WASSERSTEIN CONDITIONAL INDEPENDENCE TESTING

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Abstract. We introduce a test for the conditional independence of random variables $X$ and $Y$ given a random variable $Z$, specifically by sampling from the joint distribution $(X,Y,Z)$, binning the support of the distribution of $Z$, and conducting multiple $p$-Wasserstein two-sample tests. Under a $p$-Wasserstein Lipschitz assumption on the conditional distributions $\mathcal{L}_{X|Z}$, $\mathcal{L}_{Y|Z}$, and $\mathcal{L}_{(X,Y)|Z}$, we show that it is possible to control the Type I and Type II error of this test, and give examples of explicit finite-sample error bounds in the case where the distribution of $Z$ has compact support.

Consider random variables $X, Y, Z$. That is, $(\Omega, \mathcal{A}, \mathbb{P})$ is our sample space, and $X : \Omega \to \mathbb{R}^{d_X}$, $Y : \Omega \to \mathbb{R}^{d_Y}$, and $Z : \Omega \to \mathbb{R}^{d_Z}$ are all Borel functions, with distributions $\mathcal{L}_X := \mathbb{P} \circ X^{-1}$ (and similar for $Y$ and $Z$) as well as joint distribution $\mathcal{L}_{(X,Y,Z)} := \mathbb{P} \circ (X,Y,Z)^{-1}$. We are interested in testing the conditional dependence relations between $X$, $Y$, and $Z$. For a general overview of some of the many ways in which conditional (in)dependence arises in statistics, we refer the reader to the classic article by Dawid [Dawid79]. More recently, conditional independence testing has found a central role in the areas of causal inference and causal discovery; for a summary of this line of work, see the recent text by Peters et al. [PJS17], as well as the foundational works by Spirtes et al. [SGS01] and Pearl [Pea09].

Numerous practical methods for testing conditional independence have been proposed — for instance, Heinze-Deml et al. [HDPM18] describe six classes of conditional independence test which have been implemented in the R package CondIndTests. Nonetheless, general theoretical guarantees for conditional independence testing — consistency results for general joint distributions $\mathcal{L}_{(X,Y,Z)}$, sample complexity, power estimates, and so on — have been hard to come by. Recently, Shah and Peters [SP20] have demonstrated that this is not an accident: indeed, they show that for general joint distribution $\mathcal{L}_{(X,Y,Z)}$, any valid test of conditional independence does not have power against any alternative. (This result has also been reproved, using techniques from optimal transport, in [NBW21].) Consequently, it is of interest to find mild assumptions on $\mathcal{L}_{(X,Y,Z)}$ (or, similarly, on the various conditional distributions between the variables $X$, $Y$, and $Z$) under which a general test for conditional independence does, indeed, exist.

Here, our strategy is to present regularity conditions on the conditional distributions $\mathcal{L}_{X|Z=z}$, $\mathcal{L}_{Y|Z=z}$, and $\mathcal{L}_{(X,Y)|Z=z}$, so that if we bin the conditioning variable $Z$ using a sufficiently fine, finite partition $V_1, \ldots, V_J$ of $\text{supp}(\mathcal{L}_Z)$, then for all $j = 1, \ldots, J$ and all $z \in V_j$,

$$\mathcal{L}_{X|Z=z} \otimes \mathcal{L}_{Y|Z=z} \approx \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}, \quad \text{and} \quad \mathcal{L}_{(X,Y)|Z=z} \approx \mathcal{L}_{(X,Y)|Z \in V_j}$$

where $\approx$ denotes closeness with respect to some suitable metric on the space of probability measures.

If this holds, then we can replace the (intractable in general) problem of directly comparing the measures $\mathcal{L}_{(X,Y)|Z=z}$ and $\mathcal{L}_{X|Z=z} \otimes \mathcal{L}_{Y|Z=z}$ for every $z$ in the range of $Z$, with the (costly, but in principle tractable) problem of comparing $\mathcal{L}_{(X,Y)|Z \in V_j}$ and $\mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}$ for every bin $V_j$. In other words, we seek regularity conditions that allow for conditional independence to be tested indirectly using multiple two-sample independence tests. Of course, one must also ensure that the
two-sample tests comparing $\mathcal{L}_{(X,Y)|Z \in V_j}$ and $\mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}$ are themselves feasible (in the sense, for instance, of having explicit finite-sample control on the Type I & II error).

Our work uses the formalism of optimal transport, in particular the Wasserstein distance $W_p$, in an essential way. As a metric structure on the space of probability measures, the Wasserstein distance is only slightly stronger than weak convergence, so the stipulation that (for instance) “for small $V_j$, $W_p(\mathcal{L}_{(X,Y)|Z=z}, \mathcal{L}_{(X,Y)|Z \in V_j}) \approx 0^p$ is comparatively easy to satisfy. At the same time, it is also possible to use the Wasserstein distance to conduct two-sample tests of quite general probability measures.

The structure of the paper is as follows. In Section 1, we give an overview of the necessary background from optimal transport, and discuss how to use the Wasserstein distance to conduct two-sample independence tests. In Section 2 we review the general infeasibility of conditional independence testing, but show that if the conditional distributions $\mathcal{L}_{X|Z=z}$, $\mathcal{L}_{Y|Z=z}$, and $\mathcal{L}_{(X,Y)|Z=z}$ are Lipschitz functions of $z$ when the space of probability measures is equipped with the $W_p$ metric, then binning the conditioning variable $Z$ incurs a small, explicit error in the $W_p$ metric. We then explain how this allows for a “$W_p$ multiple two-sample” conditional independence test, with explicit finite-sample control of the Type I and Type II error, under a wide variety of mild auxiliary regularity assumptions (which are needed so that the two-sample tests are themselves feasible). Additionally, in Section 3 we give a “plug-in” estimator for the $W_p$-Lipschitz constants of $\mathcal{L}_{X|Z=z}$, $\mathcal{L}_{Y|Z=z}$, and $\mathcal{L}_{(X,Y)|Z=z}$.

Regarding recent related work by others, while the work presented in this article was in progress, the author learned of the recent article [NBW21], which also considers conditional independence testing under smoothness assumptions on the conditional distributions $\mathcal{L}_{(X,Y)|Z}$, $\mathcal{L}_{X|Z}$, and $\mathcal{L}_{Y|Z}$. The two works are similar in spirit, but complementary. On the one hand, as discussed below in Section 2, our background assumptions are weaker than those used in [NBW21]: on the other hand, [NBW21] provides delicate minimax estimates which are valid in the total variation setting.

1. Two-sample independence testing with the Wasserstein distance

We first consider testing whether $X \perp \!\!\!\perp Y$. Note that this amounts to a two-sample test between the distributions $\mathcal{L}_{(X,Y)}$ and $\mathcal{L}_X \otimes \mathcal{L}_Y$. Furthermore, note that given the ability to sample from $\mathcal{L}_{(X,Y)}$, we can always artificially sample from $\mathcal{L}_X \otimes \mathcal{L}_Y$ as well — for instance, one can sample from $\mathcal{L}_{(X,Y)} 2n$ times, and for the first $n$ samples discard the $Y$ values, and for the second $n$ samples discard the $X$ values, and then $(x_1, y_{n+1}), (x_2, y_{n+2}), \ldots, (x_n, y_{2n})$ will be drawn from $\mathcal{L}_X \otimes \mathcal{L}_Y$.

Specifically, we consider Wasserstein-based two sample tests (cf. [RGTC17], which considers some stronger results in the univariate case). We do not attempt to give a general survey on optimal transport/Wasserstein distances here (a more than sufficient background reference is [San15]; see also [PZ19] for a survey tailor to a statistical audience), but we give a short motivational discussion. Recall that for $p \in [1, \infty)$, the $p$-Wasserstein distance on the space $P_p(U)$ of Borel probability measures with finite $p$-th moments on the domain $U \subseteq \mathbb{R}^d$ is given by

$$W_p(\mu, \nu) := \inf_{\gamma \in \Pi(\mu, \nu)} \left( \int_{U^2} ||x - y||^p d\gamma(x, y) \right)^{1/p}$$

where $\Pi(\mu, \nu)$ is the space of all couplings of $\mu$ and $\nu$, namely all probability measures on $U^2$ with marginals $\mu$ and $\nu$. For $p \in [1, \infty)$, the $p$-Wasserstein distance metrizes the weak convergence of probability measures together with convergence of $p$th moments. In the jargon of optimal transport, a measure $\gamma \in \Pi(\mu, \nu)$ is said to be a transport plan between $\mu$ and $\nu$, and moreover $\gamma$ is said to be an optimal plan if the infimum in the definition of $W_p$ is attained at $\gamma$, that is, $W_p(\mu, \nu) = \inf_{\gamma \in \Pi(\mu, \nu)} \left( \int_{U^2} ||x - y||^p d\gamma(x, y) \right)^{1/p}$.
It is a basic feature of the theory that, given arbitrary measures $\mu, \nu \in \mathcal{P}_p(U)$ on a “reasonable” domain $U$ (specifically, we require that $U$ be a Polish space), there exists an optimal plan $\gamma$ between $\mu$ and $\nu$, but $\gamma$ need not be unique.

If, moreover, we restrict our attention to absolutely continuous measures (say with respect to the Lebesgue measure on $U$), then the $p$-Wasserstein distances enjoy another interpretation, in terms of optimal transport maps rather than optimal couplings. If we write $T#\mu$ for the pushforward of $\mu$ by the map $T$ (that is, the measure defined by $T#\mu(A) := \mu(T^{-1}(A))$), then it turns out that when $\mu$ is absolutely continuous,

$$W_p(\mu, \nu) = \inf_{T: T#\mu = \nu} \left( \int_U |x - T(x)|^p \, d\mu(x) \right)^{1/p}.$$ 

There is an extensive theory studying these transport maps — under what circumstances the infimum in the previous expression is attained, whether the map $T$ instantiating the infimum is unique, what regularity properties it possesses, and so on. This theoretical apparatus will not play a role in our arguments. However, there is one further feature of the $p$-Wasserstein distances that will be be very helpful for us, which is the following. Suppose that $x_1, x_2, \ldots$ are i.i.d. samples from $\mu$. Let $\mu_n := \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$ denote the $n$th empirical measure for $\mu$. (Note that $\mu_n$ is random, but $\mu$ is fixed.) One variant of the law of large numbers (namely, the Glivenko-Cantelli theorem) states that $\mu_n$ converges to $\mu$ in distribution with probability 1; accordingly, $W_p(\mu_n, \mu) \to 0$ almost surely, when $p \in [1, \infty)$ (and, it turns out, when $p = \infty$ as well). In fact, $W_p(\mu_n, \mu)$ possesses known sample complexity bounds: for instance, if the domain $U$ on which $\mu$ resides is compact, $d$-dimensional and Hausdorff regular, and (for instance) $\mu$ is absolutely continuous w.r.t. the volume measure on $U$, then for any $p \in [1, d/2]$ the $W_p$ sample complexity of $\mu$ is no worse than $O(n^{-1/d})$ [WB19, Theorem 1 and Proposition 8] (see also discussion in the introduction of [AG19] or [NWR19] for a brief overview of similar results). Significant improvements on this bound are possible in special cases, for example if $\mu$ is actually supported on a lower-dimensional surface [WB19]. Note also that if $\mu \neq \nu$, then the convergence of $W_p(\mu_n, \nu_n)$ to $W_p(\mu, \nu)$ was recently shown to occur at a faster rate than $O(n^{-1/d})$ in general [CRL+20, MNW21].

Now let’s return our focus to (two-sample) independence testing for $X$ and $Y$.

Let’s be slightly more explicit about what this test looks like. The null hypothesis $H_0$ will be that $X$ and $Y$ are indeed independent, so $L_{(X,Y)} = L_X \otimes L_Y$. We first approximate both $L_{(X,Y)}$ and $L_X \otimes L_Y$ with empirical measures based on samples, for instance

$$\frac{1}{n} \sum_{i=1}^n \delta_{(x_i, y_i)} + \frac{1}{n} \sum_{i=1}^n \delta_{(x_{n+i}, y_{2n+i})}$$

respectively. Under the null hypothesis, we use the fact that $L_{(X,Y)} = L_X \otimes L_Y$ to deduce that

$$W_p \left( \frac{1}{n} \sum_{i=1}^n \delta_{(x_i, y_i)}, \frac{1}{n} \sum_{i=1}^n \delta_{(x_{n+i}, y_{2n+i})} \right)$$

$$\leq W_p \left( \frac{1}{n} \sum_{i=1}^n \delta_{(x_i, y_i)}, L_{(X,Y)} \right) + W_p \left( L_X \otimes L_Y, \frac{1}{n} \sum_{i=1}^n \delta_{(x_{n+i}, y_{2n+i})} \right)$$

and observe that

$$W_p \left( \frac{1}{n} \sum_{i=1}^n \delta_{(x_i, y_i)}, L_{(X,Y)} \right) \xrightarrow{n \to \infty} 0, \quad W_p \left( L_X \otimes L_Y, \frac{1}{n} \sum_{i=1}^n \delta_{(x_{n+i}, y_{2n+i})} \right) \xrightarrow{n \to \infty} 0.$$
This motivates the following definition:

**Definition 1.** (\(p\)-Wasserstein Two Sample Independence Test) The null hypothesis \(H_0\) is that \(\mathcal{L}_{(X,Y)} = \mathcal{L}_X \otimes \mathcal{L}_Y\). We then set some “level” \(\varepsilon_0 > 0\), and say that we reject the null hypothesis if

\[
W_p \left( \frac{1}{n} \sum_{i=1}^{n} \delta(x_i, y_i), \frac{1}{n} \sum_{i=1}^{n} \delta(x_{n+i}, y_{2n+i}) \right) \geq \varepsilon_0,
\]

and we fail to reject otherwise.

In other words, the test above prescribes using the plug-in estimator \(W_p(\mathcal{L}_{(X,Y)}, \mathcal{L}_X \otimes \mathcal{L}_Y)\) for \(W_p(\mathcal{L}_{(X,Y)}, \mathcal{L}_X \otimes \mathcal{L}_Y)\).

**Remark.** Other finite-sample estimators for the \(W_p\) distance between two measures have been considered in the literature, and may even be more desirable in some situations (see discussion, for instance, in [CRL+20]). We restrict our attention to the plug-in estimator only in the interest of simplicity. Note also that there are theoretical obstructions to producing a finite-sample estimator which is vastly superior to the plug-in estimator, in particular the recent minimax result from [SP18].

To emphasize, the false rejection rate under the null is governed by the previously stated \(W_p\) sample complexity bounds for empirical measures. On the other hand, the false acceptance rate under the alternative (that is, the probability of the two empirical measures being within \(\varepsilon_0\) of each other, even though \(\mathcal{L}_{(X,Y)} \neq \mathcal{L}_X \otimes \mathcal{L}_Y\)) depends on which distribution \(\mathcal{L}_{(X,Y)}\) actually is; more specifically, it depends on \(W_p(\mathcal{L}_{(X,Y)}, \mathcal{L}_X \otimes \mathcal{L}_Y)\).

Before proceeding to testing procedures for conditional independence in Section 2 below, we give a more explicit analysis of the “Wasserstein two-sample” independence test described above. Namely: how must \(\varepsilon_0\) be chosen in order to ensure a given \(p\)-value and power function for the test? Morally, this is “just” an application of the sample complexity estimates for \(W_p\) already mentioned; note that \(\mathcal{L}_{(X,Y)}\) and \(\mathcal{L}_X \otimes \mathcal{L}_Y\) reside in \(\mathbb{R}^{d_X + d_Y}\), so the “off-the-shelf” \(W_p\) sample complexity for such a two-sample test is \(O(n^{-1/(d_X + d_Y)})\) (for \(p \in [1, \frac{1}{2}(d_X + d_Y))\)). However, this sample complexity is an asymptotic result, and is therefore unsuitable e.g. for the construction of an explicit confidence interval. At the same time, while there is notable recent progress on central limit theorems for the empirical Wasserstein distance, for instance for the asymptotic distribution of the Wasserstein distance \(W_p(\mu_n, \nu)\) where \(\mu_n\) is an empirical measure for \(\mu\) [DBL19, dBGSL21], the result therein are also insufficient to construct explicit confidence intervals without more information regarding the quantity \(\mathbb{E}W_p(\mu_n, \nu)\).

We therefore proceed by an alternative analysis, which has essentially two ingredients:

1. Given a measure \(\mu\) and an empirical measure \(\mu_n\) for \(\mu\), we desire an explicit upper bound on the expected error introduced by passing to the empirical measure \(\mu_n\), that is, the quantity \(\mathbb{E}W_p(\mu, \mu_n)\). In what follows, we call this the expectation bound.
2. Additionally, we would like a concentration inequality indicating how the random quantity \(W_p(\mu, \mu_n)\) is distributed around its expectation \(\mathbb{E}W_p(\mu, \mu_n)\).

If we have these two ingredients, it is straightforward to produce an upper bound on the probability that, under the null, the test indicated in Definition 1 will nonetheless be rejected.

For an example of a suitable concentration inequality, let us mention the following:

**Proposition 2** ([WB19, Proposition 20]). Let \((X, d)\) be a Polish metric space, and let \(\mu \in \mathcal{P}_p(X)\) be a measure supported on a set of diameter at most \(D\). Let \(\mu_n\) denote an empirical measure for \(\mu\).
Then,
\[ \mathbb{P} \left[ W_p^n(\mu, \mu_n) \geq EW_p^n(\mu, \mu_n) + t \right] \leq \exp \left( -\frac{2nt^2}{D^{2p}} \right). \]

Remark. Weed and Bach only state their concentration inequality in the case where \( D = 1 \). However the modification of their argument for general diameter is quite routine; for completeness, we rerun the argument with general diameter in Appendix B.

It is also possible to extend the argument for Proposition 2 to the case of a measure \( \mu \) with unbounded support on a Polish metric space \((X, d)\), at least provided \( \mu \) also lies in \( \mathcal{P}_q(X) \) for some \( q > p \). This concentration inequality, which we state as Proposition 13 below, is of independent interest; we state and prove this result in Appendix B.

It turns out that of the two ingredients — the expectation bound, and the concentration inequality — it is the former that is the more challenging one, and indeed has been the subject of ongoing investigation by numerous authors, such as [BLG14, DSS13, FG15, Lei20, WB19]. In particular, it is known that estimating the error introduced by passing to empirical measures for distributions \( L_{(X,Y)} \) and \( L_X \otimes L_Y \) depends sensitively on the dimension \( d_X + d_Y \). We note that the following theorem applies directly for the case where \( d_X + d_Y \geq 3 \); however, since there is no absolute continuity requirement, even in the (important) case where \( d_X + d_Y = 2 \), this theorem can still be employed, simply by taking \( d = \min\{3, d_X + d_Y\} \).

**Theorem 3 ([DSS13, Theorem 1]).** Let \( \mu \) be a measure on \( \mathbb{R}^d \) with \( d \geq 3 \), and let \( \mu_n \) be an empirical measure for \( \mu \). Let \( p \in [1, d/2) \) and \( q > dp/(d - p) \). Then there exists a constant \( \kappa_{p,q,d} \) depending only on \( p, q, \) and \( d \), such that
\[
E[W_p^n(\mu_n, \mu)]^{1/p} \leq \kappa_{p,q,d} \left( \int_{\mathbb{R}^d} \|x\|^q d\mu(x) \right)^{1/q} n^{-1/d}
\]
where \( \| \cdot \| \) is a norm on \( \mathbb{R}^d \) and \( \kappa_{p,q,d} \) is given explicitly in [DSS13].

Remark. While our focus in this article is to construct a test with finite-sample guarantees under very general assumptions, we also alert the reader to the fact that the rate in the theorem above can be improved significantly if \( \mu \) is known to have some additional regularity, e.g., is concentrated near a low-dimensional set or is a Gaussian mixture — see extensive consideration of these issues in [WB19].

Observe that by combining the estimates
\[
\mathbb{P} \left[ W_p^n(\mu_n, \mu) \geq t \right] \leq \exp(-2nt^2/D^{2p})
\]
and
\[
E[W_p^n(\mu_n, \mu)]^{1/p} \leq \kappa_{p,q,d} \left( \int_{\mathbb{R}^d} \|x\|^q d\mu(x) \right)^{1/q} n^{-1/d}
\]
it follows directly that in the case where \( \mu \) has support with diameter at most \( D \) (and therefore \( \int_{\mathbb{R}^d} \|x\|^q d\mu(x) < \infty \),
\[
\mathbb{P} \left[ W_p^n(\mu_n, \mu) \geq t + E[W_p^n(\mu_n, \mu)] \right] \leq \mathbb{P} \left[ W_p^n(\mu_n, \mu) \geq t + \kappa_{p,q,d} \left( \int_{\mathbb{R}^d} \|x\|^q d\mu(x) \right)^{p/q} n^{-p/d} \right]
\leq \exp(-2nt^2/D^{2p}).
\]
For instance (although this is far from the most efficient upper bound in \( n! \)), if \( n \) is large enough that 
\[
\kappa^p_{p,q,d} \left[ \int_{\mathbb{R}^d} \|x\|^q d\mu(x) \right]^{p/q} n^{-p/d} \leq \frac{1}{2} \left( \frac{\varepsilon}{2} \right)^p,
\]
then putting \( t = \frac{1}{2} \left( \frac{\varepsilon}{2} \right)^p \) gives 
\[
\mathbb{P} \left[ W^p_p(\mu_n, \mu) \geq \left( \frac{\varepsilon}{2} \right)^p \right] \leq \exp \left( -\frac{2n\varepsilon^{2p}}{4p+1D^{2p}} \right)
\]
or equivalently
\[
\mathbb{P} \left[ W_p(\mu_n, \mu) \geq \varepsilon \right] \leq \exp \left( -\frac{2n\varepsilon^{2p}}{4p+1D^{2p}} \right).
\]
Lastly, note that if \( \mu_n \) and \( \mu'_n \) are both empirical measures drawn from the same distribution \( \mu \), and \( W_p(\mu_n, \mu'_n) \geq \varepsilon \), then the case must be the case that either \( W_p(\mu_n, \mu) \geq \frac{\varepsilon}{2} \) or \( W_p(\mu'_n, \mu) \geq \frac{\varepsilon}{2} \). Hence,
\[
\mathbb{P} \left[ W_p(\mu_n, \mu'_n) \geq \varepsilon \right] \leq 2 \exp \left( -\frac{2n\varepsilon^{2p}}{4p+1D^{2p}} \right).
\]

Likewise, if \( \mu \) has unbounded support but still satisfies a higher \( q \)th moment bound, as per Theorem 3, one can combine Theorems 13 and 3 in a similar manner: see Corollary 14 below.

It is also possible to explicitly bound the type II error of the test given in Definition 1, as a function of \( W_p(L_{(X,Y)}, L_{X \otimes L_Y}) \). Indeed, suppose that \( W_p(L_{(X,Y)}, L_{X \otimes L_Y}) \geq \varepsilon_0 + \delta_0 \). Then, if a type II error occurs, namely \( W_p \left( \frac{1}{n} \sum_{i=1}^n \delta(x_i, y_i), \frac{1}{n} \sum_{i=1}^n \delta(x_{n+i}, y_{2n+i}) \right) < \varepsilon_0 \), it must be the case that at least one of the following holds:
\[
W_p \left( L_{(X,Y)}, \frac{1}{n} \sum_{i=1}^n \delta(x_i, y_i) \right) > \frac{\delta_0}{2} \quad \text{or} \quad W_p \left( L_X \otimes L_Y, \frac{1}{n} \sum_{i=1}^n \delta(x_{n+i}, y_{2n+i}) \right) > \frac{\delta_0}{2}.
\]
But we can upper bound the probability of each of these events using exactly the same analysis — expectation bound combined with concentration inequality — that we have just described.

Additionally, let us remark on the task of actually computing the estimator \( W_p(\hat{\mu}_n, \hat{\nu}_n) \) for \( W_p(\mu, \nu) \). Computing the optimal coupling for \( \hat{\mu}_n \) and \( \hat{\nu}_n \) takes the form of a classical (discrete) optimal matching problem, which has been extensively studied and is amenable to the standard methods of linear programming. State-of-the-art computational methods for this problem are surveyed, for instance, in [PC19]; for example, fast methods based on Sinkhorn’s algorithm, discussed therein, achieve a computational cost of \( O(n^2 \log n) \). Therefore, when conducting a Wasserstein two-sample test, one must take care to work with empirical measures supported on a number of points which is large enough that the test achieves a small enough \( p \)-value, but not so large that the estimator itself is infeasible to compute.

In what follows, we (to some extent) work modulo the choice of a Wasserstein two-sample (independence) test with a given \( p \)-value and power function. However, we hope that from the previous discussion, the reader is convinced that such a test is feasible, albeit subject to ongoing technical improvements, viz. in terms of expectation bounds, concentration inequalities, and computational complexity.

2. Conditional independence testing via binning

Now we consider conditional independence testing. That is, we ask whether \( X \perp\!\!\!\perp Y \mid Z \). At the level of distributions, this amounts to comparing \( L_{(X,Y)\mid Z=z} \) with \( L_{X\mid Z=z} \otimes L_{Y\mid Z=z} \) for every \( z \) in the range of \( Z \). (Note that these distributions should be understood as disintegrations of the joint distributions \( L_{(X,Y,Z)} \) and \( L_{(X,Z)} \) and \( L_{(Y,Z)} \) w.r.t \( Z \), e.g. in the sense of regular conditional distributions.) That is, conditional independence testing may be understood as (at least implicitly) requiring a continuum number of two-sample tests.
It should now be clear to the reader that without further assumptions on the random variables \(X, Y,\) and \(Z\) (and their joint distribution), finite sample conditional independence testing is futile. Indeed, it may be that for all of the (finitely many) values \(z\) of \(Z\) that we actually get to sample, it is the case that \(\mathcal{L}(X,Y)|Z=z = \mathcal{L}_X|z \otimes \mathcal{L}_Y|z=z;\) but for some \(z'\) out of our sample, \(\mathcal{L}(X,Y)|Z=z'\) and \(\mathcal{L}_X|z \otimes \mathcal{L}_Y|z=z'\) are very far apart as distributions. Compare with the analogous concern for \(\mathcal{L}(X,Y)\) versus \(\mathcal{L}_X \otimes \mathcal{L}_Y;\) here, we have a guarantee from the (convergence of measures version of the) law of large numbers that empirical measures converge to the measures they are drawn from almost surely, with a deviation rate/concentration bounds given by Sanov’s theorem or similar. We have no such luck here, simply from the fact that \(\mathcal{L}(X,Y)|Z=z\) and \(\mathcal{L}(X,Y)|Z=z'\) are different distributions with no a priori relationship. (The proof in [SP20] which shows that conditional independence testing is not feasible in general, proceeds by way of a different, but in some sense related, argument: there, they construct two joint distributions of random variables \((X, Y, Z)\) and \((\tilde{X}, \tilde{Y}, \tilde{Z})\) where each of \(\{X, \tilde{X}\}, \{Y, \tilde{Y}\},\) and \(\{Z, \tilde{Z}\}\) are close with high probability, hence costly to distinguish with finite samples, yet \((X, Y, Z)\) and \((\tilde{X}, \tilde{Y}, \tilde{Z})\) have different conditional dependence relations.)

So in order to construct a conditional independence test which, say, comes with any kind of finite sample guarantee, some auxiliary assumptions are necessary. In particular, if we knew that all the marginal distributions varied in some continuous fashion with \(z,\) we would be able to use the fact that \(\mathcal{L}(X,Y)|Z=z \approx \mathcal{L}(X,Y)|Z=z'\) whenever \(z \approx z'\) (and likewise for the families of distributions \(\mathcal{L}_X|z\) and \(\mathcal{L}_Y|z),\) to deduce some overall estimate of conditional dependence by binning the variable \(Z,\) and then performing a (possibly very large) number of separate two-sample independence tests.

In what follows, it turns out that we will need to set some small parameters (specifically the diameter of bins for the range of \(Z\)) to be small compared to the inverse of all three optimal Lipschitz constants simultaneously.

\[
\mathbb{R}^{dz} \rightarrow \mathcal{P}(\mathbb{R}^{dx+dy}) \\
z \mapsto \mathcal{L}(X,Y)|Z=z.
\]

We ask that \(z \mapsto \mathcal{L}(X,Y)|Z=z\) is Lipschitz continuous, provided we equip \(\mathcal{P}(\mathbb{R}^{dx+dy})\) with the \(W_p\) metric; in other words,

\[
\begin{align*}
z \mapsto \mathcal{L}(X,Y)|Z=z & \text{ is } L_{XY}\text{-Lipschitz} \\
\iff (\forall z, z' \in \mathbb{R}^{dz} \cap \text{supp}(\mathcal{L}_Z)) W_p(\mathcal{L}(X,Y)|Z=z, \mathcal{L}(X,Y)|Z=z') & \leq L_{XY}|z-z'|.
\end{align*}
\]

Observe that requiring that \(z \mapsto \mathcal{L}(X,Y)|Z=z\) be \(L\)-Lipschitz not only imposes that \(z \approx z' \implies \mathcal{L}(X,Y)|Z=z \approx_{W_p} \mathcal{L}(X,Y)|Z=z',\) it does so in a quantitative fashion: if we know that \(|z-z'| < \varepsilon / L_{XY},\) then we can say that \(W_p(\mathcal{L}(X,Y)|Z=z, \mathcal{L}(X,Y)|Z=z) < \varepsilon.\)

In addition, we will also require that the functions

\[
z \mapsto \mathcal{L}_X|Z=z \quad \text{and} \quad z \mapsto \mathcal{L}_Y|Z=z
\]

be Lipschitz continuous, in other words,

\[
(\forall z, z' \in \mathbb{R}^{dz} \cap \text{supp}(\mathcal{L}_Z)) \quad W_p(\mathcal{L}_X|Z=z, \mathcal{L}_X|Z=z') \leq L_X|z-z'|;
\]

\[
(\forall z, z' \in \mathbb{R}^{dz} \cap \text{supp}(\mathcal{L}_Z)) \quad W_p(\mathcal{L}_Y|Z=z, \mathcal{L}_Y|Z=z') \leq L_Y|z-z'|.
\]

In what follows, it turns out that we will need to set some small parameters (specifically the diameter of bins for the range of \(Z\)) to be small compared to the inverse of all three optimal Lipschitz constants simultaneously.
Remark. There are, of course, many inequivalent metrics of interest on the space of probability measures. Why choose the $W_p$ metric (for some $p \in [1, \infty]$) in particular? Indeed, the recent article [NBW21], also concerned with conditional independence testing, makes extensive use of the total variation ($TV$) metric rather than a metric coming from an optimal transport problem. To some extent, the choice of metric on the space of probability measures is simply a modeling decision, but let us emphasize a topological point in favor of the $W_p$ metrics. On compact sets, convergence in $W_p$ is equivalent to convergence in distribution, a.k.a. convergence in the probabilist’s weak topology; on the other hand, the TV norm metrizes strong convergence, equivalently convergence in $L^1$.

Since the strong topology is (as the name suggests) stronger than the weak topology, it follows that fewer functions from $\mathbb{R}^d$ into the space of probability measures are strongly continuous than weakly continuous. In our particular situation, this means that on a compact domain, the requirement that conditional distributions of the form $z \mapsto \mathcal{L}_{(X,Y)|Z=z}$ be $W_p$-continuous is less stringent than requiring that $z \mapsto \mathcal{L}_{(X,Y)|Z=z}$ be $TV$-continuous. This difference in strength of assumption is especially evident in the case where the conditional distributions $z \mapsto \mathcal{L}_{(X,Y)|Z=z}$ and $z \mapsto \mathcal{L}_{(X,Y)|Z=z'}$ are mutually singular for different values of $z$, as is the case, for example, when the conditional distributions are supported on disjoint hypersurfaces parametrized by $z$. For emphasis, we give a couple of concrete instances of this type in the following example.

Example 4. (examples of conditional distribution which is $W_p$-Lipschitz but not $TV$-continuous) (1) Consider the slightly trivial case where $Y = X$ and $Z = X$. In this case, $\mathcal{L}_{(X,Y)|Z=z} = \mathcal{L}_{X|Z=z} \otimes \mathcal{L}_{Y|Z=z} = \delta_z \otimes \delta_z$. In particular, if $(z_n)$ is a sequence which converges to $z$ in $\mathbb{R}^d$ (but $z_n \neq z$ for all $n \in \mathbb{N}$), then $(\delta_{z_n} \otimes \delta_{z_n})$ converges to $\delta_z \otimes \delta_z$ in the weak topology as well as in $W_p$ (for every $p \in [1, \infty]$). However, $TV(\delta_{z_n} \otimes \delta_{z_n}, \delta_z \otimes \delta_z) \to 0$, since the total variation distance between any two mutually singular measures is identically 1.

(2) Suppose that $X$ and $Y$ are both random variables in $\mathbb{R}^2$ (equipped with polar coordinates) where the radial variable for $X$ and $Y$ is deterministically coupled. In other words, there is some random variable $Z: \Omega \to \mathbb{R}^+$ where $X = (Z, \Theta_1(Z, \cdot))$ and $Y = (Z, \Theta_2(Z, \cdot))$ where $\Theta_1(r, \cdot)$ and $\Theta_2(r, \cdot)$ are both “random angles”, that is, random variables from $\Omega$ into $[0, 2\pi)$, which may depend on the radial variable $r$. In this case, $X$ and $Y$ may both have full support in $\mathbb{R}^2$; but the conditional distributions $\mathcal{L}_{X|Z=z}$ and $\mathcal{L}_{Y|Z=z}$ are always supported within the sphere of radius $z$, and so $\mathcal{L}_{X|Z=z}$ and $\mathcal{L}_{Y|Z=z}$ are mutually singular for all distinct $z$ and $z'$ (and similarly for $\mathcal{L}_{(X,Y)|Z=z}$). It follows that $z \mapsto \mathcal{L}_{(X,Y)|Z=z}$ and $z \mapsto \mathcal{L}_{X|Z=z}$ and $z \mapsto \mathcal{L}_{Y|Z=z}$ cannot be $TV$-continuous, but may still be $W_p$-continuous if $\Theta_1(r, \cdot)$ and $\Theta_2(r, \cdot)$ vary continuously with $r$ (we demonstrate this immediately below, in Example 5, in the particular case where $\Theta_1(r, \cdot)$ and $\Theta_2(r, \cdot)$ are Lipschitz continuous in $r$).

It is certainly worth asking how $W_p$-Lipschitz type assumptions relate to the candidate functional relations between $X$, $Y$, and $Z$ in the causal inference setting. For instance, if there is no deterministic functional relationship between $X$ and $Y$ but $X = f(Z) + E_1$ and $Y = g(Z) + E_2$ (where $E_1$ and $E_2$ are i.i.d. noise variables), how do the $W_p$-Lipschitz assumptions on the conditional distributions we have just detailed relate to the regularity properties of $f$ and $g$?

Example 5 (Additive noise model; $Z$ causes $X$ and $Y$ but $X \perp \perp Y \mid Z$). Suppose we are given random variables $X, Y,$ and $Z$, and we know that $X = f(Z) + E_1$ and $Y = g(Z) + E_2$, where $E_1$ and $E_2$ are independent and identically distributed noise variables (for instance, $E_1$ and $E_2$ may be (truncated) Gaussians), and $f$ and $g$ are (deterministic) Lipschitz continuous functions. We claim that in this circumstance, all of $z \mapsto \mathcal{L}_{X|Z=z}$, $z \mapsto \mathcal{L}_{Y|Z=z}$, and $z \mapsto \mathcal{L}_{(X,Y)|Z=z}$ are Lipschitz continuous with respect to $W_p$. Note that in this case, if we condition on $Z = z_0$, then $X$ has the
distribution \( f(z_0) + E_1 \) and \( Y \) has the distribution \( g(z_0) + E_2 \). Thus, if both \( f \) and \( g \) are \( L \)-Lipschitz, the distributions of \( X \mid Z = z_0 \) and \( X \mid Z = z_1 \) are identical, modulo a shift by a constant at most \( \varepsilon \), provided that \( |z_0 - z_1| < \varepsilon/L \), and similarly for \( Y \mid Z = z_0 \) and \( Y \mid Z = z_1 \) respectively. Note that since \( L_{X \mid Z = z_0} = f(z_0) + L_{E_1} \), it follows that the shift map \( x \mapsto x + f(z_1) - f(z_0) \) pushes \( L_{X \mid Z = z_0} \) onto \( L_{X \mid Z = z_1} \). Consequently, this shift is an admissible transport map in the optimal transport problem, and it follows that

\[
W_p(L_{X \mid Z = z_0}, L_{X \mid Z = z_1}) \leq \left( \int_{\Omega} |f(z_1) - f(z_0)|^p \, dL_{X \mid Z = z_0} \right)^{1/p}.
\]

But since \( |f(z_1) - f(z_0)| < \varepsilon \), it follows that \( W_p(L_{X \mid Z = z_0}, L_{X \mid Z = z_1}) < \varepsilon \). By an identical argument, it also holds that \( W_p(L_{Y \mid Z = z_0}, L_{Y \mid Z = z_1}) < \varepsilon \). And, of course, in this case, \( X \) and \( Y \) are, in fact conditionally independent given \( Z \), so since \( L_{(X,Y) \mid Z} = L_{X \mid Z} \otimes L_{Y \mid Z} \) we see that an analogous estimate applies to the joint distribution; that is, that since the product shift map

\[
(x, y) \mapsto (x + f(z_1) - f(z_0), y + g(z_1) - g(z_0))
\]
pushes \( L_{X \mid Z = z_0} \otimes L_{Y \mid Z = z_0} \) onto \( L_{X \mid Z = z_1} \otimes L_{Y \mid Z = z_1} \), we have the transport map upper bound

\[
W_p^2(L_{(X,Y) \mid Z = z_0}, L_{(X,Y) \mid Z = z_1}) \leq \int_{\Omega^2} |f(z_1, g(z_1)) - (f(z_0), g(z_0))|^p \, dL_{(X,Y) \mid Z = z_0} \otimes dL_{(X,Y) \mid Z = z_0}
\]

\[
\leq 2^{p-1} \left( \int_{\Omega} |f(z_1) - f(z_0)|^p + |g(z_1) - g(z_0)|^p \, dL_{X \mid Z = z_0} \otimes dL_{Y \mid Z = z_0} \right)
\]

\[
= 2^{p-1} \int_{\Omega} |f(z_1) - f(z_0)|^p \, dL_{X \mid Z = z_0} + 2^{p-1} \int_{\Omega} |g(z_1) - g(z_0)|^p \, dL_{Y \mid Z = z_0}
\]

\[
\leq (2\varepsilon)^p.
\]

**Remark.** On the other hand, if we consider a non-additive noise model, then it is less clear whether there is a clean relationship between the Lipschitz property of \( z \mapsto L_{(X,Y) \mid Z} \) and the functional form of the causal relations between \( X \), \( Y \), and \( Z \).

As promised, the Lipschitz assumption allows us to perform a conditional independence test on \((X,Y,Z)\) using binning. Let us now summarize how this works, before proceeding with a series of technical arguments. The idea is to divide the range of \( Z \) into cells \( V_j \) of diameter at most \( \varepsilon/L \) where \( L \) is some function of \( L_X \), \( L_Y \), and \( L_{XY} \) (here one could use, say, cubes or Voronoi cells), and compute empirical estimates of the conditional distributions \( L_{(X,Y) \mid Z = z} \) and \( L_{X \mid Z = z} \otimes L_{Y \mid Z = z} \). Then, for each cell \( V_j \), we compute the Wasserstein distance between those two empirical distributions; if for each \( V_j \) the distance between the two empirical distributions is small, then we can conclude that with high probability, \( X \) and \( Y \) are conditionally independent given “\( Z \)” discretized onto the cells \( V_j \). A fancier way to say this is that if \( \mathcal{V} \) is the \( \sigma \)-algebra in the sample space generated by the partition \( Z^{-1}\{V_j\} \), we are testing whether \( X \perp \!\!\!\perp Y \mid \mathsf{E}[Z \mid \mathcal{V}] \). Finally, our Lipschitz assumption will allow us to deduce a relationship between our test for \( X \perp \!\!\!\perp Y \mid \mathsf{E}[Z \mid \mathcal{V}] \), and whether \( X \perp \!\!\!\perp Y \mid Z \).

Crucially, we must explicitly control the error introduced by replacing \( Z \) with \( \mathsf{E}[Z \mid \mathcal{V}] \). At the heuristic level, the situation is rather straightforward. Indeed, suppose that our joint and conditional distributions have densities; consider \((x_1, y_1, z_1)\) and \((x_2, y_2, z_2)\), both samples from the joint density \( p(x, y, z) \). Suppose that \( z_1 \) and \( z_2 \) belong to the same cell, and thus \( z_2 \in B_{\varepsilon/L}(z_1) \). We want to pretend that up to some small error, \((x_2, y_2)\) is a sample from \( p(x, y \mid z_1) \) rather than
\[ p(x, y | z_2), \] as is actually the case. If we had an “optimal transport oracle”, we could ask for the optimal transport map \( T \) from \( p(x, y | z_2) \) to \( p(x, y | z_1) \), and then just compute \( T((x_2, y_2)) \); then this would be a sample from \( p(x, y | z_1) \). Instead, we do nothing to \( (x_2, y_2) \), but since \( p(x, y | z_2) \) and \( p(x, y | z_1) \) are close in the Wasserstein sense, we know that \( \| T - \text{id} \| \) is small; this will allow us to say something like

\[
W_p \left( \frac{1}{n} \sum_{i=1}^{n} \delta_{(x_i, y_i) | z_i \in V_j, p(x, y | z_1)} \right) \leq \varepsilon.
\]

Despite this pleasing heuristic motivation, phrased in terms of optimal maps and samples, it turns out to be more direct, from a technical standpoint, to work with optimal plans and population measures, which is how we will proceed in the remainder of the section. Our analysis depends on the following lemma (stated with rather general assumptions, since the proof is no more difficult):

**Lemma 6.** Let \( z \mapsto \mu_z \) be a Borel measurable function from a Polish space \( S \), to \((\mathcal{P}_p(U), W_p)\), where \((U, d)\) is a Polish metric space, and let \( V \subseteq S \) be a Borel set inside \( S \). Let \( \lambda \) be a probability measure on \( V \), and let \( \nu \in W_p(U) \). Then,

\[
W_p^p \left( \int_V \mu_z d\lambda(z), \nu \right) \leq \int_V W_p^p(\mu_z, \nu) d\lambda(z).
\]

In fact, the proof of such a result is more or less indicated by the contents of [Vil08, Ch. 4 & 5]; however, the argument therein omits a number of technical points, so we nonetheless give a rather explicit proof in Appendix A.

We can now easily prove the following:

**Proposition 7.** Suppose that \( z \mapsto L_{(X,Y)|Z=z} \) is \( L_{XY} \)-Lipschitz with respect to \( W_p \). Suppose that \( \{V_j\}_{j=1}^{J} \) is a measurable partition of the support of \( L_Z \), and that \( \text{diam}(V_j) \leq \varepsilon / L_{XY} \) for every bin \( V_j \) in the partition. Then, for all \( z_0 \in V_j \), it holds that

\[
W_p(L_{(X,Y)|Z=z} \mid V_j, \mathcal{L}_{(X,Y)|Z=z_0}) \leq \varepsilon.
\]

**Proof.** In the setting of Lemma 6, let \( V = V_j \), \( U = \mathbb{R}^{d_X} \times \mathbb{R}^{d_Y} \), and

\[
\mu_z = L_{(X,Y)|Z=z} \quad \text{and} \quad \nu = L_{(X,Y)|Z=z_0}.
\]

Furthermore, let \( \lambda = \frac{1}{\mathbb{P}(z \in V_j)} L_Z \mid V_j \). Under the assumptions of the proposition,

\[
W_p^p \left( L_{(X,Y)|Z=z} \mid V_j, L_{(X,Y)|Z=z_0} \right) \leq \varepsilon^p \quad \text{for all } z, z_0 \in V_j.
\]

Since the function \( z \mapsto \mu_z \) is Lipschitz continuous from \( supp(L_Z) \) (which is closed inside \( \mathbb{R}^{d_Z} \), hence a Polish space) to \( (\mathcal{P}_p(\mathbb{R}^{d_X} \times \mathbb{R}^{d_Y}), W_p) \), it is automatically Borel measurable. Lemma 6 then indicates that

\[
W_p^p \left( \int_{V_j} L_{(X,Y)|Z=z} dL_Z(z), L_{(X,Y)|Z=z_0} \right) \leq \int_{V_j} W_p^p \left( L_{(X,Y)|Z=z}, L_{(X,Y)|Z=z_0} \right) dL_Z(z)
\]

\[
\leq \int_{V_j} \varepsilon^p dL_Z(z)
\]

\[
= \varepsilon^p.
\]

Since \( \int_{V_j} L_{(X,Y)|Z=z} dL_Z(z) = L_{(X,Y)|Z\in V_j} \), the proposition is proved. \( \square \)
We also need an analogous proposition, but for the measures $\mathcal{L}_X|Z=z_0 \otimes \mathcal{L}_Y|Z=z_0$ and $\mathcal{L}_X|Z\in V_j \otimes \mathcal{L}_Y|Z\in V_j$.

**Proposition 8.** Suppose that $z \mapsto \mathcal{L}_X|Z=z$ and $z \mapsto \mathcal{L}_Y|Z=z$ are $L_X$- and $L_Y$-Lipschitz (resp.) with respect to $W_p$. Suppose that $\{V_j\}_{j=1}^J$ is a measurable partition of the support of $\mathcal{L}_Z$, and that for all bins $V_j$,

$$\text{diam}(V_j) \leq \frac{\varepsilon}{(2p-1)(L_X^p + L_Y^p))^{1/p}}.$$

Then

$$W_p(\mathcal{L}_X|Z\in V_j \otimes \mathcal{L}_Y|Z\in V_j, \mathcal{L}_X|Z=z_0 \otimes \mathcal{L}_Y|Z=z_0) \leq \varepsilon.$$

**Proof.** The argument is similar to that for the previous proposition, but with a couple of additional complications.

Let $\gamma_X$ be an optimal transport plan between $\mathcal{L}_X|Z\in V_j$ and $\mathcal{L}_X|Z=z_0$, and similarly for $\gamma_Y$. Then, $\gamma_X \otimes \gamma_Y$ is a transport plan between $\mathcal{L}_X|Z\in V_j \otimes \mathcal{L}_Y|Z\in V_j$ and $\mathcal{L}_X|Z=z_0 \otimes \mathcal{L}_Y|Z=z_0$; consequently,

$$W_p(\mathcal{L}_X|Z\in V_j \otimes \mathcal{L}_Y|Z\in V_j, \mathcal{L}_X|Z=z_0 \otimes \mathcal{L}_Y|Z=z_0)$$

$$\leq \int_{(\mathbb{R}^d)^2} \|(x, y) - (x_0, y_0)\|^p d(\gamma_X \otimes \gamma_Y)((x, y), (x_0, y_0))$$

$$= \int_{(\mathbb{R}^d)^2} \int_{(\mathbb{R}^d)^2} \|(x, y) - (x_0, y_0)\|^p d\gamma_X(x, x_0) d\gamma_Y(y, y_0)$$

$$= \int_{(\mathbb{R}^d)^2} \int_{(\mathbb{R}^d)^2} (\sqrt{(x - x_0)^2 + (y - y_0)^2})^p d\gamma_X(x, x_0) d\gamma_Y(y, y_0).$$

Now, since $(x - x_0)^2 + (y - y_0)^2 \leq (x - x_0)^2 + 2|x - x_0||y - y_0| + (y - y_0)^2$, it follows that

$$\sqrt{(x - x_0)^2 + (y - y_0)^2} \leq \sqrt{(|x - x_0| + |y - y_0|)^2}$$

and so

$$\int_{(\mathbb{R}^d)^2} \int_{(\mathbb{R}^d)^2} (\sqrt{(x - x_0)^2 + (y - y_0)^2})^p d\gamma_X d\gamma_Y \leq \int_{(\mathbb{R}^d)^2} \int_{(\mathbb{R}^d)^2} (|x - x_0| + |y - y_0|)^p d\gamma_X d\gamma_Y.$$

In turn, $(|x - x_0| + |y - y_0|)^p \leq 2^{p-1} (|x - x_0|^p + |y - y_0|^p)$, so

$$\int_{(\mathbb{R}^d)^2} \int_{(\mathbb{R}^d)^2} (|x - x_0| + |y - y_0|)^p d\gamma_X d\gamma_Y \leq \int_{(\mathbb{R}^d)^2} \int_{(\mathbb{R}^d)^2} 2^{p-1} (|x - x_0|^p + |y - y_0|^p) d\gamma_X d\gamma_Y$$

$$= 2^{p-1} \left( \int_{(\mathbb{R}^d)^2} |x - x_0|^p d\gamma_X + \int_{(\mathbb{R}^d)^2} |y - y_0|^p d\gamma_Y \right)$$

$$= 2^{p-1} \left( W_p^p(\mathcal{L}_X|Z\in V_j, \mathcal{L}_X|Z=z_0) + W_p^p(\mathcal{L}_Y|Z\in V_j, \mathcal{L}_Y|Z=z_0) \right).$$

Since both $z \mapsto \mathcal{L}_X|Z=z$ and $z \mapsto \mathcal{L}_Y|Z=z$ are Lipschitz continuous (with respective Lipschitz constants $L_X$ and $L_Y$), we know that for $z, z_0 \in V_j$,

$$W_p(\mathcal{L}_X|Z=z, \mathcal{L}_X|Z=z_0) \leq L_X|z - z_0| \leq \frac{L_X}{2^{p-1}(L_X^p + L_Y^p))^{1/p}} \varepsilon$$

and likewise

$$W_p(\mathcal{L}_Y|Z=z, \mathcal{L}_Y|Z=z_0) \leq L_Y|z - z_0| \leq \frac{L_Y}{2^{p-1}(L_X^p + L_Y^p))^{1/p}} \varepsilon.$$
Therefore, we can invoke Lemma 6 with \( \mu_z = \mathcal{L}_{X \mid Z = z} \), \( \nu = \mathcal{L}_{X \mid Z = z_0} \), and conclude, as in the proof of the previous proposition, that

\[
W_p^p \left( \mathcal{L}_{X \mid Z \in V_j}, \mathcal{L}_{X \mid Z = z_0} \right) \leq \int_{V_j} W_p^p \left( \mathcal{L}_{X \mid Z = z}, \mathcal{L}_{X \mid Z = z_0} \right) d\mathcal{L}_Z(z) = \left( \frac{L_X}{\left(2^{p-1} (L_X^p + L_Y^p)\right)^{1/p}} \right)^p
\]

and, by identical reasoning,

\[
W_p^p \left( \mathcal{L}_{Y \mid Z \in V_j}, \mathcal{L}_{Y \mid Z = z_0} \right) \leq \left( \frac{L_Y}{\left(2^{p-1} (L_X^p + L_Y^p)\right)^{1/p}} \right)^p.
\]

Therefore,

\[
W_p^p \left( \mathcal{L}_{X \mid Z \in V_j} \otimes \mathcal{L}_{Y \mid Z \in V_j}, \mathcal{L}_{X \mid Z = z_0} \otimes \mathcal{L}_{Y \mid Z = z_0} \right) \leq 2^{p-1} \left( \frac{L_X}{\left(2^{p-1} (L_X^p + L_Y^p)\right)^{1/p}} \right)^p + 2^{p-1} \left( \frac{L_Y}{\left(2^{p-1} (L_X^p + L_Y^p)\right)^{1/p}} \right)^p = \varepsilon^p
\]
as desired. \( \square \)

**Remark.** Using essentially the same computation as in the proof above, one can show that if \( z \mapsto \mathcal{L}_{X \mid Z = z} \) and \( z \mapsto \mathcal{L}_{Y \mid Z = z} \) are \( L_X \)- and \( L_Y \)-Lipschitz (resp.) with respect to \( W_p \), then \( z \mapsto \mathcal{L}_{X \mid Z = z} \otimes \mathcal{L}_{Y \mid Z = z} \) is Lipschitz with constant \( \left(2^{p-1} (L_X^p + L_Y^p)\right)^{1/p} \). Of course, under the null hypothesis, \( \mathcal{L}_{X \mid Z = z} \otimes \mathcal{L}_{Y \mid Z = z} = \mathcal{L}_{(X,Y) \mid Z = z} \) for all \( z \), so in particular it must be the case that \( \left(2^{p-1} (L_X^p + L_Y^p)\right)^{1/p} = L_{XY} \). Under the alternative, however, there is no *a priori* relationship between \( L_X \), \( L_Y \), and \( L_{XY} \).

**Corollary 9.** Suppose that \( z \mapsto \mathcal{L}_{(X,Y) \mid Z = z} \) be \( L_{XY} \)-Lipschitz with respect to \( W_p \), and that \( z \mapsto \mathcal{L}_{X \mid Z = z} \) and \( z \mapsto \mathcal{L}_{Y \mid Z = z} \) are \( L_X \)- and \( L_Y \)-Lipschitz (resp.) with respect to \( W_p \). Suppose that \( \{V_j\}_{j=1}^J \) is a measurable partition of the support of \( \mathcal{L}_Z \), and that for every bin \( V_j \),

\[
\text{diam}(V_j) \leq \frac{\varepsilon}{4 \max \left\{ L_{XY}, \left(2^{p-1} (L_X^p + L_Y^p)\right)^{1/p} \right\}}.
\]

Then,

\[
\left| W_p \left( \mathcal{L}_{(X,Y) \mid Z = z_0}, \mathcal{L}_{X \mid Z = z_0} \otimes \mathcal{L}_{Y \mid Z = z_0} \right) - W_p \left( \mathcal{L}_{(X,Y) \mid Z \in V_j}, \mathcal{L}_{X \mid Z \in V_j} \otimes \mathcal{L}_{Y \mid Z \in V_j} \right) \right| \leq \frac{\varepsilon}{2}.
\]

**Proof.** This follows directly from Propositions 7 and 8, together with the triangle inequality. \( \square \)

The significance of this corollary is the following. If, for every bin \( V_j \), we perform a \( W_p \) two-sample test on the measures \( \mathcal{L}_{(X,Y) \mid Z \in V_j} \) and \( \mathcal{L}_{X \mid Z \in V_j} \otimes \mathcal{L}_{Y \mid Z \in V_j} \); then (under our running assumptions) this amounts to a \( W_p \) two-sample test on the measures \( \mathcal{L}_{(X,Y) \mid Z = z_0} \) and \( \mathcal{L}_{X \mid Z = z_0} \otimes \mathcal{L}_{Y \mid Z = z_0} \), for every \( z_0 \in V_j \). Consequently, under our assumptions, “\( W_p \) conditional independence testing” is reducible to a large, but finite, number of \( W_p \) two-sample tests.
To put this more formally, we now state a “metatheorem”, indicating how to aggregate Wasserstein two-sample tests on the bins $V_j$, with given Type I and Type II error, into a conditional independence test.

**Theorem 10.** Let $X: \Omega \to \mathbb{R}^d_X$, $Y: \Omega \to \mathbb{R}^d_Y$, and $Z: \Omega \to \mathbb{R}^d_Z$ be random variables. Suppose that $z \mapsto \mathcal{L}_{(X,Y)|Z=z}$ is $L_{XY}$-Lipschitz with respect to $W_p$, and that $z \mapsto \mathcal{L}_{X|Z=z}$ and $z \mapsto \mathcal{L}_{Y|Z=z}$ are $L_X$- and $L_Y$-Lipschitz (resp.) with respect to $W_p$. Suppose the bins $\{V_j\}_{j=1}^J$ form a measurable partition of the support of $\mathcal{L}_Z$, and that for every bin $V_j$,

$$diam(V_j) \leq \frac{\varepsilon}{4 \max\{L_{XY}, (2p^{-1}(L_X^p + L_Y^p))^{1/p}\}}.$$

Let $W_p(\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j})$ denote the plug-in estimator for $W_p(\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j})$, and let $n_j$ denote the number of data points drawn from each of $\mathcal{L}_{(X,Y)|Z \in V_j}$ and $\mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}$. Then:

1. **(Control of Type I error)** Suppose that for a given $j \in \{1, \ldots, J\}$, $n_j$ is sufficiently large that for $p_j: \mathbb{N} \to [0, 1]$,

$$\mathbb{P}\left(W_p(\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}) \geq W_p(\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}) + \frac{\varepsilon}{2}\right) \leq p_j(n_j)$$

Then for all $z \in V_j$,

$$\mathbb{P}\left(W_p(\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}) \geq W_p(\mathcal{L}_{(X,Y)|Z \in z}, \mathcal{L}_{X|Z \in z} \otimes \mathcal{L}_{Y|Z \in z}) + \varepsilon\right) \leq p_j(n_j)$$

and under the null hypothesis that for all $z$ in the support of $\mathcal{L}_Z$, $W_p(\mathcal{L}_{(X,Y)|Z \in z}, \mathcal{L}_{X|Z \in z} \otimes \mathcal{L}_{Y|Z \in z}) = 0$, it holds that

$$\mathbb{P}\left(\exists j \in \{1, \ldots, J\}, W_p(\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}) \geq \varepsilon\right) \leq \sum_{j=1}^J p_j(n_j).$$

2. **(Control of Type II error)** Suppose that for a given $j \in \{1, \ldots, J\}$, $n_j$ is sufficiently large that for $\varepsilon, \delta_j > 0$ and $\alpha_j: \mathbb{R}_+ \to [0, 1]$,

$$\mathbb{P}\left(W_p(\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}) < W_p(\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}) - \delta_j + \frac{\varepsilon}{2}\right) \leq \alpha_j\left(\delta_j - \frac{\varepsilon}{2}, n_j\right).$$

Then for all $z \in V_j$,

$$\mathbb{P}\left(W_p(\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}) < W_p(\mathcal{L}_{(X,Y)|Z \in z}, \mathcal{L}_{X|Z \in z} \otimes \mathcal{L}_{Y|Z \in z}) - \delta_j + \varepsilon\right) \leq \alpha_j\left(\delta_j - \frac{\varepsilon}{2}, n_j\right)$$

and under the alternative hypothesis that for every $j \in \{1, \ldots, J\}$, there exists a $z \in V_j$ such that $W_p(\mathcal{L}_{(X,Y)|Z \in z}, \mathcal{L}_{X|Z \in z} \otimes \mathcal{L}_{Y|Z \in z}) \geq \delta_j + \varepsilon$, it holds that

$$\mathbb{P}\left(\forall j \in \{1, \ldots, J\}, W_p(\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}) < \varepsilon\right) \leq \prod_{j=1}^J \alpha_j\left(\delta_j - \frac{\varepsilon}{2}, n_j\right).$$
Proof. (1) This is immediate from Corollary 9, together with a Bonferroni correction.

(2) This is also an immediate consequence of Corollary 9, together with the fact that the bins $V_j$ are disjoint, and hence the events

$$W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) < W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) - \delta_j + \frac{\varepsilon}{2},$$

for $j \in \{1, \ldots, J\}$, are independent. Explicitly, independence implies that

$$\mathbb{P} \left( \forall j \leq J, W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) < W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) - \delta_j + \frac{\varepsilon}{2} \right)$$

$$= \prod_{j=1}^J \mathbb{P} \left( W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) < W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) - \delta_j + \frac{\varepsilon}{2} \right)$$

$$\leq \prod_{j=1}^J \alpha_j \left( \delta_j - \frac{\varepsilon}{2}, \eta_j \right)$$

and, under the stipulated alternative, namely $W_p \left( \mathcal{L}_{(X,Y)|Z = z}, \mathcal{L}_{X|Z = z} \otimes \mathcal{L}_{Y|Z = z} \right) \geq \delta_j + \varepsilon$ for some $z \in V_j$, we have by Corollary 9 that $W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) \geq \delta_j + \frac{\varepsilon}{2}$, and hence

$$\mathbb{P} \left( \forall j \leq J, W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) < \varepsilon \right)$$

$$\leq \mathbb{P} \left( \forall j \leq J, W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) < W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) - \delta_j + \frac{\varepsilon}{2} \right).$$

Hence

$$\mathbb{P} \left( \forall j \in \{1, \ldots, J\}, W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) < \varepsilon \right) \leq \prod_{j=1}^J \alpha_j \left( \delta_j - \frac{\varepsilon}{2}, \eta_j \right)$$

as desired. \qed

Remark. Note that $J$, the number of bins partitioning $\text{supp}(\mathcal{L}_Z)$, is on the order of the $\varepsilon/(4 \max\{L_{XY}, (2^{p-1}(L_X^p + L_Y^p))^{1/p}\})$-covering number of $\text{supp}(\mathcal{L}_Z)$, and so if $\text{supp}(\mathcal{L}_Z)$ is geometrically “simple” (i.e. has small isoperimetric ratio compared to a $d_Z$-ball), then $J$ is on the order of

$$\left(8 \cdot \text{diam}(\text{supp}(\mathcal{L}_Z)) \max \left\{ L_{XY}, (2^{p-1}(L_X^p + L_Y^p))^{1/p} \right\} \sqrt{d}/\varepsilon \right)^d.$$
Indeed, recall the expectation bound from Theorem 3, namely, that for \( d \geq 3 \), if \( p \in [1, d/2) \) and \( q > dp/(d - p) \), then there exists a constant \( \kappa_{p,q,d} \) depending only on \( p, q, \) and \( d \), such that

\[
\mathbb{E}[W_p^p(\mu, \mu_n)]^{1/p} \leq \kappa_{p,q,d} \left( \int_{\mathbb{R}^d} ||x||^q d\mu(x) \right)^{1/q} n^{-1/d}.
\]

So suppose that there is some uniform \( M_{XY} \) such that

\[
\left( \int_{\mathbb{R}^d} \|(x, y)||^q d\mu(x, y) \right)^{1/q} \leq M_{XY}
\]

whenever \( \mu = L(X,Y)|_{Z=z} \) and \( z \in \text{supp}(L_Z) \). We claim that the same moment bound then holds for \( L(X,Y)|_{Z \in V_j} \), also, at least provided that \( z \mapsto L(X,Y)|_{Z=z} \) is continuous w.r.t. \( W_q \) (in addition to being \( L_{XY} \)-Lipschitz w.r.t. \( W_p \); since convergence in \( W_q \) is equivalent to weak convergence plus convergence of \( q \)th moments, it suffices, for instance, to assume yet another uniform moment bound, for any \( q' > q \); see [Bil95, Corollary following Theorem 25.12]). Indeed,

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \|(x, y)||^q d\mu(x, y) = W_q^q(\mu, \delta_0)
\]

and so, by Lemma 6,

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \|(x, y)||^q d\mu(x, y) = W_q^q(L(X,Y)|_{Z \in V_j}, \delta_0)
\]

\[
\leq \int_{V_j} W_q^q(L(X,Y)|_{Z=z}, \delta_0) dL_Z(z)
\]

\[
\leq \int_{V_j} M_{XY}^q dL_Z(z)
\]

\[
= M_{XY}^q.
\]

Likewise, it is obvious that if, for all \( z \in \text{supp}L_Z \), \( L(X,Y)|_{Z=z} \) is supported inside some ball \( B(0, D) \), then the same is true for each \( L(X,Y)|_{Z \in V_j} \). And identical reasoning applies to both \( L_X|_{Z=z} \) and \( L_Y|_{Z=z} \). Finally, observe that

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \|(x, y)||^q d\mathcal{L}_X|_{Z \in V_j} \otimes \mathcal{L}_Y|_{Z \in V_j}(x, y) \leq 2^{q-1} \left( \int_{\mathbb{R}^d} ||x||^q d\mathcal{L}_X|_{Z \in V_j}(x) \right) + \int_{\mathbb{R}^d} ||y||^q d\mathcal{L}_Y|_{Z \in V_j}(y)
\]

so, if \( L_X|_{Z \in V_j} \) has \( q \)th moment bound \( M_X \) and \( L_Y|_{Z \in V_j} \) has \( q \)th moment bound \( M_Y \), it follows that \( L_X|_{Z \in V_j} \otimes L_Y|_{Z \in V_j} \) has \( q \)th moment bound \( (2^{q-1} (M_X^q + M_Y^q))^{1/q} \).

Thus, if we assume that \( z \mapsto L(X,Y)|_{Z=z} \) and \( z \mapsto L_X|_{Z=z} \) and \( z \mapsto L_Y|_{Z=z} \) are:

1. \( L_{XY} \)-, \( L_X \)-, and \( L_Y \)-Lipschitz with respect to \( W_p \) for some \( p \in [1, \infty) \),
2. continuous with respect to \( W_q \) for some \( q > dp/(d - p) \), where \( d = \min\{3, d_X + d_Y\} \), and
3. have \( q \)th moments uniformly bounded by \( M_{XY} \) and \( M_X \) and \( M_Y \) respectively, and
4. have bounded support\(^1\) with radius \( D \),

Then we can use both the expectation bound stated in Theorem 3, as well as the concentration inequality stated in Proposition 2, in the case of the empirical measures of \( L(X,Y)|_{Z \in V_j} \) and \( L_X|_{Z \in V_j} \otimes L_Y|_{Z \in V_j} \).

\(^1\) Note: this implies automatically that (3) holds, but we run the analysis with \( M_X, M_Y, M_{XY} \) given more generally, in case one has access to tighter moment bounds than those implied automatically from the diameter of the support.
Indeed, we saw in the previous section that under the null hypothesis, if \( \mu_n \) and \( \mu'_n \) are both samples from the same measure \( \mu \), and \( n \) is sufficiently large that 
\[
\left( k_{p,q,d} \left[ \int_{\mathbb{R}^d} \|x\|^q d\mu(x) \right]^{1/q} n^{-1/d} \right)^p \leq \left( \frac{1}{2} \left( \frac{\epsilon}{4} \right)^p \right),
\]
then combining the expectation bound from Theorem 3 and the concentration inequality from Proposition 2 results in the estimate
\[
\mathbb{P} \left[ W_p(\mu_n, \mu'_n) \geq \frac{\epsilon}{2} \right] \leq \mathbb{P} \left[ W_p(\mu_n, \mu) \geq \frac{\epsilon}{4} \right] + \mathbb{P} \left[ W_p(\mu'_n, \mu) \geq \frac{\epsilon}{4} \right] 
\leq 2 \exp \left( -\frac{2n^{2p}}{4^{2p+1}D^{2p}} \right).
\]
So, by the preceding theorem, it holds under the null that if for all \( j \in \{1, \ldots, J\} \), \( n_j \) is sufficiently large that (again \( d = \min\{3, dx + dy\} \))
\[
\left( k_{p,q,d} \left[ \int_{\mathbb{R}^d \times \mathbb{R}^d} \| (x,y) \|^q d\mathcal{L}_{(X,Y)|Z \in V_j} (x,y) \right]^{1/q} n_j^{-1/d} \right)^p \leq \left( k_{p,q,d} M_{XY} n_j^{-1/d} \right)^p \leq \left( \frac{1}{2} \left( \frac{\epsilon}{4} \right)^p \right),
\]
it holds that
\[
\mathbb{P} \left[ \exists j \in \{1, \ldots, J\} \right] W_p(\overline{\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}}) \geq \epsilon \leq \sum_{j=1}^J 2 \exp \left( -\frac{2n_j^{2p}}{4^{2p+1}D^{2p}} \right)
\]
which is precisely a bound on the Type I error.

Let us now turn to the Type II error. As discussed in the previous section, we reason as follows. Our alternative hypothesis is that for each \( j \in \{1, \ldots, J\} \), there exists a \( z \in V_j \) such that \( W_p(\overline{\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}}) \geq \delta_j + \epsilon \); hence \( W_p(\overline{\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}}) \geq \delta_j + \frac{\epsilon}{2} \).

If \( W_p(\overline{\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}}) \geq \frac{\delta_j}{2} - \frac{\epsilon}{4} \) or \( W_p(\overline{\mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}}) \geq \frac{\delta_j}{2} - \frac{\epsilon}{4} \)
then it must be the case that
\[
W_p(\overline{\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}}) \geq \frac{\delta_j}{2} + \frac{\epsilon}{2}
\]
In the first case, using \( t = \frac{1}{2} \left( \frac{\delta_j - \frac{\epsilon}{2}}{4} \right)^p \) in Proposition 2, we see that
\[
\mathbb{P} \left[ W_p(\overline{\mathcal{L}_{(X,Y)|Z \in V_j}, \mathcal{L}_{X,Y)|Z \in V_j}}) \geq \frac{\delta_j}{2} - \frac{\epsilon}{4} \right] \leq \exp \left( -\frac{2n_j (\delta_j - \frac{\epsilon}{2})^{2p}}{4^{2p+1}D^{2p}} \right)
\]
provided that \( n_j \) is sufficiently large that
\[
\left( k_{p,q,d} \left[ \int_{\mathbb{R}^d \times \mathbb{R}^d} \| (x,y) \|^q d\mathcal{L}_{(X,Y)|Z \in V_j} (x,y) \right]^{1/q} n^{-1/d} \right)^p \leq \left( \frac{1}{2} \left( \frac{\delta_j - \frac{\epsilon}{2}}{4} \right)^p \right).
\]
or, in terms of the moment bound \( M_{XY} \), that
\[
\left( k_{p,q,d} M_{XY} n^{-1/d} \right)^p \leq \left( \frac{1}{2} \left( \frac{\delta_j - \frac{\epsilon}{2}}{4} \right)^p \right).
\]
In the second case, similarly,
\[
\mathbb{P} \left[ W_p(\overline{\mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}, \mathcal{L}_{X|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j}}) \geq \frac{\delta_j}{2} - \frac{\epsilon}{4} \right] \leq \exp \left( -\frac{2n_j (\delta_j - \frac{\epsilon}{2})^{2p}}{4^{2p+1}D^{2p}} \right)
\]
provided that $n_j$ is sufficiently large that
\[
\left( \kappa_{p,q,d} \left[ \int_{\mathbb{R}^d \times \mathbb{R}^d} \| (x, y) \|_2^q d \mathcal{L}_X|_{Z \in V_j} \otimes \mathcal{L}_Y|_{Z \in V_j} (x, y) \right] \right)^{1/q} n^{-1/d} \leq \frac{1}{2} \left( \frac{\delta_j - \frac{\epsilon}{2}}{4} \right)^p
\]
or, in terms of our moment bound, that
\[
\left( \kappa_{p,q,d} \left( 2^{q-1}(M_X^q + M_Y^q) \right)^{1/q} n^{-1/d} \right)^p \leq \frac{1}{2} \left( \frac{\delta_j - \frac{\epsilon}{2}}{4} \right)^p.
\]
Therefore,
\[
P \left[ W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) \leq W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) - \delta_j + \frac{\epsilon}{2} \right] 
\leq 2 \exp \left( -\frac{2n_j \left( \delta_j - \frac{\epsilon}{2} \right)^{2p}}{4^{2p+1} D^{2p}} \right)
\]
provided that $n_j$ is sufficiently large that (again, $d = \min\{3, d_X + d_Y\}$)
\[
\left( \max \left\{ M_{XY}, (2^{q-1}(M_X^q + M_Y^q))^{1/q} \right\} \right)^p \kappa_{p,q,d} n^{-1/d} \leq \frac{1}{2} \left( \frac{\delta_j - \frac{\epsilon}{2}}{4} \right)^p.
\]
Combining these estimates across bins, we conclude that
\[
P \left( \forall j \in \{1, \ldots, J\}, W_p \left( \mathcal{L}_{(X,Y)|Z \in V_j} \otimes \mathcal{L}_{Y|Z \in V_j} \right) < \epsilon \right) \leq \prod_{j=1}^J 2 \exp \left( -\frac{2n_j \left( \delta_j - \frac{\epsilon}{2} \right)^{2p}}{4^{2p+1} D^{2p}} \right)
\]
provided that for all $j \in \{1, \ldots, J\}$,
\[
\left( \max \left\{ M_{XY}, (2^{q-1}(M_X^q + M_Y^q))^{1/q} \right\} \right)^p \kappa_{p,q,d} n^{-1/d} \leq \frac{1}{2} \left( \frac{\delta_j - \frac{\epsilon}{2}}{4} \right)^p.
\]

Remark. Using the concentration inequality from Proposition 13, it is also possible to extend the analysis from the previous example to the case where $\mathcal{L}_X$ and $\mathcal{L}_Y$ have unbounded support (but still satisfy a higher moment bound).

3. Plug-in estimation of the Lipschitz constant

We have seen that the role played by the Lipschitz constants $L_X$, $L_Y$, and $L_{XY}$ is that they specify a bin size which is sufficient to introduce only a small discretization error. In specific applications, there may well be domain knowledge that allows us to upper bound the $L$’s in an a priori fashion; however, testing whether a function (with continuous domain) is Lipschitz, or testing for $L$ given the fact that the function is Lipschitz with some constant, is not possible in general, at least if one requires any sort of finite-sample guarantees. (To see why this is the case, it suffices to consider some standard pathological function from real analysis, such as the Weierstrass function.)

Remark. In a situation similar to the one from Example 5 above, some a priori/expert knowledge about $L$ may come from the functional form of a causal model under investigation, e.g. if one considers an additive noise model as we did there. Additionally, it may be possible to deduce a upper bound on $L$ analytically, for instance if the conditional distributions are known to satisfy a suitable functional inequality (e.g. of Poincaré or log-Sobolev type) — for such a result, we refer the reader to [DM, Theorem 2.1].
However, it is still of interest to provide a consistent estimator of \( L \), should no guess based on domain knowledge be available.

To that end, we note that it is possible to compute the Lipschitz constant (w.r.t. the \( W_p \) metric) of the discrete function

\[
V_j \mapsto \hat{L}_{(X,Y)|Z \in V_j} := \frac{1}{|\{i : z_i \in V_j\}|} \sum_{i : z_i \in V_j} \delta_{(z_i,y_i)}
\]

which, given a bin, returns the empirical conditional distribution for that bin. Briefly, this is because the space of bins \( V_j \) can be viewed as a discrete space, and in such a setting one can simply compute the Lipschitz constant by brute force. (Note, however, that there is work on efficient estimation of Lipschitz constants for discrete functions, for instance [AJMR16].)

Therefore, we propose using the “plug-in estimator” \( \hat{L}_{XY} \) for the Lipschitz constant \( L_{XY} \), namely

\[
\hat{L}_{XY} := Lip \left( V_j \mapsto \hat{L}_{(X,Y)|Z \in V_j} \right)
\]

where \( \hat{L}_{(X,Y)|Z \in V_j} \) resides in a Wasserstein space \( W_{p}(\mathbb{R}^{d_X+d_Y}) \), and the distance between two bins \( V_j \) and \( V_{j'} \) (which we denote by \( dist(V_j,V_{j'}) \)) is given by the Euclidean distance between their centroids. In exactly the same fashion, we also define the plug-in estimators \( \hat{L}_X \) and \( \hat{L}_Y \) for \( L_X \) and \( L_Y \), respectively, by

\[
\hat{L}_X := Lip \left( V_j \mapsto \hat{L}_{X|Z \in V_j} \right); \quad \hat{L}_Y := Lip \left( V_j \mapsto \hat{L}_{Y|Z \in V_j} \right).
\]

We now claim the following result, which requires that geometry of the bins is in some sense “uniform”, and the number of samples per bin grows fast enough as the size of the bins goes to zero. (We remark however that our assumptions allow for bins which are non-convex or even disconnected.)

**Proposition 12.** Suppose that the joint distribution \( \mathcal{L}_{(X,Y,Z)} \) is compactly supported inside \( \mathbb{R}^{d_X+d_Y+d_Z} \), and that \( z \mapsto \mathcal{L}_{(X,Y)|Z=z} \) is \( L_{XY} \)-Lipschitz, and that we have drawn \( n \) i.i.d. samples from \( \mathcal{L}_{(X,Y,Z)} \). Suppose we have a set of bins \( \{V_j\}_{j=1}^J \) whose “scale” depends on a parameter \( \varepsilon > 0 \) in a sense which we specify below. Fix the following assumptions:

1. For all \( j \in \{1, \ldots, J\} \), \( \text{diam}(V_j) \leq \varepsilon / L_{XY} \).
2. For all \( j \in \{1, \ldots, J\} \), \( c_{Vol} \leq \frac{\max_{j \in \{1, \ldots, J\}} Vol(V_j)}{\min_{j \in \{1, \ldots, J\}} Vol(V_j)} \leq C_{Vol} \), where again \( c_{Vol} \) and \( C_{Vol} \) are independent of \( \varepsilon \).
3. Let \( n_{\min} \) denote the least number of samples from \( \mathcal{L}_{(X,Y,Z)} \) belonging to the same bin \( V_j \) (out of all \( j \in \{1, \ldots, J\} \)). Assume that as \( \varepsilon \to 0 \), \( \varepsilon^{2d} \exp \left( -\frac{n_{\min} \varepsilon^2}{D^2} \right) \to 0 \), where \( D \) is the diameter of the support of \( \mathcal{L}_{(X,Y)} \); and,
4. For some \( q > p \), assume \( \kappa_{q,p,d} M_q^{1/q} n_{\min}^{-1/d} \leq \varepsilon \), where \( M_q \) is a uniform \( q \)th moment bound on \( \mathcal{L}_{(X,Y)|Z=z} \), \( d = \min\{3, d_X + d_Y\} \), and \( \kappa_{q,p,d} \) is the constant from Theorem 3.

Then, \( \hat{L}_{XY} \) is a consistent estimator, in the following sense: with probability approaching 1 as \( \varepsilon \to 0 \), it holds both that for all \( j, j' \in \{1, \ldots, J\} \),

\[
W_p(\hat{L}_{(X,Y)|Z \in V_j}, \hat{L}_{(X,Y)|Z \in V_{j'}}) \leq L_{XY} \cdot dist(V_j,V_{j'}) + \left( 2 + 2^{1+1/p} \right) \varepsilon.
\]
and for all \( z, z' \in \text{supp}(\mathcal{L}_Z) \),

\[
W_p(\mathcal{L}(X,Y)|Z=z, \mathcal{L}(X,Y)|Z=z') \leq \hat{L}_{XY}|z-z'| + \left(2 + 2^{1+1/p} + 2\frac{\hat{L}_{XY}}{L_{XY}}\right)\varepsilon.
\]

The same holds true for \( \hat{L}_X \) and \( \hat{L}_Y \).

Remark. This proposition establishes that the plug-in estimator for the Lipschitz constant is accurate with high probability, provided that we restrict ourselves to considering points \( z, z' \) (resp. bins \( V_j, V_{j'} \)) which are a macroscopic distance apart as compared to the length scale parameter \( \varepsilon \). This type of restriction on the result is necessary, as binning the \( Z \) variable can, \textit{a priori}, smooth out oscillations at small length scales.

Proof. The proof is identical for all three estimators; we therefore proceed only for the estimator \( \hat{L}_{XY} \).

Let \( \varepsilon > 0 \). Let \( \{V_j\}_{j=1}^J \) be a measurable partition of \( \text{supp}(\mathcal{L}_Z) \), which we take to depend on \( \varepsilon \), such that for all \( j \in \{1, \ldots, J\} \), \( \text{diam}(V_j) \leq \varepsilon/L_{XY} \). Furthermore, we require that there exist constants \( c \) and \( C \) which are independent of \( \varepsilon \), such that

\[
c \leq \frac{\max_{j \in \{1, \ldots, J\}} \text{Vol}(V_j)}{\min_{j \in \{1, \ldots, J\}} \text{Vol}(V_j)} \leq C.
\]

Given \( n \) samples from the joint distribution \( \mathcal{L}_{(X,Y,Z)} \), we let \( n_j \) denote the number of samples for which \( Z \in V_j \). Likewise we write \( n_{\text{min}} = \min_{j \in \{1, \ldots, J\}} n_j \). We note that as \( \varepsilon \to 0 \), \( J \to \infty \); likewise, the \( n_j \)'s (and hence \( n_{\text{min}} \)) increase at a rate that depends on \( \varepsilon \).

Previously, in Proposition 7, we have seen that if \( \text{diam}(V_j) \leq \varepsilon/L_{XY} \), then

\[
W_p(\mathcal{L}(X,Y)|Z \in V_j, \mathcal{L}(X,Y)|Z=z_0) \leq \varepsilon.
\]

At the same time, for \( n_j \) sufficiently large, we have that \( \mathcal{L}(X,Y)|Z \in V_j \approx_{W_p} \mathcal{L}(X,Y)|Z \in V_j \), with probability going to 1 as \( n_j \) goes to \( \infty \), where \( n_j \) is the number of samples in the \( j \)th bin \( V_j \).

Therefore, we proceed as follows. Pick \( z_0 \) and \( z'_0 \) such that \( z_0 \in V_j \) and \( z'_0 \in V_{j'} \). We know that

\[
W_p(\mathcal{L}(X,Y)|Z=z_0, \mathcal{L}(X,Y)|Z=z'_0) \leq L_{XY}|z_0-z'_0|.
\]

At the same time, by the triangle inequality and Proposition 7, we have (still with \( z_0 \in V_j \) and \( z'_0 \in V_{j'} \)) that

\[
W_p(\mathcal{L}(X,Y)|Z \in V_j, \mathcal{L}(X,Y)|Z \in V_{j'}) \leq W_p(\mathcal{L}(X,Y)|Z=z_0, \mathcal{L}(X,Y)|Z=z'_0) + 2\varepsilon.
\]

Hence in particular,

\[
W_p(\mathcal{L}(X,Y)|Z \in V_j, \mathcal{L}(X,Y)|Z \in V_{j'}) \leq L_{XY}|z_0-z'_0| + 2\varepsilon.
\]

Using the triangle inequality again, and the fact that \( \mathcal{L}(X,Y)|Z \in V_j \approx_{W_p} \mathcal{L}(X,Y)|Z \in V_j \) and \( \mathcal{L}(X,Y)|Z \in V_{j'} \approx_{W_p} \mathcal{L}(X,Y)|Z \in V_{j'} \) for \( n_j, n_{j'} \) very large (with probability approaching 1 as \( n_j, n_{j'} \to \infty \)), we have that (also with probability approaching 1 as \( n_j, n_{j'} \to \infty \))

\[
W_p(\mathcal{L}(X,Y)|Z \in V_j, \mathcal{L}(X,Y)|Z \in V_{j'}) \lesssim L_{XY}|z_0-z'_0| + 2\varepsilon.
\]
some uniform constant $C$ volume within a fixed constant multiple of each other (that is, independent of $\epsilon$).

We therefore require that

$$\Pr\left[W_p\left(L_{(X,Y)}|Z \in V_j, L_{(X,Y)}|Z \in V_j\right) \geq \mathbb{E}W_p\left(L_{(X,Y)}|Z \in V_j, L_{(X,Y)}|Z \in V_j\right) + \epsilon\right] \leq \exp\left(-\frac{n_j \epsilon^2}{D^{2p}}\right)$$

where $D$ is the diameter of the support of $L(X,Y)$. Note that using the inequality $2^{1-p}(x+y)^p \leq x^p + y^p$, and Jensen’s inequality applied to the expectation, this implies

$$\Pr\left[W_p\left(L_{(X,Y)}|Z \in V_j, L_{(X,Y)}|Z \in V_j\right) \geq 2^{(1-p)/p}\mathbb{E}W_p\left(L_{(X,Y)}|Z \in V_j, L_{(X,Y)}|Z \in V_j\right) + \epsilon\right] \leq \exp\left(-\frac{n_j \epsilon^2}{D^{2p}}\right).$$

This shows that if $\mathbb{E}W_p\left(L_{(X,Y)}|Z \in V_j, L_{(X,Y)}|Z \in V_j\right) \leq \epsilon$ (which holds provided that $\kappa_{q,p,d} M_q^{1/q} n_j^{-1/d} \leq \epsilon$, as per Theorem 3) then we have

$$\Pr\left[W_p\left(L_{(X,Y)}|Z \in V_j, L_{(X,Y)}|Z \in V_j\right) \geq 2^{1/p}\epsilon\right] \leq \exp\left(-\frac{n_j \epsilon^2}{D^{2p}}\right).$$

Then, from the triangle inequality,

$$W_p\left(L_{(X,Y)}|Z \in V_j, L_{(X,Y)}|Z \in V_j\right) \leq L_{XY}|z_0 - z_0'| + (2 + 2^{1+1/p})\epsilon$$

with probability at least $1 - \exp\left(-\frac{n_j \epsilon^2}{D^{2p}}\right) - \exp\left(-\frac{\kappa \epsilon^2}{D^{2p}}\right)$.

Now, this analysis holds for any $z_0$ and $z_0'$; in particular we may take $z_0$ and $z_0'$ to be the centroids of $V_j$ and $V_j'$ (although note this may require us to take a smaller $\epsilon$). In this case, the “distance” between $V_j$ and $V_j'$ that we have specified, and denote by $\text{dist}(V_j, V_j')$, is none other than $|z_0 - z_0'|$.

Then, quantifying over all pairs of indices $j, j'$, we see that under the same assumptions on $\epsilon$, it holds that

$$W_p\left(L_{(X,Y)}|Z \in V_j, L_{(X,Y)}|Z \in V_j\right) \leq L_{XY} \cdot \text{dist}(V_j, V_j') + (2 + 2^{1+1/p})\epsilon$$

with probability at least

$$1 - \sum_{j, j' = 1}^J \left(\exp\left(-\frac{n_j \epsilon^2}{D^{2p}}\right) + \exp\left(-\frac{\kappa \epsilon^2}{D^{2p}}\right)\right).$$

Note that the sum has $\frac{1}{2}J(J-1)$ terms. Now, under the assumption that all of the cells $V_j$ have volume within a fixed constant multiple of each other (that is, independent of $\epsilon$), it holds that for some uniform constant $C$, $J \leq C\epsilon^d$. This implies that (changing the constant $C$ as necessary)

$$1 - \sum_{j, j' = 1}^J \left(\exp\left(-\frac{n_j \epsilon^2}{D^{2p}}\right) + \exp\left(-\frac{\kappa \epsilon^2}{D^{2p}}\right)\right) \geq 1 - C\epsilon^{2d} \exp\left(-\frac{n_{\min} \epsilon^2}{D^{2p}}\right).$$

We therefore require that $n_{\min}$ grows fast enough, as a function of $\epsilon$, that $\epsilon^{2d} \exp\left(-\frac{n_{\min} \epsilon^2}{D^{2p}}\right) \rightarrow 0$. For, given this, we have that for all $j, j'$,

$$W_p\left(L_{(X,Y)}|Z \in V_j, L_{(X,Y)}|Z \in V_j\right) \leq L_{XY} \cdot \text{dist}(V_j, V_j') + (2 + 2^{1+1/p})\epsilon$$

with probability at least $1 - C\epsilon^{2d} \exp\left(-\frac{n_{\min} \epsilon^2}{D^{2p}}\right)$.\]
It remains, therefore, to show the other inequality. The argument is very similar. Take \( V_j \) and \( V_{j'} \) to be arbitrary. We know that
\[
W_p(\mathcal{L}(X,Y)|Z \in V_j, \mathcal{L}(X,Y)|Z \in V_{j'}) \leq \hat{L}_{XY} \cdot \text{dist}(V_j, V_{j'})
\]
simply from the definition of \( \hat{L} \). For a very large number of data points \( n_j \) and \( n_{j'} \), we have that \( \mathcal{L}(X,Y)|Z \in V_j \approx W_p \mathcal{L}(X,Y)|Z \in V_j \) and \( \mathcal{L}(X,Y)|Z \in V_{j'} \approx W_p \mathcal{L}(X,Y)|Z \in V_{j'} \) (with probability approaching 1 as \( n_j, n_{j'} \to \infty \)), and so
\[
W_p(\mathcal{L}(X,Y)|Z \in V_j, \mathcal{L}(X,Y)|Z \in V_{j'}) \lesssim \hat{L}_{XY} \cdot \text{dist}(V_j, V_{j'}). 
\]
More explicitly, if \( \mathbb{E} W_p \left( \mathcal{L}(X,Y)|Z \in V_j, \mathcal{L}(X,Y)|Z \in V_{j'} \right) \leq \varepsilon \) (which holds provided that \( \kappa_{q,p,d} M_q^{1/q} n_j^{-1/d} \leq \varepsilon \), as per Theorem 3) then we have
\[
\mathbb{P} \left[ W_p \left( \mathcal{L}(X,Y)|Z \in V_j, \mathcal{L}(X,Y)|Z \in V_{j'} \right) \geq 2^{1/p} \varepsilon \right] \leq \exp \left( -\frac{n_j \varepsilon^{2p}}{D^{2p}} \right).
\]
Then, from the triangle inequality,
\[
W_p(\mathcal{L}(X,Y)|Z \in V_j, \mathcal{L}(X,Y)|Z \in V_{j'}) \leq \hat{L}_{XY} \cdot \text{dist}(V_j, V_{j'}) + 2^{1+1/p} \varepsilon
\]
with probability at least \( 1 - \exp \left( -\frac{n_j \varepsilon^{2p}}{D^{2p}} \right) - \exp \left( -\frac{n_{j'} \varepsilon^{2p}}{D^{2p}} \right) \).

Let \( z_0 \) and \( z_{0}' \) be the centroids of \( V_j \) and \( V_{j'} \). Then (still provided that \( \kappa_{q,p,d} M_q^{1/q} n_j^{-1/d} \leq \varepsilon \), and with probability at least \( 1 - \exp \left( -\frac{n_j \varepsilon^{2p}}{D^{2p}} \right) - \exp \left( -\frac{n_{j'} \varepsilon^{2p}}{D^{2p}} \right) \))
\[
W_p(\mathcal{L}(X,Y)|Z \in V_j, \mathcal{L}(X,Y)|Z \in V_{j'}) \leq \hat{L}_{XY} |z_0 - z_{0}'| + 2^{1+1/p} \varepsilon.
\]
From the triangle inequality and the binning consistency estimate, we have that
\[
W_p(\mathcal{L}(X,Y)|Z=z, \mathcal{L}(X,Y)|Z=z') \leq \hat{L}_{XY} |z_0 - z_{0}'| + (2 + 2^{1+1/p}) \varepsilon \quad \forall z \in V_j, z' \in V_{j'}.
\]
Now, note that
\[
|z_0 - z|, |z_{0}' - z'| < \varepsilon / \hat{L}_{XY}
\]
from the diameter estimate on the bins. Therefore, (still provided that \( \kappa_{q,p,d} M_q^{1/q} n_j^{-1/d} \leq \varepsilon \), and with probability at least \( 1 - \exp \left( -\frac{n_j \varepsilon^{2p}}{D^{2p}} \right) - \exp \left( -\frac{n_{j'} \varepsilon^{2p}}{D^{2p}} \right) \))
\[
W_p(\mathcal{L}(X,Y)|Z=z, \mathcal{L}(X,Y)|Z=z') \leq \hat{L}_{XY} |z - z'| + \left( 2 + 2^{1+1/p} + 2 \frac{\hat{L}_{XY}}{\hat{L}_{XY}} \right) \varepsilon \quad \forall z \in V_j, z' \in V_{j'}.
\]
Finally, quantifying over all bins, we conclude that for all \( z \) and \( z' \) in the support of \( \mathcal{L}_Z \),
\[
W_p(\mathcal{L}(X,Y)|Z=z, \mathcal{L}(X,Y)|Z=z') \leq \hat{L}_{XY} |z - z'| + \left( 2 + 2^{1+1/p} + 2 \frac{\hat{L}_{XY}}{\hat{L}_{XY}} \right) \varepsilon
\]
again with probability at least
\[
1 - \sum_{j,j'=1}^J \left( \exp \left( -\frac{n_j \varepsilon^{2p}}{D^{2p}} \right) + \exp \left( -\frac{n_{j'} \varepsilon^{2p}}{D^{2p}} \right) \right) \geq 1 - C \varepsilon^{2d} \exp \left( -\frac{n_{\min} \varepsilon^{2p}}{D^{2p}} \right) .
\]
\( \square \)
4. Discussion

It should be emphasized that the class of joint distributions \((X, Y, Z)\) for which a conditional independence test, constructed in the manner of Theorem 10, is feasible, is quite general. As we have already discussed, the \(W_p\)-Lipschitz continuity we require is a weaker condition than the \(TV\)-Lipschitz continuity assumption from [NBW21]; nor do we assume that any of the distributions involved have density with respect to the Lebesgue measure; nor do we assume that the joint distribution is produced by any sort of parametric model. Nonetheless, we mention several possible extensions of the work in this article, stated in approximate order of increasing difficulty.

1. Relaxing the Lipschitz continuity assumption. One might entertain other quantitative smoothness conditions on the maps \(z \mapsto \mathcal{L}_{(X,Y)|Z=z}\), \(z \mapsto \mathcal{L}_{X|Z=z}\), and \(z \mapsto \mathcal{L}_{Y|Z=z}\), besides Lipschitz continuity, such as Hölder continuity. Indeed, if one takes the Hölder exponent and constant as given, the proofs in Section 2 still go through with only minor adjustments to the epsilon management. Likewise, if one takes the Hölder exponent as given, it is straightforward to adapt the arguments in Section 3 so as to produce a consistent estimator for the Hölder constant.

In principle, more general quantitative smoothness assumptions (such as an explicitly given modulus of continuity) are also feasible; what our analysis ultimately demands is some sort of quantitative information about the continuity of the maps \(z \mapsto \mathcal{L}_{(X,Y)|Z=z}\), \(z \mapsto \mathcal{L}_{X|Z=z}\), and \(z \mapsto \mathcal{L}_{Y|Z=z}\), so that we can appropriately fix the diameter of the bins.

2. Allowing the support of \(L_Z\) to be unbounded. The restriction of the results in Section 2 to the case where \(L_Z\) has bounded support inside \(\mathbb{R}^{d_Z}\) excludes many natural situations (take for instance \(Z\) to be a Gaussian random variable!). We propose two possible ways to relax this assumption and work with non-compactly supported \(L_Z\), one of which amounts to “moving the goalposts” and the other of which amounts to “adding a much stronger assumption somewhere else”.

For the first, observe that since \(L_Z\) is automatically tight, for every \(\varepsilon > 0\) there exists a compact set \(K_{\varepsilon}\) such that \(L_Z(\mathbb{R}^{d_Z}\setminus K_{\varepsilon}) < \varepsilon\). Therefore, while it is not possible to form a measurable partition of \(\text{supp}(L_Z)\) with a finite number of bins and where the bins all have uniformly diameter (as is required by Theorem 10), what is possible is to form such a partition on \(K_{\varepsilon}\). Then, Theorem 10 indicates how to test the conditional independence of \(X\) and \(Y\) given \(Z\), conditional on \(Z \in K_{\varepsilon}\). This does not allow us to test whether \(L_{(X,Y)|Z=z}\) is equal to \(L_{X|Z=z} \otimes L_{Y|Z=z}\) for every nonzero \(z\), but rather for all \(z\) lying in a set \(K_{\varepsilon}\) where \(\mathbb{P}(Z \in K_{\varepsilon}) \geq 1 - \varepsilon\). Call this “\((1-\varepsilon)\)-conditional independence testing”; this discussion shows that, if we are able to come up with an explicit such \(K_{\varepsilon}\) for \(Z\), and \(X, Y\), and \(Z\) satisfy the other assumptions of Theorem 10, then \((1-\varepsilon)\)-conditional independence testing is feasible.

As for the second: suppose that, instead of \(z \mapsto L_{(X,Y)|Z=z}\) and \(z \mapsto L_{X|Z=z}\) and \(z \mapsto L_{Y|Z=z}\), merely being \(W_p\)-Lipschitz maps, we require that these maps moreover have a local Lipschitz constant which quickly goes to zero as \(|z| \to \infty\). In this situation, it becomes permissible for the bins partitioning \(L_Z\) to have larger and larger diameter as \(|z| \to \infty\); for bins \(z \in V_j\) where all \(z\) are “very far” from 0, it is even permissible for the bin to be unbounded towards infinity, and still have small discretization error. We are not aware of an application area in conditional independence testing where such an “asymptotically very \(W_p\) smooth” assumption would be natural, but from an analytical standpoint...
such an assumption is sufficient for $W_p$ conditional independence testing to be feasible with unbounded $L_Z$.

3) **Data-dependent bins.** In Section 2, we assumed that the support of $L_Z$ was first partitioned into bins, and then samples are drawn from the joint distribution $(X,Y,Z)$. In this setting, Theorem 10 then indicates how many data points must lie in each bin in order to have global control of the Type I & II error for the conditional independence test. Or (what is much the same thing), the bins are produced *independently* from the data.

In a target application where data is plentiful and the bottleneck is the computational cost of the empirical Wasserstein distance (see discussion in Section 1), this is not too concerning. However, in general it might be desirable to first collect “as many samples as one can”, and *then* partition the space where $L_Z$ resides in such a way that each bin has “enough” samples, and then seek various finite sample guarantees. In this situation, the set of bins (equivalently, the measurable partition induced by the bins) becomes a random variable which depends on the samples. This *significantly* complicates much of the analysis — see, for instance, the work Canonne et al. [CDKS18], which offers a conditional independence test for random variables which take values in a *finite set*, and which *does* offer a binning scheme where the bins are allocated in a data-dependent fashion. In our (continuous) setting, we leave such analysis to future work.

4) **Random variables taking values in spaces other than $\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d$.** We have stipulated that the random variables $X$, $Y$, and $Z$ are Euclidean-valued for concreteness. However, the general theory of Wasserstein spaces/optimal transport can be carried out in the rather general setting of complete separable metric spaces [AG13, Vil03], and some of the statistical results in, for instance, [BLG14, WB19] are stated for more general metric spaces. Most tantalizing is the recent result of Lei [Lei20], which offers an expected error bound, similar to the one of Dereich et al. from [DSS13], in an infinite-dimensional setting. (However, [Lei20] does not provide explicit constants, which our statistical applications would certainly require.)

Unfortunately, in (say) an infinite-dimensional Banach space one runs into the difficulty that (for say $\varepsilon < \frac{1}{2}$) the $\varepsilon$-covering number of the unit ball is infinite, so even if $L_Z$ has bounded support, binning the support of $L_Z$ seems challenging! (On the other hand, if we assume that $L_Z$ has *compact* support, then this essentially means that $L_Z$ resides in a finite-dimensional subspace, and the putative infinite-dimensional setting trivializes.) On possible strategy is to exploit the *tightness* of (Radon) probability measures — that is, even in an infinite dimensional space, if $L_Z$ is Radon we know that for every $\varepsilon > 0$, there exists a compact $K_\varepsilon$ with $L_Z(K_\varepsilon) > 1 - \varepsilon$. If, moreover, modeling assumptions tell us that $Z$ must e.g. be concentrated in some fashion that actually *tells us* a compact set which serves as a $K_\varepsilon$, it is conceivable that, with a suitable infinite-dimensional concentration inequality, and a more explicit error estimate resembling the one from [Lei20], that one could perform “$(1 - \varepsilon)$-conditional independence testing” as per (2). However we expect that the requisite analysis to construct such a test would be challenging.

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Before proceeding, we require the following technical measure-theoretic result, which we will use to handle the potential non-uniqueness of optimal transport plans in our setting.

**Theorem** (Arsenin-Kunugui uniformization theorem [Kec12, Theorem 35.46 (ii)]). Let $X$ and $Y$ be Polish spaces. Let $R \subseteq X \times Y$ be a Borel set. Suppose that for every $x \in X$, $\{y \in Y : (x, y) \in R\}$ is a countable union of compact sets. Then the projection of $R$ onto $X$ is a Borel subset of $X$, and there exists a uniformization of $R$, that is, a Borel function $f : \text{proj}_X R \to Y$ such that $\{x, f(x)\} \in R$ for all $x \in \text{proj}_X R$.

**Proof of Lemma 6.** Let $V \subseteq Z$ where $Z$ is some Polish space.

Given any $z \in Z$, define $\text{Opt}(\mu_z, \nu)$ to be the set of optimal transport plans between the probability measures $\mu_z$ and $\nu$. Since $\mathcal{P}(U)$ is a Polish space (when equipped with the narrow topology), it is known that for fixed $z$, $\text{Opt}(\mu_z, \nu)$ is compact inside the Polish space $\mathcal{P}(U \times U)$ [Vil08, Corr. 5.21]. Also this set is always non-empty [San15, Theorem 1.7]. Moreover, it follows from [Vil08, Theorem 5.20] that the set

$$\text{Opt}(\cdot, \nu) := \{\gamma \in \mathcal{P}(U \times U) : \exists \mu \in \mathcal{P}(U), \pi \in \text{Opt}(\mu, \nu)\}$$

is closed inside $\mathcal{P}(U \times U)$, and is therefore itself a Polish space.

Now, let consider the projection map

$$\text{proj}_1 : \text{Opt}(\cdot, \nu) \to \mathcal{P}(U)$$

which, given a transport plan $\gamma \in \text{Opt}(\mu, \nu)$, returns the first marginal of $\gamma$, namely $\mu$. It is not hard to see that $\Pi_1$ is narrowly continuous: indeed, consider some bounded continuous function $\varphi$ on $U^2$ that only depends on the first coordinate; in this case,

$$\int_{U^2} \varphi \gamma = \int_U \varphi \text{proj}_1 \gamma$$

so in particular, for any narrowly convergent sequence $\gamma_n$ of transport plans (with limit $\gamma$), we have

$$\int \varphi \gamma_n = \int \varphi \text{proj}_1 \gamma_n; \quad \int \varphi \gamma = \int \varphi \text{proj}_1 \gamma$$

which implies that $\int \varphi \text{proj}_1 \gamma_n \to \int \varphi \text{proj}_1 \gamma$ for any bounded continuous $\varphi$ on $U^2$, as desired.

Since $\Pi_1$ is narrowly continuous, it follows that the transpose of the graph of $\text{proj}_1$, namely the set

$$\text{Gr}^T \text{proj}_1 := \{(\mu, \gamma) \in \mathcal{P}(U) \times \text{Opt}(\cdot, \nu) : \mu = \text{proj}_1 \gamma\},$$

is closed (when both $\text{Opt}(\cdot, \nu)$ and $\mathcal{P}(U)$ are equipped with the narrow topology), and so, in particular, is Borel. Since both $\text{Opt}(\cdot, \nu)$ and $\mathcal{P}(U)$ are Polish, it follows from the Arsenin-Kunugui uniformization theorem that there exists a Borel function $\text{OptSelect}$ from $\text{proj}_1 \text{Opt}(\cdot, \nu)$ to $\text{Opt}(\cdot, \nu)$.
whose graph is contained within $\text{Gr}^T \text{proj}_1$. But since $\text{proj}_1 \text{Opt}(\cdot, \nu) = \mathcal{P}(U)$ (since $\text{Opt}(\mu, \nu)$ is non-empty for every $\mu, \nu \in \mathcal{P}(U)$) it follows that the domain of $\text{OptSelect}$ is all of $\mathcal{P}(U)$. In other words, $\text{OptSelect}(\mu)$ is a Borel measurable selection of a transport plan in $\text{Opt}(\mu, \nu)$.

Now, we have assumed that the function $z \mapsto \mu_z$ is Borel, so by composing $z \mapsto \mu_z$ with $\text{OptSelect}$, we get a Borel measurable mapping

$$z \mapsto \gamma_z : \text{proj}_1 \gamma_z = \mu_z.$$ 

We also make the following measure-theoretic observation. The narrow topology on probability measures has the property that for every open set $O$, the evaluation map $\mu \mapsto \mu(O)$ is continuous; in particular, this implies (by the monotone class theorem; see also [BS78, Prop. 7.25]) that for every Borel set $B$, the evaluation map $\mu \mapsto \mu(B)$ is Borel. Consequently, for our measurable selection $z \mapsto \gamma_z$, it holds simultaneously that (1) for every $z \in Z$, $\gamma_z$ is a probability measure (on the space $U \times U$), and that (2) for fixed Borel set $B$, the map $z \mapsto \gamma_z(B)$ is Borel (since it is the composition of Borel maps). In other words, our measurable selection $\gamma_z$ is a (Borel measurable) stochastic kernel.

We claim that for any Borel measurable $V \subseteq Z$, the measure

$$\int_V \gamma_z d\lambda(z)$$

is a transport plan with first marginal $\int_V \mu_z d\lambda(z)$. Indeed, take any measurable set $B \subseteq U$; then, since $\gamma_z$ is a stochastic kernel, we can use the following elementary property of stochastic kernels (see e.g. [Çın11, Thm. I.6.3]):

$$\int_{U \times U} 1_{A \times U} d \left( \int_V \gamma_z d\lambda(z) \right) = \int_V \left( \int_{U \times U} 1_A d\gamma_z \right) d\lambda(z)
= \int_V \left( \int_U 1_A d\mu_z \right) d\lambda(z)
= \int_U 1_A d \left( \int_V \mu_z d\lambda(z) \right)$$

and so $(\int_V \gamma_z d\lambda(z)) (A \times U) = (\int_V \mu_z d\lambda(z)) (A)$. Moreover, by the same reasoning, we see that the second marginal is $\nu$.

Now, compute as follows. Since $\int_V \gamma_z d\lambda(z)$ is a transport plan between $\int_V \mu_z d\lambda(z)$ and $\nu$, it holds that

$$W_p^p \left( \int_V \mu_z d\lambda(z), \nu \right) \leq \int_{U^2} d(u_1, u_2)^p d \left( \int_V \gamma_z d\lambda(z) \right)(u_1, u_2).$$

Using [Çın11, Thm. I.6.3] again, we deduce that

$$\int_{U^2} d(u_1, u_2)^p d \left( \int_V \gamma_z d\lambda(z) \right)(u_1, u_2) = \int_V \left( \int_{U^2} d(u_1, u_2)^p d\gamma_z(u_1, u_2) \right) d\lambda(z).$$

But note that

$$\int_{U^2} d(u_1, u_2)^p d\gamma_z(u_1, u_2) = W_p^p(\mu_z, \nu).$$

Therefore,

$$\int_V \left( \int_{U^2} d(u_1, u_2)^p d\gamma_z(u_1, u_2) \right) d\lambda(z) = \int_V W_p^p(\mu_z, \nu) d\lambda(z).$$
and so
\[
W^p_p \left( \int_Y \mu_z d\lambda(z), \nu \right) \leq \int_Y W^p_p(\mu_z, \nu) d\lambda(z)
\]
as desired. This completes the proof. □

Appendix B. Additional Results

B.1. Concentration of \( W^p_p(\mu_n, \mu) \). We first prove Proposition 2 in the case where the support of \( \mu \) has general diameter (as opposed to a diameter of 1, as in [WB19]). We emphasize that this is extremely close to what is already done therein; consider this proof more of a sanity check.

Proof of Proposition 2. Let \( c(x, y) = d(x, y)^p \). Kantorovich duality tells us that
\[
W^p_p(\mu_n, \mu) = \max_{f \in C_b} \left[ \int f d\mu_n - \int f^c d\mu \right]
\]
and
\[
f(x) = \inf_y \left[ f^c(y) + d(x, y)^p \right]
\]
and
\[
f^c(y) = \sup_x \left[ f(x) - d(x, y)^p \right].
\]
Chose \( f \in C_b \) so that it attains the maximum for \( \int f d\mu_n - \int f^c d\mu \). \( f \) is defined only up to a constant, so without loss of generality take \( \sup_x f(x) = D^p \). Consequently,
\[
f^c(y) \geq \sup_x \left[ D^p - d(x, y)^p \right] \geq 0
\]
and therefore
\[
f(x) \geq \inf_y \left[ 0 + d(x, y)^p \right] \geq 0.
\]
Thus, we can take the \( f \in C_b \) which attains the maximum for \( \int f d\mu_n - \int f^c d\mu \) to have the property that \( 0 \leq f(x) \leq D^p \) for all \( x \) in the domain.

Now, let \( X_1, \ldots, X_n \) be i.i.d. draws from \( \mu \), so that \( \mu_n = \frac{1}{n} \sum_{i=1}^n X_i \). Define the random function
\[
w(X_1, \ldots, X_n) := W^p_p(\mu_n, \mu)
\]
\[
= \sup_{f \in C_b} \left[ \int f d\mu_n - \int f^c d\mu \right]
\]
\[
= \sup_{f \in C_b} \left[ \frac{1}{n} \sum_{i=1}^n f(X_i) - \int f^c d\mu \right].
\]
Let \( j \in \{1, \ldots, n\} \). Observe that given any \( x_1, \ldots, x_n \) and \( x'_j \),
\[
w(x_1, \ldots, x_j, \ldots, x_n) - w(x_1, \ldots, x'_j, \ldots, x_n) \leq \sup_{f \in C_b} \left[ \frac{1}{n} \sum_{i=1}^n f(x_i) - \int f^c d\mu \right]
\]
\[
- \sup_{f \in C_b} \left[ \frac{1}{n} \sum_{i=1}^n f'(x_i) + \frac{1}{n} f'(x'_j) - \int (f')^c d\mu \right].
\]
Let
\[ \tilde{f} \in \arg \max_{\tilde{f} \in C_b, 0 \leq \tilde{f} \leq D_p} \left[ \frac{1}{n} \sum_{i=1}^{n} f(x_i) - \int f^c \, d\mu \right]. \]

Note that
\[ \left[ \frac{1}{n} \sum_{i=1}^{n} \tilde{f}(x_i) + \frac{1}{n} \tilde{f}(x'_j) - \int (\tilde{f})^c \, d\mu \right] \leq \sup_{f' \in C_b, 0 \leq f' \leq D_p} \left[ \frac{1}{n} \sum_{i=1}^{n} f'(x_i) + \frac{1}{n} f'(x'_j) - \int (f')^c \, d\mu \right] \]
and thus
\[
\sup_{f' \in C_b, 0 \leq f' \leq D_p} \left[ \frac{1}{n} \sum_{i=1}^{n} f(x_i) - \int f^c \, d\mu \right] - \sup_{f' \in C_b, 0 \leq f' \leq D_p} \left[ \frac{1}{n} \sum_{i=1}^{n} f'(x_i) + \frac{1}{n} f'(x'_j) - \int (f')^c \, d\mu \right]
\leq \left[ \frac{1}{n} \sum_{i=1}^{n} \tilde{f}(x_i) - \int \tilde{f}^c \, d\mu \right] - \left[ \frac{1}{n} \sum_{i=1}^{n} \tilde{f}(x_i) + \frac{1}{n} \tilde{f}(x'_j) - \int (\tilde{f})^c \, d\mu \right]
\leq \frac{1}{n} \left[ \tilde{f}(x_j) - \tilde{f}(x'_j) \right] \leq \frac{D_p}{n}.
\]

It therefore follows from McDiarmid’s inequality that
\[ \mathbb{P} \left[ W_p^n(\mu_n, \mu) \geq EW_p^n(\mu_n, \mu) + t \right] \leq \exp \left( -\frac{2nt^2}{D_p^2} \right) \]
as desired.

Let us now adapt the previous proof to the case where \( \mu \) is not necessarily bounded, using Combes’s variant on McDiarmid’s inequality, proved in [Com15]. Mostly we are interested in a concentration inequality under the same assumptions as in Theorem 3, namely that \( d \geq 3 \), \( p \in [1, d/2) \), and \( \mu \) has a \( q \)th moment bound for \( q \) such that \( q > dp/(d-p) \).

Let’s recall the statement of Combes’s variant on McDiarmid’s inequality.

**Theorem** (Combes [Com15]). Let \( (X_1, \ldots, X_n) \) be sets and define \( X := \prod_{i=1}^{n} X_i \). Let \( X := (X_1, \ldots, X_n) \) be independent random variables with \( X_i \in X_i \). Let \( w : X \to \mathbb{R} \), so that \( w(X) \) is a random variable.

Let \( \mathcal{Y} \subset X \). Define \( p := 1 - \mathbb{P}[X \in \mathcal{Y}] \) and \( m = \mathbb{E}[w(X) \mid X \in \mathcal{Y}] \). Let \( \bar{c} := (c_1, \ldots, c_n) \in \mathbb{R}^n_+ \) and define \( \bar{c} = \sum_{i=1}^{n} c_i \). Suppose that: for all \( j \in \{1, \ldots, n\} \), for all \( (y, y') \in \mathcal{Y}^2 \) with \( y_i = y'_i \) for all \( i \neq j \), it holds that \( |w(y) - w(y')| \leq c_j \). Then, for all \( t > 0 \), it holds that
\[ \mathbb{P}[w(X) \geq m + t] \leq p + \exp \left( -\frac{2(t - p\bar{c})^2}{\sum_{i=1}^{n} c_i^2} \right). \]

We will apply Combes’s inequality in the case where \( (X_1, \ldots, X_n) \) are i.i.d. samples from some probability measure \( \mu \) (and we denote \( \mu_n = \frac{1}{n} \sum_{i=1}^{n} X_i \)), \( \mathcal{Y} = B(e, R)^n \) for some “large” radius \( R \) and arbitrary “origin” \( e \in X \), and \( w(X) = W_p^n(\mu_n, \mu) \). In order to apply Combes’s inequality, we
must compute $c_i$, $m$, and $p$. We do so in the situation where $\mu$ has bounded $q$th moment, where $q > p$.

**Proposition 13 (Wasserstein empirical measure concentration inequality with higher moment bound).** Let $(X,d)$ be a Polish metric space with (arbitrary) distinguished point $e \in X$. Let $\mu \in \mathcal{P}(X)$ with $(\int_X d(e,x)^q d\mu(x))^{1/q} \leq M_q$ for some $q > p \geq 1$. Let $\mu_n = \sum_{i=1}^n \delta_{x_i}$ be a (random) empirical measure for $\mu$. Furthermore, let $\eta \in (0,1)$, and let

$$\bar{\mu} \mid B(e, M_q \eta^{-1/q}) := \frac{1}{\mu(B(e, M_q \eta^{-1/q}))} \mu \mid B(e, M_q \eta^{-1/q})$$

denote the normalized restriction of $\mu$ to $B(e, M_q \eta^{-1/q})$, and let $\mu_n \mid (X_1, \ldots, X_n) \in B(e, M_q \eta^{-1/q})^n$ denote the conditional empirical measure where $x_i \in B(e, M_q \eta^{-1/q})$ for all $i = 1, \ldots, n$. Then, for any $t > 0$, it holds that

$$\mathbb{P}\left[W_p^p(\mu_n, \mu) \geq E \left[\left(W_p \left(\mu_n \mid (X_1, \ldots, X_n) \in B(e, M_q \eta^{-1/q})^n, \bar{\mu} \mid B(e, M_q \eta^{-1/q})\right) + c_{p,q} M_q \eta^{1/p-1/q}\right)^p\right] + t\right]$$

$$\leq 1 - (1-\eta)^n + \exp\left(-\frac{2n \left(t - (1 - (1-\eta)^n)(M_q \eta^{-1/q})^p\right)^2}{(M_q \eta^{-1/q})^{2p}}\right)$$

where $c_{p,q} := \frac{2^{1/q} \eta^{1/p-1/q}}{2^{1/p-1/q} - 1} + \frac{\eta^{1/p}}{2^{1/p-1}}$.

**Proof.** First, recall that every (Radon) probability measure $\mu$ on a Polish space is automatically tight — that is, for every $\eta \in (0,1)$ there exists a compact $K_\eta$ such that $\mu(K_\eta) > 1 - \eta$. If, moreover, $\mu$ has bounded $q$th moment, we can say more. Indeed, suppose that $\mu(X \setminus B(e, R)) \geq \eta$. Then,

$$R \eta^{1/q} \leq \left(\int_X d(e,x)^q d\mu(x)\right)^{1/q}.$$

It follows that if we know that $(\int_X d(e,x)^q d\mu(x))^{1/q} \leq M_q$, then $R \eta^{1/q} \leq M_q$, in other words, the maximal radius at which $\mu(X \setminus B(e, R)) \geq \eta$ is $M_q \eta^{-1/q}$. Likewise, if we have $n$ i.i.d. draws from $\mu$, we know that for each draw, the probability of landing outside of $B(e, M_q \eta^{-1/q})$ is at most $\eta$. It follows that the probability of all the draws landing inside $B(e, M_q \eta^{-1/q})$ — which is the quantity $1 - p$ in the statement of Combes’s inequality — is at least $(1 - \eta)^n$. Hence $p \leq 1 - (1-\eta)^n$.

To compute $m$ from the statement of Combes’s inequality, we will need to upper bound $W_p^p(\mu, \bar{\mu} \mid B(e, M_q \eta^{-1/q}))$ in the case where $p < q$. So, compute as follows. We have seen that $\mu(B(e, M_q \left(\frac{\eta}{2}\right)^{-1/q})) \geq 1 - \frac{\eta}{2}$. It follows that

$$\mu \left(B(e, M_q \left(\frac{\eta}{2}\right)^{-1/q}) \setminus B(e, M_q \left(\frac{\eta}{2^{1-1}}\right)^{-1/q})\right) \leq \mu \left(\mathbb{R}^d \setminus B(e, M_q \left(\frac{\eta}{2^{1-1}}\right)^{-1/q})\right) < \frac{\eta}{2^{1-1}}.$$

At the same time, regardless of the choice of transport plan between $\bar{\mu} \mid B(e, M_q \eta^{-1/q})$ and $\mu$, when transporting the mass in $\mu$ which resides in $B(e, M_q \left(\frac{\eta}{2}\right)^{-1/q}) \setminus B(e, M_q \left(\frac{\eta}{2^{1-1}}\right)^{-1/q}$ onto $\bar{\mu} \mid B(e, M_q \eta^{-1/q})$, the distance traveled by this mass is at most $M_q \left(\frac{\eta}{2}\right)^{-1/q} + M_q \eta^{-1/q}$ (for each particle of mass), and the total mass transported from $B(e, M_q \left(\frac{\eta}{2}\right)^{-1/q}) \setminus B(e, M_q \left(\frac{\eta}{2^{1-1}}\right)^{-1/q})$ is less than $\frac{\eta}{2^{1-1}}$. Consequently, the $W_p$ transportation cost to transport this portion of the mass in $\mu$ is less than $\left(M_q \left(\frac{\eta}{2}\right)^{-1/q} + M_q \eta^{-1/q}\right) \left(\frac{\eta}{2^{1-1}}\right)^{1/p}$.
Furthermore, since the mass in $\frac{1}{\mu(B(e, M_q \eta^{-1/q}))}\mu \rvert B(e, M_q \eta^{-1/q})$ is everywhere greater than the mass in $\mu \rvert B(e, M_q \eta^{-1/q})$, it follows that we can choose a transport plan from $\mu$ to $\frac{1}{\mu(B(e, M_q \eta^{-1/q}))}\mu \rvert B(e, M_q \eta^{-1/q})$ will leave all of $\mu$'s mass within $B(e, M_q \eta^{-1/q})$ unmoved. Therefore, we can upper bound

$$W_p(\mu, \frac{1}{\mu(B(e, M_q \eta^{-1/q}))}\mu \rvert B(e, M_q \eta^{-1/q})) = \sum_{i=1}^{\infty} \left( M_q \frac{\eta}{2^i} \right)^{1/q} + M_q \eta^{-1/q} \left( \frac{\eta}{2^i-1} \right)^{1/p}$$

$$= M_q \eta^{1/p-1/q} \sum_{i=1}^{\infty} \left( \frac{2^i-1}{2} \frac{1}{(2^i-1)^{1/p}} + \frac{1}{(2^i-1)^{1/p}} \right)$$

$$= M_q \eta^{1/p-1/q} \sum_{i=1}^{\infty} \left( \frac{2^i}{2^{i-1}-1} \frac{2^i}{(2^i)-1^{1/p}} + \frac{1}{(2^i)-1^{1/p}} \right)$$

$$= M_q \eta^{1/p-1/q} \left( \frac{2^i}{2^{i-1}-1} \frac{1}{(2^i-1)^{1/p}} + \frac{1}{(2^i-1)^{1/p}} \right)$$

Letting $c_{p,q} := 2^{1/q} \frac{2^i}{(2^i)-1^{1/p}} + \frac{2^i}{(2^i)-1^{1/p}}$, we see that

$$W_p(\mu, \frac{1}{\mu(B(e, M_q \eta^{-1/q}))}\mu \rvert B(e, M_q \eta^{-1/q})) < c_{p,q} M_q \eta^{1/p-1/q}.$$  

Note that $c_{p,q} \to \infty$ as $q \searrow p$.

We are now in a position to compute $c_i$ and $m$ (again from the statement of Combes’ inequality). First, note that the random measure $\mu_n$, but conditioned on the event $(X_1, \ldots, X_n) = X \in B(e, M_q \eta^{-1/q})^n$, is an empirical measure for $\tilde{\mu} \rvert B(e, M_q \eta^{-1/q})$. Thus, reasoning as in the proof of Proposition 2, we see that

$$W_p^p \left( \mu_n \mid (X_1, \ldots, X_n) \in B(e, M_q \eta^{-1/q})^n, \tilde{\mu} \rvert B(e, M_q \eta^{-1/q}) \right) = \sup_{f \in C_b} \left[ \frac{1}{n} \sum_{i=1}^{n} f(X_i) - \int f \, d\mu \right]$$

and likewise, conditioned on the event $X = B(e, M_q \eta^{-1/q})$, the proof of Proposition 2 shows that for all $j \in \{1, \ldots, n\},$

$$w(x_1, \ldots, x_j, \ldots, x_n) - w(x_1, \ldots, x'_j, \ldots, x_n) \leq \frac{(M_q \eta^{-1/q})^p}{n} := c_j.$$  

Hence $\tilde{c} := \sum_{i=1}^m c_i = (M_q \eta^{-1/q})^p$, and $\sum_{i=1}^n c_i = \frac{(M_q \eta^{-1/q})^{2p}}{n}$. At the same time, by the triangle inequality,

$$m := \mathbb{E} W_p^p \left( \mu_n \mid (X_1, \ldots, X_n) \in B(0, M_q \eta^{-1/q})^n, \mu \right) \leq \mathbb{E} \left[ W_p \left( \mu_n \mid (X_1, \ldots, X_n) \in B(e, M_q \eta^{-1/q})^n, \tilde{\mu} \rvert B(e, M_q \eta^{-1/q}) \right) + W_p \left( \mu, \tilde{\mu} \rvert B(e, M_q \eta^{-1/q}) \right) \right]^p$$

$$\leq \mathbb{E} \left[ W_p \left( \mu_n \mid (X_1, \ldots, X_n) \in B(e, M_q \eta^{-1/q})^n, \tilde{\mu} \rvert B(e, M_q \eta^{-1/q}) \right) + c_{p,q} M_q \eta^{1/p-1/q} \right]^p.$$
Therefore, Combes’s inequality tells us that: for all $\eta \in (0, 1)$ and $t > 0$,

$$
P \left[ W_p^p(\mu_n, \mu) \geq \mathbb{E} \left[ \left( W_p \left( \mu_n \mid (X_1, \ldots, X_n) \in B(e, M_q \eta^{-1/q})^n, \bar{\mu} \mid B(e, M_q \eta^{-1/q}) \right) + c_{p,q} M_q \eta^{1/p-1/q} \right)^p \right] + t \right] 
\leq P \left[ W_p^p(\mu_n, \mu) \geq m + t \right] \leq 1 - (1 - \eta)^n + \exp \left( -\frac{2n \left( t - (1 - \eta)^n \right) (M_q \eta^{-1/q})^p}{(M_q \eta^{-1/q})^{2p}} \right). \tag*{□}
$$

It is possible to combine this concentration inequality with the expectation bound from Theorem 3 in a straightforward way:

**Corollary 14.** Under the same assumptions as the preceding theorem, suppose, in addition, that $X \in \mathbb{R}^d$, $p \in [1, d/2)$, and $q > dp/(d - p)$. Then, for all $\eta \in (0, 1)$ and $t > 0$,

$$
P \left[ W_p^p(\mu_n, \mu) \geq \left( \kappa_{p,q,d} M_q (1 + \eta)^{1/q} \eta^{-1/d} + c_{p,q} M_q \eta^{1/p-1/q} \right)^p + t \right] 
\leq 1 - (1 - \eta)^n + \exp \left( -\frac{2n \left( t - (1 - \eta)^n \right) (M_q \eta^{-1/q})^p}{(M_q \eta^{-1/q})^{2p}} \right). \tag*{□}
$$

**Proof.** If $\mu$ has moment bound $M_q$, then it follows that $\bar{\mu} \mid B(0, M_q \eta^{-1/q})$ has upper moment bound $M_q (1 + \eta)^{1/q}$ (because in the worst case, $\mu$ is concentrated near $\partial B(0, M_q \eta^{-1/q})$.) So, we know, using Theorem 3, that under the requisite additional assumptions of Theorem 3, namely that $p \in [1, d/2)$ and $q > dp/(d - p)$, it holds that

$$
\text{EW}_p \left( \mu_n \mid (X_1, \ldots, X_n) \in B(0, M_q \eta^{-1/q})^n, \bar{\mu} \mid B(0, M_q \eta^{-1/q}) \right) \leq \kappa_{p,q,d} M_q (1 + \eta)^{1/q} \eta^{-1/d}
$$

and so it follows, in this circumstance, that

$$
P \left[ W_p^p(\mu_n, \mu) \geq \left( \kappa_{p,q,d} M_q (1 + \eta)^{1/q} \eta^{-1/d} + c_{p,q} M_q \eta^{1/p-1/q} \right)^p + t \right] 
\leq 1 - (1 - \eta)^n + \exp \left( -\frac{2n \left( t - (1 - \eta)^n \right) (M_q \eta^{-1/q})^p}{(M_q \eta^{-1/q})^{2p}} \right). \tag*{□}
$$

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