Transport Dependency: Optimal Transport Based Dependency Measures

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Abstract

Finding meaningful ways to measure the statistical dependency between random variables \( \xi \) and \( \zeta \) is a timeless statistical endeavor. In recent years, several novel concepts, like the distance covariance, have extended classical notions of dependency to more general settings. In this article, we propose and study an alternative framework that is based on optimal transport. The transport dependency \( \tau \geq 0 \) applies to general Polish spaces and intrinsically respects metric properties. For suitable ground costs, independence is fully characterized by \( \tau = 0 \). Via proper normalization of \( \tau \), three transport correlations \( \rho_\alpha \), \( \rho_{\omega} \), and \( \rho_{\ast} \) with values in \([0, 1]\) are defined. They attain the value 1 if and only if \( \zeta = \varphi(\xi) \), where \( \varphi \) is an \( \alpha \)-Lipschitz function for \( \rho_\alpha \), a measurable function for \( \rho_{\omega} \), or a multiple of an isometry for \( \rho_{\ast} \). The transport dependency can be estimated consistently by an empirical plug-in approach, but alternative estimators with the same convergence rate but significantly reduced computational costs are also proposed. Numerical results suggest that \( \tau \) robustly recovers dependency between data sets with different internal metric structures. The usage for inferential tasks, like transport dependency based independence testing, is illustrated on a data set from a cancer study.

Keywords: transport dependency, transport correlation, optimal transport, statistical dependence, mutual information, correlation, distance correlation, lower complexity adaptation

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1 Introduction

In this article, we explore a method to quantify the statistical dependence between two random variables \( \xi \) and \( \zeta \) on Polish spaces \( X \) and \( Y \) via optimal transport (see, e.g., Rachev and
The core idea is to calculate the effort necessary to transform the joint distribution $\gamma$ of $\xi$ and $\zeta$ into the product of their marginal distributions $\mu$ and $\nu$. This motivates the definition of the transport dependency (Definition 3.1)

$$\tau(\xi, \zeta) = \tau(\gamma) = T_c(\gamma, \mu \otimes \nu) = \inf_{\pi} \int c \, d\pi,$$

(1.1)

where $T_c$ is the optimal transport cost with (non-negative) base costs $c$ on $X \times Y$. The infimum on the right is taken over the set of all couplings between $\gamma$ and $\mu \otimes \nu$, i.e., probability distributions $\pi$ on $(X \times Y)^2$ with marginals $\gamma$ and $\mu \otimes \nu$. Figure 1a illustrates this concept. If the cost function has benign properties, the transport dependency $\tau$ displays many traits that are attractive for a measure of statistical association. For instance, if $c$ is a metric, then $\tau(\gamma) = 0$ if and only if $\gamma = \mu \otimes \nu$, which means statistical independence of $\xi$ and $\zeta$.

Prior work. The idea of evaluating an optimal transport cost between a coupling $\gamma$ and the product $\mu \otimes \nu$ of its marginals has recently gained attention in the statistical and machine learning literature. For example, Móri and Székely (2020) introduced the Earth mover’s correlation, a coefficient of dependency on Polish metric spaces that is based on a special case of (1.1). As we will see later on, several open conjectures of their work – for example, the characterization of couplings $\gamma$ with maximal Earth mover’s correlation – are resolved by our theory. In Euclidean settings, variants of (1.1) have been proposed under the names Wasserstein dependence measure and Wasserstein total correlation by Ozair et al. (2019) and Xiao and Wang (2019), who applied it to beneficial effect in the context of representation learning. The same ansatz also underlies recent work by Mordant and Segers (2021), who defined Wasserstein dependency coefficients that are powered by (1.1) under squared Euclidean cost. For the purpose of normalization, the authors divide $\tau(\gamma)$ by the supremum of $\tau(\tilde{\gamma})$ over all $\tilde{\gamma}$ with fixed marginals $\mu$ and $\nu$. However, it is difficult to calculate these coefficients and quasi-Gaussian surrogates are necessary for application. In contrast, our approach relies on easily computable upper bounds that extend those in Móri and Székely (2020). Another instance of the transport dependency $\tau$ has recently been explored by Wiesel (2021), who proposed the association measure

$$\tau^Y(\xi, \zeta) = \tau^Y(\gamma) = \int T_{c_Y}(\gamma_x \nu) \, \mu(dx),$$

(1.2)

where $(\gamma_x)_{x \in X}$ denotes the disintegration of $\gamma$ with respect to the first coordinate (meaning that $\gamma_x$ is the law of $\zeta$ given $\xi = x$) and $c_Y$ is the power of a metric on the space $Y$. The author employed a similar upper bound as Móri and Székely (2020) to derive a normalized coefficient that exhibits a number of desirable properties postulated by Dee et al. (2013) and Chatterjee (2020). Integrals of the form (1.2) have previously also appeared in the context of generalization bounds for statistical learning problems (Zhang et al. 2018; Lopez and Jog 2018; Wang et al. 2019). During our investigation of the transport dependency, it will become clear that (1.1) and (1.2) are tightly related. In particular, $\tau$ reduces to $\tau^Y$ if transport in the space $X$ is forbidden by costs that assume the value $\infty$ for non-vertical movements (see Figure 1b). Moreover, $\tau^Y$
Mutual information. The general idea to compare the joint distribution of random variables to the product of their marginals dates far back. In his landmark work, Shannon (1948) introduced the mutual information $M(\gamma) = D(\gamma \mid \mu \otimes \nu)$, where $D$ denotes the Kullback-Leibler divergence. The mutual information has since become an indispensable tool for measuring the information content stored in the relation between random variables and has found application in feature selection (Estévez et al. 2009), image registration and alignment (Maes et al. 1997; Pluim et al. 2000), clustering (Kraskov et al. 2005), and independence testing (Berrett and Samworth 2019), besides others. Its immediate use for statistical data analysis, however, is complicated by several issues. For example, it is often inconvenient to estimate $M(\gamma)$ from data, as density estimates or binning / clustering methods are necessary and estimation suffers from the curse of dimensionality (Hall and Morton 1993; Paninski and Yajima 2008; Berrett et al. 2019). Furthermore, the mutual information does not respect topological or metric properties of the coupling $\gamma$, as measurable rearrangements of $\xi$ and $\zeta$ leave $M(\gamma)$ invariant. In this sense, it is not able to distinguish “chaotic” relations between $\xi$ and $\zeta$ from “well-behaved” ones (see Figure 2). Despite these potential drawbacks, the mutual information and its surrogates, such as the mutual information dimension (Sugiyama and Borgwardt 2013) or the maximal information coefficient (Reshef et al. 2011), are widely used tools for detecting and quantifying statistical dependency in data sets.

Distance covariance. A more recent approach to capture dependency by contrasting $\gamma$ to $\mu \otimes \nu$ is the distance covariance (Székely et al. 2007). The (Euclidean) distance covariance between

\[ \tau(\gamma) = T_{\epsilon}(\gamma, \mu \otimes \nu) \]

\[ \tau^{\gamma}(\epsilon) = \int T_{\epsilon}(y, \nu(x)) \mu(dx) \]

\[ \text{(a)} \]

\[ \text{(b)} \]
where \( k \) (separable) metric spaces \( p \) for \( \mathbb{R} \) ultrametric spaces, and weighted trees (Meckes 2013, Theorem 3.6). Known counter examples are \( \mu \) a separable Hilbert space. This condition asserts \( \text{dcov}^2 \) type measures a separable Hilbert space. is condition asserts \( \text{dcov} \) a performant unbiased estimator (Gao et al. 2021), and a well-understood limit theory, it is if \( \chi \) negative type characterizes independence. Examples for spaces of negative type are \( \text{dcov} \) or the distance covariance, assign a (much) lower degree of dependence to scenario (b). In contrast, dependency measures that are aware of metric or topological properties, like the transport dependency \( \tau \), \( \text{dcov} \) or the distance covariance, assign a (much) lower degree of dependence to scenario (b). This discrepancy stresses an important point: should deterministic but chaotic relations between \( \xi \) and \( \zeta \) maximize a measure for statistical dependency? Aer all, one may not be able to recover the relation in practice and distinguish it from noise if data is limited.

random vectors \( \xi \) in \( \mathbb{R}^r \) and \( \zeta \) in \( \mathbb{R}^q \) for \( r, q \in \mathbb{N} \) is a weighted \( L_2 \) distance between the joint characteristic function \( f_\gamma \) of \( \gamma \) and the product of the marginal characteristic functions \( f_\mu \) and \( f_\nu 

\[
dcov^2(\xi, \zeta) = \frac{1}{c_r c_q} \int \frac{|f_\gamma(t, s) - f_\mu(t)f_\nu(s)|^2}{\|t\|^{1+r}\|s\|^{1+q}} \lambda^d\lambda^d(ds),
\]

where \( \| \cdot \| \) is the Euclidean norm, \( c_d \) is a constant only depending on the dimensions \( d \), and \( \lambda^d \) denotes the Lebesgue measure in \( \mathbb{R}^d \). Lyons (2013) later proposed a generalization of (1.3) to (separable) metric spaces \( (X, d_X) \) and \( (Y, d_Y) \), given by

\[
dcov^2(\xi, \zeta) = \mathbb{E}
[ d_X(\xi, \xi') d_Y(\zeta, \zeta') ]
+ \mathbb{E}
[ d_X(\xi, \zeta') ]
\mathbb{E}
[ d_Y(\zeta, \zeta') ]
- 2 \mathbb{E}
[ d_X(\xi, \xi') d_Y(\zeta, \zeta') ],
\]

where \( (\xi', \zeta') \sim \gamma \) and \( \zeta'' \sim \nu \) are independent copies of \( \xi \) and \( \zeta \). If \( X \) and \( Y \) are of strong negative type \( \text{dcov}^2(\xi, \zeta) \) as defined above is indeed non-negative and vanishes if and only if \( \xi \) and \( \zeta \) are independent (Lyons 2013; Jakobsen 2017). Due to fast computability on data, a performant unbiased estimator (Gao et al. 2021), and a well-understood limit theory, it is

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1 A separable metric space \( (X, d_X) \) is of negative type \( \text{dcov}^2 \geq 0 \) if there is an isometric embedding \( \varphi \) of \( (X, d_X^{1/2}) \) into a separable Hilbert space. This condition asserts \( \text{dcov}^2 \geq 0 \). If the mean embedding \( \mu \mapsto \int \varphi d\mu \) for probability measures \( \mu \in \mathcal{P}(X) \) with finite first \( d_X \)-moment is additionally injective, the space \( (X, d_X) \) is of strong negative type and \( \text{dcov} = 0 \) characterizes independence. Examples for spaces of negative type are \( L_p \) spaces for \( 1 \leq p \leq 2 \), ultrametric spaces, and weighted trees (Meckes 2013, Theorem 3.6). Known counter examples are \( \mathbb{R}^d \) with \( L_p \) norms for \( p > 2 \) (see the references in Lyons 2013).

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Figure 2: Marginal and joint distribution of random variables \( \xi \sim \text{Unif}[0, 1] \) and \( \zeta = f_n(\xi) \sim \text{Unif}[0, 1] \) for zigzag functions \( f_n \) with \( n \) linear segments for \( n = 1 \) in (a) and \( n = 8 \) in (b). The drawn arrows illustrate how the optimal transport between \( \mu \otimes \nu \) and \( \gamma \) could look like. Note that the mutual information and related concepts that only measure the information content do not distinguish between the two scenarios. In contrast, dependency measures that are aware of metric or topological properties, like the transport dependency \( \tau \) or the distance covariance, assign a (much) lower degree of dependence to scenario (b). This discrepancy stresses an important point: should deterministic but chaotic relations between \( \xi \) and \( \zeta \) maximize a measure for statistical dependency? Aer all, one may not be able to recover the relation in practice and distinguish it from noise if data is limited.
a compelling instrument for non-parametric independence testing (Yao et al. 2016; Castro-Prado and González-Manteiga 2020; Chakraborty and Zhang 2019) and related problems, like independent component analysis (Matteson and Tsay 2017).

The distance covariance possesses the natural upper bound $\text{dcov}^2(\xi, \zeta) \leq \text{dcov}(\xi, \xi) \cdot \text{dcov}(\zeta, \zeta)$, which is utilized to define the normalized distance correlation with values in $[0, 1]$. The distance correlation $\text{dcor}$, which can serve as a more general surrogate for classical dependency coefficients like the Pearson correlation, has the following properties (Lyons 2013):

- $\text{dcor}(\xi, \zeta) = 0$ iff $\xi$ and $\zeta$ are independent,
- $\text{dcor}(\xi, \zeta) = 1$ iff there is a $\beta > 0$ and an isometry $\varphi: (X, \beta d_X) \rightarrow (Y, d_Y)$ with $\zeta = \varphi(\xi)$.

This provides a neat and tangible interpretation: the distance correlation measures a degree of isometric functional dependency (up to scalings). For the Euclidean case, this means that a value of $\text{dcor}(\xi, \zeta) = 1$ is assumed if and only if $\zeta = \beta (A\xi + a)$, where $A$ is an orthogonal matrix, $a$ an offset vector, and $\beta > 0$ (at least if the support of $\mu$ contains an open set). Other relations between $\xi$ and $\zeta$, even if they are deterministic, result in smaller values $\text{dcor}(\xi, \zeta) < 1$. Indeed, the more chaotic the relation becomes, the further away one is from an isometric dependency, and the lower the value of the distance correlation will typically be (see Figure 2). This draws a sharp distinction to other (non-parametric) concepts of dependency, like the mutual information or several recently proposed coefficients of association (Dee et al. 2013; Chaerjee 2020; Deb et al. 2020; Wiesel 2021), which assume maximal values for any measurable deterministic relation – not only for structured ones.

**Other measures of association.** Looking past classical concepts of correlation that are universally applied (like the Pearson correlation, Spearman’s $\rho$, or Kendall’s $\tau$), the literature on how to best measure dependency quickly becomes immensely broad and scattered. Besides the approaches cited above, we exemplarily mention maximal correlation coefficients (Gebelein 1941; Koyak 1987), rank or copula based methods (Schweizer and Wolff 1981; Marti et al. 2017), or various measures acting on the distribution of pairwise distances (Friedman and Rafsky 1983; Heller et al. 2013). For a survey, see Tjostheim et al. (2018). More closely related to our work, optimal transport maps have recently been utilized to define multivariate rank statistics that allow for asymptotically distribution-free independence tests (Ghosal and Sen 2019; Shi et al. 2020; Shi et al. 2021). Furthermore, optimal transport induced geometries have been explored for covariance analysis in functional data analysis (Petersen and Müller 2019; Dubey and Müller 2020).

A different class of data analysis and exploration techniques to be mentioned in this context are those that quantify how multiple data sets are spatially associated. A prominent example is Ripley’s $K$ function (Ripley 1976), for which new developments have recently been advanced (Amgad et al. 2015). A particular case of spatial association arises in colocalization problems in cell microscopy. We mention Wang et al. (2017), who propose a colocalization metric based on Kendall’s $\tau$, and Tameling et al. (2021), who suggest certain surrogates of the optimal transport plan for quantifying colocalization.
Transport dependency. A primary reason for the widely scattered literature on this topic is that the notion of “dependency” eludes the reduction to a single real number and heavily depends on the context. One important demarcation line in this regard has already been stressed: do we aim to measure dependency in a purely stochastic sense (like the mutual information), or do we also seek to impose structural conditions, like linearity (Pearson correlation), monotonicity (rank correlations), or metric compatibility (distance correlation)? Indeed, the theme of shape restrictions is central for recent efforts to find meaningful quantifiers of dependency (Cao and Bickel 2020; see also Guntuboyina, Sen, et al. 2018 for related work on shape-restricted regression).

In this article, we contribute to this topic by establishing the transport dependency as a principled tool that is flexible enough to bridge the gap between unstructured and structured dependency quantification. To begin with, \( \tau \) combines a number of attractive general properties that are desirable for a measure of association (see Section 3). For example, the condition \( \tau(y) = 0 \) fully characterizes independence under mild assumptions on the costs (Theorem 3.2). Furthermore, the value of \( \tau(y) \) only relies on the intrinsic cost structure and does not change, say, under transformations of \( x \) and \( \zeta \) that leave the cost function invariant (Proposition 3.6). The transport dependency also behaves well under perturbations: it is (Lipschitz) continuous (Proposition 3.9 and Theorem 3.10) and additive independent noise contributions (i.e., convolutions) can only decrease the value of \( \tau \) (Theorem 3.11). Moreover, if \( t \) percent of \( y \) are replaced (contaminated) by a distribution \( \tilde{y} \) with the same marginals, then \( \tau((1-t)y + t\tilde{y}) \leq (1-t)\tau(y) + t\tau(\tilde{y}) \) (Proposition 3.5). A particularly interesting theory unfolds on Polish metric spaces \( X, d_X \) and \( Y, d_Y \) under additive costs \( c(x_1, y_1, x_2, y_2) = (\alpha \cdot d_X(x_1, x_2) + d_Y(y_1, y_2))^p \) (1.5) for \( \alpha, p > 0 \), where \( x_1, x_2 \in X \) and \( y_1, y_2 \in Y \) (see Section 4). In this case, one of our core insights (Theorem 4.2) establishes that \( \tau(y) \) attains the upper bound (Proposition 3.14)

\[
\tau(y) \leq \int d_Y^p \, d(v \otimes v) \tag{1.6}
\]

if and only if \( y \) is concentrated on the graph of an \( \alpha \)-Lipschitz function \( \varphi : X \to Y \). In other words, the equality \( \tau(\xi, \zeta) = \mathbb{E}[d_Y(\zeta, \zeta')^p] \), for \( \zeta, \zeta' \sim \nu \) independent, holds if and only if \( \zeta = \varphi(\xi) \), where \( \varphi \) is an \( \alpha \)-Lipschitz map. The underlying intuition is captured in Figure 3, which shows that the cost of moving any point \( (x, y) \) in \( X \times Y \) to the graph of an \( \alpha \)-Lipschitz function \( \varphi \) is minimized by vertical movements. Transport along vertical movements, however, leads to bound (1.6).

Transport correlation. Based on the cost function (1.5) for \( \alpha > 0 \), we propose a family of coefficients \( \rho_\alpha \in [0, 1] \) that are tuned to detect \( \alpha \)-Lipschitz associations (see Section 5). The \( \alpha \)-transport correlation (Definition 5.1) is given by

\[
\rho_\alpha(\xi, \zeta) = \rho_\alpha(y) = \left( \frac{\tau(y)}{\int d_Y^p \, d(v \otimes v)} \right)^{1/p}.
\]
where the scaling by the inverse of bound (1.6), which we assume to be positive, guarantees $0 \leq \rho_\alpha \leq 1$. Two of the hallmark features of $\rho_\alpha$ are (Proposition 5.2)

- $\rho_\alpha(y) = 0$ iff $\xi$ and $\zeta$ are independent,
- $\rho_\alpha(y) = 1$ iff there is an $\alpha$-Lipschitz function $\varphi : (X, d_X) \to (Y, d_Y)$ with $\zeta = \varphi(\xi)$.

This allows us to view $\rho_\alpha$ as a generalized alternative to Pearson’s correlation coefficient that measures the degree of association in terms of best approximation by $\alpha$-Lipschitz functions (instead of linear functions). Later in the article, we will see that the idea behind $\rho_\alpha$ can fluently be extended to the limit $\alpha \to \infty$ (Theorem 3.17), in which the transport dependency $\tau$ becomes the marginal transport dependency $\tau^\gamma$. The resulting coefficient $\rho_\infty$, which we name **marginal transport correlation** (Definition 3.15), satisfies (Proposition 5.4)

- $\rho_\infty(y) = 0$ iff $\xi$ and $\zeta$ are independent,
- $\rho_\infty(y) = 1$ iff there is a measurable function $\varphi : X \to Y$ with $\zeta = \varphi(\xi)$.

Note that the marginal transport correlation is equal to the measure of association introduced by Wiesel (2021), who already recognized the above properties.

Both the $\alpha$-transport correlation and the marginal transport correlation are asymmetric concepts and only measure to what extent $\zeta$ can be understood as a function of $\xi$, not vice versa. If symmetry is desired, the coefficients can be adjusted in various ways. For example, we choose $d_{\alpha}^\gamma = \int d_Y^\gamma d(v \otimes v) / \int d_Y^\gamma d(\mu \otimes \mu)$ and set $\rho_\gamma = \rho_\alpha$, to define the **isometric transport correlation** (Definition 5.5), which has the following properties (Proposition 5.6):

- $\rho_\gamma(y) = 0$ iff $\xi$ and $\zeta$ are independent,
- $\rho_\gamma(y) = 1$ iff there is a $\beta > 0$ and an isometry $\varphi : (X, \beta d_X) \to (Y, d_Y)$ with $\zeta = \varphi(\xi)$.

This shows that $\rho_\gamma$ assumes its extremal values for exactly the same $\gamma$ as the distance correlation. For dependencies leading to non-extremal values, on the other hand, $\rho_\gamma$ can differ considerably

![Figure 3: Projection onto the graph of an $\alpha$-Lipschitz function $\varphi : X \to Y$ under costs $c = d^p$ as in (1.5). By applying the triangle inequality of $d_Y$ and the Lipschitz property $d_Y(\varphi(x_1), \varphi(x_2)) \leq \alpha d_X(x_1, x_2)$, one can see that the cost-optimal way to move any point $(x, y) \in X \times Y$ to the graph of $\varphi$ is to simply shift it up- or downwards.](image)
Figure 4: Power of independence tests under increasing levels of noise. The upper row depicts exemplary i.i.d. samples of size $n = 50$ at varying contamination noise levels $\varepsilon \in [0, 1]$ with $\xi \sim \text{Unif}[0, 1]$. The undisturbed samples ($\varepsilon = 0$) are drawn from the graph of a 3-Lipschitz zigzag function. The figure on the bottom depicts the power of level 0.1 permutation tests for independence that are based on $\rho_\alpha$, $\rho_\alpha^*$ for $\alpha = 3$, the distance correlation, the Pearson correlation, the Spearman correlation, and the maximal information coefficient. See Section 7 for more details on the numerical setting and the applied permutation tests.

from dcor (see our simulation study in Section 7). Contrary to the Earth Movers correlation proposed by Móri and Székely (2020), which is also a symmetric coefficient based on $\tau$ (see equation (5.4) in Section 5), $\rho_\alpha$ satisfies all of the axioms put forward by Móri and Székely (2019).

Estimation, computation, and application. In the presence of empirical data, the transport dependency can be estimated consistently by the plug-in estimator $\tau(\hat{\gamma}_n)$, where $\hat{\gamma}_n$ is the empirical measure of $n$ independent and identically distributed observations (see Section 6). Under mild conditions, the convergence rate of this estimator is determined by the intrinsic dimension of $\gamma$ (equation (6.3), Corollary 6.1 and Theorem B.1) and not by the potentially higher dimension of $\mu \otimes \nu$ or even $X \times Y$. This phenomenon of lower complexity adaptation (LCA) was recently uncovered and described by Hundrieser et al. (2022), extending findings by Weed and Bach (2019) and Divol (2022). Consequently, the stronger the measures $\mu$ and $\nu$ are coupled, the more LCA affects the empirical convergence rates. Since the calculation of $\tau(\hat{\gamma}_n)$ requires solving an optimal transport problem of size $n \times n^2$, which causes a high computational burden in case of large amounts of data, we also propose re-sampling based estimators (with effective size $n^\alpha$) that can be calculated by several orders of magnitude faster (for large $n$) but achieve the same LCA rates (Theorem B.3). Even though Monte-Carlo simulations (see Section 7) demonstrate a sizable bias in higher dimensions, which is inherited from the underlying optimal transport problem, the transport dependency generally performs well in the task of recognizing dependency via permutation tests. In particular, the most distinctive feature of $\tau$ is its flexibility to adapt to different environments by the freedom to work with arbitrary cost functions. In simulated settings, this is exemplified by considerable performance advantages of $\rho_\alpha$ compared to other dependency coefficients when detecting (noisy) $\alpha$-Lipschitz signals (see Figure 4 for an
Whenever convenient, we may express our arguments in terms of random elements $\zeta$ where only one marginal distribution is specified. If we want to condition on $x$ instead of probability measures, their joint law is usually $(\xi, \zeta) \sim \gamma \in C(\mu, \nu)$. Note that $\gamma(x, \cdot)$ is the conditional distribution of $\zeta$ given $\xi = x$ and vice versa for $\gamma(\cdot, y)$, and that the pushforward $f_{\*}\gamma$ equals the law of $f(\xi, \zeta)$ whenever $f : X \times Y \to Z$ is a measurable map into a Polish space.

2 Preliminaries

This section introduces the notation for the rest of the manuscript and summarizes basic definitions and results from the theory of optimal transport on Polish (i.e., separable and completely metrizable topological) spaces.

Notation. The set of all probability measures on a Polish space $X$ is denoted by $\mathcal{P}(X)$. The integration of a (Borel-)measurable function $f : X \to \mathbb{R}$ with respect to $\mu \in \mathcal{P}(Y)$ is flexibly written as $\int f(x) \mu(dx)$, $\int f \mu$, or simply $\mu f$. Every measurable function $\varphi : X \to Y$ between Polish spaces induces a pushforward map $\varphi_* : \mathcal{P}(X) \to \mathcal{P}(Y)$ via $\mu \mapsto \varphi_* \mu = \mu \circ \varphi^{-1}$. We write $\mu_n \rightharpoonup \mu$ if a sequence $(\mu_n)_{n \in \mathbb{N}} \subset \mathcal{P}(X)$ converges weakly (or in distribution) to $\mu$ in $\mathcal{P}(X)$. The product $X \times Y$ of two Polish spaces is again Polish if equipped with its product topology. We write $p^X$ and $p^Y$ for the Cartesian projections onto the spaces $X$ and $Y$, and we let

$$(\varphi, \psi)(x) = (\varphi(x), \psi(x)) \quad \text{and} \quad (\varphi \otimes \psi)(x, y) = (\varphi(x), \psi(y))$$

for suitable functions $\varphi$ and $\psi$. The notation $C(\mu, \nu) \subset \mathcal{P}(X \times Y)$ is used to denote the set of couplings (or transport plans) between measures $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$. Thus, $\gamma \in C(\mu, \nu)$ is a joint distribution on $X \times Y$ with marginals $p^X_\gamma = \mu$ and $p^Y_\gamma = \nu$. The product measure $\mu \otimes \nu$ is always an element of $C(\mu, \nu)$. We also write $C(\mu, \cdot)$ or $C(\cdot, \nu)$ for the subsets of $\mathcal{P}(X \times Y)$ where only one marginal distribution is specified. If we want to condition $\gamma \in C(\mu, \nu)$ on one of its components, we use the shorthand notation

$$\gamma(dx, dy) = \gamma(x, dy) \mu(dx)$$

to indicate a disintegration of $\gamma$ along the space $X$, where $\gamma(x, \cdot) \in \mathcal{P}(Y)$ is a probability distribution for each $x \in X$ (see Chang and Pollard [1997], Kallenberg [2006]). The family $(\gamma(x, \cdot))_{x \in X}$ is a probability kernel (or Markov kernel or stochastic kernel), which means that the mapping $x \mapsto \gamma(x, A)$ is measurable for each Borel set $A \subset Y$. Analog notation will be used for conditioning on $y \in Y$ or if products of more than two spaces are considered.

Whenever convenient, we may express our arguments in terms of random elements $\xi$ and $\zeta$ instead of probability measures. Their joint law is usually $(\xi, \zeta) \sim \gamma \in C(\mu, \nu)$. Note that $\gamma(x, \cdot)$ is the conditional distribution of $\zeta$ given $\xi = x$ and vice versa for $\gamma(\cdot, y)$, and that the pushforward $f_{\*}\gamma$ equals the law of $f(\xi, \zeta)$ whenever $f : X \times Y \to Z$ is a measurable map into a Polish space.
We call a lower semi-continuous function $c: X \times X \to [0, \infty]$ a cost function on $X$ if it is symmetric and vanishes on the diagonal, meaning $c(x_1, x_2) = c(x_2, x_1)$ and $c(x, x) = 0$ for all $x, x_1, x_2 \in X$. Sometimes we require $c(x_1, x_2) > 0$ for $x_1 \neq x_2$, in which case we call the cost function positive.

### Optimal transport

The optimal transport cost $T_c$ between measures $\mu$ and $\nu$ in $\mathcal{P}(X)$ for base costs $c$ on a Polish space $X$ is defined as

$$T_c(\mu, \nu) = \inf_{\pi \in \mathcal{C}(\mu, \nu)} \pi c. \quad (2.1)$$

An optimal transport plan $\pi^*$ that attains the infimum in equation (2.1) always exists if $c$ is lower semi-continuous (Villani [2008] Theorem 4.1). In general, optimal transport plans need not be unique. If $c = d^p$ for a metric $d$ on $X$ with $p \geq 1$, the quantity $T_c(\mu, \nu)^{1/p}$ is called the $p$-Wasserstein distance and is a metric on the probability measures on $X$ that have finite $p$-th moments (Villani [2008] Theorem 6.9).

When a transport plan $\pi \in \mathcal{C}(\mu, \nu)$ is concentrated on the graph of a function $\varphi: X \to X$, this function is called transport map and satisfies $\varphi_* \mu = \nu$ and $(\text{id}, \varphi)_* \mu = \pi$. Under certain conditions on $\mu$, $\nu$, and $c$, optimal transport plans $\pi^*$ that minimize (2.1) correspond to optimal transport maps $\varphi^*$. For example, this always holds when $\mu$ has a Lebesgue density in $\mathbb{R}^d$ for $d \in \mathbb{N}$ and $c$ is given by an $l_p$ norm with $p > 1$ (Gangbo and McCann [1996] Theorem 3.7).

The optimal transport problem (2.1) can alternatively be stated in its dual formulation,

$$T_c(\mu, \nu) = \sup_{f \oplus g \leq c} \mu f + \nu g, \quad (2.2)$$

where $(f \oplus g)(x_1, x_2) = f(x_1) + g(x_2)$ and where the supremum is taken over bounded and continuous functions $f$ and $g$. This fact is commonly known as Kantorovich-duality, dating back to Kantorovich (1942). Like for the existence of transport plans, the cost function $c$ being lower semi-continuous is sufficient for (2.1) and (2.2) to coincide (Villani [2008] Theorem 5.10). If $c$ is a metric, (2.2) takes the particular form

$$T_c(\mu, \nu) = \sup_{f \in \text{Lip}_1(X)} \mu f - \nu f, \quad (2.3)$$

where $\text{Lip}_1(X)$ denotes all real valued 1-Lipschitz functions on $X$ with respect to $c$. In particular, this is a special case of an integral probability metric (Müller [1997]; Sriperumbudur et al. [2012]).

### 3 Transport dependency: general properties

The transport dependency features several desirable traits for a measure of statistical association. In this section, we formally define it and discuss some of its generic properties, including convexity, symmetry, continuity, and the behavior under convolutions. We also establish three distinct upper bounds, one of which corresponds to a special case of $\tau$ when movement of mass...
along the space $X$ is forbidden. This naturally leads to the definition of the marginal transport dependency later on. Most of the proofs in this section are delegated to Appendix A.

**Definition 3.1 (transport dependency):** Let $X$ and $Y$ be Polish spaces and $c$ a cost function on $X \times Y$. The (c-)transport dependency $\tau_c : \mathcal{P}(X \times Y) \rightarrow [0, \infty]$ is defined via

$$
\tau(y) = \tau_c(y) = T_c(y, p^X_x \otimes p^Y_y).
$$

We usually omit the cost function $c$ in the subscript if it is apparent from the context, and we write $\tau(\xi, \zeta) = \tau(\gamma)$ for random elements $\xi$ and $\zeta$ with joint distribution $\gamma$. One can easily see that $\tau(\xi, \zeta) = 0$ in case of statistical independence. If $c$ is a positive cost function, this criterion is even sufficient for independence of $\xi$ and $\zeta$.

**Theorem 3.2 (independence):** Let $X$ and $Y$ be Polish spaces and $c$ a positive cost function on $X \times Y$. Then $\tau(\gamma) = 0$ if and only if $\gamma = \mu \otimes \nu$ for some $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$.

**Proof.** If $\gamma = \mu \otimes \nu$, the transport plan $\pi = (id, id)_* (\mu \otimes \nu) \in C(\gamma, \mu \otimes \nu)$ satisfies $0 \leq \tau(\gamma) \leq \pi c = 0$, where we used that $c \geq 0$ and that $c$ vanishes on the diagonal. Conversely, if $\tau(\gamma) = 0$ for some $\gamma \in C(\mu, \nu)$, we find $\pi^* c = 0$ for the optimal plan $\pi^*$, so $c = 0$ holds $\pi^*$-almost surely. Since $c$ is positive, this implies $\pi^* \{(x, y, x, y) \mid x \in X, y \in Y\} = 1$. Consequently, it follows that $\pi^* = (id, id)_* (\mu \otimes \nu) \in C(\mu \otimes \nu, \mu \otimes \nu)$, where id denotes the identity map on $X \times Y$. This establishes $\gamma = \mu \otimes \nu$. \hfill $\square$

**Example 3.3 (multivariate Gaussian):** Let $(\xi, \zeta)$ be a pair of real valued and normally distributed random vectors on $X \times Y = \mathbb{R}^r \times \mathbb{R}^q$ that follow a joint distribution $\gamma = \mathcal{N}(\eta, \Sigma)$ so that

$$
\eta = \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}
$$

with $\eta_1 \in \mathbb{R}^r, \eta_2 \in \mathbb{R}^q, \Sigma_{11} \in \mathbb{R}^{r \times r}, \Sigma_{22} \in \mathbb{R}^{q \times q}, \Sigma_{12} \in \mathbb{R}^{r \times q}$ and $\Sigma_{21} = \Sigma_{12}^T$. Since independence of normal random variables is characterized by zero correlation, the independent coupling is given by

$$
\mu \otimes \nu = \mathcal{N}(\eta, \Sigma_{\text{ind}}) \quad \text{with} \quad \Sigma_{\text{ind}} = \begin{pmatrix} \Sigma_{11} & 0 \\ 0 & \Sigma_{22} \end{pmatrix}.
$$

As costs on the space $X \times Y$, we consider the squared Euclidean distance

$$
c(x_1, y_1, x_2, y_2) = ||x_1 - x_2||^2 + ||y_1 - y_2||^2
$$

for $(x_1, y_1), (x_2, y_2) \in \mathbb{R}^r \times \mathbb{R}^q$. In this setting, evaluating the transport dependence of $\gamma$ corresponds to computing the square of the 2-Wasserstein distance between two normal...
distributions. We obtain (Dowson and Landau 1982)

\[
\tau(y) = 2 \text{trace}(\Sigma_{11}) + 2 \text{trace}(\Sigma_{22}) - 2 \text{trace}\left(\begin{pmatrix} \Sigma_{11}^2 & \Sigma_{11}\Sigma_{12} \\ \Sigma_{22}\Sigma_{21} & \Sigma_{22}^2 \end{pmatrix}^{1/2}\right).
\]  

(3.1)

If \( \xi \) and \( \zeta \) are univariate random variables, a more explicit formula can easily be derived. Let the covariance matrix be given by

\[
\Sigma = \begin{pmatrix} \sigma_1^2 & \rho \sigma_1 \sigma_2 \\ \rho \sigma_1 \sigma_2 & \sigma_2^2 \end{pmatrix}
\]

with \( \rho \in [0, 1) \) and \( \sigma_1, \sigma_2 > 0 \). Then, using an identity provided in (Levinger 1980), we can compute the square root of the \( 2 \times 2 \) matrix appearing in (3.1) and obtain

\[
\tau(y) = 2 \left( \sigma_1^2 + \sigma_2^2 - \sqrt{\sigma_1^4 + \sigma_2^4 + 2\sigma_1^2\sigma_2^2\sqrt{1 - \rho^2}} \right).
\]  

(3.2)

If \( \sigma_1 = \sigma_2 = \sigma \) for some \( \sigma > 0 \), this expression simplifies to

\[
\tau(y) = 2\sigma^2 \left( 2 - 2\sqrt{2\sqrt{1 - \rho^2}} \right).
\]

As to be expected, the transport dependency between \( \xi \) and \( \zeta \) is a strictly increasing function of the correlation \( \rho^2 \). Its minimal value is 0 for \( \rho = 0 \) and its maximal value is \((4 - 2\sqrt{2})\sigma^2 \approx 1.2\sigma^2\) for \( \rho = \pm 1 \) (if \( \sigma_1 = \sigma_2 = \sigma \)).

The mutual information is given by \( M(y) = -\log(1 - \rho^2)/2 \) (Gelfand 1959) and the Euclidean distance covariance by (Székely et al. 2007)

\[
dcov^2(y) = \frac{4\sigma^2}{\pi} \left( \rho \arcsin \rho + \sqrt{1 - \rho^2} - \rho \arcsin(\rho/2) - \sqrt{4 - \rho^2} + 1 \right).
\]

See Figure 5 for a comparison.

**Convexity and invariance.** The optimal transport cost \( T_c \) in (2.1) is a convex functional in both of its arguments (Villani 2008 Theorem 4.8). Similarly, the transport dependency \( \tau \) can be shown to be convex on subsets of \( \mathcal{P}(X \times Y) \) that share (at least) one marginal.

**Proposition 3.4 (convexity):** Let \( X \) and \( Y \) be Polish spaces and \( c \) a cost function on \( X \times Y \). Fix marginal distributions \( \mu \in \mathcal{P}(X) \) and \( \nu \in \mathcal{P}(Y) \). Then the transport dependency \( \tau \) is convex when restricted to \( C(\mu, \cdot) \) or \( C(\cdot, \nu) \).

Note that \( \tau \) is not convex on its whole domain, save for trivial exceptions. In fact, convexity on all of \( \mathcal{P}(X \times Y) \) would imply \( 0 \leq 2 \tau(\delta_{z_1}/2 + \delta_{z_2}/2) \leq \tau(\delta_{z_1}) + \tau(\delta_{z_2}) = 0 \) for point masses \( \delta_{z_i} \) with \( z_1, z_2 \in X \times Y \). By induction, \( \tau \) would have to vanish on all empirical measures. For
**Figure 5:** Selected dependency measures in the bivariate case $\xi, \zeta \sim N(0, 1)$ with $\text{cov}(\xi, \zeta) = \rho$, see Example 3.3. Graph (a) shows the mutual information (which diverges as $\rho^2 \to 1$), the Euclidean distance covariance (1.3), the marginal transport dependency (1.2), and the general transport dependency as function of $\rho^2$. Graph (b) shows the latter three quantities normalized such that their respective maximal value equals 1 for $\rho^2 = 1$. See Example 3.18 for a closed form of the marginal transport dependency $\tau^Y$ in this setting.

reasonable costs, like metrics on $X \times Y$, this only happens if $X$ and $Y$ are singletons.

Proposition 3.4 can be used to show that replacing a part of $\gamma$ with independent contributions consistently decreases the transport dependency.

**Proposition 3.5 (convex contamination):** Let $X$ and $Y$ be Polish spaces and $c$ a cost function on $X \times Y$. For $\gamma \in C(\mu, \nu)$ with $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$ define $\gamma_t = (1-t)\gamma + t(\mu \otimes \nu)$. Then the mapping $t \mapsto \tau(\gamma_t)$ is convex, monotonically decreasing, and satisfies
\[
\tau(\gamma_t) \leq (1-t) \tau(\gamma).
\]

When $c$ is a metric, (3.3) holds with equality.

We next formulate a symmetry result for $\tau$ that is based on a fundamental invariance property of optimal transport (Lemma A.1 in Appendix A). It can easily be generalized to cost preserving maps between distinct Polish spaces, but we restrict to the presented setting for simplicity.

**Proposition 3.6 (invariance):** Let $X$ and $Y$ be Polish spaces and $c$ a cost function on $X \times Y$ of the form
\[
c(x_1, y_1, x_2, y_2) = h(c_X(x_1, x_2), c_Y(y_1, y_2))
\]
for marginal costs $c_X$ and $c_Y$ on $X$ and $Y$ and a measurable function $h : [0, \infty)^2 \to [0, \infty]$. If $f_X : X \to X$ and $f_Y : Y \to Y$ are measurable maps that leave $c_X$ and $c_Y$ invariant, then
any $\gamma \in \mathcal{P}(X \times Y)$ satisfies
\[ \tau_c(f \gamma) = \tau_c(\gamma). \]

If $c_X$ and $c_Y$ are (based on) metrics and $\xi$ and $\zeta$ are random elements on $X$ and $Y$, we conclude that applying isometries to either $\xi$ or $\zeta$ does not change the value $\tau(\xi, \zeta)$. In other words, $\tau$ measures dependency in a way that is indifferent to isometric transformations on the margins. This property is shared by the distance covariance (1.4).

Example 3.7 (invariance in Euclidean space): Let $\xi$ and $\zeta$ be random vectors in $X = \mathbb{R}^r$ and $Y = \mathbb{R}^q$. If $c_X$ and $c_Y$ denote the respective Euclidean metrics and $c$ takes the form $h(c_X, c_Y)$, for example $c = c_X^2 + c_Y^2$ as in Example 3.3, Proposition 3.6 asserts that
\[ \tau(\xi, \zeta) = \tau(A \xi + a, B \zeta + b) \]
for all orthogonal matrices $A \in \mathbb{R}^{r \times r}$, $B \in \mathbb{R}^{q \times q}$ as well as vectors $a \in \mathbb{R}^r$, $b \in \mathbb{R}^q$.

**Continuity and convergence.** The optimal transport cost $T_c$ with lower semi-continuous base costs $c$ is again lower semi-continuous with respect to the weak convergence of measures. This property carries over to the transport dependency.

**Proposition 3.8 (lower semi-continuity):** Let $X$ and $Y$ be Polish spaces and let $c$ be a cost function on $X \times Y$. Then $\tau$ is lower semi-continuous with respect to weak convergence.

To show proper continuity of $\tau$, we need stronger assumptions, since the optimal transport cost $T_c$ is in general not continuous under weak convergence (Santambrogio [2015] Proposition 7.4). To this end, we equip the Polish space $X$ with a compatible metric $d_X$ that completely metrizes its topology. For $p \geq 1$, we define the set of probability distributions with finite $p$-th moment by
\[ \mathcal{P}_p(X) = \{ \mu \in \mathcal{P}(X) \mid \mu d_X^p(\cdot, x_0) < \infty \text{ for some } x_0 \in X \}, \]
and we say that a sequence $(\mu_n)_{n \in \mathbb{N}}$ in $\mathcal{P}_p(X)$ converges $p$-weakly to $\mu \in \mathcal{P}_p(X)$ if
\[ \mu_n \rightharpoonup \mu \quad \text{and} \quad \mu_n d_X(\cdot, x_0)^p \to \mu d_X(\cdot, x_0)^p \quad (3.4) \]
as $n \to \infty$ for some $x_0 \in X$. It is a well known fact (Mallows [1972]) that the $p$-Wasserstein distance metrizes this particular form of convergence (see Villani [2008] Theorem 6.9 for a general proof), so (3.4) is equivalent to $T_c(\mu_n, \mu) \to 0$ as $n \to \infty$ with $c = d_X^p$. Note that the anchor point $x_0$ in these definitions does not matter and can be replaced by any other element of $X$.

On products $X \times Y$ of two Polish metric spaces $(X, d_X)$ and $(Y, d_Y)$, there are many different ways to choose a compatible metric. For simplicity, we pick
\[ d(x_1, y_1, x_2, y_2) = d_X(x_1, x_2) + d_Y(y_1, y_2) \quad (3.5) \]
for \((x_1, y_1), (x_2, y_2) \in X \times Y\) in the following statement, even though any equivalent metric, like 
\[ d = \max(d_X, d_Y), \]
works as well.

**Proposition 3.9 (continuity):** Let \((X, d_X)\) and \((Y, d_Y)\) be Polish metric spaces and let \(c\) be 
a continuous cost function on \(X \times Y\) bounded by \(c \leq d^p\) for \(p \geq 1\) and \(d\) as in (3.5). If the 
sequence \((y_n)_{n \in \mathbb{N}}\) converges \(p\)-weakly to \(y\) in \(\mathcal{P}_p(X \times Y)\), then \(\tau(y_n) \to \tau(y)\).

An important consequence of Proposition 3.9 is the guarantee of consistency when \(\tau(y)\) is 
empirically estimated (see Section 6 for more details on estimation). We also present a continuity 
statement with explicit bounds in case that \(c\) is equal to the power of a metric. This time, since 
we only rely on the triangle inequality, the metric does not have to metrize the Polish topology. In 
fact, it suffices if \(d\) is a pseudo-metric on \(X \times Y\).

**Theorem 3.10 (continuity):** Let \(X\) and \(Y\) be Polish spaces and let \(c = d^p\) for a continuous 
pseudo-metric \(d\) on \(X \times Y\). Assume that \(y, y' \in \mathcal{P}(X \times Y)\) with \(\tau(y), \tau(y') < \infty\). Then, 
for any \(p \geq 1\),

\[
|\tau(y)^{1/p} - \tau(y')^{1/p}| \leq T_c(y, y')^{1/p} + T_c(\mu \otimes v, \mu' \otimes v')^{1/p}.
\]

If the metric \(d\) on \(X \times Y\) in the statement above is given in terms of marginal metrics \(d_X\) and \(d_Y\) 
on \(X\) and \(Y\), like \(d = d_X + d_Y\), one can apply the triangle inequality to derive

\[
T_c(\mu \otimes v, \mu' \otimes v')^{1/p} \leq T_c(\mu \otimes v, \mu' \otimes v)^{1/p} + T_c(\mu' \otimes v, \mu' \otimes v')^{1/p} \\
\leq T_{c_X}(\mu, \mu')^{1/p} + T_{c_Y}(v, v')^{1/p} \\
\leq 2T_c(y, y')^{1/p},
\]

where \(c_X = d_X^p\) and \(c_Y = d_Y^p\). In this case, Theorem 3.10 implies that \(\tau^{1/p}\) is \(3\)-Lipschitz continuous 
with respect to the \(p\)-Wasserstein distance: for any \(y_1, y_2 \in \mathcal{P}(X \times Y)\), it holds that

\[
|\tau(y_1)^{1/p} - \tau(y_2)^{1/p}| \leq 3T_c(y_1, y_2)^{1/p}.
\] (3.6)

**Convolutions.** The sum of independent random variables plays a distinguished role in many 
applications. If \(\xi \sim \mu \in \mathcal{P}(X)\) and \(\epsilon_X \sim \kappa_X \in \mathcal{P}(X)\) is an independent noise variable in a vector 
space \(X\), the distribution of \(\xi + \epsilon_X\) equals the convolution \(\mu * \kappa_X\). The latter is defined by

\[
(\mu * \kappa_X)(A) = \int \mathbb{1}_A(x_1 + x_2) \, (\mu \otimes \kappa_X)(dx_1, dx_2)
\]

for any Borel set \(A \subset X\). If \(\zeta \sim \nu \in \mathcal{P}(Y)\) is also contaminated by an independent additive 
noise contribution \(\epsilon_Y \sim \kappa_Y \in \mathcal{P}(Y)\), the joint distribution of \((\xi + \epsilon_X, \zeta + \epsilon_Y)\) is given by \(\gamma * \kappa\) for \(\kappa = \kappa_X \otimes \kappa_Y\).

The following theorem provides insights into how the transport dependency of \(\gamma * \kappa\) is related 
to the value \(\tau(y)\) for translation invariant costs. We work in Polish vector spaces, by which we 
mean topological vector spaces that are Polish; examples include separable Banach spaces.
Theorem 3.11 (convolution): Let $X$ and $Y$ be Polish vector spaces and let $c$ be a cost function on $X \times Y$ that satisfies $c(x_1, y_1, x_2, y_2) = h(x_1 - x_2, y_1 - y_2)$ for $(x_1, y_1), (x_2, y_2) \in X \times Y$ and some $h: X \times Y \to [0, \infty]$. For any $\gamma \in \mathcal{P}(X \times Y)$ and $\kappa = \kappa_X \otimes \kappa_Y$ with $\kappa_X \in \mathcal{P}(X)$ and $\kappa_Y \in \mathcal{P}(Y)$, it holds that

$$\tau(\gamma) \leq \tau(\gamma).$$

If additionally $c = d^p$ and $\tau(\gamma) < \infty$ for a continuous pseudo-metric $d$ on $X \times Y$ with $p \geq 1$, then

$$\tau(\gamma)^{1/p} - \tau(\gamma \ast \kappa)^{1/p} \leq 2(\kappa h)^{1/p}.$$

Theorem 3.11 unveils a fundamental property of the transport dependency: if a coupling $\gamma$ is blurred by the convolution with a product kernel, then $\tau$ never increases (and typically decreases). Intuitively, this is a desirable trait. For Gaussian noise, for example, it guarantees that $\tau$ monotonically decreases with increasing standard deviation of the noise.

Example 3.12 (Gaussian additive noise): Let $X = \mathbb{R}^r$ and $Y = \mathbb{R}^q$ and consider the squared Euclidean cost of the form $c(x_1, y_1, x_2, y_2) = h(x_1 - x_2, y_1 - y_2) = \|x_1 - x_2\|^2 + \|y_1 - y_2\|^2$, where $x_1, x_2 \in X$ and $y_1, y_2 \in Y$. Under Gaussian noise contributions $\kappa_X \sim \mathcal{N}(0, \Sigma_X)$ and $\kappa_Y \sim \mathcal{N}(0, \Sigma_Y)$, where $\Sigma_X$ and $\Sigma_Y$ are covariance matrices in $\mathbb{R}^{r \times r}$ and $\mathbb{R}^{q \times q}$, Theorem 3.11 states that

$$\tau(\gamma)^{1/2} \geq \tau(\gamma \ast \kappa)^{1/2} \geq \tau(\gamma)^{1/2} - 2(\text{trace } \Sigma_X + \text{trace } \Sigma_Y)^{1/2}$$

for any $\gamma \in \mathcal{P}(X \times Y)$ with $\tau(\gamma) < \infty$.

Example 3.13 (Manhattan-type costs): If $(X, \| \cdot \|_X)$ and $(Y, \| \cdot \|_Y)$ are separable Banach spaces and the costs $c$ are given by $h = \| \cdot \|_X + \| \cdot \|_Y$, application of Theorem 3.11 yields

$$\tau(\gamma) \geq \tau(\gamma \ast \kappa) \geq \tau(\gamma) - 2 \left( \int \|x\|_X \kappa_X(dx) + \int \|y\|_Y \kappa_Y(dy) \right)$$

for any $\gamma \in \mathcal{P}(X \times Y)$, $\kappa_X \in \mathcal{P}(X)$, and $\kappa_Y \in \mathcal{P}(Y)$, as long as $\tau(\gamma) < \infty$ holds.

**Upper bounds.** Our next goal is to derive upper bounds for the transport dependency. To this end, we bound the infimum in the optimal transport problem 2.1 by explicitly constructing feasible transport plans $\pi \in C(\mu, \nu)$ that may or may not be optimal. The idea behind these plans is to restrict the transport in $X \times Y$ to the fibers $X \times \{y\}$ and $\{x\} \times Y$ for $x \in X$ and $y \in Y$. Consequently, we often deal with costs of the form $c(x, y_1, x, y_2)$ or $c(x_1, y, x_2, y)$, and will thus assume that $c$ is controlled by suitable marginal costs $c_X$ and $c_Y$ on $X$ and $Y$ via

$$c_X(x_1, x_2) \geq \sup_{y \in Y} c(x_1, y, x_2, y) \quad \text{and} \quad c_Y(y_1, y_2) \geq \sup_{x \in X} c(x, y_1, x, y_2)$$

(3.7)
Figure 6: Different transport plans between $\gamma \in C(\mu, v)$ and $\mu \otimes v$ for $\gamma = \text{Unif}\{(1, 6), (2, 1), (4, 2), (4, 5)\}$. Each arrow corresponds to the movement of 1/16 parts of mass. The first graph shows the optimal transport plan $\pi^*$ under $l_2$ (or $l_1$) costs on $X \times Y = \mathbb{R}^2$, while the plans $\pi^{(a)}$ to $\pi^{(c)}$ correspond to the plans behind the three upper bounds established in Proposition 3.14 and 3.16. The example was chosen such that all bounds are different, and we find $\pi^* c < \pi^{(a)} c < \pi^{(b)} c < \pi^{(c)} c$. The difference between $\pi^{(b)}$ and $\pi^{(c)}$ is that the vertical movement of mass restricted to the fiber $x = 4$ is optimal in case of $\pi^{(c)}$, while $\pi^{(b)}$ transports along the product coupling on this fiber. The plan $\pi^{(a)}$ corresponds to the best assignment possible if transport is restricted to vertical and horizontal movements only.

For all $(x_1, y_1), (x_2, y_2) \in X \times Y$. To gain intuition for the three upper bounds we introduce in the following (and the transport plans $\pi^{(a)}$ to $\pi^{(b)}$ behind them), Figure 6 can be consulted. The first two of them, corresponding to the plans $\pi^{(a)}$ and $\pi^{(b)}$, are established in the following result.

**Proposition 3.14 (upper bounds, diameter):** Let $\gamma \in C(\mu, v)$ for $\mu \in \mathcal{P}(X)$ and $v \in \mathcal{P}(Y)$ in Polish spaces $X$ and $Y$. If the cost function $c$ on $X \times Y$ satisfies (3.7), then

$$
\tau(\gamma) \leq (\gamma \otimes \gamma) c_{XY} \leq \min((\mu \otimes \mu) c_X, (v \otimes v) c_Y), \tag{3.8a}
$$

where $c_{XY} : (X \times Y)^2 \to [0, \infty]$ is the cost function defined by

$$
c_{XY}(x_1, y_1, x_2, y_2) = \min(c_X(x_1, x_2), c_Y(y_1, y_2)).
$$

For convenience, we refer to integrals of the form $(v \otimes v) c_Y$ as the ($c_Y$)-diameter of $v$. Hence, inequality (3.8b) shows that the transport dependency $\tau(\gamma)$ can be bounded in terms of the diameters of the marginals $\mu$ and $v$.

The third upper bound, which is based on the improvement $\pi^{(c)}$ of the plan $\pi^{(b)}$ in Figure 6, is a worthwhile measure of association in its own right and receives its own definition.
Definition 3.15 (marginal transport dependency): Let $X$ and $Y$ be Polish spaces and $c_Y$ a continuous cost function on $Y$. The $(c_Y)$-marginal transport dependency is defined via

$$
\tau^Y(y) = \tau^Y_{c_Y}(y) = \int T_{c_Y}(y(x, \cdot), \nu) \mu(dx).
$$

Again, we typically suppress the dependency on $c_Y$ in our notation if the costs are apparent from the context. Note also that we have to assume that the mapping $x \mapsto T_{c_Y}(y(x, \cdot), \nu)$ is measurable for this definition to make sense. When $c_Y$ is continuous, measurability is guaranteed by Villani (2008, Corollary 5.22). Since $\tau^Y$ disregards the cost landscape on $X$, it is especially suited to quantify dependency in asymmetric settings where points in $X$ cannot be transported from one to another in a meaningful way, for instance if $X$ is categorical.

Proposition 3.16 (upper bounds, marginal transport): Let $\gamma \in C(\mu, \nu)$ for $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$ in Polish spaces $X$ and $Y$. If the cost function $c$ on $X \times Y$ satisfies the marginal bounds (3.7) for a continuous $c_Y$, then

$$
\tau(\gamma) \leq \tau^Y(\gamma) \leq (\nu \otimes \nu) c_Y.
$$

It is worth pointing out that the marginal transport dependency is in fact a special case of the (general) transport dependency under costs of the form

$$
c_{\infty}(x_1, y_1, x_2, y_2) = \begin{cases} 
c_Y(y_1, y_2) & \text{if } x_1 = x_2, \\
c_{\infty} & \text{else.}
\end{cases}
$$

This indicates that $\tau^Y$ arises as limit case if movements within the space $X$ become prohibitively expensive, such that all transport eventually withdraws to the fibers $\{x\} \times Y$ for $x \in X$. The following result confirms this intuition to be accurate.

Theorem 3.17 (marginal transport dependency as limit): Let $X$ and $Y$ be Polish spaces. For $\alpha > 0$, let $c_{\alpha}$ be a cost function on $X \times Y$ that satisfies

$$
c_{\alpha}(x_1, y_1, x_2, y_2) = \begin{cases} 
c_Y(y_1, y_2) & \text{if } x_1 = x_2, \\
\max(\alpha c_X(x_1, x_2), c_Y(y_1, y_2)) & \text{else,}
\end{cases}
$$

where $c_Y$ is a continuous cost function on $Y$ and $c_X$ a positive cost function on $X$. Then, for any $\gamma \in \mathcal{P}(X \times Y)$,

$$
\lim_{\alpha \to \infty} \tau_{c_{\alpha}}(\gamma) = \tau_{c_{\infty}}(\gamma) = \tau^Y_{c_Y}(\gamma).
$$

Example 3.18 (multivariate Gaussian, part 2): We revisit the Gaussian setting of Example 3.3. Recall that $(\xi, \zeta) \sim \gamma = N(\eta, \Sigma)$, where $\eta$ is a mean vector and $\Sigma$ a covariance
matrix with blocks $\Sigma_{11}$, $\Sigma_{12}$, $\Sigma_{21}$ = $\Sigma_{12}^T$ and $\Sigma_{22}$. This time, we work with costs of the form

$$c_\alpha(x_1, y_1, x_2, y_2) = \alpha \|x_1 - x_2\|^2 + \|y_1 - y_2\|^2$$

for $\alpha > 0$. Since these costs can be interpreted as scaling $\xi$ by the factor $\sqrt{\alpha}$ under the usual squared Euclidean distance $c_1$, we can employ the same arguments as in Example 3.3 and find expressions for $\tau_{c_\alpha}$ via replacing $\Sigma_{11}$ by $\alpha \Sigma_{11}$ and $\Sigma_{12}$ by $\sqrt{\alpha} \Sigma_{12}$. Adapting equation (3.1) in this way yields

$$\tau_{c_\alpha}(y) = 2\alpha \text{trace}(\Sigma_{11}) + 2 \text{trace}(\Sigma_{22}) - 2 \text{trace}\left(\begin{pmatrix} \alpha^2 \Sigma_{11}^2 & \alpha^{3/2} \Sigma_{11} \Sigma_{12} \\ \alpha^{1/2} \Sigma_{22} \Sigma_{21} & \Sigma_{22}^2 \end{pmatrix}^{1/2}\right).$$

According to Theorem 3.17, the right-hand side converges to the marginal transport dependency $\tau_{c_\alpha}^Y(y)$ as $\alpha \to \infty$, where $c_Y$ is the squared Euclidean distance. In the bivariate case (3.2), this limit can readily be calculated and reads

$$\tau_{c_\alpha}^Y(y) = \lim_{\alpha \to \infty} \tau_{c_\alpha}(y)$$

$$= \lim_{\alpha \to \infty} 2 \left(\alpha \sigma_1^2 + \sigma_2^2 - \sqrt{\alpha^2 \sigma_1^4 + \sigma_2^4 + 2\alpha \sigma_1^2 \sigma_2^2 \sqrt{1 - \rho^2}}\right)$$

$$= 2\sigma_2^2 \left(1 - \sqrt{1 - \rho^2}\right).$$

From this, it becomes apparent that $\tau_{c_\alpha}^Y$ “loses” the metric information on the space $X$ carried via $\sigma_1$.

The three upper bounds (3.8a) to (3.8c) established above play a crucial role for the remainder of the manuscript. In Section 4, we investigate under which conditions the inequalities in (3.8) are actually equalities. This uncovers an intimate relation between maximal values of transport dependency on the one hand and contracting couplings on the other. Afterwards, in Section 5, we apply this understanding to derive normalized coefficients of dependency.

## 4 Transport dependency: contractions and maximal values

Up to this point, we were concerned with general properties of the transport dependency for generic cost functions. We now focus on a particular additive cost structure that enables us to characterize under which conditions the upper bounds of the previous section are attained. All proofs in this section are delegated to Appendix A.

We equip the Polish space $X$ with a (general) cost function $k_X$ and the Polish space $Y$ with a lower semi-continuous (pseudo-)metric $d_Y$, and we consider costs of the form

$$c(x_1, y_1, x_2, y_2) = h(k_X(x_1, x_2) + d_Y(y_1, y_2))$$

for $(x_1, y_1), (x_2, y_2) \in X \times Y$, where $h: [0, \infty) \to [0, \infty)$ is a strictly increasing function that
satisfies $h(0) = 0$. We also fix the marginal costs

$$c_X = h \circ k_X \quad \text{and} \quad c_Y = h \circ d_Y, \quad (4.1b)$$

which fulfill condition (3.7). Therefore, $c_X$ and $c_Y$ are suited for the upper bounds in Proposition 3.14. To state our findings, we need to define couplings that describe contractions between $X$ and $Y$. We say that $\gamma \in \mathcal{P}(X \times Y)$ is contracting (on its support) if

$$d_Y(y_1, y_2) \leq k_X(x_1, x_2) \quad \text{for all} \quad (x_1, y_1), (x_2, y_2) \in \text{supp} \gamma. \quad (4.2)$$

We also need a slightly weaker condition and say that $\gamma$ is almost surely contracting if (4.2) holds $\gamma$-almost surely (but not necessarily on each single pair of points of the support).

**Theorem 4.1 (contracting couplings):** Let $X$ and $Y$ be Polish spaces, $c$ be a cost function on $X \times Y$ of the form (4.1), and $\gamma \in C(\cdot, \nu) \subset \mathcal{P}(X \times Y)$ for $\nu \in \mathcal{P}(Y)$. If $\gamma$ is contracting,

$$\tau(\gamma) = (\nu \otimes \nu) c_Y. \quad (4.3)$$

Conversely, if $(\nu \otimes \nu) c_Y < \infty$ and (4.3) holds, then $\gamma$ is almost surely contracting.

This theorem reveals that vertical movements of mass, which the upper bound $(\nu \otimes \nu) c_Y$ is based on, are optimal when mass is transported to a contracting coupling $\gamma$ (recall Figure 3 in this context). Conversely, vertical movements are not optimal whenever $\gamma$ is not (almost surely) contracting. Note that the distinction between “contracting” and “almost surely contracting” in Theorem 4.1 is necessary, as one can construct almost surely contracting couplings $\gamma$ such that $\tau(\gamma) = 0$ and $(\nu \otimes \nu) c_Y > 0$. If $d_Y$ and $k_X$ are continuous, the two concepts coincide (see Lemma A.8 in Appendix A). In this case, Theorem 4.1 implies the equivalence

$$\gamma \in C(\cdot, \nu) \quad \text{is contracting} \iff \tau(\gamma) = (\nu \otimes \nu) c_Y.$$

Under mild assumptions, contracting couplings are always deterministic and correspond to contracting functions. We say that a measurable function $\varphi: X \to Y$ is $\mu$-almost surely contracting if there is a Borel set $A \subset X$ with $\mu(A) = 1$ and

$$d_Y(\varphi(x_1), \varphi(x_2)) \leq k_X(x_1, x_2) \quad \text{for all} \quad x_1, x_2 \in A. \quad (4.4)$$

Combining the previous observations with Theorem 4.1 yields the following statement.

**Theorem 4.2 (contracting deterministic couplings):** Let $X$ and $Y$ be Polish spaces and $c$ be a cost function on $X \times Y$ of the form (4.1), where $h$ and $k_X$ are continuous and $d_Y$ is a continuous metric. Let $\gamma \in C(\mu, \nu)$ with $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$, and $(\nu \otimes \nu) c_Y < \infty$. Then

$$\tau(\gamma) = (\nu \otimes \nu) c_Y$$

holds if and only if $\gamma = (\text{id}, \varphi)_\ast \mu$ for a $\mu$-almost surely contracting function $\varphi: X \to Y$. 

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A point deserving emphasis is that Theorem 4.2 actually provides a characterization of Lipschitz and Hölder functions, as well as of isometries. If \( k_X \) is set to \( \alpha \cdot d_X \) for a metric \( d_X \) on \( X \), then condition (4.4) is equivalent to \( \varphi \) being \( \alpha \)-Lipschitz \( \mu \)-almost surely. Similarly, under the choice \( k_X = \alpha \cdot d_X \) for \( \beta \in (0, 1) \), condition (4.4) coincides with the \( \beta \)-Hölder criterion for \( \varphi \) (with constant \( \alpha \)). Finally, the simultaneous equality

\[
\tau(\gamma) = (\mu \otimes \mu) c_X = (v \otimes v) c_Y
\]

for \( k_X = d_X \) holds if and only if \( \varphi \) is \( \mu \)-almost surely an isometry from \( (X, d_X) \) to \( (Y, d_Y) \). In this context, we highlight that a \( \mu \)-almost sure contraction \( \varphi \) in the sense of Theorem 4.2 can always be uniformly extended to the full support of \( \mu \) if \( (Y, d_Y) \) is a Polish metric space (see Lemma A.9 in Appendix A).

It is interesting to contrast the condition \( \tau(\gamma) = (v \otimes v) c_Y \) at the heart of Theorem 4.2 to the weaker condition \( \tau^Y(\gamma) = (v \otimes v) c_Y \), where \( \tau^Y \) denotes the marginal transport dependency established in Definition 3.15. In the following statement, \( c_Y \) can be a general cost function and does not have to satisfy (4.1b).

**Theorem 4.3 (measurable deterministic couplings):** Let \( X \) and \( Y \) be Polish spaces and \( c_Y \) a positive continuous cost function on \( Y \). Let \( \gamma \in C(\mu, v) \) with \( \mu \in \mathcal{P}(X) \), \( v \in \mathcal{P}(Y) \), and \( (v \otimes v) c_Y < \infty \). Then

\[
\tau^Y(\gamma) = (v \otimes v) c_Y
\]

holds if and only if \( \gamma = (\text{id}, \varphi)_\# \mu \) for a measurable function \( \varphi : X \to Y \).

In this context, we note that Conjecture 2 of Móri and Székely (2020) states that the equality \( \tau(\gamma) = \min(\tau^Y(\gamma), \tau^X(\gamma)) \) holds under “general conditions” for costs \( c = d_X + d_Y \) in Polish metric spaces. If, however, \( \gamma \) is concentrated on the graph of a bijective function \( \varphi : X \to Y \) such that \( \varphi \) and \( \varphi^{-1} \) are both not 1-Lipschitz, combining Theorem 4.2 and Theorem 3.17 shows \( \tau(\gamma) < \min(\tau^Y(\gamma), \tau^X(\gamma)) \). In fact, we believe (and numerical tests suggest) that the claimed equality only holds in somewhat special situations.

To conclude this section, we want to highlight that the preceding results equip the transport dependency with a meaningful interpretation as quantifier of dependence: the larger the transport dependency \( \tau(\xi, \zeta) \) between two random variables \( \xi \) and \( \zeta \) is, the more they have to be associated in a contracting manner. Intuitively, this means that the conditional law of \( \zeta | \xi = x \) must behave well as a function of \( x \in X \), judged in terms of \( k_X \) and \( d_Y \). In fact, the highest possible degree of transport dependency for fixed marginals is (under continuity assumptions) only assumed if \( \xi \) and \( \zeta \) are deterministically related by \( \zeta = \varphi(\xi) \) for a contraction \( \varphi \). Other deterministic relations between \( \zeta \) and \( \xi \), which exhibit rapid changes that break condition (4.4), are assigned a lower degree of dependency. This way of dependency quantification can often be desirable, especially in situations where quickly oscillating or chaotic relations between \( \xi \) and \( \zeta \) practically cannot (or should not) be distinguished from actual noise.
Figure 7: Example for which the upper bounds (3.8) are not sharp. The marginal distributions are \( \mu = \nu = \text{Unif}\{1, 2, 3\} \). (a) One can show that \( \gamma^* = \text{Unif}\{(1, 1), (2, 2), (3, 3)\} \) maximizes \( \tau(\gamma) \) over \( \gamma \in \mathcal{C}(\mu, \nu) \), assuming the value \( \tau^* = 2(2 + \sqrt{2})/9 \) if \( c \) is the Euclidean distance on \( \mathbb{R}^2 \). The visualized plan \( \pi^* \) is optimal. (b) All of the established upper bounds move mass along a plan \( \pi \) that is restricted to vertical or horizontal transports. The total transportation cost is \( 8/9 > \tau^* \). Note that the Euclidean distance on \( X \times Y \) can not be expressed in the additive form (4.1a).

5 Transport correlation

In this section, we introduce several coefficients of association that are based on the transport dependency. The central ingredient is upper bound (3.8b) in Proposition 3.14, which can be used to scale \( \tau \) to the interval \([0, 1]\) in a way that only depends on the marginal distributions. Without further assumptions, however, bound (3.8b) is not necessarily sharp, and values close to 1 may be impossible (see Figure 7). We therefore focus on costs of the form (4.1a), for which the sharpness of the upper bounds is well understood (Theorem 4.2 in Section 4). Detailed proofs of the statements in this section can be found in Appendix A.

For the sake of clarity, we work in a slightly less general setting than in Section 4 and right away assume \( (X, d_X) \) and \( (Y, d_Y) \) to be Polish metric spaces, restricting to costs

\[
c(x_1, y_1, x_2, y_2) = (\alpha \cdot d_X(x_1, x_2) + d_Y(y_1, y_2))^p
\]  

(5.1)

for \( x_1, x_2 \in X \), \( y_1, y_2 \in Y \), and \( \alpha, p > 0 \). In what follows, \( d_X \), \( d_Y \), and \( p \) are usually considered to be fixed, and we mainly explore the influence of \( \alpha \). We call a map \( \varphi: X \to Y \) a dilatation if there exists some \( \beta > 0 \) such that

\[
d_Y(\varphi(x_1), \varphi(x_2)) = \beta d_X(x_1, x_2)
\]

for all \( x_1, x_2 \in X \). A dilatation can be thought of as an isometry from \( (X, \beta d_X) \) to \( (Y, d_Y) \), i.e., an isometry up to the correct scaling. We also recall the notion of \( p \)-weak convergence on \( \mathcal{P}_p(X \times Y) \), which was introduced and discussed in the context of continuity (Section 5).
Definition 5.1 (α-transport correlation): Let \((X, d_X)\) and \((Y, d_Y)\) be Polish metric spaces and consider costs \(c\) of the form \(\|x\|\) for \(\alpha, p > 0\). For \(\gamma \in C(\mu, \nu)\) with \(\mu \in P(X)\) and \(\nu \in P(Y)\) such that \(0 < (\nu \otimes v) d_Y^p < \infty\), the α-transport correlation is defined via

\[
\rho_\alpha(y) = \left( \frac{\tau(y)}{\nu \otimes v} d_Y^p \right)^{1/p}.
\] (5.2)

Proposition 5.2: The α-transport correlation \(\rho_\alpha\) in Definition 5.1 satisfies

1. \(\rho_\alpha(y) = 0\) if \(y = \mu \otimes \nu\),
2. \(\rho_\alpha(y) = 1\) if \(y = (\text{id}, \varphi) \circ \mu\) for an α-Lipschitz function \(\varphi : X \to Y\),
3. \(\rho_\alpha(y) = \rho_\alpha(y')\) if \(y' = (f_X, f_Y) \circ y\) for isometries \(f_X : X \to X\) and \(f_Y : Y \to Y\),
4. \(y \mapsto \rho_\alpha(y)^p\) is convex when restricted to \(C(\cdot, \nu) \subset P(X \times Y)\) for fixed \(\nu\),
5. \(\rho_{\alpha_n}(y_n) \to \rho_\alpha(y)\) as \(n \to \infty\) if \((y_n)_{n \in N}\) converges p-weakly to \(y\) and \(\alpha_n \to \alpha\),
6. \(\alpha \mapsto \rho_\alpha(y)^p\) is monotonically increasing for all \(\rho > 0\) and concave if \(\rho \leq 1\),

where the functions \(\varphi, f_X,\) and \(f_Y\) only have to be defined \(\mu\)- or \(\nu\)-almost surely.

Properties 1 and 2 lend the transport correlation a distinctive interpretation as dependency coefficient that identifies Lipschitz relations between random variables \(\xi\) and \(\zeta\). Based on our earlier findings (Theorems 3.17 and 4.3) on the marginal transport dependency \(\tau^Y\) (see Definition 3.15), it is possible to extend \(\rho_\alpha(y)\) to \(\alpha = \infty\).

Definition 5.3 (marginal transport correlation): Let \(X\) and \((Y, d_Y)\) be Polish (metric) spaces and \(c_Y = d_Y^p\) for \(p > 0\). For \(\gamma \in C(\mu, \nu)\) with \(\mu \in P(X)\) and \(\nu \in P(Y)\) such that \(0 < (\nu \otimes v) d_Y^p < \infty\), the marginal transport correlation is defined via

\[
\rho_\infty(y) = \left( \frac{\tau^Y(y)}{\nu \otimes v} d_Y^p \right)^{1/p}.
\]

Proposition 5.4: The marginal transport correlation \(\rho_\infty\) in Definition 5.3 satisfies

1. \(\rho_\infty(y) = 0\) if \(y = \mu \otimes \nu\),
2. \(\rho_\infty(y) = 1\) if \(y = (\text{id}, \varphi) \circ \mu\) for a measurable function \(\varphi : X \to Y\),
3. \(\rho_\infty(y) = \rho_\infty(y')\) if \(y' = (f_X, f_Y) \circ y\) for a measurable injection \(f_X : X \to X\) and a dilatation \(f_Y : Y \to Y\),
4. \(y \mapsto \rho_\infty(y)^p\) is convex when restricted to \(C(\cdot, \nu) \subset P(X \times Y)\) for fixed \(\nu\),

where the functions \(\varphi, f_X,\) and \(f_Y\) only have to be defined \(\mu\)- or \(\nu\)-almost surely.
The differences in Proposition 5.2 and 5.4 reflect that \( \rho_\alpha \) progressively loses the sense for metrical structure in \( X \) when \( \alpha \) is increased. In the limit \( \alpha = \infty \), the Lipschitz restrictions appearing in Proposition 5.2 are dissolved and only conditions of measurability remain.

Since we normalize with the diameter of \( \nu \) instead of the one of \( \mu \) in Definition 5.1, the transport correlation \( \rho_\alpha \) singles out functional relations in the direction \( X \rightarrow Y \). One possibility to compensate for this asymmetry is to adapt the value of \( \alpha \) to the diameters.

**Definition 5.5 (isometric transport correlation):** Let \((X, d_X)\) and \((Y, d_Y)\) be Polish metric spaces. For \( \gamma \in C(\mu, \nu) \) with \( \mu \in \mathcal{P}(X) \) and \( \nu \in \mathcal{P}(Y) \), consider costs of the form (5.1) with \( p > 0 \) and

\[
\alpha = \alpha_\gamma = \left(\frac{(\nu \otimes \nu) d_Y^n}{(\mu \otimes \mu) d_X^n}\right)^{1/p}.
\]

(5.3)

For \( 0 < \alpha_\gamma < \infty \), the isometric transport correlation is defined via \( \rho_\gamma(\gamma) = \rho_{\alpha_\gamma}(\gamma) \).

**Proposition 5.6:** The isometric transport correlation \( \rho_\gamma \) in Definition 5.5 satisfies

1. \( \rho_\gamma(\gamma) = 0 \) iff \( \gamma = \mu \otimes \nu \),
2. \( \rho_\gamma(\gamma) = 1 \) iff \( \gamma = (id, \varphi)_* \mu \) or \( \gamma = (\psi, id)_* \nu \) for dilatations \( \varphi : X \rightarrow Y \) or \( \psi : Y \rightarrow X \),
3. \( \rho_\gamma(\gamma) = \rho_\gamma(\gamma') \) if \( \gamma' = (f_X, f_Y)_* \gamma \) for dilatations \( f_X : X \rightarrow X \) and \( f_Y : Y \rightarrow Y \),
4. \( \gamma \mapsto \rho_\gamma(\gamma)^p \) is convex when restricted to \( C(\mu, \nu) \subset \mathcal{P}(X \times Y) \) for fixed \( \mu \) and \( \nu \),
5. \( \rho_\gamma(\gamma_n) \rightarrow \rho_\gamma(\gamma) \) as \( n \rightarrow \infty \) if \( (\gamma_n)_{n \in \mathbb{N}} \) converges \( p \)-weakly to \( \gamma \),
6. \( \rho_\gamma(\gamma) = \rho_\gamma(\gamma') \) if \( \gamma' = f_* \gamma \) for the symmetry map \( f(x, y) = (y, x) \),

where the functions \( \varphi, \psi, f_X, \) and \( f_Y \) only have to be defined \( \mu \)- or \( \nu \)-almost surely.

We can interpret this choice of \( \alpha_\gamma \) as first normalizing the metric measure spaces \((X, d_X, \mu)\) and \((Y, d_Y, \nu)\) by their \( p \)-diameters before calculating the transport dependency.

To conclude, we mention another symmetric coefficient of association which can be derived from the transport dependency. Instead of dividing by the diameter of \( \nu \) in (5.2), one can divide by the minimum of the diameters of \( \nu \) and \( \mu \). Setting \( \alpha = 1 \) in (5.1), this results in the coefficient

\[
\left(\frac{\tau_\gamma(\gamma)}{\min \left((\mu \otimes \mu) d_X^n, (\nu \otimes \nu) d_Y^n\right)}\right)^{1/p},
\]

(5.4)

which has, for \( p = 1 \), been introduced as Earth mover’s correlation by Móri and Székely (2020). It enjoys similar properties to the isometric transport correlation. In Conjecture 3 of Móri and Székely (2020) it is speculated that the expression in (5.4) is 1 if and only if \( \gamma = (id, \varphi)_* \mu \) for a dilatation \( \varphi : X \rightarrow Y \). However, our results in Section 4 clarify that this is the case if and only if \( \gamma \) is concentrated on the graph of a 1-Lipschitz function from \( X \) to \( Y \) or a 1-Lipschitz function from \( Y \) to \( X \).
6 Estimation and computation

We now discuss various strategies to estimate the transport dependency \( \tau(\gamma) \) in the presence of \( n \in \mathbb{N} \) empirical i.i.d. observations \( (\xi_i, \zeta_i)_{i=1}^n \sim \gamma^{\otimes n} \) for \( \gamma \in \mathcal{P}(X) \) and \( \nu \in \mathcal{P}(Y) \). The general approach will be to construct an estimator \( \hat{\gamma}_n \) of \( \gamma \) as well as an estimator \( \hat{\mu} \otimes \hat{\nu} \) of \( \mu \otimes \nu \) and plug them into the optimal transport functional, yielding estimates of the general form

\[
\hat{\tau}_n = T_c(\hat{\gamma}_n, (\mu \otimes \nu)_n).
\]

A striking observation, which we substantiate below, is that such estimators naturally seem to exhibit lower complexity adaptation (LCA, Hundrieser et al. 2022), meaning that the intrinsic dimension of \( \gamma \) determines the statistical convergence rate to the true value – and not the dimension of the product \( \mu \otimes \nu \) that is potentially higher.

**Product estimator.** The most immediate estimates of the probability measures \( \gamma \) and \( \mu \) and \( \nu \) are given by their empirical counterparts

\[
\hat{\tau}_n = \tau(\hat{\gamma}_n) = T_c(\hat{\gamma}_n, \hat{\mu} \otimes \hat{\nu}).
\]

We call this the **product estimator** as it relies on the product of the empirical measures \( \hat{\mu} \) and \( \hat{\nu} \) to estimate \( \mu \otimes \nu \). Since this estimator is simply the transport dependency of \( \hat{\gamma}_n \), several properties follow immediately from established results. For example, strong consistency, meaning that \( \lim_{n \to \infty} \hat{\tau}_n = \tau(\gamma) \) almost surely, follows from Proposition 3.9 under modest moment requirements. Further continuity-related properties can be derived from Theorem 3.10 or, for additive costs, equation (3.6). If the latter can be applied, the product estimator satisfies

\[
|\tau(\hat{\gamma}_n)^{1/p} - \tau(\gamma)^{1/p}| \leq T_c(y, \hat{\gamma}_n)^{1/p},
\]

which implies a convergence rate that only depends on \( \gamma \) (and not on \( \mu \otimes \nu \)). This demonstrates lower complexity adaptation. Indeed, as we explore in Appendix B, LCA of \( \tau(\hat{\gamma}_n) \) holds for non-metric and non-additive costs as well. For instance, the following statement is a corollary of Theorem B.1 together with metric entropy bounds derived in Hundrieser et al. (2022).

**Corollary 6.1 (lower complexity adaptation):** Let \( X \) and \( Y \) be smooth manifolds and \( \gamma \in \mathcal{P}(X \times Y) \) such that \( \text{supp} \, \gamma \) is contained in a compact smooth manifold of dimension \( s \in \mathbb{N} \). If the cost function \( c \) on \( X \times Y \) is twice continuously differentiable, then

\[
\mathbb{E} |\tau(\hat{\gamma}_n) - \tau(\gamma)| \leq n^{-2/s}.
\]

The major practical drawback of the product estimator consists of the associated computational burden. Its calculation relies on solving an optimal assignment problem between \( n^2 \) and \( n \) points. Even for fast algorithms like the network simplex or cost scaling, this implies a (worst-case) runtime of \( O(n^5) \) (up to logarithmic factors, see Peyré and Cuturi 2019). We next discuss alternative estimators that use only \( O(n) \) instead of \( n^2 \) points to estimate \( \mu \otimes \nu \), reducing the worst-case time complexity to \( O(n^3) \) (again, up to logarithmic factors).
Splitting estimators. Using a suitable sample splitting procedure, i.i.d. observations can be constructed to estimate $\gamma$ and $\mu \otimes \nu$. In a setting with $2n$ observations $(\xi_i, \zeta_j)_{i,j=1}^{2n} \sim \gamma^\otimes 2n$, for example, this can be realized by letting $\gamma_n$ be the empirical measure of the first $n$ data points and $(\mu \otimes \nu)_n$ be the empirical measure of $(\xi_i, \zeta_{n+i})_{i=1}^{n} \sim (\mu \otimes \nu)^\otimes n$ in the estimator (6.1). The resulting estimator is of the form of an empirical optimal transport cost, so the LCA framework developed in Hundrieser et al. (2022) is applicable. However, splitting estimators are inefficient from a practical point of view and primarily serve as a proof-of-concept that the LCA-rates of the product estimator can also be expected when $(\mu \otimes \nu)_n$ is estimated by $O(n)$ points only.

Sampling estimators. A more efficient approach to estimate $\mu \otimes \nu$ is to randomly sample $N = O(n)$ times from $A$ either with or without replacement. Alternatively, samples of the form $(\xi_i, \zeta_{\sigma(i)})_{i=1}^{n}$, where $\sigma$ is uniformly distributed over the set of permutations of $\{1, \ldots, n\}$, can be employed. To improve the estimate, we can also repeat this scheme for $k$ different random permutations $\sigma = (\sigma_1, \ldots, \sigma_k)$, ending up with a total of $N = kn$ sampled points. This procedure yields estimators of the form

$$\hat{\tau}_n^\sigma = T_c(\hat{\gamma}_n, (\mu \otimes \nu)_n^\sigma) \quad \text{where} \quad (\mu \otimes \nu)_n^\sigma = \frac{1}{kn} \sum_{r=1}^{k} \sum_{i=1}^{n} \delta_{(\xi_i, \zeta_{\sigma_r(i)})}, \quad (6.4)$$

which we call permutation estimators. In Appendix B we prove that these estimators satisfy the LCA property as well (Theorem B.3 and Corollary B.4) and thus exhibit no worse convergence rates than the product estimator. In particular, Corollary 6.1 still holds when the estimate $\tau(\hat{\gamma}_n)$ is replaced by $\hat{\tau}_n^\sigma$.

Other estimators. All of the previous proposals for estimates of $\tau(\gamma)$ are based on (randomly) picking points in the set $A = (\xi_i, \zeta_j)_{i,j=1}^{n} \subset X \times Y$. This can be done in various ways, for example by drawing $N = O(n)$ times from $A$ either with or without replacement. Alternatively, instead of randomly sampling from $A$, the estimator $(\mu \otimes \nu)_n$ may be based on a systematic approximation of $A$ with $O(n)$ weighted support points, e.g., realized via clustering. Based on our previous observations, it is to be expected that estimates of this form should display LCA properties as well.

Still, the comparably large bias of optimal transport costs in high dimensions will cause the expected statistical convergence rate to be slow in complex settings. As a remedy, further steps to exploit the potential smoothness of the measure $\gamma$ could be pursued, like kernel density or wavelet estimators for $\gamma$ and $\mu \otimes \nu$ (Weed and Berthet 2019; Deb et al. 2021; Manole and Niles-Weed 2021; Divol 2022). Presently, these types of estimators are mostly confined to the realm of theory, however, as their computation poses several difficulties.

Estimating the marginal transport dependency. We finally want to discuss estimation strategies for the marginal transport dependency $\tau^Y(\gamma)$, see Definition 3.15, for which the plug-in approach is often not feasible: in settings where $\mu$ is diffuse, the empirical data $\hat{\gamma}_n$
likely obeys functional relations \( \hat{y}_n = (\text{id}, \hat{\phi}_n)_{\hat{\mu}_n} \) for \( \hat{\phi}_n : X \rightarrow Y \). Thus, \( r^Y(\hat{y}_n) \) always equals \( (\hat{\nu}_n \otimes \hat{\mu}_n)_{\hat{\nu}_n} \) and is not informative (recall Theorem 4.3).

Similar problems also affect other quantifiers of (unstructured) dependency, like the mutual information, and the usual remedy is to preprocess the data. In Euclidean settings, for example, one can first estimate a smooth kernel-density or to bin the data with a kernel size or bin width \( h_n \) that decreases to 0 as \( n \) grows in order to obtain a consistent estimator (see Tsybakov [2008]). In a certain sense, the limiting procedure of \( \alpha \rightarrow \infty \) in Theorem 3.17 has a similar effect: a finite \( \alpha < \infty \) allows for some leeway along the space \( X \) when matching \( \hat{y}_n \) with \( \hat{\nu}_n \otimes \hat{\mu}_n \), and this leeway becomes progressively smaller as \( \alpha \) increases. Indeed, it is possible to find suitable sequences \( \alpha_n \rightarrow \infty \) so that \( \tau_{\alpha_n}(\hat{y}_n) \) is a consistent estimator of \( r^Y(\gamma) \) under mild assumptions.

Proposition 6.2 (consistent estimation of \( r^Y \)): Let \( (X, d_X) \) and \( (Y, d_Y) \) be Polish metric spaces, \( c_Y = d_y^p \), and \( c_\alpha = (\alpha d_X + d_Y)^p \) for \( p \geq 1 \) and \( \alpha > 0 \). Moreover, assume \( \gamma \in \mathcal{P}(X \times Y) \) to have a finite \( p \)-moment with respect to \( d = d_X + d_Y \). If \( (\alpha_n)_{n \in \mathbb{N}} \) is a positive diverging sequence that satisfies \( \alpha_n \cdot \mathbb{E} T_{c_\alpha}(\hat{\gamma}_n, \gamma)^{1/p} \rightarrow 0 \) as \( n \rightarrow \infty \), then

\[
\mathbb{E} \left| \tau_{\alpha_n}(\hat{\gamma}_n)^{1/p} - \tau^Y(\gamma)^{1/p} \right| \rightarrow 0.
\]

Another route to consistently estimate the marginal transport dependency from data is described in Wiesel [2021], who derives convergence rates if \( r^Y(\gamma) \) is estimated by \( r^Y(\hat{y}_n) \) for a so-called adapted empirical measure \( \hat{y}_n \). An example for such an adaption is the projection of the individual observations \( \xi_i \) and \( \zeta_i \) to a grid in the unit cube (see Backhoff et al. [2020]).

7 Simulations

We now investigate the performance of the transport dependency on simulated data. After briefly outlining our settings and numerical methodologies, we proceed to compare the product and permutation estimators introduced in the previous section. In particular, we confirm the LCA property for both of them and show that their rates of convergence are identical. Afterwards, we conduct a series of benchmarks that illuminate properties of the coefficients \( \rho_u \) and \( \rho_s \) in Euclidean spaces. We also investigate commonalities as well as differences to other coefficients of association, for example by comparing their performance in permutation tests for independence. Additional simulations that cover alternative parameter choices and adopt different dependency models can be found in Appendix D.

Setting. In the following, we restrict to Euclidean spaces \( X = \mathbb{R}^r \) and \( Y = \mathbb{R}^q \) for \( r, q \in \mathbb{N} \), and equip them with their respective Euclidean metrics \( d_X \) and \( d_Y \). We focus on joint distributions \( \gamma \in \mathcal{P}(\mathbb{R}^r \times \mathbb{R}^q) \) that are either given deterministically via \( \gamma = (\text{id}, \phi)_*\mu \) for \( \phi : [0, 1]^r \rightarrow [0, 1]^q \) and \( \mu = \text{Unif}[0, 1]^r \) (i.e., concentrated on the graph of the function \( \phi \)), or by placing (uniform) mass on more general shapes in \( [0, 1]^{r+q} \). The number of samples independently drawn from \( \gamma \) for the purpose of empirical estimation is denoted by \( n \in \mathbb{N} \), and we write \( \hat{y}_n \) to refer to the corresponding empirical measure, see Section 6. To study the influence of statistical noise, we
Later in the section also consider convex contamination models of the form
\[ y^\epsilon = (1 - \epsilon) y + \epsilon (\mu \otimes \nu), \]  
(7.1)
where \( \epsilon \in [0, 1] \) denotes the noise level distorting \( y \in \mathcal{C}(\mu, \nu) \). Observations \((x, y) \in \mathbb{R}^r \times \mathbb{R}^q \) sampled from \( y^\epsilon \) are with probability \((1 - \epsilon)\) randomly drawn from \( y \) and with probability \(\epsilon\) randomly drawn from \(\mu \otimes \nu\). Further simulations that use additive Gaussian noise instead are provided in Appendix D.

**Computation.** Depending on the size of the optimal transport problem, we alternate between two different computational approaches. In sufficiently small settings, like \( n \leq 100 \) for the product estimator (6.2) and all simulated \( n \) with the permutation estimator (6.4), we employ a network simplex based solver provided by the python optimal transport (POT) package (Flamary and Courty 2017). To still be able to capture the behavior of the product estimator for larger values of \( n \) (up to \( n = 1000 \)), we additionally employ our own implementation\(^2\) of an approximation scheme proposed by Schmitzer (2019). It is based on the Sinkhorn algorithm for entropically regularized optimal transport (Cuturi 2013) and operates by successively decreasing the regularization constant \( \eta > 0 \) until a suitable approximation of the non-regularized problem is obtained. While \( \eta \) is scaled down, in our case from \( \eta = 10^{-1} \) to \( \eta = 10^{-3} \), the increasing sparsity of the transport plan (after negligible entries are removed) is exploited by using sparsity-optimized data structures. On systems equipped with a decent GPU, the product estimator can thereby be calculated accurately for \( n = 1000 \) (as is done in Figure 13 below) within a couple of seconds to minutes for generic costs.

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\(^2\)The code is available in the julia programming language under [gitlab.gwdg.de/thomas.staudt/otter.jl](gitlab.gwdg.de/thomas.staudt/otter.jl)
Lower complexity adaptation. In order to investigate the convergence behavior of the estimators proposed in Section 6, we have to operate in a setting where \( \tau(\gamma) \) can be calculated explicitly (or at least be approximated very well). This is trivially the case for independent couplings \( \gamma = \mu \otimes \nu \) with \( \tau(\gamma) = 0 \), but since the dimensionality of \( \gamma \) and \( \mu \otimes \nu \) coincides for such \( \gamma \), we would not be able to discern lower complexity adaptation of the estimators. Instead, we consider the case \( \gamma = \text{id} \times \text{id} \) and \( \mu \sim \text{Unif}[0, 1]^r \), where analytical solutions are feasible for squared Euclidean costs (see Appendix C). The intrinsic dimensionality of \( \gamma \) is equal to \( r \). Therefore, according to Corollary 6.1 and the associated results in Appendix B, we expect that

\[
\mathbb{E} |\hat{\tau}_n - \tau(\gamma)| \leq n^{-2/r} \tag{7.2}
\]

if \( r > 4 \) for both the product estimator \( \hat{\tau}_n = \tau(\hat{\gamma}_n) \) and the permutation estimator \( \hat{\tau}_n = \hat{\tau}_n^\sigma \). Figure 8 depicts the results of Monte-Carlo simulations of \( \mathbb{E} |\hat{\tau}_n - \tau(\gamma)| \) for \( r \in \{1, 5\} \) under different choices of \( \hat{\tau}_n \). As expected, the product estimator performs best. However, it is only marginally better than the permutation estimator with \( k = 5 \) random permutations. The simulations confirm that the upper bound (7.2) correctly characterizes the decay of the mean absolute error, and show that the LCA property of the estimators affects the finite sample regime considered in Figure 8.

Dependency coefficients. We continue our numerical study by comparing different dependency coefficients that assume values in \( [0, 1] \). Besides the isometric and \( \alpha \)-Lipschitz transport correlations \( \rho_\alpha \) and \( \rho_\alpha \) for \( \alpha > 0 \) (see Section 5), which we estimate via the product estimator (6.2) unless specified otherwise, we consider the following commonly applied coefficients:

- **cor**: the Pearson correlation. It is only applicable if \( r = q = 1 \). Since it assumes values in \([-1, 1]\), we always report its absolute value.

- **spe**: the Spearman rank correlation coefficient. It is only applicable if \( r = q = 1 \) and is comparable to Kendall’s \( \tau \), another popular rank based correlation coefficient.

- **dcor**: the Euclidean distance correlation (Székely et al. 2007), based on the distance covariance defined in equation (1.3). It is applicable for all \( r, q \in \mathbb{N} \). In its generalized form (1.4), it is also applicable in generic (separable) metric spaces of (strong) negative type. As discussed previously, some of its properties make it comparable to \( \rho_\alpha \). Note that we use the vanilla empirical distance correlation in our simulations. Related estimators, like an unbiased estimator of \( \text{dcor}^2 \) proposed by Székely and Rizzo (2013), showed a comparable performance when testing for independence and are not included in this study.

- **mic**: the maximal information coefficient (Reshef et al. 2011). It is only applicable if \( r = q = 1 \). For its estimation, we use the estimator \( \text{mic}_\epsilon \) (Reshef et al. 2016), which we compute via the tools provided by Albanese et al. (2012). The two algorithmic parameters \( c \) and \( \alpha \) were set to 5 and 0.75, respectively (as recommended in Albanese et al. 2018).

For each of these coefficients, generically called \( \rho \) for the moment, we are interested in several features. Apart from the actual value of \( \rho(\gamma) \), which signifies the amount of dependency attributed to \( \gamma \), we look at the variance and bias of \( \hat{\rho}(\hat{\gamma}_n) \) as an estimator of \( \rho(\gamma) \) when data is
limited.

To check how well the coefficients are able to distinguish structure from noise, we also include the results of permutation tests for independence (see Lehmann and Romano, 2006, Section 15.2, or Janssen and Pauls, 2003 for background on permutation based tests). The $\rho$-based permutation test we employ works as follows: for given data $z = (x_i, y_i)_{i=1}^n \in (X \times Y)^n$, assumed to be sampled from $\gamma^n$, we write $\rho(z)$ for the empirical estimate of $\rho(y)$ based on $z$. Furthermore, we denote $z_\sigma = (x_i, y_{\sigma(i)})_{i=1}^n$, where $\sigma$ is a permutation of $n$ elements. For the test, we randomly select $m$ permutations $\sigma_1, \ldots, \sigma_m$ and reject the null hypothesis that $z$ is sampled from an independent coupling $\gamma = \mu \otimes \nu$ if

$$\left| \left\{ i : \rho(z_{\sigma_i}) > \rho(z) \right\} \right| \leq k$$

(7.3)

for some $k \in \{0, \ldots, m\}$. Since a permutation of the second components does not affect the distribution of $\gamma^n$ if $\gamma = \mu \otimes \nu$ is a product coupling, this leads to a level $\frac{k}{m}$ test. In all of our applications, we choose $k$ and $m$ such that this level is $\leq 0.1$. Note that the power of the permutation test will usually increase if $m$ is increased while the level is held constant.

**Recognizing shapes.** We begin with an investigation of the behavior of the aforementioned coefficients in two dimensional settings, meaning $r = q = 1$. Figure 9 contains box plots depicting the coefficients’ performance on simple geometries, like lines or circles, for $n = 50$ samples. As a point of reference, we also include uniform noise on $[0,1]^2$.

To showcase the Lipschitz-selectivity of $\rho_\alpha$, we chose to include the coefficient $\rho_3$ for $\alpha = 3$. Recall that this implies $\rho_3(\gamma) = 1$ whenever $\gamma$ is concentrated on the graph of a function whose slope is at most 3. Figure 9 confirms this property of $\rho_3$, which is the only coefficient to assign maximal dependency to the zigzag function with slope 3 and the polynomial. On the zigzag function with 5 segments (and thus slope 5), it has already decreased to about 0.7. In this context, the mic, which generally achieves high values on all geometries, performs notably well. It is also the coefficient that most clearly distinguishes the pretzel example from noise. Another noteworthy observation is that $\rho_3$ and $\text{dcor}$ indeed behave comparably, especially on functional relations. On non-functional patterns, like the circle or the cross, $\rho_3$ assumes somewhat higher values than $\text{dcor}$. At the same time, the bias of $\rho_3$ on independent noise (for which values of 0 are expected in the limit of large $n$) is slightly higher than the one of $\text{dcor}$, albeit with a smaller variance. Finally, as to be expected, the Pearson and Spearman correlation coefficients do a poor job at discerning non-monotonic structures. In case of the circle, for example, the values of these coefficients are systematically lower than when confronted with random noise.

**Behavior under noise.** Our next simulations concern the performance under convex noise models $\gamma^\epsilon$ as defined in equation (7.1). Figure 10 and 11 illustrate the coefficients’ empirical estimates and their power when used for independence testing in case that $\gamma$ is deterministically given in terms of the identity (Figure 10) or the zigzag function with maximal slope 5 (Figure 11). In Appendix D, this type of comparison can be found for all other distributions considered in Figure 9 as well, and we also present results under additive Gaussian noise.

In case of the identity, all coefficients seem to behave roughly similar, especially for small noise
Figure 9: Comparison of several dependency coefficients on two dimensional geometries. As reference, independent $\text{Unif}(0, 1)^2$ noise has also been simulated (bottom right). For each geometry, the scatter plot on top displays an exemplary sample of size $n = 50$. The box plots below summarize the values of the empirically estimated coefficients based on 100 such samples. For the sake of visualization, boxes in the box plot are replaced by single dots if their extent would be smaller than 0.1.

levels. Under pure noise ($\epsilon = 1$), for which the coefficients should attain the value 0 in the limit of large $n$, the transport correlation exhibits a comparably large bias at a relatively small variance. This trend of high biases becomes even more serious in higher dimensions and is further investigated below (Figure 13). Regarding the test performance, the power curves in Figure 10 reveal that all coefficients except $\rho_s$ and mic perform comparably. The power of $\rho_s$ is consistently higher than its competitors’, while mic performs notably worse.

The picture changes substantially for the zigzag example in Figure 11. Due to the absence of monotonicity, cor and spe are not able to distinguish data points originated from the zigzag function from the ones coming from the independence coupling of its marginals. The coefficient dcor and, to a lesser extent, $\rho_s$ also assume lower values and can only partially discern the dependency structure under noise. Meanwhile, the coefficients mic and specifically $\rho_3$ lie systematically higher and are still able to recognize dependency under high noise levels.
Figure 10: Dependency coefficients applied to increasingly noisy datasets according to the convex noise model in (7.1), where $\gamma$ is given in terms of the identity on $[0, 1]$. The scatter plots on the top show exemplary samples drawn from $\gamma^\epsilon$ of size $n = 50$. The box plots are based on 100 such samples. The power curves on the bottom display the results of the permutation tests described in (7.3). To estimate the power, 1000 tests were conducted per value of $\epsilon$ for each coefficient. The significance level (dashed line) of these tests is 10%.

The role of $\alpha$. In Figure 4 of the introduction, we already noted that $\rho_3$ performs very well on a 3-Lipschitz functional relation. Additionally, Figure 11 testifies that $\rho_3$ also outperforms all other considered coefficients when applied to a 5-Lipschitz relation. It stands to reason, however, that $\rho_5$ would do even better than $\rho_3$ in this setting. To further examine the claim that adapting $\alpha$ to the slopes inherent to $\gamma$ improves the performance, we conducted a series of numerical experiments with functions of different maximal slope and varying $\alpha$. The findings are displayed in Figure 12, where the power of $\rho_\alpha$-based permutation tests is plotted as a function of $\alpha$ (for fixed noise levels $\epsilon = 0.75$). The results clearly suggest that choosing a value of $\alpha$ close to the Lipschitz constant of the actual functional relation in $\gamma$ can significantly improve the test performance. If $\alpha$ is chosen too small or too large, the power systematically declines.

Bias and high dimensions. Another prevalent trend in the numerical results so far is the notable bias of $\rho_\epsilon$ and $\rho_\alpha$ on independent noise (i.e., for $\epsilon = 1$), where we expect a value of 0 for $n \to \infty$. In fact, empirical estimators of optimal transport distances are known to be susceptible to a certain degree of bias, especially in high dimensions. In Figure 13 we therefore compare the empirical estimation of $\rho_\epsilon$ and dcor in settings of different dimensions for sample sizes $n$ running from 10 to 1000. We observe that the bias of $\rho_\epsilon$ and dcor seem comparable for
$r = q = 1$. If the dimensions are chosen higher, the bias increases much quicker for $\rho_\gamma$ than for $dcor$. At the same time, the variance of the $\rho_\gamma$ estimates is (in part much) smaller for all choices of dimensions. Indeed, in case of $r = q = 5$ and $n = 1000$, the estimated standard deviation of $\rho_\gamma$ is multiple times smaller than the one of $dcor$, even though the bias is substantial ($\rho_\gamma \approx 0.72$, while $dcor \approx 0.13$).

A high bias in itself does not necessarily mean that $\rho_\gamma$ is blind to dependencies in high dimensions, however. Figure [14] reveals that simple linear structures with noise of the form $(7.1)$ are still recognized somewhat better via $\rho_\gamma$ than via $dcor$ for $n = 50$, particularly in the setting $r = q = 5$.

To examine a more involved example, we also look at spherical dependencies, where $\gamma$ is the uniform distribution on the sphere $S^{r+q-1} \subset \mathbb{R}^r \times \mathbb{R}^q$. In this case, the results are more unintuitive and prompt several questions. First of all, spherical dependencies are separated from noise (much) better by the transport correlation than by $dcor$ in settings with $r, q \in \{1, 2\}$. At the same time, for $r = q = 5$, both the distance correlation and the transport correlation consistently exhibit test powers that are smaller than 0.1, meaning that a random sample from the sphere regularly results in lower estimates of $\rho_\gamma$ and $dcor$ than drawing from the corresponding marginals $\mu \otimes \nu$ would. This effect is particularly severe in case of the transport dependency. Even though this observation could in part be caused by the small sample size $n = 50$ and the rather weak dependency in the spherical setting, it demonstrates that detecting dependency in more complex situations remains an open issue that merits further investigation.
Figure 12: Influence of $\alpha$ on the test performance of $\rho_\alpha$ for linear (a) and sine (b) dependencies at a noise level of $\epsilon = 0.75$, see (7.1). The graphs on the top display exemplary samples together with the actual functional relations encoded in $\gamma$ for different slopes. From left to right, the respective curves have maximal slopes of 1, 3, and 5 in both (a) and (b). The respective values of $\alpha \in \{1, 3, 5\}$ are marked as vertical lines in the power plot below. For each value of $\alpha$, the power is estimated based on 500 samples of size $n = 50$.

Figure 13: Empirical estimates of the isometric transport correlation and the distance correlation as a function of the sample size $n$ in different dimensions $r$ and $q$. The true distribution in the respective graphs is given by the product measure $\gamma = \text{Unif}[0, 1]^r \otimes \text{Unif}[0, 1]^q$. Therefore, $\rho_\star(\gamma) = \text{dcor}(\gamma) = 0$ is the (unbiased) value to be expected for $n \to \infty$. The shaded error regions correspond to $\pm$ three times the estimated standard deviation. The number of samples employed for the estimation of the mean and variance was adaptively decreased from 500 for $n = 10$ to 20 for $n = 1000$. 

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Figure 14: Test performance of the isometric transport correlation and the distance correlation in different dimensions $r$ and $q$. Shown are results for both linear and spherical relations under the noise model (7.1). In the former case, $\gamma$ is given by $(\text{id, id})\text{Unif}[0,1]^r$ if $r = q$ and by $(\text{id, pr}_1)\text{Unif}[0,1]^r$ in case of $r = 2$ and $q = 1$, where $\text{pr}_1$ denotes the projection on the first coordinate. In case of the sphere, $\gamma$ is uniformly distributed on the surface $S^{r+q-1} \subset \mathbb{R}^{r+q}$. For all power curves, 1000 samples of size $n = 50$ were used.

In fact, the data application in the next section showcases that the transport dependency can yield meaningful results even for $r = 5000$ and $n < 100$.

8 Application to gene expression data

In this section, we re-analyze a breast cancer gene expression study (Van’t Veer et al. 2002) using the transport dependency, confirming the findings by Behr et al. (2020), who developed a specialized method for this data set. Our results demonstrate that the transport dependency is able to sensibly detect structural relations even when relying on non-metric similarity criteria in high dimensions.

In the original study (Van’t Veer et al. 2002), gene expression levels of breast cancer samples were collected from 98 patients along with six clinical responses: BRCA mutation ($k = 1$), estrogen receptor expression ($k = 2$), histological grade ($k = 3$), lymphocytic infiltration ($k = 4$), angioinvasion ($k = 5$), and development of distant metastasis within 5 years ($k = 6$). We model the genetic data as i.i.d. random variables $\xi = (\xi_1, \ldots, \xi_{98})$, each taking values in the high dimensional space $X = \mathbb{R}^{5000}$. The components in this space correspond to the expression levels of 5000 different genes. We furthermore let $\zeta^k = (\zeta^k_1, \ldots, \zeta^k_{98})$ for $k \in \{1, \ldots, 6\}$ denote the $k$-th responses with values in $Y = \mathbb{R}$, again assumed to be i.i.d. To quantify the similarity between the gene expressions of different patients, Van’t Veer et al. (2002) employ a biologically motivated
Visually, the presence of dependency between the respective tree structure and the binary responses particularly strongly related to the gene expressions. Moreover, from the \( p \)-values, we conclude that the estrogen receptor expression \((k = 2)\) is particularly strongly related to the gene expressions. Moreover, from the \( p \)-values, we conclude
that we can decidedly reject the null-hypothesis of independence between the gene expression and all the response variables, with the exception of the angioinvasion response ($k = 5$), which has also a low transport dependency value. This conclusion coincides with the findings by Behr et al. (2020), demonstrating that the transport dependency can be used to detect and quantify dependencies even when the data is high dimensional, provided that meaningful criteria of similarity are available on the marginal spaces.

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A Omitted statements and proofs

This appendix provides detailed proofs for all statements that are not proven in the main text. Note that we rely on disintegration arguments to construct or destruct transport plans on several occasions. This is often not the only viable method, however, and several of our results could alternatively be tackled by other techniques, like exploiting the cyclical monotonicity of optimal transport plans (see Villani [2008]).

Convexity and invariance. In the following, we provide proofs for Proposition 3.4 and Proposition 3.5 (related to the convexity of the transport dependency). We furthermore establish a fundamental invariance property of optimal transport (Lemma A.1), which then powers the proof of Proposition 3.6.

Proof of Proposition 3.4. Let \( \gamma_0, \gamma_1 \in \mathcal{C}(\mu, \cdot) \) with second marginals \( \nu_i \in \mathcal{P}(Y) \) for \( i \in \{0, 1\} \), and let \( \pi_t^* \) be an optimal transport plan between \( \gamma_t \) and \( \mu \otimes \nu_t \) with respect to \( c \). Then, defining \( \gamma_t = (1-t)\gamma_0 + t\gamma_1 \) for \( t \in [0, 1] \) (and similarly \( \nu_t \)), we find \( \gamma_t \in \mathcal{C}(\mu, \nu_t) \) and \( \pi_t = (1-t)\pi_0^* + t\pi_1^* \in \mathcal{C}(\gamma_t, \mu \otimes \nu_t) \). Hence,

\[
\tau(\gamma_t) = T_c(\gamma_t, \mu \otimes \nu_t) \leq \pi_t c = (1-t) \tau(\gamma_0) + t \tau(\gamma_1),
\]

which establishes convexity on \( \mathcal{C}(\mu, \cdot) \). The result on \( \mathcal{C}(\cdot, \nu) \) follows analogously. \( \square \)

Proof of Proposition 3.5. Since \( \tau(\mu \otimes \nu) = 0 \), the first part of the statement follows from Proposition 3.4. For equality in (3.3) if \( c \) is a metric, we consider the dual formulation (2.3) and deduce

\[
\tau(\gamma_t) = \sup f \in \mathcal{L} \tau(f, \gamma_t) = (1-t) \sup f \in \mathcal{L} \tau(f, \gamma_0) + t \sup f \in \mathcal{L} \tau(f, \gamma_1),
\]

where both suprema are taken over \( f \in \mathcal{L}(X \times Y) \) with respect to \( c \). \( \square \)

Lemma A.1: Let \( X \) and \( Y \) be Polish spaces and let \( c \) be a cost function on \( Y \). Consider a measurable function \( f : X \to Y \) and let \( c_f : X^2 \to [0, \infty] \) be defined by \( c_f(x, x') = c(f(x), f(x')) \). Then for any \( \mu, \nu \in \mathcal{P}(X) \),

\[
T_c(f_*\mu, f_*\nu) = T_{c_f}(\mu, \nu).
\]

Proof of Lemma A.1. By a change of variables, we can immediately establish \( \pi c_f = (f \otimes f)_* \pi c \) for any \( \pi \in \mathcal{C}(\mu, \nu) \), where \( (f \otimes f)_* \pi \in \mathcal{C}(f_*\mu, f_*\nu) \). This shows

\[
T_{c_f}(\mu, \nu) = \inf_{\pi \in \mathcal{C}(\mu, \nu)} \pi c_f = \inf_{\pi \in \mathcal{C}(\mu, \nu)} (f \otimes f)_* \pi c \geq \inf_{\tilde{\pi} \in \mathcal{C}(f_*\mu, f_*\nu)} \tilde{\pi} c = T_c(f_*\mu, f_*\nu).
\]

To prove the reverse inequality, we fix some \( \tilde{\pi} \in \mathcal{C}(f_*\mu, f_*\nu) \) and explicitly construct a measure \( \pi \in \mathcal{C}(\mu, \nu) \) that satisfies \( \pi c_f = \tilde{\pi} c \).
We construct $\pi$ in two steps. First, we define an intermediate measure $\pi'$ by the relation $\pi'(dx_1, dy_2) = \tilde{\pi}(f(x_1), dy_2) \mu(dx_1)$. In the second step, we set $\pi(dx_1, dx_2) = \pi'(dx_1, f(x_2)) \nu(dx_2)$.

It is straightforward to check $\pi' \in C(\mu, f_\nu \nu)$ and $\pi \in C(\mu, \nu)$ by applying substitution and utilizing the properties of conditioning. In a similar vein, consecutive steps of substitution also show

$$\pi c_f = \int c_f(x_1, x_2) \pi(dx_1, dx_2)$$
$$= \int c(f(x_1), f(x_2)) \pi'(dx_1, f(x_2)) \nu(dx_2)$$
$$= \int c(f(x_1), y_2) \pi'(dx_1, y_2) (f_\nu \nu)(dy_2)$$
$$= \int c(f(x_1), y_2) \pi'(dx_1, dy_2)$$
$$= \int c(f(x_1), y_2) \tilde{\pi}(f(x_1), dy_2) \mu(dx_1)$$
$$= \int c(y_1, y_2) \tilde{\pi}(y_1, dy_2) (f_\mu \nu)(dy_1) = \tilde{\pi}c.$$

This establishes $T_{c_f}(\mu, \nu) \leq T_c(f_\mu, f_\nu \nu)$ and thus the equality of the two transport costs. Note that $T_c(f_\mu, f_\nu \nu)$ and $T_{c_f}(\mu, \nu)$ do not have to be finite for this result to hold, as all integrands are non-negative. \hfill $\square$

**Proof of Proposition 3.9**

For $y \in C(\mu, v)$ with $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$, we observe that $c_f = c$ as well as $f_\mu \otimes \nu = f_{X+\mu} \otimes f_{Y+\nu}$ and $f_{X+\mu} \otimes f_{Y+\nu} \in C(f_{X+\mu}, f_{Y+\nu})$. The conclusion then follows from Lemma \[A.4\] \hfill $\square$

**Continuity.** This section covers the proofs for Proposition 3.8, Proposition 3.9, and Theorem 5.1 (continuity of the transport dependency). We furthermore provide two auxiliary results (Proposition \[A.3\] and Lemma \[A.4\]) that control optimal transport costs under uniform changes of the base costs. These are needed in Section 5.

**Proof of Proposition 3.8** Let $(y_n)_{n \in \mathbb{N}} \subset \mathcal{P}(X \times Y)$ be a sequence of probability measures that weakly converges to $y \in C(\mu, v)$ for $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$. By the continuous mapping theorem, the respective marginals $(\mu_n)_{n \in \mathbb{N}}$ and $(\nu_n)_{n \in \mathbb{N}}$ weakly converge to $\mu$ and $\nu$. According to Billingsley (2016, Theorem 2.8), this implies weak convergence of the product measures $\mu_n \otimes \nu_n$ to $\mu \otimes \nu$. The result of the proposition now follows along the lines of the proof of the lower semi-continuity of the optimal transport cost (see for example Santambrogio 2015, Proposition 7.4, which requires only slight adaptations to make it work for sequences in both arguments of $T_c$). \hfill $\square$

**Proof of Proposition 3.9** In order to prove this claim, we first establish an auxiliary result.
Lemma A.2: Let $X$ be a Polish space and $f, g: X \to [0, \infty)$ continuous functions with $g \leq f$. For a sequence $(\mu_n)_{n \in \mathbb{N}} \subset \mathcal{P}(X)$ converging weakly to $\mu \in \mathcal{P}(X)$, it holds that
\[
\lim_{n \to \infty} \mu_n f = \mu f < \infty \quad \text{implies} \quad \lim_{n \to \infty} \mu_n g = \mu g < \infty.
\]

Proof. Assume $\mu_n f \to \mu f < \infty$ as $n \to \infty$. According to Ambrosio et al. (2008, Lemma 5.1.7), this implies that $f$ is uniformly integrable with respect to $(\mu_n)_{n \in \mathbb{N}}$. Fix some $k > 0$. Since $g(x) > k$ implies $f(x) > k$ for all $x \in X$, we find $\mu_n (\mathbb{1}_{g \geq k} g) \leq \mu_n (\mathbb{1}_{f \geq k} f)$ for all $n$ and conclude that $g$ is also uniformly integrable with respect to $(\mu_n)_{n \in \mathbb{N}}$. This in turn asserts that $\mu_n g \to \mu g$ as $n \to \infty$. \(\Box\)

We now return to the proof of Proposition 3.9. We know that $\liminf_{n \to \infty} \tau(y_n) \geq \tau(y)$ due to the semi-continuity of $\tau$ (Proposition 3.8). Thus, it is enough to show $\limsup_{n \to \infty} \tau(y_n) = \bar{\tau} \leq \tau(y)$. By passing to a (not explicitly named) subsequence, we can assume that $\tau(y_n)$ converges to $\bar{\tau}$.

Let $y_n \in C(\mu_n, \nu_n)$ and $y \in C(\mu, \nu)$ for suitable marginal distributions $\mu, \mu_n \in \mathcal{P}(X)$ and $\nu, \nu_n \in \mathcal{P}(Y)$. Since $y_n \to y$ by assumption, we note that $\mu_n \to \mu$ and $\nu_n \to \nu$ as $n \to \infty$ by the continuous mapping theorem. Like in the proof of Proposition 3.8, we conclude that $\mu_n \otimes \nu_n$ converges weakly to $\mu \otimes \nu$. Next, we fix a point $(x_0, y_0) \in X \times Y$. According to Lemma A.2. $\mu_n d_X(\cdot, x_0)^p = \nu_n d_X(\cdot, x_0)^p \to \gamma d_X(\cdot, x_0)^p = \mu d_X(\cdot, x_0)^p$ as $n \to \infty$, where we set $g(x, y) = d_X(x, x_0)^p, f(x, y) = d((x, y), (x_0, y_0))^p$, and used that $y_n f \to y f < \infty$ (by assumption). Therefore, $\mu_n$ converges $p$-weakly to $\mu$, and the same holds for $\nu_n$ by a similar argument.

In the next step, we bound the metric $d$ on $X \times Y$ by applying the triangle inequality and using that $(\sum_{i=1}^4 a_i)^p \leq 4^p \sum_{i=1}^4 a_i^p$ for numbers $a_i \geq 0$ with $1 \leq i \leq 4$. We find
\[
d(x_1, y_1, x_2, y_2)^p \leq (d_X(x_1, x_0) + d_X(x_2, x_0) + d_Y(y_1, y_0) + d_Y(y_2, y_0))^p
\leq 4^p(d_X(x_1, x_0)^p + d_X(x_2, x_0)^p + d_Y(y_1, y_0)^p + d_Y(y_2, y_0)^p)
\]
\[= : \delta(x_1, y_1, x_2, y_2).
\]

Let $\pi^*_n$ denote an (arbitrary) optimal transport plan between $y_n$ and $\mu_n \otimes \nu_n$, meaning $\tau(y_n) = \pi^*_n c$. Applying the previous inequality yields
\[
\pi^*_n c \leq \pi^*_n d^p \leq \pi^*_n \delta = 2 \cdot 4^p(\mu_n d_X(\cdot, x_0)^p + \nu_n d_Y(\cdot, y_0)^p),
\]
where the right-hand side converges as $n \to \infty$, since we have established that $\mu_n$ and $\nu_n$ converge $p$-weakly. As the cost $c$ is continuous, we can use the stability result in (Villani 2008, Theorem 5.20) and conclude that there is a subsequence $\pi^*_{n_k}$ of optimal transport plans weakly converging to some optimal $\pi^* \in C(\gamma, \mu \otimes \nu)$, such that $\tau(y) = \pi^* c$. Exploiting that
\[
\pi^*_{n_k} \delta \to 2 \cdot 4^p(\mu d_X(\cdot, x_0)^p + \nu d_Y(\cdot, y_0)^p) = \pi^* \delta < \infty
\]
as $k \to \infty$, we can apply Lemma A.2 with $f = \delta$ and $g = c$ to finally conclude
\[
\bar{\tau} = \lim_{n \to \infty} \pi^*_n c = \lim_{k \to \infty} \pi^*_{n_k} c = \pi^* c = \tau(y),
\]
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which completes the proof.

Proof of Theorem 3.10. Since \( d \) satisfies the triangle inequality, so does \( \rho = T_1^{1/p} \) (see Villani 2008, Definition 6.1). Furthermore, the stated inequality is trivial if the right-hand side is \( \infty \). Thus, we can assume \( \rho(y, y') < \infty \) and \( \rho(\mu \otimes v, \mu' \otimes v') < \infty \). Then also \( \rho(y', \mu \otimes v) \leq \rho(y', \mu' \otimes v') + \rho(\mu \otimes v, \mu' \otimes v') < \infty \). Now, the result follows from applying the reverse triangle inequality:

\[
|\tau(y)^{1/p} - \tau(y')^{1/p}| = |\rho(y, \mu \otimes v) - \rho(y', \mu' \otimes v')| \\
\leq |\rho(y, \mu \otimes v) - \rho(y', \mu \otimes v)| + |\rho(y', \mu \otimes v) - \rho(y', \mu' \otimes v')| \\
\leq \rho(y, y') + \rho(\mu \otimes v, \mu' \otimes v').
\]

\[\square\]

We write \( \| \cdot \|_\infty \) to denote the sup-norm of a real valued function and use the convention \( 0/0 = 1 \) in the following statement.

Proposition A.3 (varying costs): Let \( X \) and \( Y \) be Polish spaces and let \( c \) and \( c_n \) be cost functions on \( X \times Y \) that satisfy \( \|c/c_n - 1\|_\infty \rightarrow 0 \) as \( n \rightarrow \infty \). Let \( (y_n)_{n \in \mathbb{N}} \) be a sequence in \( \mathcal{P}(X \times Y) \) and \( y \in \mathcal{P}(X \times Y) \) such that \( \tau_c(y) < \infty \). Then

\[
\lim_{n \rightarrow \infty} \tau_c(y_n) = \tau_c(y) \quad \text{implies} \quad \lim_{n \rightarrow \infty} \tau_c(y_n) = \tau_c(y).
\]

Proof. We set \( a_n = \max (\|c/c_n - 1\|_\infty, \|c_n/c - 1\|_\infty) \) and observe \( a_n \rightarrow 0 \) as \( n \rightarrow \infty \) by the assumption of uniform convergence. Applying Lemma A.4 below, we can control the deviation of \( \tau_c(y_n) \) from \( \tau_c(y) \)

\[
|\tau_c(y_n) - \tau_c(y)| \leq |\tau_c(y_n) - \tau_c(y_n) + |\tau_c(y_n) - \tau_c(y)|| \\
\leq a_n(1 + a_n) \tau_c(y_n) + |\tau_c(y_n) - \tau_c(y)| \rightarrow 0.
\]

\[\square\]

Lemma A.4: Let \( X \) be a Polish space and let \( c_1 \) and \( c_2 \) be cost functions on \( X \) that satisfy

\[
\max (\|c_1/c_2 - 1\|_\infty, \|c_2/c_1 - 1\|_\infty) \leq a
\]

under the convention \( 0/0 = 1 \), where \( \| \cdot \|_\infty \) is the sup norm and \( a > 0 \). Then for all \( \mu, v \in \mathcal{P}(X) \) with \( T_{c_1}(\mu, v) < \infty \), we find \( T_{c_1}(\mu, v) \leq (1 + a)T_{c_2}(\mu, v) < \infty \) and

\[
|T_{c_1}(\mu, v) - T_{c_2}(\mu, v)| \leq a \max (T_{c_1}(\mu, v), T_{c_2}(\mu, v)) \leq a(1 + a) T_{c_2}(\mu, v).
\]

Proof of Lemma A.4. We first note that \( c_1 \leq (1 + a)c_2 \), which implies \( T_{c_1}(\mu, v) \leq (1 + a)T_{c_2}(\mu, v) \). Furthermore, if \( \pi_1^* \) and \( \pi_2^* \) denote optimal transport plans between \( \mu \) and \( v \) under the costs \( c_1 \) and \( c_2 \), then

\[
T_{c_1}(\mu, v) - T_{c_2}(\mu, v) = \pi_1^* c_1 - \pi_2^* c_2 \leq \pi_2^* |c_1 - c_2| \leq a \pi_2^* c_2 = a T_{c_2}(\mu, v)
\]

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Convolutions. In the following, a general statement about the behavior of the optimal transport cost under convolution is formulated and proved (Lemma A.5). This result is then applied to prove Theorem 3.11.

Lemma A.5: Let $X$ be a Polish vector space and $c(x_1, x_2) = h(x_1 - x_2)$ for $x_1, x_2 \in X$ a translation invariant cost function on $X$. For any probability measures $\mu, \nu$, and $\kappa$ in $\mathcal{P}(X)$,

$$T_c(\mu \ast \kappa, \nu \ast \kappa) \leq T_c(\mu, \nu) \quad \text{and} \quad T_c(\mu, \mu \ast \kappa) \leq \kappa h.$$

Proof of Lemma A.5. To prove the first inequality, we reach for the dual formulation (2.2) of optimal transport. For any continuous and bounded potential $f : X \rightarrow \mathbb{R}$, we define $f_\kappa(x) = \kappa f(x + \cdot)$ for $x \in X$. It is easy to check that $f_\kappa$ is again continuous and bounded. If $g$ is another potential such that $f \otimes g \leq c$, we find

$$f_\kappa(x_1) + g_\kappa(x_2) = \kappa \left( f(x_1 + \cdot) + g(x_2 + \cdot) \right) \leq \int c(x_1 + y, x_2 + y) \kappa(dy) = c(x_1, x_2)$$

for any $x_1, x_2 \in X$ due to the translation invariance of $c$. Therefore, $f_\kappa \otimes g_\kappa \leq c$. This implies

$$(\mu \ast \kappa) f + (\nu \ast \kappa) g = \mu f_\kappa + \nu g_\kappa \leq \sup \mu f' + \nu g' = T_c(\mu, \nu),$$

where the supremum is taken over continuous and bounded potentials $f'$ and $g'$ with $f' \otimes g' \leq c$. Since $f$ and $g$ were arbitrary, $T_c(\mu \ast \kappa, \nu \ast \kappa) \leq T_c(\mu, \nu)$ follows. Note that this arguments holds even if $T_c(\mu, \nu) = \infty$, so there are no restrictions on $\mu, \nu \in \mathcal{P}(X)$.

For the upper bound in the second result, we construct an explicit transport plan $\pi$ between $\mu$ and $\mu \ast \kappa$. It is defined by $\pi f = \int f(x_1, x_1 + x_2) \mu(dx_1) \kappa(dx_2)$ for any measurable map $f : X \times X \rightarrow [0, \infty)$. It is straightforward to check that $\pi \in C(\mu, \mu \ast \kappa)$, and we can conclude

$$T_c(\mu, \mu \ast \kappa) \leq \pi c = \int c(x_1, x_1 + x_2) \mu(dx_1) \kappa(dx_2) = \kappa h,$$

where we made use of the translation invariance $c(x_1, x_2) = h(x_1 - x_2)$ and the symmetry $c(x_1, x_2) = c(x_2, x_1)$ of $c$ for any $x_1, x_2 \in X$. Again, the argument stays valid even if $T_c(\mu, \mu \ast \kappa) = \infty$, so the results holds for any $\mu \in \mathcal{P}(X)$.

Proof of Theorem 3.11. One can easily check that $\gamma \ast \kappa \in C(\mu \ast \kappa_X, \nu \ast \kappa_Y)$ and $(\mu \otimes \nu) \ast \kappa = (\mu \ast \kappa_X) \otimes (\nu \ast \kappa_Y)$. Therefore, $\tau(\gamma \ast \kappa) = T_c(\gamma \ast \kappa, (\mu \otimes \nu) \ast \kappa)$ and Lemma A.5 can be applied, which yields the first result. For the second result, we recall Theorem 3.10 and use the second part of Lemma A.5 to find

$$\tau(\gamma)^{1/p} - \tau(\gamma \ast \kappa)^{1/p} \leq T_c(\gamma, \gamma \ast \kappa)^{1/p} + T_c(\mu \otimes \nu, (\mu \otimes \nu) \ast \kappa)^{1/p} \leq 2(\kappa h)^{1/p},$$

which finishes the proof.
Upper bounds and marginal transport dependency. This segment establishes the upper bounds in Proposition 3.14 and 3.16 and contains proofs for Theorem 3.17 and Proposition 6.2 concerning the marginal transport dependency.

Proof of Proposition 3.14 It is evident that $c_{XY}$ is a cost function (non-negative, symmetric, lower semi-continuous). Furthermore, the second inequality in (3.8a) follows trivially. To prove the first inequality, we construct a coupling $\pi_2 \in C(\gamma, \mu \otimes \nu)$ that aims to prevent either horizontal or vertical movements, depending on which of the associated marginal costs is larger. We therefore define the set

$$S = \{(x_1, y_1, x_2, y_2) \mid c_X(x_1, x_2) \geq c_Y(y_1, y_2)\} \subset (X \times Y)^2,$$

and note that $S$ is symmetric under exchanging $(x_1, y_1)$ and $(x_2, y_2)$ due to the symmetry of the costs $c_X$ and $c_Y$. We write $R$ to denote the complement of $S$, which is also symmetric. Next, we introduce the function $r: (X \times Y)^2 \to (X \times Y)^2$ given by

$$r(x_1, y_1, x_2, y_2) = \begin{cases} (x_1, y_1, x_2, y_2) & \text{if } (x_1, y_1, x_2, y_2) \in S, \\ (x_2, y_2, x_1, y_1) & \text{else.} \end{cases}$$

The proof is completed once we show that the coupling defined by $\pi_2 = r_* (\gamma \otimes \gamma)$ has the correct marginals, meaning $\pi_2 \in C(\gamma, \mu \otimes \nu)$, and that $\pi_2 c$, which is an upper bound for $\tau(\gamma)$, is in turn upper bounded by $(\gamma \otimes \gamma) c_{XY}$. The second marginal $\mu \otimes \nu$ is an immediate consequence of the definition of $r$ and $\pi_2$. To check the first marginal, we consider an arbitrary positive and measurable function $f: X \times Y \to \mathbb{R}$. Then, if $q$ denotes the two first components of $r$,

$$\int f(x_1, y_1) \, d\pi_2(x_1, y_1, x_2, y_2) = \int f(q(x_1, y_1, x_2, y_2)) \, d\gamma(x_1, y_1) \, d\gamma(x_2, y_2)$$

$$= \int 1_S(x_1, y_1, x_2, y_2) \, f(x_1, y_1) \, d\gamma(x_1, y_1) \, d\gamma(x_2, y_2)$$

$$+ \int 1_R(x_1, y_1, x_2, y_2) \, f(x_2, y_2) \, d\gamma(x_1, y_1) \, d\gamma(x_2, y_2)$$

$$= \int f(x_1, y_1) \, d\gamma(x_1, y_1) = \gamma f,$$

where we swapped the roles of $(x_1, y_1)$ and $(x_2, y_2)$ to establish the third equality. This is permissible due to the symmetry of $S$ (and $R$). Similarly, we observe

$$\tau(\gamma) \leq \pi_2 c$$

$$= \int_S c(x_1, y_1, x_2, y_2) \, d\gamma(x_1, y_1) \, d\gamma(x_2, y_2) + \int_R c(x_2, y_2, x_1, y_1) \, d\gamma(x_1, y_1) \, d\gamma(x_2, y_2)$$

$$\leq \int_S c_Y(y_1, y_2) \, d\gamma(x_1, y_1) \, d\gamma(x_2, y_2) + \int_R c_X(x_1, x_2) \, d\gamma(x_1, y_1) \, d\gamma(x_2, y_2)$$

$$= \int \min(c_X(x_1, x_2), c_Y(y_1, y_2)) \, d\gamma(x_1, y_1) \, d\gamma(x_2, y_2) = (\gamma \otimes \gamma) c_{XY},$$

where we bounded $c$ by $c_Y$ and $c_X$ via condition (3.7).
Proof of Proposition 3.16: In order to prove this result, we first introduce an alternative characterization of the measurability of probability kernels that is employed in Villani (2008).

Lemma A.6 (measurability of kernels): Let $X$ be Polish and let $(\mu_\omega)_{\omega \in \Omega} \subset \mathcal{P}(X)$ be a family of probability measures indexed in a measurable space $(\Omega, \mathcal{F})$. Then

$$\omega \mapsto \mu_\omega(A) \text{ is measurable for all Borel sets } A \subset X \iff \omega \mapsto \mu_\omega \text{ is measurable},$$

where $\mathcal{P}(X)$ is equipped with the Borel $\sigma$-algebra with respect to the topology of weak convergence of measures.

Proof. Theorem 17.24 in Kechris (2012) asserts that the Borel $\sigma$-algebra of $\mathcal{P}(X)$ is generated by functions $r_A: \mathcal{P}(X) \to [0, 1]$ of the form $\nu \mapsto \nu(A)$ for Borel sets $A \subset X$. This means that $\mathcal{G} = \left\{ r_A^{-1}(B) \mid B \in [0, 1] \text{ Borel and } A \subset X \text{ Borel} \right\}$ is a generator of the Borel $\sigma$-algebra of $\mathcal{P}(X)$. In particular, each $r_A$ is measurable.

Thus, if $\mu: \omega \mapsto \mu_\omega$ is measurable, then $\omega \mapsto (r_A \circ \mu)(\omega) = \mu_\omega(A)$ is also measurable as composition of measurable functions. Conversely, if $\omega \mapsto \mu_\omega(A)$ is measurable for each Borel set $A \subset X$, then $\mu^{-1}(G) \in \mathcal{F}$ for each $G \in \mathcal{G}$. Since $\mathcal{G}$ is a generator, this suffices to show that $\omega \mapsto \mu_\omega$ is measurable. \qed

We now return to the proof of Proposition 3.16. Let $\pi_x^* \in C(Y(x, \cdot), \mu)$ be an optimal transport plan with respect to the base costs $c_Y$ for each $x \in X$. Corollary 5.22 in Villani (2008) together with the continuity of $c_X$ and Lemma A.6 above guarantee that $\pi_x^*$ can be selected such that $(\pi_x^*)_{x \in X}$ is a probability kernel. We can thus define $\pi_3 \in \mathcal{P}(X \times Y)$ via

$$d\pi_3(x_1, y_1, x_2, y_2) = \pi_x^*(dy_1, dy_2) \delta_{x_1}(dx_2) \nu(dx_1).$$

It can easily be checked that the marginals of $\pi_3$ match $\gamma$ and $\mu \otimes \nu$. Using condition (3.7), we find

$$\tau(\gamma) \leq \tau_3 \leq \int \left( \int c_Y(y_1, y_2) \pi_x^*(dy_1, dy_2) \right) \mu(dx) = \int (\pi_x^* c_Y) \mu(dx),$$

which shows the first inequality of the proposition. To assert the second inequality, one just has to note that $\pi_x^* c_Y \leq (\gamma(x, \cdot) \otimes \nu) c_Y$ for each $x \in X$ by construction of $\pi_x^*$ as optimal plan. \qed

Proof of Theorem 3.17: We begin by defining a set that contains all vertical movements along the fibers $\{x\} \times Y$, given by $S = \{(x, y_1, x, y_2) \mid x \in X, y_1, y_2 \in Y\} \subset (X \times Y)^2$. Due to the definition of $c_{\infty}$, it is evident that

$$\tau_{c_{\infty}}(\gamma) = \inf_{\pi \in C(\gamma, \mu \otimes \nu)} \pi c_Y.$$  \hspace{1cm} (A.1)

We use this characterization to show that the equality $\tau_{c_{\infty}}(\gamma) = \tau_Y^T(\gamma)$ holds. First, we define $f: S \to X \times Y^2$ via $f(x, y_1, x, y_2) = (x, y_1, y_2)$. For each $\pi$ that is feasible in the infimum in (A.1), we furthermore define $\pi_x = (f_2 \pi)(x, \cdot, \cdot) \in \mathcal{P}(Y \times Y)$ for $x \in X$. One can check
that \( \pi_x \in C(y(x, \cdot), \nu) \) holds \( \mu \)-almost surely due to the (almost sure) uniqueness property of disintegrations. If \( \pi_x^* \in C(y(x, \cdot), \nu) \) are a measurable selection of optimal transport plans for the problem \( T_c(y(x, \cdot), \nu) \) as in the proof of Proposition 5.16, we observe

\[
\pi c_Y = \int \int c_Y d\pi = \int \int c_Y d(f_x \mu) = \int (\pi_x c_Y) \mu(dx) = \int (\pi_x c_Y) \mu(dx) = \tau^Y_c(y).
\]

Taking the infimum on the left-hand side and applying (A.1) implies \( \tau_{cw}(y) \geq \tau^Y_c(y) \). Since we already know \( \tau_{cw}(y) \leq \tau^Y_c(y) \) by Proposition 5.16, this proves equality.

It is left to show that \( \tau_{cw}(y) \rightarrow \tau_{cw}(y) \) as \( \alpha \rightarrow \infty \). Since \( c_{cw} \geq c_{\alpha} \) for all \( \alpha > 0 \), we know that \( \tau_{cw}(y) \geq \tau_{ca}(y) \) and it is accordingly sufficient to show \( \lim \inf_{\alpha \rightarrow \infty} \tau_{ca}(y) = \tau_{cw}(y) \). We thus fix \( \overline{\tau} = \lim \inf_{\alpha \rightarrow \infty} \tau_{ca}(y) \) and consider a diverging sequence \( (\alpha_n)_{n \in \mathbb{N}} \subset (0, \infty) \) such that \( \tau_{ca}(y) \rightarrow \overline{\tau} \). Due to Prokhorov’s theorem and the existence of optimal transport plans, we can assume that there are couplings \( \pi_n^* \) and \( \pi_{\infty} \) in \( C(y, \mu \otimes \nu) \) that satisfy \( \tau_{c_{\alpha n}}(y) = \pi_n^* \otimes c_{\alpha n} \) and \( \pi_{\infty} \). We use these properties to lead the assumption \( \tau_{c_{\infty}}(y) \geq \overline{\tau} \) to a contradiction. If this assumption were true, observe that for any \( k > 0 \),

\[
\lim_{n \rightarrow \infty} \pi_n^* \otimes c_{\alpha n} \geq \lim_{n \rightarrow \infty} \alpha_n \pi_n^* c_{\alpha n} \geq k \lim_{n \rightarrow \infty} \pi_n^* c_{\alpha n} \geq k \pi_{\infty} c_{\alpha n},
\]

where the final inequality follows from the lower semi-continuity of the mapping \( \pi \mapsto \pi h \) under weak convergence for lower semi-continuous integrands \( h \) that are bounded from below (Santambrogio 2015, Proposition 7.1). Since \( k \) is arbitrary, we conclude \( \pi_{\infty} c_{\alpha n} = 0 \), which implies \( \pi_{\infty}(S) = 1 \) due to the positivity of \( c_{\alpha n} \). Employing representation (A.1) of \( \tau_{c_{\infty}}(y) \), we find the contradiction

\[
\tau_{c_{\infty}}(y) > \overline{\tau} = \lim_{n \rightarrow \infty} \pi_n^* \otimes c_{\alpha n} \geq \lim_{n \rightarrow \infty} \pi_n^* c_Y \geq \pi_{\infty} c_Y \geq \tau_{c_{\infty}}(y).
\]

This establishes \( \overline{\tau} = \tau_{c_{\infty}}(y) \) and finishes the proof.

\[
\text{Proof of Theorem 4.3} \quad \text{We begin the proof by showing the following auxiliary statement.}
\]

**Lemma A.7:** Let \( X \) be a Polish space and \( c \) a positive continuous cost function on \( X \). For \( \mu, \nu \in P(X) \) with \( \text{supp} \mu \subset \text{supp} \nu \) and \( T_c(\mu, \nu) < \infty \), it holds that

\[
T_c(\mu, \nu) = (\mu \otimes \nu) c \quad \iff \quad \mu = \delta_x \text{ for some } x \in X.
\]

**Proof:** The implication from right to left is trivial, since \( \mu \otimes \nu \) is the only feasible coupling if \( \mu \) is a point mass. To show the reverse direction, we assume that \( \mu \neq \delta_x \) for any \( x \in X \) and show that \( T_c(\mu, \nu) = (\mu \otimes \nu) c \) is impossible. First, we pick two distinct points \( x_1 \neq x_2 \) from the support of \( \mu \). By assumption, these points also lie in the support of \( \nu \). To show that \( \mu \otimes \nu \) cannot be an optimal transport plan, it is sufficient to show that \( \text{supp}(\mu \otimes \nu) = \text{supp} \mu \times \text{supp} \nu \) is not \( c \)-cyclically monotone (Villani 2003). This is easy to see, since for \( (x_1, x_2), (x_2, x_1) \in \text{supp}(\mu \otimes \nu) \), we find

\[
c(x_1, x_2) + c(x_2, x_1) > c(x_1, x_1) + c(x_2, x_2) = 0
\]

due to the positivity of \( c \).
Returning to the proof of Theorem 4.3 we note that $\tau^Y(y)$ and $(v \otimes v) c_Y$ are equal iff
\[
\int T_{c_Y} (\gamma(x, \cdot), v) \mu(dx) = \int (\gamma(x, \cdot) \otimes v) c_Y \mu(dx).
\] (A.2)
Evidently, these two values are the same if $\gamma = (\text{id}, \varphi)_* \mu$, since this implies $\gamma(x, \cdot) = \delta_{\varphi(x)}$ for $\mu$-almost all $x \in X$. So it only remains to show that equality in (A.2) implies $\gamma = (\text{id}, \varphi)_* \mu$ for some $\mu$-almost surely defined measurable function $\varphi : X \to Y$.

Since the right-hand side in (A.2) is by assumption finite and $0 \leq T_{c_Y} (\gamma(x, \cdot), v) \leq (\gamma(x, \cdot) \otimes v) c_Y$ holds for each $x \in X$, we find that equality in (A.2) can only hold if
\[
T_{c_Y} (\gamma(x, \cdot), v) = (\gamma(x, \cdot) \otimes v) c_Y
\]
for $\mu$-almost all $x \in X$. As $\operatorname{supp} \gamma(x, \cdot) \subset \operatorname{supp} \nu$ also holds for $\mu$-almost all $x \in X$ (see below), we can apply Lemma A.7 and find that $\gamma(x, \cdot) = \delta_{\varphi(x)}$ for a $\mu$-almost surely defined function $\varphi$. The measurability of $\varphi$ follows from the measurability of the maps $x \mapsto \gamma(x, A)$ for all Borel sets $A \subset Y$, since $x \in \varphi^{-1}(A)$ is equivalent to $\gamma(x, A) = 1$ for all $x \in X$ for which $\varphi$ is defined by the construction above.

A brief argument to see that $\operatorname{supp} \gamma(x, \cdot) \subset \operatorname{supp} \nu$ for $\mu$-almost all $x \in X$ goes as follows: note that $\operatorname{supp} \gamma \subset \operatorname{supp} (\mu \otimes \nu) = \operatorname{supp} \mu \times \operatorname{supp} \nu$ and write
\[
1 = \int d\gamma = \int 1_{\operatorname{supp} \nu}(y) \gamma(dx, dy) = \int 1_{\operatorname{supp} \nu}(y) \gamma(x, dy) \mu(dx),
\]
which proves that $\gamma(x, \operatorname{supp} \nu) = 1$ for $\mu$-almost all $x \in X$. \qed

Proof of Proposition 6.2. We first note that $\tau_{c_{\text{cov}}} (\gamma) < \infty$ for all $0 < \alpha \leq \infty$ due to the finite $p$-th moment of $\gamma$. Next, we observe
\[
\mathbb{E} \left[ |\tau_{c_{\text{cov}}} (\hat{y}_n)^{1/p} - \tau^Y_{c_{\text{cov}}} (\gamma)^{1/p}| \right] \leq \mathbb{E} \left[ |\tau_{c_{\text{cov}}} (\hat{y}_n)^{1/p} - \tau_{c_{\text{cov}}} (\gamma)^{1/p}| \right] + |\tau_{c_{\text{cov}}} (\gamma)^{1/p} - \tau^Y_{c_{\text{cov}}} (\gamma)^{1/p}|.
\]
By Theorem 3.17 the second summand converges to zero as $n \to \infty$. The first summand can be controlled by Theorem 3.10 and bound (3.6), yielding
\[
\mathbb{E} \left[ |\tau_{c_{\text{cov}}} (\hat{y}_n)^{1/p} - \tau_{c_{\text{cov}}} (\gamma)^{1/p}| \right] \leq 3 \mathbb{E} \left[ T_{c_{\text{cov}}} (\gamma, \hat{y}_n)^{1/p} \right] \leq 3 \alpha_n \mathbb{E} \left[ T_{c_1} (\gamma, \hat{y}_n)^{1/p} \right].
\] \qed

Contracting couplings and maps. We next provide proofs and statements that were omitted in our work on contractions in Section 4. This includes the proof of our main results, Theorem 4.1 and 4.2, as well as the formulation of two auxiliary statements (Lemma A.8 and A.9), which simplify Theorem 4.1 if sufficient regularity is imposed on the involved costs.
Proof of Theorem 4.1. We first show the second part. Assuming that \(\tau(y) = (\nu \otimes \nu)_{cY} < \infty\), we use the upper bound in Proposition 3.14 to conclude \((\gamma \otimes \gamma)_{c_{XY}} = (\nu \otimes \nu)_{cY}\), which can be stated as
\[
\int \min(c_X(x_1, x_2), c_Y(y_1, y_2)) \, d(\gamma \otimes \gamma)(x_1, y_1, x_2, y_2) = \int c_Y(y_1, y_2) \, d(\nu \otimes \nu)(y_1, y_2).
\]
This implies \((\gamma \otimes \gamma)(c_Y \leq c_X) = 1\), since the left-hand side in the equality above would otherwise be strictly smaller than the right-hand side. Recalling that \(c_X = h \circ k_X\) and \(c_Y = h \circ d_Y\) for a strictly increasing \(h\), we find \((\gamma \otimes \gamma)(d_Y \leq k_X) = 1\), meaning that \(\gamma\) is almost surely contracting.

To prove the first statement, we show that \(\tau(y) \geq (\nu \otimes \nu)_{cY}\), which is sufficient to assert equality due to Proposition 3.14. Let \(\pi \in C(\mu, \nu)\) be arbitrary. We define \(\hat{\lambda} \in \mathcal{P}((X \times Y)^2 \times Y)\) via the relation \(d\hat{\lambda}(x_1, y_1, x_2, y_2, y) = \gamma(x_2, dy) \, d\pi(x_1, y_1, x_2, y_2)\). One can readily establish that integrating out \(y_2 \in Y\) yields a measure \(\lambda \in C(\gamma, Y) \subset \mathcal{P}((X \times Y)^2)\). In particular, \(\text{supp } \lambda \subset \text{supp } \gamma \times \text{supp } \gamma\), which implies \(\lambda(d_Y \leq k_X) = 1\) by the assumption that \(\gamma\) is contracting on its support. Combining this insight with the strict monotonicity of \(h\) and the triangle inequality for \(d_Y\), we find
\[
\pi c = \int h(k_X(x_1, x_2) + d_Y(y_1, y_2)) \, d\hat{\lambda}(x_1, y_2, x_1, y, y_2)
\geq \int h(d_Y(y_1, y) + d_Y(y_1, y_2)) \, d\hat{\lambda}(x_1, y_2, x_1, y, y_2)
\geq \int h(d_Y(y, y_2)) \, d\hat{\lambda}(x_1, y_2, x_1, y, y_2)
= \int c_Y(y, y_2) \, d\nu(y) \, d\nu(y_2) = (\nu \otimes \nu)_{c_Y}.
\]
One can check that the independence in the final line follows from the definition of \(\hat{\lambda}\). Taking the infimum over \(\pi \in C(\gamma, \mu \otimes \nu)\) now yields the desired result. \(\square\)

Lemma A.8. Let \(X\) and \(Y\) be Polish spaces and let \(k_X\) and \(d_Y\) be continuous cost functions on \(X\) and \(Y\). Then \(\gamma\) is contracting on its support iff it is almost surely contracting (with respect to \(k_X\) and \(d_Y\)).

Proof of Lemma A.8. It is clear that a contracting coupling \(\gamma\) is almost surely contracting since the set \((X \times Y)^2 \setminus (\text{supp } \gamma)^2\) is a null set for \(\gamma \otimes \gamma\). Let \(\gamma\) therefore be almost surely contracting. If \(k_X\) and \(d_Y\) are continuous and there are \((x_1, y_1), (x_2, y_2) \in \text{supp } \gamma\) with \(d_Y(y_1, y_2) > k_X(x_1, x_2)\), then we also find an open neighbourhood \(U \subset (X \times Y)^2\) of \((x_1, y_1, x_2, y_2) \in (\text{supp } \gamma)^2\) such that \(\supp (\gamma \otimes \gamma) = \supp (\gamma \otimes \gamma)\) where this inequality is true. By the definition of the support, we conclude \((\gamma \otimes \gamma)(U) > 0\) and \(\gamma\) thus fails to be almost surely contracting. \(\square\)
Lemma A.9 (uniform extension): Let $X$ be Polish and $(Y, d_Y)$ a Polish metric space, and let $k_X : X \times X \to [0, \infty)$ be a continuous cost function on $X$. Any function $\varphi : D \to Y$ defined on a subset $D \subset X$ that satisfies
\[ d_Y(\bar \varphi(x_1), \bar \varphi(x_2)) \leq k_X(x_1, x_2) \quad \text{(A.3)} \]
for all $x_1, x_2 \in D$ can uniquely be extended to a function $\varphi : \bar D \to Y$ on the closure $\bar D$ of $D$ that satisfies (A.3) for all $x_1, x_2 \in \bar D$. In particular, $\varphi$ is continuous.

Proof of Lemma A.9: Let $x \in \bar D \setminus D$ and $(x_n)_{n \in \mathbb{N}}$ be a sequence in $D$ converging to $x$. Set $y_n = \bar \varphi(x_n)$ for $n \in \mathbb{N}$ and observe that $d_Y(y_n, y_m) \leq k_X(x_n, x_m)$ for all $n, m \in \mathbb{N}$. In particular, the sequence $(y_n)$ is Cauchy: if it were not Cauchy, there would exist an $\epsilon > 0$ and values $n_r, m_r \geq r$ for each $r \in \mathbb{N}$ such that $d_Y(y_n, y_m) \geq \epsilon$. However, observing $\lim_{n \to \infty} k_X(x_n, x_m) \to 0$ due to continuity of $k_X$ leads this to a contradiction. Consequently, the sequence $(y_n)_{n \in \mathbb{N}}$ converges to a unique limit $y \in Y$ due to the completeness of $(Y, d_Y)$.

The limit point $y$ does not depend on the chosen sequence: if $(x'_n)_{n}$ is another sequence converging to $x$, and $y'$ is the corresponding limit in $Y$, continuity of $d_Y$ and $k_X$ make sure that
\[ 0 \leq d_Y(y, y') = \lim_{n \to \infty} d_Y(y_n, y'_n) \leq \lim_{n \to \infty} k_X(x_n, x'_n) = 0. \]
Therefore, a well-defined extension of $\bar \varphi$ to $\bar D$ exists. For any $x, x' \in \bar D$, this extension $\varphi$ satisfies
\[ d_Y(\varphi(x), \varphi(x')) = \lim_{n \to \infty} d_Y(\bar \varphi(x_n), \bar \varphi(x'_n)) \leq \lim_{n \to \infty} k_X(x_n, x'_n) = k_X(x, x') \]
as $n \to \infty$ for any sequence $(x_n, x'_n)_{n \in \mathbb{N}} \subset D \times D$ that converges to $(x, x') \in \bar D \times \bar D$. \hfill $\square$

Proof of Theorem 4.2: Let $\varphi : X \to Y$ be $\mu$-almost surely contracting such that $\gamma = (\text{id}, \varphi)_\# \mu$. By a change of variables,
\[ (\gamma \otimes \gamma)(d_Y) \leq k_X = (\mu \otimes \mu)(d_\varphi) \leq k_X = 1, \]
where $d_\varphi(x_1, x_2) = d_Y(\varphi(x_1), \varphi(x_2))$ for any $x_1, x_2 \in X$. Therefore, $\gamma$ is almost surely contracting. Since $k_X$ and $d_Y$ are continuous, we can apply Lemma A.8 to conclude that $\gamma$ is contracting on its support. By Theorem 4.1, $\tau(\gamma) = (v \otimes v) c_Y$ follows.

For the reverse direction, we consult the upper bound in Proposition 3.16 to find that $\tau(\gamma) = (v \otimes v) c_Y$ implies $\tau^Y(\gamma) = (v \otimes v) c_Y$. Consequently, Theorem 4.3 establishes the existence of a measurable function $\varphi : X \to Y$ with $\gamma = (\text{id}, \varphi)_\# \mu$. It is left to show that $\varphi$ is $\mu$-almost surely contracting. According to Lemma A.8 and Theorem 4.1, $\gamma$ is contracting on its support. We can therefore consider the set $A = (\text{id}, \varphi)^{-1}(\text{supp } \gamma)$ and conclude that both $\mu(A) = \gamma(\text{supp } \gamma) = 1$ and
\[ d_Y(\varphi(x_1), \varphi(x_2)) \leq d_X(x_1, x_2) \quad \text{for all } x_1, x_2 \in A, \]
since all tuples $(x, \varphi(x)) \in X \times Y$ for $x \in A$ are elements of the support of $\gamma$. \hfill $\square$
Properties of the transport correlation. We next present proofs of Proposition \ref{prop:5.2} to \ref{prop:5.6} regarding basic properties of the transport correlation. Most of the claimed properties are direct consequences of previously established results. Additional arguments are mainly required for properties 5 and 6 in Proposition \ref{prop:5.2} and property 2 in Proposition \ref{prop:5.6}. Recall from Section \ref{sec:5} that we focus on additive costs of the form
\[ c = (ad_X + d_Y)^p \]
on Polish metric spaces \((X, d_X)\) and \((Y, d_Y)\) for \(a, p > 0\).

Proof of Proposition \ref{prop:5.2}. Properties 1 and 2, which characterize when \(\rho_n(\gamma)\) equals 0 and 1, follow from Theorem \ref{thm:3.2} in Section \ref{sec:2} and from Theorem \ref{thm:4.2} in Section \ref{sec:4}. The invariance in property 3 is a consequence of Proposition \ref{prop:3.6}. If \(\gamma\) is restricted to a set with fixed marginal \(p_n^X \gamma = \nu\), then \((\nu \otimes \nu) d^p_{d_{d}^p}\) is constant and convexity of \(\gamma \mapsto \rho_n(\gamma)^p = \tau(\gamma)/(\nu \otimes \nu) d^p_{d_{d}^p}\) is guaranteed by convexity of \(\tau\) as stated in Proposition \ref{prop:3.4}. This shows property 4.

We now turn to the continuity in property 5. Let \(v_n\) and \(v\) denote the respective second marginals of \(\gamma_n\) and \(\gamma\). For convenience, we write \(\delta_n := (v_n \otimes v_n) d^p_{d_{d}^p}\). Our first goal is to show that \(p\)-weak convergence of \(\gamma_n\) to \(\gamma\) implies \(\delta_n \rightarrow \delta = (v \otimes v) d^p_{d_{d}^p}\) as \(n \rightarrow \infty\). To do so, we fix some \(y_0 \in Y\) and define the function
\[ f(y_1, y_2) = 2^p (d_Y(y_1, y_0)^p + d_Y(y_0, y_2)^p) \]
for \(y_1, y_2 \in Y\). Noting that \((a + b)^p \leq 2^p(a^p + b^p)\) for \(a, b \geq 0\), we find \(d^p_{d_{d}^p} \leq f\) by application of the triangle inequality. Consequently,
\[ \delta_n = (v_n \otimes v_n) d^p_{d_{d}^p} \leq (v_n \otimes v_n) f = 2^{p+1} v_n d_Y(\cdot, y_0)^p \rightarrow 2^{p+1} v d_Y(\cdot, y_0)^p \]
as \(n \rightarrow \infty\). The convergence in this inequality follows from the fact that \(v_n\) converges \(p\)-weakly if \(\gamma_n\) converges \(p\)-weakly, which was shown in the proof of Proposition \ref{prop:3.9}. Reaching back to Lemma \ref{lem:A.2} (setting \(g = d^p_{d_{d}^p}, f = f\), and \(\mu_n = v_n \otimes v_n\), we conclude that \(\delta_n\) indeed converges to \(\delta\) as \(n \rightarrow \infty\).

Next, since \(c = (ad_X + d_Y)^p \leq max(1, \alpha)^p (d_X + d_Y)^p\), we can apply Proposition \ref{prop:5.9} and find \(\tau_c(\gamma_n) \rightarrow \tau_c(\gamma)\). Setting \(c_n = (\alpha_n d_X + d_Y)^p\), it is straightforward to see that \(\|c/c_n - 1\|_\infty \rightarrow 0\) due to \(\alpha_n \rightarrow \alpha > 0\) for \(n \rightarrow \infty\), which lets us use Proposition \ref{prop:A.3} to obtain
\[ \lim_{n \rightarrow \infty} \rho_{\alpha_n}(\gamma_n)^p = \lim_{n \rightarrow \infty} \frac{\tau_{c_n}(\gamma_n)}{\delta_n} = \frac{\tau_{\alpha}(\gamma)}{\delta} = \rho_{\alpha}(\gamma)^p. \]

Finally, the monotonicity of \(\alpha \mapsto \rho_{\alpha}(\gamma)\) in property 6 is trivial, since \(c\) increases with \(\alpha\). The concavity of \(\alpha \mapsto \rho_{\alpha}(\gamma)^p\) for \(p \leq 1\) and fixed \(\gamma \in C(\mu, \nu)\) with marginals \(\mu \in \mathcal{P}(X)\) and \(\nu \in \mathcal{P}(Y)\) follows from the fact that pointwise infima over concave functions are again concave. Indeed, we have that
\[ \rho_{\alpha}(\gamma)^p = \frac{1}{(\nu \otimes \nu) d^p_{d_{d}^p}} \inf_{\pi \in C(\gamma; \mu \otimes \nu)} \pi(ad_X + d_Y)^p, \]
where the mapping \(\alpha \mapsto \pi(ad_X + d_Y)^p\) is concave for any fixed \(\pi\) if \(p \leq 1\). \(\square\)
Proof of Proposition 5.4. Due to Theorem 3.17 results established for $\tau$ under generic lower semi-continuous costs $c$ also hold for the marginal transport dependency with $\alpha = \infty$. Therefore, properties 1, 3, and 4 follow from the general results stated in Theorem 3.2, Proposition 3.6, and Proposition 5.4. Note that we can allow dilatations $f_Y$ in property 3 (instead of just isometries), since we normalize by $(v \otimes v) \mathring{d}_Y$ in Definition 5.3 of $\rho_{\infty}$, which neutralizes the dilatation factor $\beta > 0$. Property 2 relies on the specific cost structure for $\alpha = \infty$ and was derived separately in Theorem 4.3.

Proof of Proposition 5.6. Properties 1, 4, and 5 follow in the same way as in the proof of Proposition 5.2. The symmetry property 6 is trivial and directly visible from the definition of $\rho$. Property 3 is a consequence of the general invariance of the transport dependence under isometries (Proposition 3.6). We can extend this to dilatations $f_X$ and $f_Y$ since we divide by the respective diameters in Definition 5.5 of $\rho$, which nullifies any scaling factors.

Regarding property 2, let $\gamma \in C(\mu, v)$ for $\mu \in \mathcal{P}(X)$ and $v \in \mathcal{P}(Y)$. We equip the spaces $X$ and $Y$ with the scaled metrics

$$\hat{d}_X = d_X / ((\mu \otimes \mu) \mathring{d}_X)^{1/p} \quad \text{and} \quad \hat{d}_Y = d_Y / ((v \otimes v) \mathring{d}_Y)^{1/p}.$$

According to Theorem 4.2 (combined with Lemma A.9), a value of $\rho(\gamma) = 1$ is equivalent to there being a contraction $\varphi$ from $(\text{supp} \mu, \hat{d}_X)$ to $(\text{supp} \nu, \hat{d}_Y)$ that satisfies $(\text{id}, \varphi)_* \mu = \gamma$. In particular means $\varphi_* \mu = \nu$. Defining $\hat{d}_\varphi(x_1, x_2) = \hat{d}_Y(\varphi(x_1), \varphi(x_2))$ for any $x_1, x_2 \in \text{supp} \mu$, we know that $\hat{d}_\varphi \leq d_X$ since $\varphi$ is a contraction. By a change of variables, we calculate

$$(\mu \otimes \mu) \hat{d}_\varphi^p = (v \otimes v) \hat{d}_Y^p = 1 = (\mu \otimes \mu) \hat{d}_X^p$$

and assert $\hat{d}_\varphi = \hat{d}_X$ to hold $(\mu \otimes \mu)$-almost surely. Since $\hat{d}_X$ and $\hat{d}_\varphi$ are continuous, we can conclude that $\varphi : (\text{supp} \mu, \hat{d}_X) \to (Y, \hat{d}_Y)$ is an isometry. Thus, $\varphi$ is a dilatation under the metrics $d_X$ and $d_Y$. Note that its dilatation factor $\beta$ is uniquely given by $\alpha$, defined in equation 5.3. Due to the symmetry of the setting, the same arguments also hold for $\psi$ instead of $\varphi$ by exchanging the roles of $X$ and $Y$.

B Lower complexity adaptation

In the following, we derive the property of lower complexity adaptation (LCA) for the estimators proposed in Section 6. We restrict our analysis to bounded and continuous cost functions $c : (X \times Y)^2 \to [0, 1]$. The proof strategy is inspired by Hundrieser et al. (2022), but we use adapted arguments to exploit the additional randomness introduced by the sampling procedure. As preparation, we revisit the dual formulation for the optimal transport cost and introduce some tools from empirical process theory.

Preliminaries. The duality theory of optimal transport crucially depends on the notion of the $c$-conjugacy of functions. We present a selection of definitions and results on this topic,
adapted to the above setting. For a given $g: X \times Y \to \mathbb{R}$ bounded from above, we define its c-transform to be

$$g^c(x, y) = \inf_{(x', y') \in X \times Y} c(x, y, x', y') - g(x', y')$$  \hspace{1cm} (B.1)

for any $(x, y) \in X \times Y$. Each function that can be written as a c-transform is called c-concave. Since $c$ is continuous, all c-concave functions are measurable. The set of (standardized) c-concave functions is denoted by

$$\mathcal{F}_c = \{g^c \mid g: X \times Y \to \mathbb{R}, \sup_{x \in X} g(x) = 0\}.$$

Based on the boundedness of the cost function, it is possible to show that both $f$ and $f^c$ are absolutely bounded by 1 for each $f \in \mathcal{F}_c$. Since we need to restrict $\mathcal{F}_c$ to the support of the coupling $\gamma \in \mathcal{P}(X \times Y)$ in order to exploit the LCA property, we also define the domain-restricted function classes

$$\mathcal{F}_{c}(\gamma) = \{f|_{\text{supp}\, \gamma} \mid f \in \mathcal{F}_c\}$$

for $\gamma \in \mathcal{P}(X \times Y)$. A function $f \in \mathcal{F}_{c}(\gamma)$ can be c-transformed via definition (B.1) by taking the infimum over $(x', y') \in \text{supp}\, \gamma$. For any $\eta_1, \eta_2 \in \mathcal{P}(X \times Y)$, it now follows from standard optimal transport theory (Villani [2008], Theorem 5.10) that strong duality in the form

$$T_c(\eta_1, \eta_2) = \sup_{f \in \mathcal{F}_c} \eta_1 f + \eta_2 f^c$$

holds. If $\text{supp} \, \eta_1 \subset \text{supp} \, \gamma$, then the consistent behavior of optimal transport under restriction of the base spaces (see, e.g., Villani [2008], Theorem 5.19, or Staudt et al. [2022], Lemma 3) even allows us to conclude

$$T_c(\eta_1, \eta_2) = \sup_{f \in \mathcal{F}_{c}(\gamma)} \eta_1 f + \eta_2 f^c.$$

The fact that we can optimize over $\mathcal{F}_{c}(\gamma)$ instead of $\mathcal{F}_c$ is what gives rise to the lower complexity adaptation of statistical optimal transport, since it enables us to reason about the optimal transport problem in terms of the support of $\gamma$.

Another tool we require is the uniform metric entropy of a class $\mathcal{F}$ of real-valued functions. It is defined as the logarithm of the uniform covering number $\mathcal{N}(\epsilon, \mathcal{F})$, which denotes the minimal number of sets with diameter $2\epsilon$ required to cover $\mathcal{F}$ in the uniform norm for $\epsilon > 0$. Our results are formulated under the assumption that the uniform metric entropy of $\mathcal{F}_{c}(\gamma)$ is upper bounded by

$$\log \mathcal{N}(\epsilon, \mathcal{F}_{c}(\gamma)) \leq \epsilon^{-k}$$  \hspace{1cm} (B.2)

for some $k > 0$. Then, we will deduce upper bounds on the convergence rates of the form

$$r_k(n) := \begin{cases} n^{-1/2} & \text{if } k < 2 \\ n^{-1/2} \log(n) & \text{if } k = 2 \\ n^{-1/k} & \text{if } k > 2. \end{cases}$$
Clearly, the value of $k$ depends on the properties of $c$ as well as the support of $\gamma$. For example, if $X$ and $Y$ are smooth manifolds and $c$ is twice continuously differentiable while the support of $\gamma$ is a compact subset of a smooth submanifold of $X \times Y$ of dimension $s \in \mathbb{N}$, one can derive $k = 2/s$. As a general rule of thumb, we find $k = s/\alpha$ if $\alpha \in (0, 2]$ denotes the Hölder-smoothness of $c$ and $s$ the intrinsic dimension of $\gamma$ (unfortunately, higher degrees of smoothness of $c$ than $\alpha = 2$ cannot be exploited). For precise definitions and results along those lines, see Section 3 in Hundrieser et al. (2022).

**LCA for various estimators.** We start with proving the LCA property of the plug-in estimator $\tau(\hat{\gamma})$, where $\hat{\gamma}$ is the empirical measure $\frac{1}{n} \sum_{i=1}^{n} \delta_{(\xi_i, \zeta_i)}$ for $(\xi_1, \zeta_1), (\xi_2, \zeta_2), \ldots, (\xi_n, \zeta_n)$. According to inequality (6.3), this estimator exhibits lower complexity adaptation under additive metric costs. The result below confirms this property also for general bounded costs.

**Theorem B.1 (LCA, product estimator):** Let $X$ and $Y$ be Polish spaces, $c : X \times Y \rightarrow [0, 1]$ continuous, and $\gamma \in \mathcal{P}(X \times Y)$. If bound (B.2) holds for $k > 0$, then

$$E |\tau(\hat{\gamma}_n) - \tau(\gamma)| \leq r_k(n).$$

**Proof.** Let $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$ be the marginal distributions of $\gamma$. We introduce the random variables $(\xi, \zeta) \sim \mu \otimes \nu$, assumed to be independent of the samples $(\xi_1, \zeta_1), (\xi_2, \zeta_2), \ldots, (\xi_n, \zeta_n)$. Since supp $\hat{\gamma}_n \subseteq$ supp $\gamma$ with probability 1, we can use the same argument as in the proof of Hundrieser et al. (2022, Theorem 2.2), to derive

$$|T_c(\hat{\gamma}_n, \hat{\gamma}_n) - T_c(\gamma, \mu \otimes \nu)| \leq \sup_{f \in \mathcal{F}_c(\gamma)} |(\hat{\gamma}_n - \gamma) f| + \sup_{f \in \mathcal{F}_c(\gamma)} |(\hat{\mu} \otimes \hat{\nu}_n - \mu \otimes \nu) f|.$$ 

Note that the class $\mathcal{F}_c(\gamma)$ equipped with the sup norm is separable since it has finite covering numbers, which means that the right hand side is measurable. The expectation term on the right hand side can be treated like in Hundrieser et al. (2022) and we find

$$E \sup_{f \in \mathcal{F}_c(\gamma)} |(\hat{\gamma}_n - \gamma) f| \leq r_k(n)$$

with a universal constant. To address the second term, we write $\mathcal{F}_c^\gamma(\gamma) = \{ f_c^\gamma \mid f \in \mathcal{F}_c(\gamma) \}$ and apply Lemma 2.1 in Hundrieser et al. (2022) to establish that $\mathcal{N}(\epsilon, \mathcal{F}_c(\gamma)) = \mathcal{N}(\epsilon, \mathcal{F}_c^\gamma(\gamma))$. Noting that $(\xi_i, \zeta_i)$ is equal to $(\xi, \zeta)$ in distribution for $i \neq j$, we conclude

$$E \sup_{f \in \mathcal{F}_c(\gamma)} |(\hat{\mu} \otimes \hat{\nu}_n - \mu \otimes \nu) f| = E \sup_{g \in \mathcal{F}_c^\gamma(\gamma)} \left| \frac{1}{n^2} \sum_{i,j=1}^{n} g(\xi_i, \zeta_j) - E g(\xi, \zeta) \right|$$

$$\leq \frac{1}{n} \sum_{i=1}^{n} E \sup_{g \in \mathcal{F}_c^\gamma(\gamma)} \left| \frac{1}{n} \sum_{j=1}^{n} g(\xi_i, \zeta_j) - E g(\xi, \zeta) \right|$$

$$\leq E \sup_{g \in \mathcal{F}_c^\gamma(\gamma)} \left| \frac{1}{n} \sum_{j=1}^{n} g(\xi, \zeta_j) - E g(\xi, \zeta) \right| + \frac{2}{n}.$$
where we have exploited that \(\|g\|_\infty \leq 1\) in the last inequality in order to replace the diagonal terms corresponding to \(j = i\) in the sum. Consequentially, the random variables \(g(\xi, \zeta_j)\) for \(j \in \{1, \ldots, n\}\) are i.i.d. distributed and bounded. Denoting \(Z_g = \frac{1}{\sqrt{n}} \sum_{i=1}^n g(\xi, \zeta_j)\), we can apply Hoeffding’s inequality to derive sub-Gaussianity

\[
P(|Z_g - \mathbb{E}Z_g| \geq t) \leq 2 e^{-t^2/2\|g\|_\infty^2},
\]

with respect to the uniform norm \(\|\cdot\|_\infty\). Therefore, we can resort to chaining arguments like in Theorem 5.22 in Wainwright (2019) to deduce

\[
\mathbb{E} \sup_{f \in \mathcal{F}_c(y)} |(\hat{\mu}_n \otimes \hat{v}_n - \mu \otimes v)f^c| \\
\leq O(n^{-1}) + \frac{1}{\sqrt{n}} \mathbb{E} \sup_{g \in \mathcal{F}_c(y)} |Z_g - \mathbb{E}Z_g| \\
\leq O(n^{-1}) + \frac{1}{\sqrt{n}} \int_{\delta/4}^{1} \sqrt{\log N(\epsilon, \mathcal{F}_c(y))} \, d\epsilon + \frac{1}{\sqrt{n}} \mathbb{E} \sup_{g, g' \in \mathcal{F}_c(y)} |Z_g - Z_{g'}| \\
\leq O(n^{-1}) + \frac{1}{\sqrt{n}} \int_{\delta/4}^{1} \sqrt{\log N(\epsilon, \mathcal{F}_c(y))} \, d\epsilon + \delta
\]

for any \(\delta > 0\). We remark that the statement in Wainwright (2019) is not explicitly formulated for the absolute value of \(Z_g - \mathbb{E}Z_g\). However, this can easily be adapted by enlarging the function class the supremum is taken over by the functions \(\{-g \mid g \in \mathcal{F}_c(y)\}\), which at most increases the covering number by a factor of two. Theorem 2.2 in Hundrieser et al. (2022) now shows that the right hand side in the display above is bounded by a multiple of \(r_k(n)\) for a suitable choice of \(\delta\), which establishes the claim of the theorem.

We now turn to the sampling based estimators proposed in Section 6. Our proof strategy allows for both sampling with and without replacement. The proof works by exploiting sub-Gaussianity of sums with randomly sampled indices.

**Lemma B.2:** Let \(a = (a_{ij})_{i,j=1}^n \in \mathbb{R}^{n \times n}\) for \(n \in \mathbb{N}\) and consider the random variable \(Z = \frac{1}{\sqrt{n}} \sum_{i=1}^n a_{ij,k}\) with (random) indices \(I = (I_i)_{i=1}^n\) and \(J = (J_i)_{i=1}^n\) that satisfy either

1) \(I_i = i\) for all \(i \in \{1, \ldots, n\}\) and \(J\) is sampled from \(\{1, \ldots, n\}\), or
2) \((I, J)\) is sampled from \(\{(1, \ldots, n)^2\}\),

where the sampling is uniform with or without replacement and the roles of \(I\) and \(J\) in case 1) can also be exchanged. Then there is a constant \(b > 0\) only depending on the sampling scheme such that

\[
P(|Z - \mathbb{E}Z| \geq t) \leq 2 e^{-t^2/2\|a\|_\infty^2}, \tag{B.3}
\]

where \(\|a\|_\infty = \max_{i,j} |a_{ij}|\) denotes the absolute value of the largest entry.
Proof. In case of sampling with replacement, \( Z \) is the (normalized) sum of \( n \) independent random variables with values in \([-\|a\|_\infty, \|a\|_\infty] \). Thus, the classical Hoeffding inequality suffices to derive inequality (B.3) for \( b = 1 \). For sampling without replacement in both components (scenario 2), the Hoeffding inequality holds as well (see, e.g., Bardenet and Maillard [2015]). Finally, sampling without replacement in only one component is, for example, treated in Chaerjee [2007], where Proposition 1.1 implies the desired result after shifting and scaling the data (rough estimates show \( b \leq 12 \)).

**Theorem B.3 (LCA, sampling estimators):** Let \( X \) and \( Y \) be Polish spaces and \( c: X \times Y \to [0, 1] \) be continuous. For \( y \in C(\mu, \nu) \) with \( \mu \in \mathcal{P}(X) \) and \( \nu \in \mathcal{P}(Y) \), assume that bound (B.2) holds for \( k > 0 \). Define the estimator

\[
(\mu \otimes \nu)_n = \frac{1}{n} \sum_{i=1}^n \delta_{(\xi_i, \zeta_i)}
\]

with (random) indices \( I = (I_i)_{i=1}^n \) and \( J = (J_i)_{i=1}^n \) as in Lemma B.2 independent of the data. Then

\[
\mathbb{E} \left| T_c(\hat{\gamma}_n, (\mu \otimes \nu)_n) - \tau(\gamma) \right| \leq r_k(n).
\]

Proof. Let \( \hat{\mathbb{E}} \) denote the expectation with respect to the random sampling \((I, J)\) only. We will show that

\[
\hat{\mathbb{E}} \left| T_c(\hat{\gamma}_n, (\mu \otimes \nu)_n) - T_c(\hat{\gamma}_n, \hat{\mu}_n \otimes \hat{\nu}_n) \right| \leq r_k(n) \tag{B.4}
\]

holds for all realizations of the data (with a common constant), which, in combination with Theorem B.1, suffices to show the claim. We first note

\[
\hat{\mathbb{E}} (\mu \otimes \nu)_n = \hat{\mu}_n \otimes \hat{\nu}_n,
\]

which follows from the observation that \( \hat{\mathbb{E}} (\mu \otimes \nu)_n \) places the same amount of mass on any point \((\xi_i, \zeta_i)_{i=1}^n\) due to the symmetry of the sampling procedure. Denoting \( Z_g = \frac{1}{\sqrt{n}} \sum_{i=1}^n g(\xi_i, \zeta_i) \) for \( g \in \mathcal{F}_c^e(\gamma) \), we apply analogous arguments as in the proof of Theorem B.1 to derive

\[
\hat{\mathbb{E}} \left| T_c(\hat{\gamma}_n, (\mu \otimes \nu)_n) - T_c(\hat{\gamma}_n, \hat{\mu}_n \otimes \hat{\nu}_n) \right| \leq \frac{1}{\sqrt{n}} \hat{\mathbb{E}} \sup_{g \in \mathcal{F}_c^e(\gamma)} |Z_g - \hat{\mathbb{E}} Z_g|.
\]

According to Lemma B.2, the process \((Z_g)_{g \in \mathcal{F}_c^e(\gamma)}\) is sub-Gaussian with respect to the uniform norm (scaled by a constant \(b > 0\)) when conditioned on the observations. Following the remaining argumentation in the proof of Theorem B.1 (with \( \mathbb{E} \) replaced by \( \hat{\mathbb{E}} \)), bound (B.4) follows, where we emphasize that the right hand side does not depend on the data anymore. Note also that the value of \( b \), which amounts to a scaling in the radius of the covering, only affects (B.4) in the implicit constant.

Finally, we want to highlight the fact that repeated sampling from the observations does not deteriorate the convergence rate of the proposed sampling estimators. In practice, combining
several (independent) samples leads to a reduced variability of the estimate. This effect is especially pronounced for small to moderate values of \( n \) (see Section 7).

**Corollary B.4 (LCA, repeated sampling):** Let \( X \) and \( Y \) be Polish spaces and \( c : X \times Y \to [0, 1] \) be continuous. For \( \gamma \in C(\mu, \nu) \) with \( \mu \in \mathcal{P}(X) \) and \( \nu \in \mathcal{P}(Y) \), assume that bound (B.2) holds for \( k > 0 \). For \( j \in \{1, \ldots, r\} \) with \( r \in \mathbb{N} \), let \( (\mu \otimes \nu)_{n,j} \) be one of the sampling estimators defined in Theorem B.3 and set

\[
(\mu \otimes \nu)^r_n = \frac{1}{r} \sum_{j=1}^r (\mu \otimes \nu)_{n,j}.
\]

Then

\[
\mathbb{E} \left| T_c(\hat{\gamma}_n, (\mu \otimes \nu)^r_n) - \tau(\gamma) \right| \leq r_k(n).
\]

**Proof.** With the same argument from the proof of Hundrieser et al. (2022, Theorem 2.2), that has already been applied in Theorem B.1 and B.3 to bound the difference of optimal transport costs, we find

\[
\begin{align*}
\mathbb{E} \left| T_c(\hat{\gamma}_n, (\mu \otimes \nu)^r_n) - T_c(\hat{\gamma}_n, \hat{\mu}_n \otimes \hat{\nu}_n) \right| &\leq \mathbb{E} \sup_{f \in \mathcal{F}_c(\gamma)} \left| ((\mu \otimes \nu)^r_n - \hat{\mu}_n \otimes \hat{\nu}_n) f^r \right| \\
&\leq \frac{1}{r} \sum_{j=1}^r \mathbb{E} \sup_{f \in \mathcal{F}_c(\gamma)} \left| ((\mu \otimes \nu)_{n,j} - \hat{\mu}_n \otimes \hat{\nu}_n) f^r \right| \\
&\leq r_k(n),
\end{align*}
\]

where we made use of the triangle inequality of the absolute value and reused the proof of Theorem B.3 in the final step. By Theorem B.1 which shows that \( T_c(\hat{\gamma}_n, \hat{\mu}_n \otimes \hat{\nu}_n) \) approaches \( \tau(\gamma) \) with rate \( r_k(n) \), we can conclude the claim.

\( \square \)

### C Analytic computation of the transport dependency

In this appendix, we present a simple setting where the transport dependency can be calculated explicitly. Let \( c_r \) for \( r \in \mathbb{N} \) denote the squared Euclidean cost in \( \mathbb{R}^r \) and let \( \delta : \mathbb{R}^r \to \mathbb{R}^{2r} \) be the mapping to the diagonal, \( \delta(x) = (x, x) \). Consider \( \gamma = \delta_n \mu \in C(\mu, \nu) \) for \( \mu = \nu = \bigotimes_{i=1}^r \mu_i \in \mathcal{P}(\mathbb{R}^r) \), where \( \mu_i \in \mathcal{P}(\mathbb{R}) \) for each \( 1 \leq i \leq r \). Expressed in random variables, this joint distribution corresponds to the case \( \xi = \zeta \). We assume that \( \tau(\gamma) = \tau_{c_{2r}}(\gamma) < \infty \). By construction, the support of \( \gamma \) is contained in the affine subspace

\[
\delta(\mathbb{R}^r) = \{ \delta(x) \mid x \in \mathbb{R}^r \} \subset \mathbb{R}^{2r},
\]

and the orthogonal projection \( p : \mathbb{R}^{2r} \to \delta(\mathbb{R}^r) \) onto this subspace is \( p(y) = \delta(\tilde{y}) \) with \( \tilde{y} \in \mathbb{R}^r \), \( \tilde{y}_i = (y_i + y_{r+i})/2 \). According to Hundrieser et al. (2022) Proposition 2.3, we find that the optimal
transport cost in this scenario can be decomposed as
\[
\tau(y) = T_{c_2}(y, \mu \otimes \mu) = T_{c_2}(y, p_\delta(\mu \otimes \mu)) + \int \|y - p(y)\|^2 \, d(\mu \otimes \mu)(y).
\]

Moreover, letting \( \tilde{\mu}_i = t_\delta(\mu_i \otimes \mu_i) \) with \( t(a, b) = (a + b)/2 \) and setting \( \tilde{\mu} = \bigotimes_{i=1}^r \tilde{\mu}_i \), it follows that \( p_\delta(\mu \otimes \mu) = \delta_{\tilde{\mu}} \). Observing \( c_2(\delta(x), \delta(y)) = 2 c_r(x, y) \) for any \( x, y \in \mathbb{R}^r \), we now apply Lemma \([A.1]\) to conclude
\[
T_{c_2}(y, p_\delta(\mu \otimes \mu)) = T_{c_2}(\delta_{\tilde{\mu}}, \delta_{\tilde{\mu}}) = 2 T_{c_r}(\mu, \tilde{\mu}) = 2 \sum_{i=1}^r T_{c_1}(\mu_i, \tilde{\mu}_i).
\]

Combining the previous two equations yields
\[
\tau(y) = T_{c_2}(y, p_\delta(\mu \otimes \mu)) + \int \|y - p(y)\|^2 \, d(\mu \otimes \mu)(y)
= 2 \sum_{i=1}^r T_{c_1}(\mu_i, \tilde{\mu}_i) + \frac{1}{2} \sum_{i=1}^d \int (y_1 - y_2)^2 \, d(\mu_i \otimes \mu_i)(y_1, y_2),
\]
which reduces calculating \( \tau(y) \) to one-dimensional optimal transport problems and integrals over \( \mu_i \otimes \mu_i \). If \( \mu_i = \text{Unif}[0, 1] \) for all \( i \), for example, the involved quantities can be calculated explicitly and we find
\[
\tau(y) = \frac{r}{60} + \frac{r}{12} = \frac{r}{10}.
\]
D Additional Simulations

This appendix contains a range of figures that supplement Section 7 and further illustrate the behaviour of the transport correlation on noisy datasets.

Convex noise. Like Figure 10 and 11 in Section 7, the upcoming Figures 16 to 22 compare \( \rho \), \( \rho_3 \), and several other dependency coefficients under the convex noise model (7.1) for different geometries \( \gamma \). One particularly noteworthy observation is that \( \rho_3 \) has a higher (or at least the same) discriminative power compared to the distance correlation, Pearson correlation, and Spearman correlation for all geometries considered.

Gaussian additive noise. We repeated our previous simulations under a Gaussian additive noise model instead of convex noise (Figure 23 to Figure 31). For a given level of noise \( \sigma > 0 \) and a given base distribution \( \gamma \), we consider the noisy relationships \( (\xi, \zeta) \sim \gamma^{\sigma} \), where 
\[
\gamma^{\sigma} = \gamma * \kappa \quad \text{with} \quad \kappa = \mathcal{N}(0, \sigma I_d).
\]
In this setting, we notice that the Pearson and Spearman correlations as well as the distance correlation have a higher power than \( \rho \) if \( \gamma \) exhibits a clear monotonic tendency. If, on the other hand, the linear correlation of the underlying distribution \( \gamma \) is low, then we observe similar trends as for the convex noise model.

Influence of \( p \). Finally, we use the same distributions and noise models as above to study the effect of the parameter \( p \) on the transport correlation coefficient \( \rho_\pi \), see Definition 5.5. From Figure 32 to Figure 49, we compare the values of \( \rho_\pi \) when the parameter \( p \) is set equal to 0.5, 1, and 2, respectively. The setting is the same as for the previous comparisons, the only difference being that just 9 (instead of 29) random permutations are used for the permutation tests. One observation that holds for all geometries \( \gamma \) is that the box plots of the estimates of \( \tau \) are generally very similar for all \( p \). In contrast, we observe that the parameter \( p = 0.5 \) often provides a (slightly) higher discriminative power against independence than the choices \( p = 1 \) or \( p = 2 \).
Figure 18

Figure 19
Figure 20

Figure 21
Figure 22

Figure 23
Figure 24

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Figure 31
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