MEASURING ASSOCIATION WITH WASSERSTEIN DISTANCES

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Abstract. Let $\pi \in \Pi(\mu, \nu)$ be a coupling between two probability measures $\mu$ and $\nu$ on a Polish space. In this article we propose and study a class of nonparametric measures of association between $\mu$ and $\nu$, which we call Wasserstein correlation coefficients. These coefficients are based on the Wasserstein distance between $\nu$ and the disintegration $\pi_{x_1}$ of $\pi$ with respect to the first coordinate. We also establish basic statistical properties of this new class of measures: we develop a statistical theory for strongly consistent estimators and determine their convergence rate in the case of compactly supported measures $\mu$ and $\nu$. Throughout our analysis we make use of the so-called adapted/bicausal Wasserstein distance, in particular we rely on results established in [Backhoff, Bartl, Beiglböck, Wiesel. Estimating processes in adapted Wasserstein distance. 2020]. Our approach applies to probability laws on general Polish spaces.

1. Introduction

Given a sample of $(X_1^1, X_1^2), (X_2^1, X_2^2), \ldots, (X_N^1, X_N^2)$ generated from a probability measure $\pi$ with marginals $\mu$ and $\nu$ on a product $X \times Y$ of topological spaces, a number of works have recently asked whether it is possible to define a simple empirical measure $T_N$, which provides an estimate for a non-parametric measure of association between $\mu$ and $\nu$. More concretely, [Chatterjee, 2020, Abstract] states the following desirable conditions:

“Is it possible to define a coefficient of correlation which is:
(i) simple as the classical coefficients like Pearson’s correlation or Spearman’s correlation, and yet
(ii) Consistently estimates some simple and interpretable measure of the degree of dependence between the variables, which is 0 if and only if the variables are independent and 1 if and only if one is a measurable function of the other, and
(iii) Has a simple asymptotic theory under the hypothesis of independence, like the classical coefficients?”

As is argued in [Chatterjee 2020], none of the various past works based on joint cumulative distribution functions and ranks, kernel-based methods, information theoretic coefficients, coefficients based on copulas or on pairwise distances (see e.g., Rényi 1959, Linfoot 1957, Blum et al. 1961, Rosenblatt 1975, Schweizer et al. 1981, Friedman and Raškaý 1983, Scarsini 1984, Székely et al. 2007),...
Lyons et al. [2013], Gamboa et al. [2018], Zhang [2019], Puccetti [2019] and the references therein) satisfy all three properties stated above. It turns out that the articles Trutschnig [2011], Junker et al. [2021] and later also Dette et al. [2013] and Chatterjee [2020] are the first to answer Chatterjee’s question above in the affirmative for spaces $X = \mathbb{R}^{d_1}$ and $Y = \mathbb{R}^{d_2}$, where $d_2 = 1$. Since then their correlation coefficient has attracted a lot of attention, see e.g. Shi et al. [2020b], Cao and Bickel [2020] and Griessenberger et al. [2021] for a very recent extension. Complementary to this approach, Deb et al. [2020] (see also Ke and Yin [2019]) show how to build a corresponding estimator $T_N$ for general $d_2 \geq 1$. The analysis in Deb et al. [2020] is restricted to estimators arising from reproducing kernel Hilbert spaces with specific requirements on the kernel and thus cannot be applied to arbitrary Polish spaces $X, Y$. In this article we offer an alternative construction of $T_N$ based on adapted Wasserstein distances. The idea of using tools from optimal transport to measure dependence of measures is not new and can be traced back at least to Gini [1915], see also Cifarelli and Regazzini [2017]. Recently, this subject has seen a spike in research activity: current works comprise Ozair et al. [2019], Xiao and Wang [2019], Móri and Székely [2020], Mordant and Segers [2021], Nies et al. [2021] amongst others. However, to the best of our knowledge this article is the first to define a coefficient of correlation based on adapted Wasserstein distances for general Polish spaces and to derive its analytical and statistical properties from adapted optimal transport. Indeed, directly utilising the underlying compatible metric structure of the space $X$, the above properties (i)-(iii) hold without further assumptions. Furthermore, by varying the metric $d$ and the Wasserstein exponent $p$, one can naturally construct a whole family of different Wasserstein correlation coefficients, while directly exploiting the theory of optimal transportation. In fact, it will turn out that once we have defined the Wasserstein correlation $\widetilde{W}$, our estimators can be computed via the plug-in approach $\widetilde{W}_N = \widetilde{W}(\widehat{\pi}_N)$ for the so-called adapted empirical measure $\widehat{\pi}_N$. In this article we derive consistency and convergence rates of the estimator $\widetilde{W}(\widehat{\pi}_N)$ under different assumptions.

2. Notation and main results

Let $\mathcal{X}$ be a Polish space with a compatible metric $d$ and let us denote by $\text{Prob}(\mathcal{X})$ the set of Borel probability measures on $\mathcal{X}$. Let us take $\mu, \nu \in \text{Prob}(\mathcal{X})$ and denote by $\Pi(\mu, \nu)$ the set of couplings between $\mu$ and $\nu$ as, i.e.

$$\Pi(\mu, \nu) = \{ \pi \in \text{Prob}(\mathcal{X} \times \mathcal{X}) : \pi(\cdot \times \mathcal{X}) = \mu(\cdot), \pi(\mathcal{X} \times \cdot) = \nu(\cdot) \}.$$ 

The Wasserstein distance $W(\mu, \nu)$ is defined via

$$W(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int d(x_1, x_2) \pi(dx_1, dx_2).$$

The pushforward of the measure $\mu$ via a function $f : \mathcal{X} \to \mathcal{X}$ is denoted by $f_#\mu$, i.e.

$$(f_#\mu)(A) := \mu(\{ x \in \mathcal{X} : f(x) \in A \})$$

for all Borel sets $A \subseteq \mathcal{X}$. Generalising the above definition to Borel probability measures on $\mathcal{X}^2 := \mathcal{X} \times \mathcal{X}$, we often write $\pi_1 = (x_1)_#\pi$ and $\pi_2 = (x_2)_#\pi$ for $\pi \in \text{Prob}(\mathcal{X}^2)$, where $(x_1, x_2) \mapsto x_1$ and $(x_1, x_2) \mapsto x_2$ are the canonical projection maps from $\mathcal{X}^2$ to the first and second coordinates respectively. We also recall that
any coupling $\pi \in \Pi(\mu, \nu)$ has a $\mu$-a.s. unique disintegration with respect to the first coordinate, i.e. there exists a Borel measurable function $x_1 \mapsto \pi_{x_1}$ such that

$$\pi(A \times B) = \int_A \pi_{x_1}(B) \, \mu(dx_1) \quad \text{for all Borel sets } A, B \subseteq \mathcal{X}.$$ 

The product coupling with marginals $\mu$ and $\nu$ is denoted by $\mu \otimes \nu$.

One of the key notions used in this article is the so-called adapted Wasserstein distance. It can be introduced as follows: for Borel probability measures $\pi, \tilde{\pi}$ on $\mathcal{X}^2$ we define the adapted (sometimes also called nested or bicausal) Wasserstein distance $\text{AW}(\pi, \tilde{\pi})$ via

$$\text{AW}(\pi, \tilde{\pi}) = \inf_{\gamma \in \Pi(\pi_1, \tilde{\pi}_1)} \int [d(x_1, y_1) + W(\pi_{x_1}, \tilde{\pi}_{y_1})] \, \gamma(dx_1, dy_1). \quad (1)$$

On an intuitive level, the nested Wasserstein distance only considers those couplings $\gamma \in \Pi(\pi, \tilde{\pi})$, which respect the information flow formalised by the canonical (i.e. coordinate) filtration $(\mathcal{F}_t)_{t \in \{1, 2\}}$: in (1) this is achieved by first taking an infimum over couplings of $\pi_1, \tilde{\pi}_1$ (i.e. “couplings at time one”) and then a second (nested) infimum with respect to the respective disintegrations (i.e. “conditional couplings at time two”). This feature distinguishes $\text{AW}$ from the Wasserstein distance $W$, which also includes “anticipative couplings”. We refer to Backhoff-Veraguas et al. to appear pp. 2-3 for a well-written introduction to this topic. The nested distance was introduced in Pfug [2009], Pfug and Pichler [2012] in the context of multistage stochastic optimisation and was independently analysed in Lassalle [2018].

Let us also remark here that we always have the inequality

$$W(\pi, \tilde{\pi}) \leq \text{AW}(\pi, \tilde{\pi}), \quad (2)$$

where the Wasserstein distance $W(\pi, \tilde{\pi})$ is correspondingly defined as

$$W(\pi, \tilde{\pi}) = \inf_{\gamma \in \Pi(\pi, \tilde{\pi})} \int [d(x_1, y_1) + d(x_2, y_2)] \, \gamma(dx_1, x_2, dy_1, y_2)$$

and

$$\Pi(\pi, \tilde{\pi}) = \{ \gamma \in \Pi(\pi, \tilde{\pi}) : \gamma(\cdot \times \mathcal{X}^2) = \pi(\cdot), \gamma(\mathcal{X}^2 \times \cdot) = \tilde{\pi}(\cdot) \}.$$ 

For the rest of this article we fix two measures $\mu, \nu \in \text{Prob}(\mathcal{X})$. We now introduce the following measure of association, which will be the main concept discussed in this article:

**Definition 2.1.** For any $\pi \in \text{Prob}(\mathcal{X}^2)$ we define the Wasserstein correlation coefficient $\pi \mapsto \widehat{W}(\pi)$ by

$$\widehat{W}(\pi) := \frac{\int W(\pi_{x_1}, \pi_{x_2}) \pi_1(dx_1)}{\int d(y, z) \, \pi_2(dy) \pi_2(dz)}.$$ 

If $\pi \in \Pi(\mu, \nu)$, then in particular

$$\widehat{W}(\pi) = \frac{\int W(\pi_{x_1}, \nu) \mu(dx_1)}{\int d(y, z) \, \nu(dy) \nu(dz)},$$

where throughout we assume that $\nu$ is not a singleton, i.e.

$$\int d(y, z) \, \nu(dy) \nu(dz) \neq 0.$$
The key idea for the definition of $\vec{W}(\pi)$ is the following insight: in order to capture association between $\mu$ and $\nu$ for a coupling $\pi \in \Pi(\mu, \nu)$, it is sufficient to compare the disintegration $\pi_{x_1}$ with $\nu$ via the term $W(\pi_{x_1}, \nu)$. Indeed, this term is zero for $\mu$-a.e. $x_1$ if and only if $\pi_{x_1} = \nu$ or equivalently $\pi = \mu \otimes \nu$. On the other hand, if $\mu$ and $\nu$ are completely dependent then $\pi_{x_1} = \delta_{f(x_1)}$ for some function $f$. In this case there is only one coupling between $\pi_{x_1}$ and $\nu$ and the value of the denominator and the numerator in the above definition align, yielding $\vec{W}(\pi) = 1$.

More generally, defining $\pi^\lambda = \lambda \pi^1 + (1 - \lambda) \pi^2$ for some measures $\pi^1, \pi^2 \in \Pi(\mu, \nu)$ and $\lambda \in [0, 1]$, we conclude by convexity of Wasserstein distances that $\vec{W}(\pi^\lambda) \leq \lambda \vec{W}(\pi^1) + (1 - \lambda) \vec{W}(\pi^2)$, i.e. $\pi \mapsto \vec{W}(\pi)$ is convex on $\Pi(\mu, \nu)$. We discuss further properties of the Wasserstein correlation in the upcoming sections. In particular we show that $\vec{W}$ indeed satisfies the main requirement (ii) stated in [Chatterjee, 2020, Abstract], as cited in the introduction:

**Theorem 2.2.** For any $\pi \in \Pi(\mu, \nu)$ the functional $\pi \mapsto \vec{W}(\pi)$ satisfies:

(i) $\vec{W}(\pi) \in [0, 1]$.

(ii) $\vec{W}(\pi) = 0$ if and only if $\pi = \mu \otimes \nu$.

(iii) $\vec{W}(\pi) = 1$ if and only if $\pi = f_{#} \mu$ for some measurable function $f : \mathcal{X} \to \mathcal{X}$.

A natural estimator for $\vec{W}$ is given via the following plugin approach:

**Theorem 2.3.** Let $\pi \in \Pi(\mu, \nu)$ such that

$$\int d(x_2, x_0) \nu(dx_2) < \infty$$

for any $x_0 \in \mathcal{X}$ and let $\hat{\pi}^N$ be an $AW$-consistent estimator of $\pi$. Then $\vec{W}(\hat{\pi}^N)$ is a consistent estimator of $\vec{W}(\pi)$.

One such $AW$-consistent estimator of $\pi$ has recently been constructed in [Backhoff et al., 2021+] and throughout this article, we will make use of results established there. In particular continuity of $\vec{W}$ in $AW$ will directly enable us to establish convergence rates for $\vec{W}(\hat{\pi}^N)$.

Let us also also remark that our analysis can easily be extended to consider $p$-Wasserstein distances $W_p$ for $p > 1$ by correspondingly considering the $p$-Wasserstein correlation coefficient

$$\vec{W}_p(\pi) := \left( \frac{\int W_p(\pi_{x_1}, \nu)^p \pi_1(dx_1)}{\left( \int d(x_2, y)^p \pi_2(dx_2) \pi_2(dy) \right)^{1/p}} \right)^{1/p}$$

and replacing $\vec{W}, AW$ by the (adapted) $p$-Wasserstein distances $W_p, AW_p$ in all results. The restriction to $p = 1$ is thus only chosen for notational simplicity.

This article is structured as follows: in Section 3 we derive basic properties of $\vec{W}$ and compare it to other measures of association derived in [Chatterjee, 2020, Deb et al., 2020] as well as Pearson’s correlation coefficient in the case of a bivariate Gaussian distribution $\pi$. In Section 4 we state general continuity properties of the functional $\pi \mapsto \vec{W}(\pi)$ with respect to $AW$ and give a first consistency result. Section 5 and 6 then exhibit convergence rates for the independent case $\pi = \mu \otimes \nu$.
and the general case respectively. Lastly Section exhibits numerical simulations, while Section discusses open research questions. We relegate longer proofs to the appendix.

3. Discussion and literature review

Recall that the Wasserstein correlation coefficient is given by

\[ \overrightarrow{W}(\pi) = \frac{\int W(\pi_1, \nu) \mu(dx_1)}{\int d(y, z) \nu(dy) \nu(dz)}. \]

We start with some preliminary comments: we first note that \( \overrightarrow{W} \) is not symmetric in the order of marginals, i.e. \( \overrightarrow{W}(\pi) \neq \overleftarrow{W}(\pi) \) in general, where

\[ \overleftarrow{W}(\pi) := \frac{\int W(\pi_2, \mu) \nu(dx_2)}{\int d(x, z) \mu(dx) \mu(dz)}. \]

This is showcased in the following example:

**Example 3.1.** Take \((X, d) = (\mathbb{R}, |\cdot|_2)\) and set

\[ \pi = \frac{\delta_{(1,0)} + \delta_{(1,1)} + \delta_{(2,2)}}{3}. \]

Then

\[ \mu = \frac{2\delta_1 + \delta_2}{3}, \quad \nu = \frac{\delta_0 + \delta_1 + \delta_2}{3} \]

as well as

\[ \pi_1 = \frac{\delta_0 + \delta_1}{2}, \quad \pi_2 = \delta_2, \]

so that \( W(\pi_1, \nu) = 1/2, W(\pi_2, \nu) = 1 \) and

\[ \overrightarrow{W}(\pi) = \frac{3}{4}, \quad \overleftarrow{W}(\pi) = \frac{2/3}{8/9} = \frac{3}{4}. \]

while \( \overleftarrow{W}(\pi) \) equals 1 by an obvious modification of Theorem (iii) for \( \overrightarrow{W} \). In conclusion \( \overrightarrow{W}(\pi) \neq \overleftarrow{W}(\pi) \).

The lack of symmetry is intentional: as we have already stated in Theorem we have \( \overrightarrow{W} = 1 \) iff \( \nu = f\#\mu \) for some measurable function \( f \). The above example shows that this does not imply \( \mu = g\#\nu \) for some measurable function \( g \). Nevertheless, in order to obtain a symmetric expression we could simply consider \( \overrightarrow{W}(\pi) \lor \overleftarrow{W}(\pi) \) instead of merely \( \overrightarrow{W}(\pi) \). For notational simplicity we will only state our estimates for \( \overrightarrow{W}(\pi) \) and remark instead that all of them also hold for \( \overrightarrow{W}(\pi) \) as well as \( \overrightarrow{W}(\pi) \lor \overleftarrow{W}(\pi) \), adjusting constants correspondingly.

Apart from the properties (i)-(iii) stated in the introduction, [Móri and Székely 2019] Property (F) also asks for invariance properties of measures of association. In our case, the following can be directly derived from the definition of Wasserstein distances:

**Lemma 3.2.** Let \( I : (X, d) \to (X, d) \) be a isometric isomorphism. Then

\[ \overrightarrow{W}(\pi) = \overrightarrow{W}((I, I)\#\pi). \]
We now compare the Wasserstein correlation $\widehat{W}$ to several other measures of association. We start with the one proposed in\cite{Trutschnig2011, Dette2013, Chatterjee2020, Junker2021}.

**Lemma 3.3.** \cite{Trutschnig2011, Dette2013, Chatterjee2020, Junker2021}'s coefficient of correlation can be rewritten as

$$T^C(\pi) = \frac{\int f_{\nu}^\pi \left( F_{\nu}^{-1}(y) \right)^2 \, dy \, \mu(dx_1)}{\int \text{Var}(\mathbb{1}_{\{Y \geq y\}}) \, \nu(dy)}$$

where $F_{\mu_x}$ and $F_{\nu}^{-1}$ denotes the cdf of $\mu_x$ and $\nu$ respectively. In particular

$$\left( \int W(\pi, \mathcal{U}([0,1])) \mu(dx_1) \right)^2 \leq T^C(\pi) \leq 2 \left( \int W(\pi, \mathcal{U}([0,1])) \mu(dx_1) \right)$$

for $\pi \colon = (F_{\nu})_{\#} \pi_x$ and $\mathcal{U}([0,1])$ is the uniform distribution on $[0,1]$.

In particular $T^C$ can be estimated by the Wasserstein distance between $\pi_x$ and $\mathcal{U}([0,1])$. We note that compared to $\hat{W}$, $\pi_x$ is always compactly supported on $[0,1]$.

Next we compare $\widehat{W}$ to the functional obtained in\cite{Deb2020} for the specific case $(\mathcal{X}, d) = (\mathbb{R}^d, \| \cdot \|_2)$:

**Lemma 3.4.** The coefficient of correlation obtained in\cite{Deb2020} is given by

$$T^{\text{DGS}}(\pi) = 1 - \left( \int \frac{|x_2 - y_2| \pi_x_1(dx_2) \pi_x_1(dy) \mu(dx_1)}{\int |y - z_2| \nu(dy) \nu(dz)} \right) = \frac{\int |y - z| \nu(dy) \nu(dz) - \int |x_2 - y_2| \pi_x_1(dx_2) \pi_x_1(dy) \mu(dx_1)}{\int |y - z| \nu(dy) \nu(dz)}$$

and $T^{\text{DGS}}(\pi) \leq 2 \widehat{W}(\pi)$.

By a similar reasoning, we can derive the following corollary:

**Corollary 3.5.** Let $(\mathcal{X}, \| \cdot \|)$ be a normed space and let us define the measure of association derived from the norm $\| \cdot \|$ by

$$T^{\| \cdot \|}(\pi) = 1 - \left( \int \frac{\|y - z\| \pi_x_1(dy) \pi_x_1(dz) \mu(dx_1)}{\|y - z\| \nu(dy) \nu(dz)} \right).$$

Then we have $T^{\| \cdot \|}(\pi) \leq 2 \widehat{W}(\pi)$.

In particular all upper bounds derived in this article also hold for $T^{\| \cdot \|}(\pi)$, adjusting by a factor of 2. However, the relation

$$T^{\| \cdot \|}(\pi) = 0 \text{ if and only if } \pi = \mu \otimes \nu$$

might not hold, e.g. if $T^{\| \cdot \|}(\pi)$ only depends on a finite number of moments of $\pi$.

Thus in general, the functional $\pi \mapsto \widehat{W}(\pi)$ offers greater flexibility than $\pi \mapsto T^{\| \cdot \|}(\pi)$ as it can be defined for any metric $d$ instead of just any norm $\| \cdot \|$, while it always satisfies the properties (i)-(iii) of Theorem 2.2.
Next we compare $\hat{W}(\pi)$ to a (non-normalised version) of the Hellinger correlation introduced in [Geenens and Lafaye de Micheaux, 2020] for $\mu, \nu \in \text{Prob}(\mathbb{R})$. As this correlation is based on the Hellinger distance, singular measures are slightly intricate to handle. To avoid technicalities we thus only consider the following simple case:

**Lemma 3.6.** Assume that the probability measures $\mu, \nu \in \text{Prob}(\mathbb{R})$ and $\pi \in \Pi(\mu, \nu)$ have densities $f_\mu, f_\nu, f_\pi$ wrt. the Lebesgue measure. Then the Hellinger correlation $T^H(\pi)$ of [Geenens and Lafaye de Micheaux, 2020, Section 4] can be written as

$$T^H(\pi) = \int \int \left( \sqrt{f_\pi(x_1, x_2)} - \sqrt{f_\mu(x_1)f_\nu(x_2)} \right)^2 dx_1 dx_2.$$

If $\mu, \nu$ have bounded support, then there exists a constant $C > 0$ such that

$$\hat{W}(\pi) \leq C \int |y-z|^2 \nu(dy) \nu(dz).$$

Lastly let us compare the Wasserstein correlation to a classical benchmark: recall that if $\pi$ is a bivariate Gaussian distribution, then the association between $\mu$ and $\nu$ is famously quantified via Pearson’s correlation coefficient. It turns out that we can also compute $\hat{W}(\pi)$ explicitly in this case:

**Lemma 3.7 (Comparison with Pearson’s correlation coefficient in the case $p = 2$).** Let $(\mathcal{X}, d) = (\mathbb{R}, | \cdot |)$ and let $\pi = \mathcal{N}(a, \Sigma)$, where $a = (a_1, a_2)$ is the mean and

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \rho \sigma_1 \sigma_2 \\ \rho \sigma_1 \sigma_2 & \sigma_2^2 \end{bmatrix}$$

is the variance of the bivariate normal distribution $\pi$. Here we assume $\sigma_1, \sigma_2 > 0$ and note that $\rho \in [-1, 1]$ is Pearson’s correlation coefficient. Then $\hat{W}_2(\pi) = 1 - \sqrt{1 - \rho^2}$.

We now compare different coefficients of correlation for the bivariate standard normal case in Figure 3. As anticipated in Section 2 the Wasserstein correlation is convex in $\rho$.

**Remark 3.8.** It turns out that the term $\sqrt{1 - \rho^2}$ is the geometric mean of the eigenvalues of $\Sigma$, which can be interpreted as a geometric proxy for dependence. Unfortunately such an interpretation is no longer obvious in higher dimensions. Indeed for a bivariate normal distribution with covariance matrix

$$\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}$$

we still have

$$\pi_{x_1} = \mathcal{N}\left( a_2 + \Sigma_{21} \Sigma_{11}^{-1}(x_1 - a_1), \Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12} \right),$$

but in general dimensions we obtain

$$\hat{W}_2(\pi_{x_1}, \nu)^2 = \left| \Sigma_{21} \Sigma_{11}^{-1}(x_1 - a_1) \right|^2 + \text{tr}(\Sigma_{22}) + \text{tr}(\Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12})$$

$$- 2\text{tr}\left( (\Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12})^{1/2} \right).$$
4. AN ESTIMATOR FOR THE WASSERSTEIN CORRELATION AND ITS ASYMPTOTIC CONSISTENCY

We now investigate continuity properties of the functional $\pi \mapsto \overrightarrow{W}(\pi)$, which will enable us to construct a plugin estimator. We then check its asymptotic consistency.

Let us first state that the functional $\pi \mapsto \overrightarrow{W}(\pi)$ is continuous in the adapted Wasserstein distance $\mathcal{AW}$:

**Theorem 4.1.** For $\pi \in \Pi(\mu, \nu)$ and $\tilde{\pi} \in \Pi(\tilde{\mu}, \tilde{\nu})$ we have

$$\left| \int W(\pi_{x_1}, \nu) \mu(dx_1) - \int W(\tilde{\pi}_{y_1}, \tilde{\nu}) \tilde{\mu}(dy_1) \right| \leq \mathcal{AW}(\pi, \tilde{\pi}) + W(\nu, \tilde{\nu}) \leq 2\mathcal{AW}(\pi, \tilde{\pi})$$

and thus in particular

$$\left| \overrightarrow{W}(\pi) - \overrightarrow{W}(\tilde{\pi}) \right| \leq \frac{1}{f(\tilde{\nu})} \left( \mathcal{AV}(\pi, \tilde{\pi}) + W(\nu, \tilde{\nu}) + g(\nu, \tilde{\nu}) \right) \leq \frac{1}{f(\tilde{\nu})} \left( \mathcal{AW}(\pi, \tilde{\pi}) + 3W(\nu, \tilde{\nu}) \right) \leq \frac{4}{f(\tilde{\nu})} \mathcal{AW}(\pi, \tilde{\pi}),$$

where

$$f(\tilde{\nu}) := \int d(y, z) \tilde{\nu}(dy) \tilde{\nu}(dz),$$

$$g(\nu, \tilde{\nu}) := \left| \int d(y, z) \tilde{\nu}(dy) \tilde{\nu}(dz) - \int d(y, z) \nu(dy) \nu(dz) \right|.$$

We have the following immediate corollary:
Corollary 4.2. Let \( \pi \in \Pi(\mu, \nu) \) such that
\[
\int d(x_2, x_0) \nu(dx_2) < \infty
\]
for any \( x_0 \in \mathcal{X} \) and let \( \hat{\pi}^N \) be an AW-consistent estimator of \( \pi \). Then \( \hat{\mathcal{W}}(\hat{\pi}^N) \) is an asymptotically consistent estimator of \( \hat{\mathcal{W}}(\pi) \).

Proof. Theorem 4.1 yields
\[
\left| \mathcal{W}(\pi) - \hat{\mathcal{W}}(\hat{\pi}^N) \right| \leq \frac{4}{f(\hat{\pi}^N)} \mathcal{AW}(\pi, \hat{\pi}^N).
\]
By assumption we have \( \lim_{N \to \infty} \mathcal{AW}(\pi, \hat{\pi}^N) = 0 \). By the proof of Theorem 4.1 in the appendix we conclude that \( g(\nu, \hat{\pi}^N) \leq 2 \mathcal{AW}(\pi, \hat{\pi}^N) \) so that
\[
\lim_{N \to \infty} f(\hat{\pi}^N) = f(\nu),
\]
where \( f(\nu) > 0 \) by assumption. This concludes the proof.

We now give an explicit example of an AW-consistent estimator \( \hat{\pi}^N \), which will then naturally facilitate a plugin estimator \( \mathcal{W}(\hat{\pi}^N) \) for \( \mathcal{W}(\pi) \). We only discuss here the case where \( \pi \) is a probability measure on \( [0, 1]^d \), where we equip \( [0, 1]^d \) with the Euclidean metric \(|\cdot|_2\). Of course, our analysis can then easily be extended to probability measures on any compact subset of \( \mathbb{R}^d \). Determining an explicit AW-consistent estimator for non-compactly supported \( \pi \) is still an open question and left for future research.

Before we explain the details of the construction, we need to introduce some additional notation: for a subset \( F \) of \( \mathbb{R}^d \) let \( \text{diam}(F) := \sup_{x, y \in F} |x - y|_2 \) and for any set \( A \), let \(|A|\) denote the number of elements in \( A \). Lastly, for any \( \pi \in \text{Prob}([0, 1]^d) \) and any Borel set \( G \subseteq [0, 1]^d \) we define the conditional probability
\[
\pi_G(\cdot) = \frac{1}{\pi_1(G)} \int_G \pi_{x_1}(\cdot) \pi_1(dx_1) \in \text{Prob}([0, 1]^d),
\]
where we make the convention that \( \pi_G := \delta_0 \) if \( \pi_1(G) = 0 \).

Let us assume that we are given i.i.d. samples \( (X_1^1, X_2^1), (X_1^2, X_2^2), \ldots, (X_1^N, X_2^N) \) of \( \pi \). Let us partition the unit cube \([0, 1]^d\) into a disjoint union of a finite number of cubes and let \( \varphi^N : [0, 1]^d \to [0, 1]^d \) map each cube to its center. Then in particular \( \varphi^N \) has a finite range for each \( N \geq 1 \). We now set
\[
\hat{\pi}^N := \frac{1}{N} \sum_{n=1}^N \delta_{\varphi^N(X_1^n), \varphi^N(X_2^n)}
\]
for each \( N \geq 1 \). In other words, if we define
\[
\Phi^N := \{(\varphi^N)^{-1}(\{x\}) : x \in \varphi^N([0, 1]^d)\},
\]
then
\[
[0, 1]^d = \bigcup_{G \in \Phi^N} G \quad \text{disjoint}.
\]
One of the main results of Backhoff et al. [2021(+) is the following:
Lemma 4.3 ([Backhoff et al., 2021(+, Theorem 1.3]). Assume that \( \lim_{N \to \infty} |\Phi^N|/N = 0 \). Then the adapted empirical measures is a strongly consistent estimator, that is,
\[
\lim_{N \to \infty} AW(\pi, \hat{\pi}^N) = 0
\]
P-almost surely.

5. The case of independent marginals: \( \pi = \mu \otimes \nu \)

In this section we discuss convergence rates of \( \hat{\pi}^N \) for the case \( \pi = \mu \otimes \nu \). We then show how to construct a test for independence of \( \mu \) and \( \nu \) using the estimator \( \hat{\pi}^N \). As \( \hat{\pi} \in [0,1] \) for all \( \pi \in \Pi(\mu, \nu) \) we cannot hope for a CLT as in [Deb et al., 2020, Theorem 4.1]. However, we can still obtain parametric convergence rates. Indeed, the main insight of this section is the following result:

**Theorem 5.1.** If \( \pi = \mu \otimes \nu \) then we have for all \( \varepsilon > 0 \)
\[
P \left( \int \mathcal{W} \left( \hat{\pi}_1^N, \hat{\pi}_2^N \right) \hat{\pi}_1^N(dx) \geq \varepsilon \right) \leq \exp \left( \log(2) \left( \frac{|\Phi^N| + 1}{2d} \right) \right)
\]
and consequently
\[
\hat{\pi}^N = O_P \left( \frac{|\Phi^N|}{\sqrt{N}} \right).
\]

In particular, if
\[
\lim_{N \to \infty} \frac{|\Phi^N|}{\sqrt{N}} = 0 \quad \text{and} \quad \lim_{N \to \infty} \frac{|\Phi^N|^2}{\log N} = \infty,
\]
then there exists \( C = C(\nu) > 0 \) such that the test: reject \( \pi = \mu \otimes \nu \) if
\[
\hat{\pi}^N > C \frac{|\Phi^N|}{\sqrt{N}},
\]
satisfies the following:

- if \( \pi = \mu \otimes \nu \) then there exists \( N_0 = N_0(\omega) \in \mathbb{N} \) such that \( \hat{\pi}^N \leq C \frac{|\Phi^N|}{\sqrt{N}} \)
  for all \( N \geq N_0 \).
- if \( \pi \neq \mu \otimes \nu \), then there exists \( N_0 = N_0(\omega) \in \mathbb{N} \) such that \( \hat{\pi}^N > C \frac{|\Phi^N|}{\sqrt{N}} \)
  for all \( N \geq N_0 \).

We note here that as the construction of \( \hat{\pi}^N \) is fully explicit and no additional assumptions on the measure \( \pi \) are necessary, which makes the above result conceptually easy to apply.

Lastly, we can construct the following simple test statistic for independence of \( \mu \) and \( \nu \):

**Corollary 5.2.** Under the assumptions that \( \mu \) and \( \nu \) are non-atomic and \( \pi = \mu \otimes \nu \), there exists a constant \( C(\nu) \) such that the test: reject \( \pi = \mu \otimes \nu \) if
\[
\hat{\pi}^N > C(\nu) \left( \frac{2 |\Phi^N|}{\sqrt{\pi \frac{\sigma}{\sqrt{N}}} + \frac{\sigma}{\sqrt{N}} \Phi^{-1}(1 - \alpha)} \right),
\]
where \( \Phi^{-1} \) denotes the quantile function of the standard normal distribution and \( \sigma = 1 - 2/\pi \), has asymptotic significance level \( \alpha \).
Proof. As in the proof of Theorem 5.1 this follows from the inequality

\[ \tilde{W}(\hat{\pi}^N) \leq \frac{\sqrt{d} \tilde{T}_N(\pi)}{\int |x_2 - y| \, \hat{\pi}^N_2(dx_2) \, \hat{\pi}^N_2(dy)} \leq C(\nu) \tilde{T}_N(\pi) \]

for some \( C(\nu) > 0 \), which holds for all sufficiently large \( N \in \mathbb{N} \). Here \( \tilde{T}_N \) is given by

\[ \tilde{T}_N(\pi) := \sum_{G \in \Phi^N} \sum_{H \in \Phi^N} \left| \frac{|\{ n \in \{1, \ldots, N\} \text{ s.t. } X_n^1 \in G \}}{N} \cdot \frac{|\{ n \in \{1, \ldots, N\} \text{ s.t. } X_n^2 \in H \}}{N} \right| \]

We then conclude by Lemma \[Wiesel, 2021, Lemma 1.1\]. \( \square \)

6. General convergence rates for the Wasserstein correlation

We now derive general rates of convergence for \( \tilde{W}(\pi) \), using results recently obtained in \[Backhoff et al., 2021(+)\]. In particular we slightly refine the definition of \( \varphi^N \) and thus the adapted empirical measure \( \hat{\pi}^N \) given in Section 4 as follows: we set \( r = 1/3 \) for \( d = 1 \) and \( r = 1/(2d) \) for all \( d \geq 2 \). For all \( N \geq 1 \), let us now partition the cube \([0, 1]^d\) into the disjoint union of \( N^{-r} \) cubes with edges of length \( N^{-r} \) and let \( \varphi^N : [0, 1]^d \to [0, 1]^d \) map each such small cube to its center. As before we then set

\[ \hat{\pi}^N := \frac{1}{N} \sum_{n=1}^{N} \delta_{\varphi^N(X_n^1), \varphi^N(X_n^2)} \]

for each \( N \geq 1 \).

In order to quantify the speed of convergence, we assume the following regularity property on the disintegration of \( \pi \) for the remainder of this section:

**Assumption 6.1 (Lipschitz kernels).** There is a version of the (\( \mu \)-a.s. uniquely defined) disintegration such that the mapping

\[ ([0, 1]^d) \ni x_1 \mapsto \pi_{x_1} \in \text{Prob}([0, 1]^d) \]

is Lipschitz continuous, where \( \text{Prob}([0, 1]^d) \) is endowed with its usual Wasserstein distance \( W \).

\[Wiesel, 2021\] Lemma 1.3] and \[Wiesel, 2021\] Lemma 1.4] stated in the appendix together with Theorem 4.1 immediately enable us to deduce average convergence rates and a deviation result for the plugin estimator \( \tilde{W}(\hat{\pi}^N) \). More concretely we obtain the following:

**Theorem 6.2.** Under Assumption 6.1 there is a constant \( C > 0 \) such that

\[ \mathbb{E} \left| \int W(\hat{\pi}_1^N, \hat{\pi}_2^N) \, \hat{\pi}_1^N(dx_1) - \int W(\pi_{x_1}, \nu) \, \mu(dx_1) \right| \]

\[ \leq C(\nu) \cdot \begin{cases} 
N^{-1/3} & \text{for } d = 1, \\
N^{-1/4} \log(N + 1) & \text{for } d = 2, \\
N^{-1/(2d)} & \text{for } d \geq 3.
\end{cases} \]
In particular we have

\[ |\tilde{W}(\hat{\pi}^N) - \tilde{W}(\pi)| = \begin{cases} O_P(N^{-1/3}) & \text{for } d = 1, \\ O_P(N^{-1/(2d)}) & \text{for } d \geq 2. \end{cases} \]

**Remark 6.3.** We note that both [Dette et al., 2013, Theorem 5.1] as well as [Chatterjee, 2020, Theorem 2.2] (under the assumption that \( \pi = \mu \otimes \nu \)) derive a CLT for their corresponding estimators of the correlation coefficient \( T_{DGSC} \), while our convergence rates suffer from the “curse of dimensionality” – a by now well-studied phenomenon for Wasserstein distances (see e.g. Fournier and Guillin [2015], Weed and Bach [2019]). In particular [Dette et al. 2013, Chatterjee 2020] achieve strictly better convergence rates than we do even if \( d = 1 \), at least if \( \pi \neq \mu \otimes \nu \). We recall however that \( T_{DGSC} \) is only well-defined for a 1-dimensional distribution \( \nu \in \text{Prob}(\mathbb{R}) \) and cannot easily be generalised. In contrast, the main goals of this article was to provide a correlation coefficient which can be defined on arbitrary Polish spaces \( X \).

**Proof.** By Theorem 4.1 we have

\[ \int W\left(\hat{\pi}^N_{x_1}, \hat{\pi}^N_{x_2}\right) \hat{\pi}^N_{x_1}(dx_1) - \int W\left(\pi_{x_1}, \nu\right) \mu(dx_1) \leq 2AW(\pi, \hat{\pi}^N), \]

so the first claim follows from [Wiesel, 2021, Lemma 1.3] replacing \( C \) by \( 2C \). Moreover, Theorem 4.1 also states that

\[ |\tilde{W}(\pi) - \tilde{W}(\hat{\pi}^N)| \leq \frac{4}{f(\hat{\pi}^N)^2} AW(\pi, \hat{\pi}^N) \]

Combining this with [Wiesel, 2021] Lemma 1.2, which states that

\[ \left(\sqrt{N} \wedge 2 \cdot \sup_x \frac{1}{|\hat{\phi}^N(x) - x|}\right) \left(f(\hat{\pi}^N_2) - f(\nu)\right) = \left(\sqrt{N} \wedge \frac{N^r}{2}\right) \left(f(\hat{\pi}^N_2) - f(\nu)\right) = N^r \left(f(\hat{\pi}^N_2) - f(\nu)\right) = O_P(1), \]

and as \( f(\nu) > 0 \), we again obtain the claim from [Wiesel, 2021, Lemma 1.3]. This concludes the proof. \( \square \)

In a similar fashion we can derive concentration bounds from [Wiesel, 2021] Lemma 1.4:

**Theorem 6.4.** Under Assumption 6.1 there are constants \( c, C > 0 \) such that

\[ P \left[ \left| \int W\left(\hat{\pi}^N_{x_1}, \hat{\pi}^N_{x_2}\right) \hat{\pi}^N_{x_1}(dx_1) - \int W\left(\pi_{x_1}, \nu\right) \mu(dx_1) \right| \geq 2C \text{rate}(N) + \varepsilon \right] \leq 4 \exp\left( -cN\varepsilon^2 \right) \]

for all \( N \geq 1 \) and all \( \varepsilon > 0 \).
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Proof. Using again Theorem 4.1, this time together with Lemma [Wiesel, 2021, Lemma 1.4], we obtain the existence of two constants $c, C > 0$

$$P \left[ \left| \int W \left( \hat{\pi}^N_1, \hat{\pi}^N_2 \right) (dx_1) - \int W \left( \pi_1, \nu \right) \mu(dx_1) \right| \geq 2C \text{rate}(N) + \varepsilon \right]$$

$$\leq P \left[ 2AW(\mu, \hat{\pi}^N) \geq 2C \text{rate}(N) + \varepsilon \right]$$

$$\leq 4 \exp \left( -cN\varepsilon^2 \right)$$

replacing $c$ by $c/4$ in [Wiesel, 2021, Lemma 1.4]. This concludes the proof. □

7. NUMERICAL EXAMPLES

In this section we numerically compare the Wasserstein correlation with other measures of dependence. In particular we exhibit the behaviour of the Pearson, Spearman, Chatterjee, distance and Wasserstein correlation. The code for the numerical implementation can be found under https://github.com/johanneswiesel/Wasserstein-correlation. In particular we use the Xicor package (https://github.com/czbiohub/xicor/) to compute Chatterjee’s correlation coefficient. We use the GitHub depository satra/distcorr.py (https://gist.github.com/satra/aa3d19a12b74e9ab7941) to compute the distance correlation and the POT package (https://pythonot.github.io) to compute the Wasserstein correlation efficiently using entropic penalisation. For simplicity we keep the penalisation parameter fixed at level $\varepsilon = 0.01$. While entropic penalisation considerably speeds up the computation compared to the exact solution of the optimal transport problem, the computational burden of the Wasserstein correlation is nevertheless non-negligible compared to the other measures of association discussed here. Mitigating these computational disadvantages (particularly in high dimensions) is however an active topic of research. In the case of $\tilde{W}$ it might also be overcome by using an estimation procedure specifically adapted for the Wasserstein correlation.

In order to compare the behaviour of the correlation coefficients listed above for different kinds of dependence between $X_1$ and $X_2$, we plot four examples in Figures 2 and 3. In all cases we take $X_1$ to be uniformly distributed on the interval $[0, 1]$, while $X_2 = f(\rho X_1 + \sqrt{1 - \rho^2} U)$ for an independent random variable $U$ with the same law as $X_1$. We consider the functions $f(x) = x$, $f(x) = |x - 0.5|$, $f(x) = (x - 0.5)^3$ and $f(x) = \sin(3x)$. We take $N = 1000$ samples and plot the average over 30 different draws below.

While the traditional coefficients perform slightly better for near-linear relationships between $X_1$ and $X_2$, the strength of the Wasserstein correlation becomes evident in the non-linear setting: for the functions $f(x) = |x - 0.5|$ and $f(x) = \sin(3x)$, where Pearson and Spearman’s correlation do not pick up any functional relationship, the Wasserstein correlation increases faster than distance correlation and Chatterjee’s correlation.

Next we discuss an application to historical data: we compare our estimate for the Wasserstein correlation with other correlation coefficients on Sir Francis Galton’s peas data. The estimator $T^C$ was already computed in [Chatterjee, 2020, Section 3] and we refer to the exposition there for a historical discussion. The data consists of
700 pairs \((X_1, X_2)\) of mean diameters of sweet peas of mother plants and daughter plants. We list the results in Figure 4.

| Correlation coefficient   | Value   | Correlation coefficient   | Value   |
|---------------------------|---------|---------------------------|---------|
| Pearson’s correlation     | 0.3463  | Pearson’s correlation     | 0.3463  |
| Spearman’s correlation    | 0.3615  | Spearman’s correlation    | 0.3615  |
| Distance correlation      | 0.3216  | Distance correlation      | 0.3216  |
| Chatterjee’s correlation  | 0.1186  | Chatterjee’s correlation  | 0.9224  |
| Wasserstein correlation   | 0.3124  | Wasserstein correlation   | 0.9409  |

Figure 4. Correlation between \(X_1\) and \(X_2\) (left) and \(X_2\) and \(X_1\) (right) for different correlation coefficients.

We observe that the Wasserstein correlation between \(X_1\) and \(X_2\) is only slightly lower than classical coefficients like Pearson’s or Spearman’s correlation, while Chatterjee’s correlation with a value of 0.12 (averaged over 10\(^5\) samples) is quite low. When reversing the roles of \(X_1\) and \(X_2\), both the Wasserstein correlation and
Chatterjee’s correlation increase decisively, hinting at the deterministic relationship $X_1 = f(X_2)$ for some function $f$. As in [Chatterjee 2020], this can be made plausible by the specific structure of the data.

Now we consider the case of independent marginals $\pi = \mu \otimes \nu$ of Section 5 and compare the power functions of four different tests for independence: these are derived from our Corollary 5.2, [Chatterjee 2020, Theorem 2.1], [Szekely et al. 2007, Theorem 6] and [Shi et al. 2020a, Theorem 3.1] respectively. We estimate the power function on 1500 samples over 200 draws. We remind the reader however that all four tests only have a theoretical foundation for the asymptotic regime $N \to \infty$. Despite our best efforts we have not been able to resolve the numerical instabilities occurring in the power of Chatterjee’s test using the Xicor package.

In Figure 5 we again plot the corresponding power functions for the uniform distribution on the unit interval $[0, 1]$ with the correlated random variable $X_2 = \rho X_1 + \sqrt{1 - \rho^2} U$ for an independent uniform random variable $U$. We also consider the transform $\log(X_1^2)$ vs $\log(X_2^2)$. In both cases, the tests discussed in [Szekely et al. 2007, Theorem 6] and [Shi et al. 2020a, Theorem 3.1] seem to yield slightly superior behaviour of the corresponding power function, while our results as well as [Chatterjee 2020, Theorem 2.1] exhibit a less spiked shape.

8. Outlook

While the theoretical properties of the Wasserstein correlation established in Sections 3 and 4 hold in great generality, the development of an estimation procedure for $\tilde{W}$ on general Polish spaces is still an open problem. In this paper we have exhibited a viable estimation approach for compactly supported probability measures, leveraging results from [Backhoff et al. 2021(+)]. It is however a non-trivial task to extend their framework to general Polish spaces and show consistency of the adapted empirical measure. We leave this extension to future work.

In a similar vein, the test of independence derived in Section 5 relies on non-optimal convergence rates even for compactly supported probability measures $\pi$ (for a numerical example see Appendix [Wiesel 2021, Section 2]). We believe that these can
be improved once a deeper understanding of the exact distribution of $\overrightarrow{W}_N$ in the asymptotic regime is available. We remark however that this a difficult task: obtaining convergence rates even for the (non-adapted) Wasserstein distance is still an active research field and recent works often rely on intricate probabilistic estimates (see e.g. Fournier and Guillin [2015], Sommerfeld and Munk [2016]).

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References

Julio Backhoff, Daniel Bartl, Mathias Beiglböck, and Johannes Wiesel. Estimating processes in adapted Wasserstein distance. *Ann. Apl. Prob.*, available at arXiv:2002.07261, 2021(+).

Julio Backhoff-Veraguas, Daniel Bartl, Mathias Beiglböck, and Manu Eder. Adapted Wasserstein Distances and Stability in Mathematical Finance. *Financ. Stoch.*, January to appear.

Julius Blum, Jack Kiefer, and Murray Rosenblatt. Distribution free tests of independence based on the sample distribution function. *Ann. Math. Stat.*, pages 485–498, 1961.

Sky Cao and Peter J Bickel. Correlations with tailored extremal properties. *arXiv preprint arXiv:2008.10177*, 2020.

S Chatterjee. A new coefficient of correlation. *J. Amer. Statist. Assoc.*, pages 1–21, 2020.

Donato Michele Cifarelli and Eugenio Regazzini. On the centennial anniversary of gini’s theory of statistical relations. *Metron*, 75(2):227–242, 2017.

Nabarun Deb, Promit Ghosal, and Bodhisattva Sen. Measuring association on topological spaces using kernels and geometric graphs. *arXiv preprint arXiv:2010.01768*, 2020.

Holger Dette, Karl Siburg, and Pavel Stoimenov. A copula-based non-parametric measure of regression dependence. *Scand. J. Stat.*, 40(1):21–41, 2013.

Nicolas Fournier and Arnaud Guillin. On the rate of convergence in Wasserstein distance of the empirical measure. *Probab. Theory Related Fields*, 162(3-4):707–738, 2015.

Jerome Friedman and Lawrence Rafsky. Graph-theoretic measures of multivariate association and prediction. *Ann. Statist.*, 11(2):377–391, 1983.

Fabrice Gamboa, Thierry Klein, and Agnès Lagnoux. Sensitivity analysis based on Cramér–von Mises distance. *SIAM/ASA J. Uncertain. Quantif.*, 6(2):522–548, 2018.

Gery Geenens and Pierre Lafaye de Micheaux. The Hellinger correlation. *J. Amer. Statist. Assoc.*, pages 1–15, 2020.

Alison L Gibbs and Francis Edward Su. On choosing and bounding probability metrics. *Int. Stat. Rev.*, 70(3):419–435, 2002.

Corrado Gini. *Nuovi contributi alla teoria delle relazioni statistiche*. Premiate Officine Grafiche di Carlo Ferrari, 1915.
Arthur Gretton and László Györfi. Consistent nonparametric tests of independence. *J. Mach. Learn. Res.*, 11:1391–1423, 2010.

Florian Griesenberger, Robert R Junker, and Wolfgang Trutschnig. On a multivariate copula-based dependence measure and its estimation. *arXiv preprint arXiv:2109.12883*, 2021.

Robert R Junker, Florian Griesenberger, and Wolfgang Trutschnig. Estimating scale-invariant directed dependence of bivariate distributions. *Computational Statistics & Data Analysis*, 153:107058, 2021.

Chenli Ke and Xiangrong Yin. Expected conditional characteristic function-based measures for testing independence. *J. Amer. Statist. Assoc.*, 2019.

Martin Knott and Cyril S Smith. On the optimal mapping of distributions. *J. Optim. Theory Appl.*, 43(1):39–49, 1984.

Rémi Lassalle. Causal transport plans and their Monge-Kantorovich problems. *Stoch. Anal. Appl.*, 36(3):452–484, 2018.

Edward H Linfoot. An informational measure of correlation. *Inf. Control*, 1(1):85–89, 1957.

Russell Lyons et al. Distance covariance in metric spaces. *Ann. Probab.*, 41(5):3284–3305, 2013.

Gilles Mordant and Johan Segers. Measuring dependence between random vectors via optimal transport. *arXiv preprint arXiv:2104.14023*, 2021.

Tamás F Móri and Gábor J Székely. Four simple axioms of dependence measures. *Metrika*, 82(1):1–16, 2019.

Tamás F Móri and Gábor J Székely. The earth mover’s correlation. *Ann. Univ. Sci. Budapest, Sect. Comput.*, 50:208–349, 2020.

Thomas Giacomo Nies, Thomas Staudt, and Axel Munk. Transport dependency: Optimal transport based dependency measures. *arXiv preprint arXiv:2105.02073*, 2021.

Sherjil Ozair, Corey Lynch, Yoshua Bengio, Aaron van den Oord, Sergey Levine, and Pierre Sermanet. Wasserstein dependency measure for representation learning. *arXiv preprint arXiv:1903.11780*, 2019.

Georg Pflug. Version-independence and nested distributions in multistage stochastic optimization. *SIAM J. Optim.*, 20(3):1406–1420, 2009.

Georg Pflug and Alois Pichler. A distance for multistage stochastic optimization models. *SIAM J. Optim.*, 22(1):1–23, 2012.

Giovanni Puccetti. Measuring linear correlation between random vectors. *Available at SSRN 3116066*, 2019.

Alfréd Rényi. On measures of dependence. *Acta Math. Acad. Sci. Hungar.*, 10(3-4):441–451, 1959.

Murray Rosenblatt. A quadratic measure of deviation of two-dimensional density estimates and a test of independence. *Ann. Statist.*, pages 1–14, 1975.

Marco Scarsini. On measures of concordance. *Stochastica*, 8(3):201–218, 1984.

Berthold Schweizer, Edward F Wolff, et al. On nonparametric measures of dependence for random variables. *Ann. Statist.*, 9(4):879–885, 1981.

Hongjian Shi, Mathias Drton, and Fang Han. Distribution-free consistent independence tests via center-outward ranks and signs. *J. Amer. Statist. Assoc.*, pages 1–16, 2020a.

Hongjian Shi, Mathias Drton, and Fang Han. On the power of Chatterjee rank correlation. *arXiv preprint arXiv:2008.11619*, 2020b.
Max Sommerfeld and Axel Munk. Inference for empirical Wasserstein distances on finite spaces. arXiv preprint arXiv:1610.03287, 2016.
Gábor J Székely, Maria L Rizzo, Nail K Bakirov, et al. Measuring and testing dependence by correlation of distances. Ann. Statist., 35(6):2769–2794, 2007.
Wolfgang Trutschnig. On a strong metric on the space of copulas and its induced dependence measure. Journal of mathematical analysis and applications, 384(2):690–705, 2011.
A. Van der Vaart. Asymptotic statistics, volume 3. Cambridge University Press, 1998.
C. Villani. Optimal Transport: Old and New, volume 338. Springer, 2008.
Jonathan Weed and Francis Bach. Sharp asymptotic and finite-sample rates of convergence of empirical measures in Wasserstein distance. Bernoulli, 4(A):2620–2648, 2019.
Johannes Wiesel. Supplement to “measuring association with wasserstein distances”. 2021.
Yijun Xiao and William Yang Wang. Disentangled representation learning with wasserstein total correlation. arXiv preprint arXiv:1912.12818, 2019.
Kai Zhang. Bet on independence. J. Amer. Statist. Assoc., 114(528):1620–1637, 2019.

Appendix A. Remaining proofs

Proof of Theorem 2.2

(i) Clearly $\overline{W}(\pi) \geq 0$. Furthermore, replacing the $W(\pi_{x_1}, \nu)$-optimal coupling in the numerator of $\overline{W}(\pi)$ by the the product coupling $\pi_{x_1} \otimes \nu$ we obtain the upper bound

$$
\int W(\pi_{x_1}, \nu) \mu(dx_1) \leq \int \int d(y, z) \pi_{x_1}(dy) \nu(dz) \mu(dx_1)
$$

(3)

(ii) If $\overline{W}(\pi) = 0$ then $W(\pi_{x_1}, \nu) = 0$ $\mu$-a.s. and thus $\pi_{x_1} = \nu$ $\mu$-a.s. by positive definiteness of the Wasserstein distance. In particular

$$
(4) \quad \pi(A \times B) = \int_A \pi_{x_1}(B) \mu(dx_1) = \int_A \nu(B) \mu(dx_1) = (\mu \otimes \nu)(A \times B)
$$

for any Borel subsets $A, B \subseteq \mathcal{X}$ and thus $\pi = \mu \otimes \nu$. On the other hand, if $\pi = \mu \otimes \nu$, then using again (4) we conclude that $\pi_{x_1} = \nu$ $\mu$-a.s. by $\mu$-a.s. uniqueness of disintegrations. Thus $W(\pi_{x_1}, \nu) = 0$ $\mu$-a.s., which in turn implies $\overline{W}(\pi) = 0$. This shows the claim.

(iii) Note that cyclical monotonicity of optimal transport for the cost function $c(x, y) = d(x, y)$ (see e.g. Villani [2008, Def. 5.1]) implies that inequality (3) is strict unless $\pi_{x_1} = \delta_{f(x_1)}$ for some function $f : \mathcal{X} \to \mathcal{X}$: indeed, consider the product coupling $\pi_{x_1} \otimes \nu$ and define the set

$$
A := \{ x_1 \in \mathcal{X} : \exists y_1, \tilde{y}_1 \in \text{supp}(\pi_{x_1}), \ y_1 \neq \tilde{y}_1 \}.
$$

Let us assume towards a contradiction that $\mu(A) > 0$. By the definition of the disintegration $x_1 \mapsto \pi_{x_1}$ and tightness of probability measures we then obtain

$$
\mu \left( \{ x_1 \in \mathcal{X} : \exists y_1, \tilde{y}_1 \in \text{supp}(\pi_{x_1}) \cap \text{supp}(\nu), \ y_1 \neq \tilde{y}_1 \} \right) > 0.
$$
Next, by the definition of the product coupling $\pi_x \otimes \nu$ we have that
$$\mu(\{x_1 \in X : \exists (y_1, \tilde{y}_1), (\tilde{y}_1, y_1) \in \text{supp}(\pi_x \otimes \nu), y_1 \neq \tilde{y}_1\}) > 0.$$ 
Now we note that
$$d(y_1, \tilde{y}_1) + d(\tilde{y}_1, y_1) > d(y_1, y_1) + d(\tilde{y}_1, \tilde{y}_1) = 0,$$
so that
$$\mu(\{x_1 \in X : \text{supp}(\pi_x \otimes \nu) \text{ is not cyclically monotone}\}) > 0,$$
a contradiction. On the other hand for $\pi_x = \delta_{f(x_1)}$ we have
$$\int \mathcal{W}(\pi_x, \nu) \mu(dx_1) = \int d(f(x_1), z) \mu(dx_1) \nu(dz)$$
$$\quad = \int d(y, z) \nu(dy) \nu(dz).$$
This concludes the proof.

\[ \square \]

**Proof of Lemma 3.3** According to \cite{Chatterjee} [Theorem 1.1] we have
$$T^C(\pi) = \frac{\int \text{Var} \left( \mathbb{E} \left[ \mathbb{1}_{\{Y \geq y\}} \mid X \right] \right) \nu(dy)}{\int \text{Var} \left( \mathbb{1}_{\{Y \geq y\}} \right) \nu(dy)}$$
$$\quad = \frac{\int \int (\pi_{x_1}[y, \infty) - \int \pi_{x_1}[y, \infty) \mu(dx_1))^2 \mu(dx_1) \nu(dy)}{\int \text{Var} \left( \mathbb{1}_{\{Y \geq y\}} \right) \nu(dy)}$$
$$\quad = \int \int (\pi_{x_1}[y, \infty) - \nu[y, \infty))^2 \mu(dx_1) \nu(dy).$$
In particular we now note that by Fubini’s theorem
$$\int \int (\pi_{x_1}[y, \infty) - \nu[y, \infty))^2 \mu(dx_1) \nu(dy) = \int \int (\pi_{x_1}[y, \infty) - \nu[y, \infty))^2 \nu(dy) \mu(dx_1)$$
$$\quad = \int \int (F_{\pi_{x_1}}(y) - F_{\nu}(y))^2 \nu(dy) \mu(dx_1)$$
$$\quad = \int \int (F_{\pi_{x_1}}(F_{\nu}^{-1}(y)) - F_{\nu}(F_{\nu}^{-1}(y)))^2 dy \mu(dx_1)$$
$$\quad = \int \int (F_{\nu}(F_{\nu}^{-1}(y)) - y)^2 dy \mu(dx_1)$$
$$\quad \leq \int \int |F_{\nu}(F_{\nu}^{-1}(y)) - y| dy \mu(dx_1)$$
$$\quad = \mathcal{W}(\tilde{\pi}_{x_1}, \mathcal{U}([0, 1])) \mu(dx_1)$$
for $\tilde{\pi}_{x_1} := (F_{\nu})_{\pi_{x_1}}$, and $\mathcal{U}([0, 1])$ is the uniform distribution on $[0, 1]$. On the other hand we also obtain from the above that
$$\left(\int \int (\pi_{x_1}[y, \infty) - \nu[y, \infty))^2 \mu(dx_1) \nu(dy) \right)^{1/2} \geq \int \int |F_{\mu_{x_1}}(F_{\nu}^{-1}(y)) - y| dy \mu(dx_1)$$
$$\quad = \mathcal{W}(\tilde{\pi}_{x_1}, \mathcal{U}([0, 1])) \mu(dx_1).$$
This concludes the proof.
Proof of Lemma 3.4: Choosing $\gamma \in \Pi(\nu, \pi_{x_1})$ such that

$$\mathcal{W}(\nu, \pi_{x_1}) = \int |y - z|_2 \gamma^{x_1}(dy, dz)$$

for each $x_1 \in \mathcal{X}$, it is not hard to see that

$$T^{DGS}(\pi) = \int \frac{(|y - z|_2 - |\tilde{y} - \tilde{z}|) \gamma^{x_1}(dy, d\tilde{y}) \gamma^{x_1}(dz, d\tilde{z}) \mu(dx_1)}{\int |y - z|_2 \nu(dy) \nu(dz)}$$

$$\leq \int \frac{|y - z - (\tilde{y} - \tilde{z})|_2 \gamma^{x_1}(dy, d\tilde{y}) \gamma^{x_1}(dz, d\tilde{z}) \mu(dx_1)}{\int |y - z|_2 \nu(dy) \nu(dz)}$$

$$\leq \int \frac{|y - \tilde{y}|_2 \gamma^{x_1}(dy, d\tilde{y}) \mu(dx_1) + |z - \tilde{z}|_2 \gamma^{x_1}(dz, d\tilde{z}) \mu(dx_1)}{\int |y - z|_2 \nu(dy) \nu(dz)}$$

$$= \int \frac{2 \mathcal{W}(\pi_{x_1}, \nu) \mu(dx_1)}{\int |y - z|_2 \nu(dy) \nu(dz)} = 2\overrightarrow{\mathcal{W}}(\pi).$$

In conclusion, in the case $(\mathcal{X}, d) = (\mathbb{R}^d, \cdot_2)$, the functional $T^{DGS}(\pi)$ is dominated by $2\overrightarrow{\mathcal{W}}(\pi)$. \qed

Proof of Lemma 3.6: Recall from Geenens and Lafaye de Micheaux \citeyear{Geenens2020}, Section 4 that

$$T^H(\pi) = \int \int \left( \sqrt{f_\pi(x_1, x_2)} - \sqrt{f_\nu(x_1, x_2)} \right)^2 dx_1 dx_2.$$

If $\mu, \nu$ have bounded support, then $\pi \in \Pi(\mu, \nu)$ also has bounded support and standard results on comparing metrics on $\text{Prob}(\mathbb{R})$ (see e.g. \cite{Gibbs2002}) imply that there exists a constant $C > 0$ such that

$$\mathcal{W}(\pi_{x_1}, \nu) \leq C \int \left( \sqrt{f_{\pi_{x_1}}(x_2)} - \sqrt{f_\nu(x_2)} \right)^2 dx_2.$$

In particular

$$\int \mathcal{W}(\pi_{x_1}, \nu) f_\mu(x_1) dx_1 \leq C \int \int \left( \sqrt{f_{\pi_{x_1}}(x_2)} - \sqrt{f_\nu(x_2)} \right)^2 dx_2 f_\mu(x_1) dx_1$$

$$\leq C \int \int \left( \sqrt{f_\mu(x_1)} f_{\pi_{x_1}}(x_2) - \sqrt{f_\mu(x_1)} f_\nu(x_2) \right)^2 dx_2 dx_1$$

$$= C \int \int \left( \sqrt{f_\pi(x_1, x_2)} - \sqrt{f_\mu(x_1)} f_\nu(x_2) \right)^2 dx_2 dx_1 = CT^H(\pi)$$

by Tonelli’s theorem and the definition of the conditional density $f_{\pi_{x_1}}(x_2)$. \qed

Proof of Lemma 3.7: Note that we can immediately read off the marginal distributions $\mu = \mathcal{N}(a_1, \sigma_1)$ and $\nu = \mathcal{N}(a_2, \sigma_2^2)$, as well as

$$\pi_{x_1} = \mathcal{N} \left( a_2 + \frac{\sigma_2^2}{\sigma_1} \rho(x_1 - a_1), (1 - \rho^2)\sigma_2^2 \right).$$
Furthermore, by the explicit formula for the 2-Wasserstein distance between Gaussians (see e.g. [Knott and Smith, 1984, Simple example]) one can compute

\[ W_2(\pi_x, \nu)^2 = \left( a + \frac{\sigma^2}{\sigma_1^2} \rho(x_1 - a_1) - a_2 \right)^2 + \sigma_1^2 \left( 1 - \rho^2 \right) \sigma_2^2 - 2 \sqrt{(1 - \rho^2) \sigma_2^4} \]

so that

\[ \int W_2(\pi_x, \nu)^2 \mu(dx_1) = \rho^2 \sigma_2^2 + \sigma_1^2 + (1 - \rho^2) \sigma_2^2 - 2 \sigma_2^2 \sqrt{1 - \rho^2} \]

Lastly

\[ \left| \int W_2(\pi_x, \nu)^2 \mu(dx_1) - \int W_2(\pi_\tilde{x}, \tilde{\nu}) \tilde{\mu}(dy_1) \right| \]

and the claim follows. \( \square \)

**Proof of Theorem 4.1.** Fix \( \delta > 0 \) and take \( \gamma \in \Pi(\mu, \tilde{\mu}) \) such that

\[ \int [d(x_1, y_1) + W(\pi_{x_1}, \tilde{\pi}_{y_1})] \gamma(dx_1, dy_1) \leq AW(\pi, \tilde{\pi}) + \delta. \]

A repeated application of the triangle inequality now yields

\[ \left| \int W(\pi_x, \nu) \mu(dx_1) - \int W(\pi_{x_1}, \tilde{\nu}) \tilde{\mu}(dy_1) \right| \]

where the last inequality follows from the particular choice of \( \gamma \) in (5). As \( \delta > 0 \) was arbitrary and noting that

\[ W(\nu, \tilde{\nu}) \leq W(\pi, \tilde{\pi}) \leq AW(\pi, \tilde{\pi}), \]

we conclude that

\[ \left| \int W(\pi_x, \nu) \mu(dx_1) - \int W(\pi_{x_1}, \tilde{\nu}) \tilde{\mu}(dy_1) \right| \leq AW(\pi, \tilde{\pi}) + W(\nu, \tilde{\nu}) \]

\[ \leq 2AW(\pi, \tilde{\pi}), \]
which shows the first claim. Let us define
\[ f(\nu, \tilde{\nu}) := \int d(y, z) \nu(dy) \nu(dz) \cdot \int d(y, z) \tilde{\nu}(dy) \tilde{\nu}(dz) \]
and recall
\[ f(\tilde{\nu}) = \int d(y, z) \tilde{\nu}(dy) \tilde{\nu}(dz). \]
The second claim now follows from writing
\[
\begin{align*}
\left| \tilde{\mathcal{W}}(\pi) - \mathcal{W}(\tilde{\pi}) \right| &= \frac{1}{f(\nu, \tilde{\nu})} \left| \int \mathcal{W}(\pi_{x_1}, \nu) \mu(dx_1) \int d(y, z) \nu(dy) \nu(dz) 
- \int \mathcal{W}(\tilde{\pi}_{y_1}, \tilde{\nu}) \tilde{\mu}(dy_1) \int d(y, z) \nu(dy) \nu(dz) \right| \\
&\leq \frac{1}{f(\nu, \tilde{\nu})} \left[ \int d(y, z) \nu(dy) \nu(dz) - \int d(y, z) \nu(dy) \nu(dz) \right] \\
&\quad \cdot \int \mathcal{W}(\pi_{x_1}, \nu) \mu(dx_1) \\
&\quad + \left| \int \mathcal{W}(\pi_{x_1}, \nu) \mu(dx_1) - \int \mathcal{W}(\tilde{\pi}_{y_1}, \tilde{\nu}) \tilde{\mu}(dy_1) \right| \\
&\quad \cdot \int d(y, z) \nu(dy) \nu(dz) \\
&\leq \frac{1}{f(\nu, \tilde{\nu})} [g(\nu, \tilde{\nu}) + \mathcal{A} \mathcal{W}(\pi, \tilde{\pi}) + \mathcal{W}(\nu, \tilde{\nu})] \\
&\leq \frac{1}{f(\nu, \tilde{\nu})} [g(\nu, \tilde{\nu}) + 2 \mathcal{A} \mathcal{W}(\pi, \tilde{\pi})]
\end{align*}
\]
for any \( x_0 \in X \), where we have used the estimate \( \int \mathcal{W}(\pi_{x_1}, \nu) \mu(dx_1) \leq \int d(y, z) \nu(dy) \nu(dz) \)
and the definition of \( f \) in the second inequality. Now let \( \gamma \in \Pi(\tilde{\nu}, \nu) \) be an \( \mathcal{W} \)-optimal coupling between \( \tilde{\nu} \) and \( \nu \). Using again the triangle inequality we then conclude that
\[
\begin{align*}
g(\nu, \tilde{\nu}) &= \left| \int d(y, z) \nu(dy) \nu(dz) - \int d(y, z) \nu(dy) \nu(dz) \right| \\
&\leq \left| \int d(y, z) \nu(dy) \nu(dz) - \int d(y, \tilde{z}) \tilde{\nu}(dy) \nu(d\tilde{z}) \right| \\
&\quad + \left| \int d(\tilde{y}, z) \tilde{\nu}(d\tilde{y}) \nu(dz) - \int d(y, z) \nu(dy) \nu(dz) \right| \\
&\leq \int |d(y, z) - d(y, \tilde{z})| \nu(dy) \gamma(dz, d\tilde{z}) \\
&\quad + \int |d(\tilde{y}, z) - d(y, z)| \nu(dz) \gamma(d\tilde{y}, dy) \\
&\leq \int d(z, \tilde{z}) \tilde{\nu}(dy) \gamma(dz, d\tilde{z}) + \int d(\tilde{y}, y) \tilde{\nu}(dz) \gamma(d\tilde{y}, dy) \\
&= 2 \mathcal{W}(\nu, \tilde{\nu}) \leq 2 \mathcal{A} \mathcal{W}(\pi, \tilde{\pi}).
\end{align*}
\]
This concludes the proof. \( \Box \)
Proof of Lemma 4.3. The proof follows from the same arguments as in [Backhoff et al., 2021] Proof of Theorem 1.3 with a few minor changes. We first remark that it is enough to show the claim for $\pi$ with continuous disintegration $x_1 \mapsto \pi_{x_1}$.

Indeed, the general case then follows exactly as in [Backhoff et al., 2021] Proof of Theorem 1.3.

We now note that [Backhoff et al., 2021] Proof of Lemma 3.4 states explicitly that

$$E \left[ W \left( \pi_1, \hat{\pi}_1^N \right) \right] \leq CR(N),$$

where the function $R$ is defined as

$$R : [0, +\infty) \to [0, +\infty], \quad R(u) := \begin{cases} 
    u^{-1/2} & \text{if } d = 1 \\
    u^{-1/2} \log(u + 3) & \text{if } d = 2 \\
    u^{-1/d} & \text{if } d \geq 3.
\end{cases}$$

Furthermore [Backhoff et al., 2021] also states that

$$E \left[ \sum_{G \in \Phi^N} \hat{\pi}_G^N(G) W \left( \mu_G, \hat{\mu}_G^N \right) | G_i^N \right] \leq R \left( \frac{N}{\Phi^N} \right),$$

so that we can conclude as in [Backhoff et al., 2021] Proof of Lemma 5.3 that

$$\mathcal{W} \left( \pi, \hat{\pi}_N \right) \leq \delta + C(\delta) \left( \Delta_N + R \left( \frac{N}{\Phi^N} \right) \right)$$

for all $N \in \mathbb{N}$ large enough, where

$$\Delta_N := \sum_{f,n} \Delta_{nf}^N,$$

$$\Delta_{nf}^N := \hat{\mu}_G^N(G) \left( W \left( \pi_G, \hat{\pi}_G^N \right) - E \left[ W \left( \pi_G, \hat{\pi}_G^N \right) | G_i^N \right] \right).$$

We can now follow the arguments in [Backhoff et al., 2021] Proof of Theorem 5.3, noting that

$$\lim_{N \to \infty} R \left( \frac{N}{\Phi^N} \right) = 0$$

as $\lim_{N \to \infty} |\Phi^N|/N = 0$ by assumption. This concludes the proof. \hfill \Box

Proof of Theorem 5.1. We first bound the Wasserstein distance $W(\hat{\pi}_G^N, \hat{\pi}_2^N)$ from above by quantities, whose distributions are easier to control. This goes back to a classical argument, see e.g. [Fournier and Guillin, 2015, Lemma 5], or also [Weed and Bach, 2019, Appendix A] for a detailed discussion. In our specific case we can write

$$\vec{W} \left( \hat{\pi}_N \right) = \sum_{G \in \Phi^N} \left[ \frac{\sum_{n \in \{1, \ldots, N\} \text{ s.t. } X_{n}^N \in G} W(\hat{\pi}_G^N, \hat{\pi}_2^N)}{N^2} \right] \sum_{n,m=1}^{N} \left| \phi^N(X^n_2) - \phi^N(X^m_2) \right|$$

and use the fact that both $\hat{\pi}_G^N$ and $\hat{\pi}_2^N$ are finitely supported on $\phi^N([0, 1]^d)$. Together with the observation that $\text{diam}([0, 1]^d) = \sqrt{d}$ we can thus bound the Wasserstein distance in (7) from above as follows:
\[
W(\hat{\pi}^N_G, \hat{\pi}^N_2) \leq \sqrt{d} \sum_{H \in \Phi^N} |\hat{\pi}^N_G(H) - \hat{\pi}^N_2(H)| \\
\leq \sqrt{d} \sum_{H \in \Phi^N} \left| \frac{1}{N} \sum_{n \in \{1, \ldots, N\} \text{ s.t. } X^n_1 \in G, X^n_2 \in H} - \frac{1}{N} \sum_{n \in \{1, \ldots, N\} \text{ s.t. } X^n_2 \in H} \right|, 
\]
so that
\[
\sum_{G \in \Phi^N} \frac{1}{N} \sum_{n \in \{1, \ldots, N\} \text{ s.t. } X^n_1 \in G} W(\hat{\pi}^N_G, \hat{\pi}^N_2) \\
\leq \sqrt{d} \sum_{G \in \Phi^N} \left| \frac{1}{N} \sum_{n \in \{1, \ldots, N\} \text{ s.t. } X^n_1 \in G} \right| \\
\cdot \left| \sum_{H \in \Phi^N} \frac{1}{N} \sum_{n \in \{1, \ldots, N\} \text{ s.t. } X^n_1 \in G, X^n_2 \in H} - \frac{1}{N} \sum_{n \in \{1, \ldots, N\} \text{ s.t. } X^n_2 \in H} \right| \\
= \sqrt{d} \sum_{G \in \Phi^N} \sum_{H \in \Phi^N} \left| \frac{1}{N} \sum_{n \in \{1, \ldots, N\} \text{ s.t. } X^n_1 \in G, X^n_2 \in H} - \frac{1}{N} \sum_{n \in \{1, \ldots, N\} \text{ s.t. } X^n_2 \in H} \right| \\
=: \sqrt{d} \hat{T}_N(\pi).
\]

Up to the constant \(\sqrt{d}\) the term \(\hat{T}_N(\pi)\) is a classical non-parametric estimator for independence of \(\mu\) and \(\nu\), see e.g. [Gretton and Györfi 2010]. More precisely, [Gretton and Györfi 2010, Theorem 1] states that under the assumption \(\pi = \mu \otimes \nu\) one has

\[
P(\hat{T}_N(\pi) \geq \epsilon) \leq 2^{(|\Phi^N| + 1)^2} \exp \left( - \frac{N\epsilon^2}{2} \right) \\
= \exp \left( \log(2)(|\Phi^N| + 1)^2 - \frac{\epsilon^2 N}{2} \right)
\]
for any \(\epsilon > 0\). We thus conclude that

\[
P \left( \int W(\hat{\pi}^N_{\pi_1}, \hat{\pi}^N_{\pi_2}) \hat{\pi}^N_1(dx_1) \geq \epsilon \right) \leq P(\sqrt{d} \hat{T}_N(\pi) \geq \epsilon) \\
\leq \exp \left( \log(2)(|\Phi^N| + 1)^2 - \frac{\epsilon^2 N}{2d} \right).
\]

This shows the first claim.

In particular choosing \(\epsilon = 2\sqrt{d \log(2)}(|\Phi^N| + 1)/\sqrt{N}\) in (8) yields

\[
P \left( \hat{T}_N(\pi) \geq 2\sqrt{d \log(2)} \frac{|\Phi^N| + 1}{\sqrt{N}} \right) \leq \exp(-|\Phi^N|^2),
\]
which is summable by assumption. Thus a Borel-Cantelli argument implies that

$$\tilde{T}_N(\pi) \leq 2\sqrt{d\log(2)} \frac{|\Phi^N| + 1}{\sqrt{N}}$$

for all sufficiently large $N \in \mathbb{N}$. Lastly, noting that by the law of large numbers

$$\lim_{N \to \infty} \int |y - z| \hat{\pi}_2^N(dy) \hat{\pi}_2^N(dz) = \int |y - z| \nu(dy) \nu(dz),$$

where the term on the right is positive by assumption, we can choose an appropriate constant $C(\nu) > 0$ in order to obtain

$$\overrightarrow{W}(\hat{\pi}^N) \leq C(\nu) \frac{|\Phi^N|}{\sqrt{N}}$$

for all $N \in \mathbb{N}$ sufficiently large. On the other hand, if $\pi \neq \mu \otimes \nu$, then $\mathcal{AW}$-consistency of $\hat{\pi}^N$ implies that

$$\int \mathcal{W}(\hat{\pi}^N_G, \hat{\pi}^N_2, \hat{\pi}^N_1(dx_1)$$

does not converge to zero, so that there exists $\delta > 0$ such that $\overrightarrow{W}(\hat{\pi}^N) \geq \delta$ for all $N \in \mathbb{N}$ sufficiently large. □

Let us next recall the following lemma, which is used in the proof of Corollary 5.2.

**Lemma A.1** ([Gretton and Gyorfi, 2010, Theorem 3]). Under the assumption that $\mu$ and $\nu$ are non-atomic and $\pi = \mu \otimes \nu$, there exists a centering sequence

$$C_N = C_N(\mu, \nu) \leq \sqrt{\frac{2|\Phi^N|}{\pi \sqrt{N}}}$$

such that

$$\sqrt{N}(\tilde{T}_N(\pi) - C_N)/\sigma \Rightarrow \mathcal{N}(0, 1),$$

where $\sigma = 1 - 2/\pi$ and

$$\tilde{T}_N(\pi) := \sum_{G \in \Phi^N} \sum_{H \in \Phi^N} \left| \frac{n \in \{1, \ldots, N\}}{N} \text{s.t. } X_1^n \in G, X_2^n \in H \right| \\
- \left| \frac{n \in \{1, \ldots, N\}}{N} \text{s.t. } X_1^n \in G \right| \left| \frac{n \in \{1, \ldots, N\}}{N} \text{s.t. } X_2^n \in H \right|.$$

While the estimate of $|f((\hat{\pi}^N)^2) - f(\nu)|$ in terms of $\mathcal{W}(\pi, \hat{\pi}^N)$ is useful for the proof of Corollary 4.2, the following result provides sharper convergence rates for the case $\hat{\pi}^N = \hat{\pi}^N$:

**Lemma A.2.** We have

$$\left( \sqrt{N} \wedge \frac{1}{2 \cdot \sup_x |\varphi^N(x) - x|} \right) \left( f(\hat{\pi}_2^N) - f(\nu) \right) = O_p(1).$$
Proof. We note that 
\[
f(\hat{\pi}_2^N) - f(\nu) = \int |y - z|^2 \hat{\pi}_2^N(dy) \hat{\pi}_2^N(dz) - \int |y - z|^2 \nu(dy) \nu(dz)
\]
\[
= \frac{1}{N^2} \sum_{i,j=1}^{N} |\varphi^N(X_i^j) - \varphi^N(X_2^j)| - \int |y - z|^2 \nu(dy) \nu(dz)
\]
\[
= \frac{1}{N^2} \sum_{i,j=1, i \neq j}^{N} |\varphi^N(X_i^j) - \varphi^N(X_2^j)| - \int |y - z|^2 \nu(dy) \nu(dz)
\]
\[
\leq 2 \cdot \sup_x |\varphi^N(x) - x| + \frac{1}{N^2} \sum_{i,j=1, i \neq j}^{N} |X_i^j - X_2^j| - \int |y - z|^2 \nu(dy) \nu(dz).
\]
Using the CLT for U-statistics for the kernel \(h(y_1, y_2) = |y_1 - y_2|\) (see e.g. [Van der Vaart, 1998, Theorem 12.3]) we conclude that 
\[
\sqrt{N} \left( \frac{1}{N^2} \sum_{i,j=1, i \neq j}^{N} |X_i^j - X_2^j| - \int |x_1 - y_2| \nu(dx) \nu(dy) \right) = O_P(1),
\]
which shows the claim. \(\square\)

In the following sections we discuss convergence rates of the estimator \(\hat{W}(\hat{\pi}^N)\), first for the independent case \(\pi = \mu \otimes \nu\) and subsequently for the general case.

Lastly, for the proofs in Section 6 we state here some of the main results from Backhoff et al. [2021(+) for the convience of the reader:

**Lemma A.3** (Average rate of \(A\mathcal{W}(\pi, \hat{\pi}^N)\), see [Backhoff et al., 2021(+) Theorem 1.5]). Under Assumption 6.1 there is a constant \(C > 0\) such that 
\[
E\left[ A\mathcal{W}(\mu, \hat{\pi}^N) \right] \leq C \cdot \begin{cases} 
N^{-1/3} & \text{for } d = 1, \\
N^{-1/4} \log(N + 1) & \text{for } d = 2, \\
N^{-1/(2d)} & \text{for } d \geq 3,
\end{cases}
\]
\[
= C \cdot \text{rate}(N)
\]
for all \(N \geq 1\).

In the theorem above, the constant \(C\) depends on \(d\) and the Lipschitz-constant in Assumption 6.1. Furthermore, Backhoff et al. [2021(+) also show the following concentration inequality:

**Lemma A.4** (Deviation of \(A\mathcal{W}(\pi, \hat{\pi}^N)\), see [Backhoff et al., 2021(+) Theorem 1.7]). Under Assumption 6.1 there are constants \(c, C > 0\) such that 
\[
P\left[ A\mathcal{W}(\mu, \hat{\pi}^N) \geq C \text{rate}(N) + \varepsilon \right] \leq 4 \exp \left( -cN\varepsilon^2 \right)
\]
for all \(N \geq 1\) and all \(\varepsilon > 0\).

As above, the constants \(c, C\) depend on \(d\), and the Lipschitz constant in Assumption 6.1.


Lastly we consider the distribution of
\[
\frac{\sqrt{N}}{\sigma} \left( \int \mathcal{W} \left( \hat{\pi}^N_{x_1}, \hat{\pi}^N_{x_2} \right) \hat{\pi}^N_1 (dx_1) - C_N(\nu) \right),
\]
which we bounded stochastically by a standard normal distribution in Corollary 5.2. The empirical study in Figure 6 shows that even if the constant $C_N(\mu, \nu)$ from Lemma A.1 is chosen such that the distribution is approximately centralised, (10) seems to possess slimmer tails than the standard normal distribution. In conclusion it seems unlikely that a CLT holds.

Figure 6. Comparison of the (shifted) histogram of (10) for 500 samples and $10^4$ draws with a standard normal density function.