of } Q_W \text{ can be restricted to be no larger than 2, (87) follows by Lemma 35, and (88) follows by the minimax theorem since the objective function is convex in } \eta.
\]

Proof of Corollary 21: By the monotonicity of } \psi, \text{ lim}_{\alpha' \uparrow \alpha} \lim_{\tau' \downarrow \tau} \psi(\alpha', \tau') \leq \psi(\alpha, \tau). \text{ So, we only need to focus on the case that } \lim_{\alpha' \uparrow \alpha} \lim_{\tau' \downarrow \tau} \psi(\alpha', \tau') < \infty. \text{ By the monotonicity of } \psi, \text{ it holds that
\[
\begin{align*}
\lim \sup_{\alpha' \uparrow \alpha, \tau' \downarrow \tau} \psi(\alpha', \tau') &= \sup_{\alpha' < \alpha, \tau' > \tau} \psi(\alpha', \tau')
= \sup_{\alpha' < \alpha, \tau' > \tau} \sup_{f_w + g_w \leq c, \forall w \in \{0,1\}} \inf_{\lambda \geq 0} \lambda(E_{Q_W}[C(Q_{XW}|W, Q_Y|W)]) - \tau
- \log P_Y(\tau)
\end{align*}
\]
(87)

where
\[
\text{by the continuous extension of } \eta \log P_X(\tau) \text{ to } \eta = 0, \text{ inf}_{\eta > 0} \text{ in (87) is replaced by inf}_{\eta > 0} \text{ in (89);}
\]
(88)
\[
\text{the sup}_{\alpha' < \alpha, \tau' > \tau} \text{ and inf}_{\eta > 0} \text{ are swapped in (90) which follows by the general minimax theorem [29, Theorem 5.2.2] by identifying that 1) the optimal value of the sup-inf in (89) is finite since it is upper bounded by } \lim_{\alpha' \uparrow \alpha} \lim_{\tau' \downarrow \tau} \psi(\alpha', \tau'), \text{ and 2) given } \alpha' > 0, \text{ the objective function in (89) goes to infinity as } \eta \rightarrow \infty, \text{ and hence, its sublevels are compact.}
\]

VIII. PROOF OF THEOREM 22

Let } (B_n) \text{ be the optimal sets given in Part (a) of Assumption 4. By the optimality of } B_n, \text{ for any } A \text{ it holds that
\[
\begin{align*}
(p^{\otimes n})^+(A) &= \sup_{\tau \in [0,1]} \inf_{r \in [0,1]} F_r^{(n)}(B_n)
= n^{-1/p} e^{-\alpha \tau} \liminf_{r \in [0,1]} F_r^{(n)}(B_n).
\end{align*}
\]
(91)

By Part (a) of Assumption 4,
\[
\liminf_{r \in [0,1]} F_r^{(n)}(B_n) \geq F_{\epsilon}^{(n)}(B_n) - \delta(\epsilon, n).
\]
Hence,

\[
\lim \inf_{n \to \infty} \lim \inf_{r \to 0} F_r^{(n)}(B_n) \geq \lim \inf_{n \to \infty} F_r^{(n)}(B_n) - \delta(\epsilon, \infty)
\]

\[
\geq \lim \inf_{n \to \infty} F_r^{(n)}(B_n) - \delta(\epsilon, \infty)
\]

\[
\geq \lim \inf_{n \to \infty} \alpha - E_r^{(n)}(\alpha, \epsilon^p) - \delta(\epsilon, \infty)
\]

\[
\geq \alpha - \lim_{r' \to 0} \lim_{r \to 0^+} \psi(\alpha', r^p) - \delta(\epsilon, \infty)
\]

\[
= \inf_{r' \in (0, \epsilon)} \alpha - \lim_{r \to 0^+} \psi(\alpha', r^p) - \delta(\epsilon, \infty)
\]

\[
= \inf_{r' \in (0, \epsilon)} \alpha - \lim_{r \to 0^+} \psi(\alpha', r^p) - \delta(\epsilon, \infty)
\]

where \(\delta(\epsilon, \infty) := \limsup_{n \to \infty} \delta(\epsilon, n)\), (92) follows by Theorem 12, (93) follows by since the monotonicity of \(\psi\),

\[
\lim \sup_{\alpha' | \alpha' \leq r' \leq \epsilon} \psi(\alpha', r^p) = \sup_{\alpha' \in (0, \alpha)} \sup_{r' \in (0, \epsilon)} \psi(\alpha', r^p)
\]

\[
= \sup_{r' \in (0, \epsilon)}\sup_{\alpha' \in (0, \alpha)} \psi(\alpha', r^p)
\]

\[
= \sup_{r' \in (0, \epsilon)} \lim_{\alpha' \to 0^+} \psi(\alpha', r^p).
\]

Taking \(\epsilon \downarrow 0\), we obtain that

\[
\lim \inf_{n \to \infty} \lim \inf_{r \to 0} F_r^{(n)}(B_n) \geq \xi(\alpha).
\]

Substituting this into (91) yields the desired inequality.

We next prove the sharpness. By Part (b) of Assumption 4, there is a family of sets \(A_{n,\epsilon} \subseteq X^n\) of probability \(e^{-n\alpha}\) such that

\[
\lim \inf_{r \to 0} F_r^{(n)}(A_{n,\epsilon}) \leq \lim \inf_{n \to \infty} F_r^{(n)}(A_{n,\epsilon}) + \delta(\epsilon, n).
\]

Hence,

\[
\lim \sup_{n \to \infty} \lim \inf_{r \to 0} F_r^{(n)}(A_{n,\epsilon}) \leq \lim \sup_{n \to \infty} \lim \inf_{r \to 0} F_r^{(n)}(A_{n,\epsilon}) + \delta(\epsilon, n)
\]

\[
\leq \lim \sup_{n \to \infty} \lim \inf_{r \to 0} F_r^{(n)}(A_{n,\epsilon}) + \delta(\epsilon, n)
\]

\[
= \alpha - \lim \inf_{n \to \infty} E_r^{(n)}(\alpha, \epsilon^p) + \delta(\epsilon, \infty)
\]

\[
\leq \alpha - \lim_{r \to 0^+} \psi(\alpha, r^p) + \delta(\epsilon, \infty),
\]

where (94) follows by Theorem 12. Taking \(\epsilon \downarrow 0\), we obtain that

\[
\lim \sup_{n \to \infty} \lim \sup_{r \to 0} F_r^{(n)}(A_{n,\epsilon}) \leq \xi(\alpha).
\]

Substituting this into (32) yields

\[
(P^{\otimes n})^+(A_{n,\epsilon}) \leq n^{1 - 1/p} e^{-n\alpha}(\xi(\alpha) + \delta(\epsilon, n)),
\]

where

\[
\lim \sup_{\epsilon \to 0} \lim \sup_{n \to \infty} \hat{\delta}(\epsilon, n) = 0.
\]

By basic analysis, the condition in (95) implies that there exists a sequence \(\epsilon_n\) such that \(\epsilon_n \to 0\) and \(\hat{\delta}(\epsilon_n, n) \to 0\) as \(n \to \infty\). For such a sequence,

\[
(P^{\otimes n})^+(A_{n,\epsilon_n}) \leq n^{1 - 1/p} e^{-n\alpha}(\xi(\alpha) + o_n(1)).
\]
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