

THE EARTH MOVER'S CORRELATION

Tamás F. Móri (Budapest, Hungary)

Gábor J. Székely (Alexandria, VA, USA)

Dedicated to the memory of Professor János Galambos

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Abstract. Since Pearson's correlation was introduced at the end of the 19th century many dependence measures have appeared in the literature. In [26] we suggested four simple axioms for dependence measures of random variables that take values in Hilbert spaces. We showed that distance correlation (see [34]) satisfies all these axioms. We still need a new measure of dependence because existing measures either do not work in general metric spaces (that are not Hilbert spaces) or they do not satisfy our four simple axioms. The *earth mover's correlation* introduced in this paper applies in general metric spaces and satisfies our four axioms (two of them in a weaker form).

1. Introduction: What is our goal?

Let S be a nonempty set of pairs of nondegenerate random variables X, Y taking values in Euclidean spaces or in real, separable Hilbert spaces H . (Non-degenerate means that the random variable is not constant with probability 1.)

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In [26] we called $\Delta(X, Y) : S \rightarrow [0, 1]$ a dependence measure on S if the following four axioms hold.

In the axioms below we need similarity transformations of H . Similarity H is defined as a bijection (1–1 correspondence) from H onto itself that multiplies all distances by the same positive real number (scale). Similarities in Hilbert spaces are known to be compositions of a translation, an orthogonal linear mapping, and a uniform scaling. We assume that if $(X, Y) \in S$ then $(f(X), g(Y)) \in S$ for all similarity transformations f, g of H .

In [26] we introduced the following axioms.

- (i) $\Delta(X, Y) = 0$ if and only if X and Y are independent.
- (ii) $\Delta(X, Y)$ is invariant with respect to all similarity transformations of H ; that is, $\Delta(f(X), g(Y)) = \Delta(X, Y)$ where f, g are similarity transformations of H .
- (iii) $\Delta(X, Y) = 1$ if and only if $Y = f(X)$ with probability 1, where f is a similarity transformation of H .
- (iv) $\Delta(X, Y)$ is continuous; that is, if for some positive constants K we have $E(|X_n|^2 + |Y_n|^2) \leq K$, $n = 1, 2, \dots$ and (X_n, Y_n) converges weakly (converges in distribution) to (X, Y) then $\Delta(X_n, Y_n) \rightarrow \Delta(X, Y)$.

In fact, what we really need is not the boundedness of the second moments but the convergence of the expectations: $\mathbb{E}(X_n) \rightarrow \mathbb{E}(X)$ and $\mathbb{E}(Y_n) \rightarrow \mathbb{E}(Y)$; so in axiom (iv) the condition on the boundedness of second moments can be replaced by any other condition that guarantees the convergence of expectations. Such a condition is uniform integrability of X_n, Y_n which follows from the boundedness of second moments. The reason of using a more restrictive condition is that it can be more easily checked.

If S is the set of bivariate Gaussian random variables then Pearson's correlation satisfies all these axioms. For more general S Pearson's correlation typically does not satisfy (i) but distance correlation does satisfy all of them if the expectations are finite.

First of all recall the definition of the sample distance correlation, see also [34] and [35]. Take all pairwise distances between sample values of one variable, and do the same for the second variable. Rigid motion invariance is automatically guaranteed if instead of sample elements we work with their distances. Another advantage of working with distances is that they are always real numbers even when the data are vectors of possibly different dimensions. Once we have computed the distance matrices of both samples, double-center them (so each has column and row means equal to zero). Then average the entries of the matrix which holds componentwise products of the two centered distance

matrices. This is the square of the sample distance covariance. If we denote the centered distances by A_{ij} , $i, j = 1, \dots, n$ and B_{ij} , $i, j = 1, \dots, n$ where n is the sample size, then the squared sample distance covariance is

$$\frac{1}{n^2} \sum_{i,j=1}^n A_{i,j} B_{i,j}.$$

This definition is very similar to, and almost equally simple as, the definition of Pearson's covariance, except that here we have double indices.

If $\mathbb{E}|X|^2$ and $\mathbb{E}|Y|^2$ are finite then the population squared distance covariance can be reduced to the following form [34].

If (X, Y) , (X', Y') , (X'', Y'') denote independent and identically distributed copies then the distance covariance is the square root of

$$\begin{aligned} \text{dCov}^2(X, Y) := & \mathbb{E}(|X - X'| |Y - Y'|) + \mathbb{E}(|X - X'|) \mathbb{E}(|Y - Y'|) - \\ & - \mathbb{E}(|X - X'| |Y - Y''|) - \mathbb{E}(|X - X''| |Y - Y'|). \end{aligned}$$

In the above referenced paper we proved that the distance variance, $\text{dCov}(X, X)$ is zero if and only if X is constant with probability 1. Once we defined distance covariance and distance variance we can define distance correlation the same way as we defined correlation with the help of covariance and variance. If the random variables X, Y have finite expected values and they are not constant with probability 1 then the definition of *population distance correlation* is the following:

$$\text{dCor}(X, Y) := \frac{\text{dCov}(X, Y)}{\sqrt{\text{dCov}(X, X) \text{dCov}(Y, Y)}}.$$

If $\text{dCov}(X, X) \text{dCov}(Y, Y) = 0$ then we do not define $\text{dCor}(X, Y)$. (If we define $\text{dCor}(X, Y) = 0$ then this would lead to a violation of (iv).)

Distance correlation equals zero if and only if the variables are independent, whatever be the underlying distributions and whatever be the dimension of the two variables (for a transparent explanation see below). This fact and the simplicity of the statistic make distance correlation an attractive candidate for measuring dependence. For generalizations to certain metric spaces see [20], [22], and [15]. These metric spaces include all separable Hilbert spaces, all real hyperbolic spaces [21], and all open hemispheres [23]. On some related information see [7].

In [34] an alternative formula for $\text{dCov}^2(X, Y)$ was given in terms of characteristic functions $f_{X,Y}$, f_X and f_Y of (X, Y) , X , and Y respectively. If the

random variable X takes values in a p -dimensional Euclidean space \mathbb{R}^p and Y takes values in \mathbb{R}^q and both variables have finite expectations we have

$$\text{dCov}^2(X, Y) := \frac{1}{c_p c_q} \int_{\mathbb{R}^{p+q}} \frac{|f_{X,Y}(t, s) - f_X(t)f_Y(s)|^2}{|t|_p^{1+p} |s|_q^{1+q}} dt ds.$$

where c_p and c_q are constants. This formula clearly shows that independence of X and Y is equivalent to $\text{dCov}(X, Y) = 0$. On a generalization to dependence measures for more than two random vectors see [8].

If the expectations of X, Y do not exist, we can generalize distance correlation for random variables with finite moments of order $\alpha > 0$, see [34, 35]. It is easy to see that the population distance correlation, $\text{dCor}(X, Y)$, satisfies axioms (ii) and (iv). For the proof that $\text{dCor}(X, Y)$ satisfies (i) and (iii), see [34].

An important generalization of distance correlation is [32]. This is related to a generalized distance correlation where the distance is a more general metric than the Euclidean one. These generalizations under some natural conditions like scale invariance also satisfy our axioms.

In [26] we proved the following theorem which shows that in our axioms similarity cannot be replaced by stronger invariances like affine invariance (except in case $\dim H = 1$).

Theorem 1.1. *Suppose S is a set of pairs of nondegenerate random variables, and if $(X, Y) \in S$ then $(f(X), g(Y)) \in S$ for all affine transformations of H .*

If the dependence measure $\Delta(X, Y)$ on S is invariant with respect to all affine transformations f, g of H where $\dim H > 1$ then axiom (iv) cannot hold. If $\dim H = 1$ then affinity is the same as similarity and in this case distance correlation is affine invariant. On the other hand, if $\Delta(X, Y)$ is invariant with respect to all 1–1 Borel measurable functions of H then even if $\dim H = 1$, axiom (iv) cannot hold.

For an “almost affine invariant” version of distance correlation see [12]. If we want to generalize the axioms from Hilbert spaces H to general metric spaces (\mathcal{M}, δ) then first we need a general definition of similarity in metric spaces.

Definition 1.1. A mapping $f : \mathcal{M} \rightarrow \mathcal{M}$ is a *similarity* if there exists a constant $c > 0$ such that for all $x \in \mathcal{M}, y \in \mathcal{M}$ we have $\delta(f(x), f(y)) = c\delta(x, y)$.

A reformulation of our axioms to arbitrary metric spaces is the following.

- (a) $\Delta(X, Y) = 0$ if and only if X and Y are independent.
- (b) $\Delta(X, Y)$ is invariant with respect to all similarity transformations of (\mathcal{M}, δ) ; that is, $\Delta(f(X), g(Y)) = \Delta(X, Y)$ where f, g are similarity transformations of (\mathcal{M}, δ) .

- (c) $\Delta(X, Y) = 1$ if and only if $Y = f(X)$ with probability 1, where f is a similarity transformation of (\mathcal{M}, δ) .
- (d) $\Delta(X, Y)$ is continuous; that is, if for some positive constant K and $x_0 \in \mathcal{M}$, $y_0 \in \mathcal{M}$ we have $\mathbb{E}(\delta^2(X_n, x_0) + \delta^2(Y_n, y_0)) \leq K$, $n = 1, 2, \dots$ and (X_n, Y_n) converges weakly (i.e., converges in distribution) to (X, Y) then $\Delta(X_n, Y_n) \rightarrow \Delta(X, Y)$.

Again, the condition on the boundedness of second moments can be replaced by any other condition that guarantees the convergence of expectations: $\mathbb{E}\delta(X_n, x_0) \rightarrow \mathbb{E}\delta(X, x_0)$ and $\mathbb{E}\delta(Y_n, y_0) \rightarrow \mathbb{E}\delta(Y, y_0)$; the uniform integrability of $\delta(X_n, x_0), \delta(Y_n, y_0)$, which follows from the boundedness of second moments, would equally do.

We will also need the following weaker forms of axioms (b) and (c):

- (b*) $\Delta(X, Y) = \Delta(f(X), f(Y))$ for every similarity transformation f of (\mathcal{M}, δ) .
- (c*) $\Delta(X, Y) = 1$ if $Y = f(X)$ with probability 1, where f is a similarity transformation of (\mathcal{M}, δ) .

Our goal is to find a dependence measure that satisfies these axioms in arbitrary metric spaces.

2. How far can we go with distance correlation?

Distance correlation can be generalized to metric spaces (\mathcal{M}, δ) that are of negative type [20]. A metric space (\mathcal{M}, δ) is called of negative type if the metric possesses the “conditional negative definite” property, namely that for all integers $n \geq 1$ and for all sets of n points $x_i \in \mathcal{M}$ and $x'_i \in \mathcal{M}$ ($i = 1, 2, \dots, n$) and for all real numbers a_1, a_2, \dots, a_n such that their sum is 0 we have

$$\sum_{i,j} a_i a_j \delta(x_i, x'_j) \leq 0.$$

Strong negative type metric spaces satisfy this with equality iff $a_1 = \dots = a_n = 0$. However, for the strong negative type property we need somewhat more, namely for all probability measures μ and ν defined on the Borel sets of \mathcal{M}

$$\int \delta(x, y) d(\mu - \nu)^2(x, y) \leq 0$$

with equality iff $\mu = \nu$.

According to a classical theorem of Schoenberg [30, 31] a necessary and sufficient condition for negative type of (\mathcal{M}, δ) is that $(\mathcal{M}, \sqrt{\delta})$ is isometrically

embeddable into a Hilbert space. Obviously this property does not hold for every metric space. When it does then in these “nice” metric spaces we can apply distance correlation, for all others we need to make new efforts.

We can try to work with functions of δ , say $\delta^*(\delta)$, that satisfies our axioms. If the only problem is that the metric is not of strong negative type, only of negative type then it is easy to find a remedy: take the square root (or any other power $0 < r < 1$) of the metric and this new metric becomes of strong negative type, see [20].

For arbitrary finite \mathcal{M} we can show, see [36], that for a suitably large number K the new distance $\delta^*(x, y) = \delta(x, y) + K$ whenever $x \neq y$ and 0 otherwise, is always conditionally negative definite. On top of that, this simple transformation of the metric does not change the unbiased estimator of dCov which is simply invariant with respect to this additive constant K .

For infinite \mathcal{M} there does not always exist a strictly monotone increasing function $\delta^*(\delta)$ such that (\mathcal{M}, δ^*) is of negative type. Take e.g. two disjoint infinite sets, A and B , and let \mathcal{M} be their union. Define the distance of two distinct elements to be 1 if they are in different sets, and 2 if they are in the same set. The function δ^* must have the following form: $\delta^*(1) = u$, $\delta^*(2) = v$, $0 < u < v$. Define $a_i := 1$ for n elements of A and $a_i := -1$ for n elements of B . Then the sum we need to check is $n(n-1)v - n^2u$, which is positive for large enough n .

Another approach is this. If all we want from our dependence measure is to test independence then it is acceptable to change the distances in (\mathcal{M}, δ) and thus change the distance correlation so long as we do not change $\text{dCor}(X, Y) = 0$. If f is an arbitrary 1–1 Borel function on (\mathcal{M}, δ) and X, Y are (\mathcal{M}, δ) valued random variables then they are independent iff $f(X), f(Y)$ are independent. But every metric space is Borel isomorphic to a “nice” metric space that is embeddable isomorphically into a Hilbert space. According to Kuratowski’s theorem two complete separable Borel spaces are Borel isomorphic iff they have the same cardinality. They are Borel isomorphic either to \mathbb{R} , or to \mathbb{Z} or to a finite metric space. Denote this Borel isomorphism by f . If we can construct it then we can check the independence of the real valued random variables $f(X), f(Y)$ via distance correlation and this is equivalent to testing the independence of X, Y that take values in general metric spaces. We might want to make f continuous to avoid the negative effect of minor noise. In this case we can choose f to be a homeomorphism between our metric space and a subspace of a Hilbert cube. This f exists if and only if our metric space is separable. Here is how to construct such an f .

Assume $\delta \leq 1$ (otherwise, use $\delta/(\delta+1)$). Choose a dense countable sequence (x_n) from \mathcal{M} which exists because the metric space is separable, and define $f(x) := (\delta(x, x_n)/n)_{n \geq 1}$, a point in the Hilbert cube and here we can apply distance correlation for testing independence.

These tricks can help to solve some of the problems in testing independence but they do not solve the problem of finding a general measure of dependence applicable to general metric space valued random variables. To use one of John von Neumann's favorite expressions, our goal here is to define a dependence measure that applies to the "rest of the universe".

3. The population value of the earth mover's correlation

First of all recall the definition of the earth mover's distance for probability measures μ, ν on general metric spaces (\mathcal{M}, δ) . We suppose that the topology of this metric space and the probability measures on the Borel sets are "compatible", that is, we suppose that the probability measures are Radon measures (finite on compact sets, outer regular and inner regular).

Heuristically, if we have two (Radon) probability distributions, μ and ν on (\mathcal{M}, δ) then the earth mover's distance is the minimum cost of turning one pile of dust or dirt with distribution μ into the other with distribution ν . The cost is proportional to the transport distance and also to the amount of dirt we transport.

This distance was considered by [25], [16], [17], [39], [28], [38], and many others, and in mathematical circles it is typically called Wasserstein distance. Most statisticians and computer scientists call it earth mover's distance. On a recent survey see [27]. On some recent advances see [5], [29], and [33].

Denote by $\mathcal{P}(\mathcal{M})$ the set of all (Radon) probability measures μ on \mathcal{M} . Suppose that for some $x_0 \in \mathcal{M}$ we have

$$\int_{\mathcal{M}} \delta(x, x_0) d\mu(x) < +\infty.$$

Then the earth mover's distance or Wasserstein distance of the probability measures μ and ν can be equivalently defined as

$$e(\mu, \nu) := \inf_{\gamma \in \Gamma(\mu, \nu)} \int_{\mathcal{M} \times \mathcal{M}} \delta(x, y) d\gamma(x, y),$$

where $\Gamma(\mu, \nu)$ is the set of all possible couplings of probability measures μ and ν , that is, the set of all joint distributions γ of (X, Y) with marginal distributions μ and ν , respectively. Equivalently,

$$e(\mu, \nu) = e(X, Y) := \inf_{\gamma \in \Gamma(\mu, \nu)} \mathbb{E}[\delta(X, Y)],$$

where again the infimum is taken for all joint distributions of (X, Y) with marginal distributions μ and ν , respectively.

Mathematically this is not an easy minimization problem to solve. Even if (\mathcal{M}, δ) is an Euclidean space where the transportation cost is the Euclidean distance the solution is related to the so-called Monge–Ampère difference equation [6, 9, 10]. For real valued random variables X, Y , however, there is a simple formula for the earth mover distance. Denote $F(x) = \mathbb{P}(X \leq x)$ and $G(y) = \mathbb{P}(Y \leq y)$ the cdf's of X and Y and consider their generalized inverses $F^{-1}(u), G^{-1}(u)$, defined as $F^{-1}(u) = \sup\{t : F(t) \leq u\}$. Then

$$\begin{aligned} e(X, Y) &= \mathbb{E}|F^{-1}(U) - G^{-1}(U)| = \\ &= \int_0^1 |F^{-1}(u) - G^{-1}(u)| du = \int_{-\infty}^{\infty} |F(t) - G(t)| dt. \end{aligned}$$

Define a metric d on the space $\mathcal{M} \times \mathcal{M}$, e.g. d can be the Manhattan distance: $d[(x, y), (u, v)] = \delta(x, u) + \delta(y, v)$.

Definition 3.1. The earth mover's covariance of random variables X, Y taking values in (\mathcal{M}, δ) is the earth mover's distance between the joint distribution and the product of its marginals:

$$e\text{Cov}(X, Y) = \inf_{\gamma \in \Gamma} \mathbb{E}d[(X, Y), (X', Y')] = e[(X, Y), (X', Y')],$$

where Γ is the set of all possible joint distributions of the random variables X, Y, X', Y' such that X' and X are identically distributed, Y' and Y are also identically distributed, and X', Y' are independent (and the joint distribution of X and Y is given).

In the following we do not really need that d is a Manhattan distance, what we need is more general, namely that $(\mathcal{M} \times \mathcal{M}, d)$ with a metric d is a metric space such that

$$d[(x, u), (x, v)] = \delta(u, v), \quad d[(x, u), (y, u)] = \delta(x, y), \quad d[(x, x), (u, v)] \geq \delta(u, v).$$

The following inequality is of Cauchy–Bunyakovsky–Schwarz type.

$$e^2[(X, Y), (X', Y')] \leq e[(X, X), (X, X')] e[(Y, Y), (Y, Y')],$$

where X and X' are iid, as well as Y and Y' , and X', Y' are independent.

In fact, we can show more, namely that

Theorem 3.1.

$$(3.1) \quad e[(X, Y), (X', Y')] \leq \min \{e[(X, X), (X, X')], e[(Y, Y), (Y, Y')]\}.$$

Proof. Suppose that the right-hand side is equal to $e[(Y, Y), (Y, Y')]$. In the sequel all random variables denoted by X with or without subscripts or superscripts will be equidistributed with X , and the same holds for Y . Let Y_2 and Y_3 be independent, then

$$\mathbb{E}d[(Y_1, Y_1), (Y_2, Y_3)] \geq \mathbb{E}\delta(Y_2, Y_3) = \mathbb{E}d[(X_2, Y_2), (X_2, Y_3)],$$

where X_2 is chosen in such a way that (X_2, Y_2) and (X, Y) are identically distributed, and Y_3 is independent of (X_2, Y_2) . Then the right-hand side is greater than or equal to $e[(X, Y), (X', Y')]$, while the infimum of the left-hand side as Y_1 varies is just $e[(Y, Y), (Y, Y')]$. ■

On the right-hand side of (3.1) $e[(X, X), (X, X')] = \text{eCov}(X, X)$ will be called *the earth mover's variance*.

Definition 3.2. The earth mover's variance of the distribution of X is

$$(3.2) \quad \text{eVar}(X) := \text{eCov}(X, X) = e[(X, X), (X, X')].$$

Theorem 3.2. *The earth mover variance is the same as Gini's mean difference:*

$$(3.3) \quad \text{eVar}(Y) = \mathbb{E}\delta(Y, Y'),$$

where Y and Y' are iid.

Proof. We have seen above that

$$\text{eVar}(Y) = \inf_{Y_1} \mathbb{E}d[(Y_1, Y_1), (Y_2, Y_3)] \geq \mathbb{E}\delta(Y_2, Y_3),$$

and equality is attained for $Y_1 = Y_2$. ■

Example 3.3. Let X be an iid sample of size n from the uniform distribution $U[0; 1]$, apply the Euclidean metric in \mathbb{R}^n and the Manhattan distance for pairs. Then by Remark 3.1 below $\text{eVar}(X) = \mathbb{E}|X - X'|$, where X and X' are independent uniform random points of the n dimensional unit cube. For $n = 1$ we get $\text{eVar}(X) = 1/3$. For general n it is known that using the notation $\text{erf}(u)$ for the "error function", i.e. the integral from $-u$ to u of the Gaussian probability density function with 0 expectation and variance 1/2 we have

$$\text{eVar}(X) = \frac{1}{\sqrt{\pi}} \int_0^\infty \left\{ 1 - \left(\frac{\sqrt{\pi} \text{erf}(u)}{u} - \frac{1 - e^{-u^2}}{u^2} \right)^n \right\} \frac{du}{u^2}.$$

We do not know any simple analytic expressions for $\text{eVar}(X)$ if n is arbitrary. However, by the inequality $|X - X'| \geq n^{-1/2} \sum_{i=1}^n |X_i - X'_i|$ it easily follows

that $\text{eVar}(X) \geq \sqrt{n}/3$. On the other hand, since the diameter of the unit cube is \sqrt{n} , we clearly have $\text{eVar}(X) \leq \sqrt{n}$. A somewhat better upper estimate is

$$\begin{aligned} \mathbb{E}|X - X'| &\leq [\mathbb{E}|X - X'|^2]^{1/2} = [n\mathbb{E}(X_1 - X'_1)^2]^{1/2} \\ &= [2n \text{Var}(X_1)]^{1/2} = \sqrt{n/6}. \end{aligned}$$

Based on Theorem 3.1 we can now introduce the definition of a new type of correlation.

Definition 3.3. The *earth mover's correlation* of the distributions of X and Y is defined as

$$\text{eCor}(X, Y) = \frac{\text{eCov}(X, Y)}{\min \{ \text{eVar}(X), \text{eVar}(Y) \}}.$$

We do not define $\text{eCor}(X, Y)$ when $\min \{ \text{eVar}(X), \text{eVar}(Y) \} = 0$.

Remark 3.1. By the previous theorem in the formula for eCor the denominator $\min \{ \text{eVar}(X), \text{eVar}(Y) \} = \min \{ \mathbb{E}\delta(X, X'), \mathbb{E}\delta(Y, Y') \} = 0$ iff at least one of X, Y is constant with probability 1. In this case we do not define eCor . It is interesting to note that for real valued random variables eVar is easy to compute. It is known, see e.g. [40], that

$$\text{eVar}(X) = 2 \int_{-\infty}^{\infty} F(x)(1 - F(x)) dx,$$

where $F(x) = \mathbb{P}(X \leq x)$ is the cdf of the random variable X .

Remark 3.2. Let us apply the Manhattan distance for pairs. Then by the triangle inequality for δ we have $\delta(X, X') + \delta(Y, Y') \geq |\delta(X, Y) - \delta(X', Y')|$, thus

$$\text{eCov}(X, Y) \geq \inf_{(X', Y')} \mathbb{E}|\delta(X, Y) - \delta(X', Y')| \geq |\mathbb{E}\delta(X, Y) - \mathbb{E}\delta(X', Y')|.$$

Example 3.4. Let X and Y be indicators, $\mathbb{P}(X = 1) = 1 - \mathbb{P}(X = 0) = p_X$, $\mathbb{P}(Y = 1) = 1 - \mathbb{P}(Y = 0) = p_Y$, $\mathbb{P}(X = Y = 1) = p_{XY}$. Let us apply the Euclidean metric in \mathbb{R} and the Manhattan distance for pairs. Then

$$\text{eCor}(X, Y) = \frac{|p_{XY} - p_X p_Y|}{\min \{ p_X(1 - p_X), p_Y(1 - p_Y) \}}.$$

Indeed, in the lower bound of Remark 3.2 we have

$$\begin{aligned}
\mathbb{E}|X - Y| - \mathbb{E}|X' - Y'| &= \\
&= \mathbb{P}(X \neq Y) - \mathbb{P}(X' \neq Y') = \\
&= \mathbb{P}(X' = Y') - \mathbb{P}(X = Y) = \\
&= p_X p_Y + (1 - p_X)(1 - p_Y) - p_{XY} - (1 - p_X - p_Y + p_{XY}) = \\
&= 2(p_X p_Y - p_{XY}),
\end{aligned}$$

thus $\text{eCov}(X, Y) \geq 2|p_{XY} - p_X p_Y|$.

On the other hand, we will construct random variables X, Y, X', Y' with the desired distribution in such a way that

$$\mathbb{E}(|X - X'| + |Y - Y'|) = 2|p_{XY} - p_X p_Y|.$$

Let U, V be independent and uniformly distributed on $[0, 1]$, and define

$$\begin{aligned}
X = X' &= I(U \leq p_X), \quad Y' = I(V \leq p_Y), \\
Y &= I\left(U \leq p_X, V \leq \frac{p_{XY}}{p_X}\right) + I\left(U > p_X, V \leq \frac{p_Y - p_{XY}}{1 - p_X}\right)
\end{aligned}$$

Then $\mathbb{P}(X \neq X') = 0$ and $\mathbb{P}(Y \neq Y') = \mathbb{P}(Y = 1, Y' = 0) + \mathbb{P}(Y = 0, Y' = 1)$. Here

$$\begin{aligned}
\mathbb{P}(Y = 1, Y' = 0) &= \\
&= \mathbb{P}\left(U \leq p_X, p_Y < V \leq \frac{p_{XY}}{p_X}\right) + \mathbb{P}\left(U > p_X, p_Y < V \leq \frac{p_Y - p_{XY}}{1 - p_X}\right),
\end{aligned}$$

and similarly,

$$\begin{aligned}
\mathbb{P}(Y = 0, Y' = 1) &= \\
&= \mathbb{P}\left(U \leq p_X, \frac{p_{XY}}{p_X} < V \leq p_Y\right) + \mathbb{P}\left(U > p_X, \frac{p_Y - p_{XY}}{1 - p_X} < V \leq p_Y\right).
\end{aligned}$$

Altogether we have

$$\mathbb{P}(Y \neq Y') = p_X \left| p_Y - \frac{p_{XY}}{p_X} \right| + (1 - p_X) \left| p_Y - \frac{p_Y - p_{XY}}{1 - p_X} \right| = 2|p_{XY} - p_X p_Y|,$$

thus $\text{eCov}(X, Y) = 2|p_{XY} - p_X p_Y|$.

Finally, $\text{eVar}(X) = 2p_X(1 - p_X)$ is straightforward, a special case of the previous formula.

The absolute value of Pearson's correlation ρ for indicators is

$$|\rho(X, Y)| = \frac{|p_{XY} - p_X p_Y|}{\sqrt{p_X(1-p_X)p_Y(1-p_Y)}}$$

thus for indicators X and Y we have $|\rho(X, Y)| \leq \text{eCor}(X, Y)$ (and we have equality iff $p_X = p_Y$).

Based on this observation one can suspect that $|\rho(X, Y)| \leq \text{eCor}(X, Y)$ for all real valued random variables with finite variance. This conjecture is also supported by the fact that the independence of X, Y implies their uncorrelatedness. In the other extreme case when $\rho(X, Y) = \pm 1$ we know that $Y = f(X)$ where f is a similarity (here a linear function) and by Theorem 3.8 below in this case we have $\text{eCor}(X, Y) = 1$.

The conjecture that $|\rho(X, Y)| \leq \text{eCor}(X, Y)$ holds for all real valued random variables with finite variance, however, can easily be disproved. The following theorem shows that if the joint distribution of X, Y is bivariate normal, the opposite inequality holds.

Theorem 3.5. *Let (X, Y) be bivariate normal with correlation $\varrho(X, Y) = \varrho$. Then*

$$\text{eCor}(X, Y) \leq \left[1 - \sqrt{1 - \varrho^2}\right]^{1/2} \leq |\varrho|,$$

and the last inequality is strict unless $\varrho = 0$ or $\varrho = \pm 1$.

Actually we have the following

Conjecture 1. *Let (X, Y) be bivariate normal with correlation $\varrho(X, Y) = \varrho$.*

Then $\text{eCor}(X, Y) = \left[1 - \sqrt{1 - \varrho^2}\right]^{1/2}$.

Proof of Theorem 3.5. Let (X, Y) be bivariate normal with $\text{Var}(X) = \sigma_X^2$, $\text{Var}(Y) = \sigma_Y^2$ and $\varrho(X, Y) = \varrho$. We can suppose $\mathbb{E}X = \mathbb{E}Y = 0$ and $\sigma_X^2 \geq \sigma_Y^2$. Let X' and Y' be independent zero mean normal with variances σ_X^2 and σ_Y^2 , respectively. Finally, set $X = X'$ and $Y = (\sigma_Y/\sigma_X)\varrho X' + \sqrt{1 - \varrho^2} Y'$. Then X, Y have the prescribed joint distribution, and $Y - Y'$ is normal with mean 0 and variance

$$\sigma_Y^2 \left[\varrho^2 + \left(1 - \sqrt{1 - \varrho^2}\right)^2 \right] = 2\sigma_Y^2 \left[1 - \sqrt{1 - \varrho^2}\right],$$

hence

$$\text{eCov}(X, Y) \leq \mathbb{E}|Y - Y'| = \frac{2\sigma_Y}{\sqrt{\pi}} \left[1 - \sqrt{1 - \varrho^2}\right]^{1/2}.$$

In the denominator of eCor we have $e\text{Var}(Y) = \frac{2\sigma_Y}{\sqrt{\pi}} \leq \frac{2\sigma_X}{\sqrt{\pi}} = e\text{Var}(X)$, thus

$$e\text{Cor}(X, Y) \leq \left[1 - \sqrt{1 - \varrho^2}\right]^{1/2} \leq |\varrho|,$$

and the last inequality is strict unless $\varrho = 0$ or $\varrho = \pm 1$. ■

Concerning the lower bound of $e\text{Cor}(X, Y)$, if $\sigma_X = \sigma_Y$ then Remark 3.2 provides the following inequality:

$$|1 - \sqrt{1 - \varrho}| \leq e\text{Cor}(X, Y).$$

The arguments in the proofs support the next conjecture.

Conjecture 2. *In computing the infimum $e\text{Cov}(X, Y) = \inf_{(X', Y')} \mathbb{E}[\delta(X, X') + \delta(Y, Y')]$, under “general conditions” we can suppose $X = X'$ or $Y = Y'$.*

On the above mentioned “general conditions” see below. But first we show by an example that the conjecture is not true without some restrictions.

Example 3.6. If X and Y are 1–1 functions of each other then the conjecture would imply that $e\text{Cor}(X, Y) = 1$ because Y is a function of $X = X'$ thus Y is independent of Y' . Hence $e\text{Cov}(X, Y) = \min\{e\text{Var}(X), e\text{Var}(Y)\}$. Thus in case of continuous marginals the empirical eCor would always be 1 because for continuous marginals no vertical or horizontal lines can contain more than one sample points with probability one. This is, however, not true as is shown by the following sample of four elements: $(1, 4), (2, 2), (3, 3), (4, 1)$. Here $e\text{Var} = 5/4$ for both coordinates but $e\text{Cov} = 1$.

Theorem 3.7. *Conjecture 2 implies Conjecture 1.*

Proof. The infimum in the theorem can be computed by applying conditional quantile transformations. Suppose $X = X'$. Let $F(x), G(y)$ denote the cdf of X and Y , resp., and $G(y|x) = \mathbb{P}(Y \leq y | X = x)$, the conditional cdf of Y . Then the infimum of $\mathbb{E}|Y - Y'|$ under the condition that $Y = Y'$ in distribution, but X', Y' are independent, equals

$$\mathbb{E}\left(\int_{-\infty}^{\infty} |G(y|X) - G(y)| dy\right) = \int_{-\infty}^{\infty} \mathbb{E}|G(y|X) - G(y)| dy.$$

Note that $G(y) = \mathbb{E}G(y|X)$, thus the integrand on the right hand side is a kind of a mean absolute difference. An alternative formula for eCov is

$$e\text{Cov}(X, Y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |G(y|x) - G(y)| dF(x) dy.$$

In the case of jointly normal X, Y the conditional quantile transformation leads to the same representation of Y as a linear combination of X' and Y' that we used in the proof of Theorem 3.5. Thus our Conjecture 1 would follow from Conjecture 2. ■

Unfortunately we could not find simple “general conditions” for the validity of Conjecture 2.

It is easy to see that eCor as a new measure of dependence satisfies at least two of our axioms for dependence measures. Axioms (a), and (d) hold. Concerning (b) and (c) we can only prove the weaker (b*) and (c*).

Theorem 3.8.

$e\text{Cor}(X, Y) = e\text{Cor}(f(X), f(Y))$ for every similarity transformation f of our metric space.

If $Y = f(X)$ where f is a similarity transformation then $e\text{Cor}(X, Y) = 1$.

Proof. From the definition it is obvious that $e\text{Cov}(f(X), f(Y)) = c \cdot e\text{Cov}(X, Y)$. Therefore we also have $e\text{Var}(f(X)) = c \cdot e\text{Var}(X)$, and finally $e\text{Cor}(f(X), f(Y)) = e\text{Cor}(X, Y)$.

For independent X_1, X_2, X_3 we have

$$\begin{aligned} d[(X_1, f(X_1)), (X_2, f(X_3))] &= \delta(X_1, X_2) + \delta(f(X_1), f(X_3)) = \\ &= \delta(X_1, X_2) + c \cdot \delta(X_1, X_3) \geq \\ &\geq \min\{1, c\} [\delta(X_1, X_2) + \delta(X_1, X_3)] = \\ &= \min\{1, c\} d[(X_1, X_1), (X_2, X_3)] \geq \\ &\geq \min\{1, c\} e\text{Var}(X) = \\ &= \min\{e\text{Var}(X), e\text{Var}(f(X))\}. \end{aligned}$$

The infimum of the left hand side as X_2 and X_3 remain independent is equal to $e\text{Cov}(X, f(X))$. Thus $e\text{Cor}(X, f(X)) \geq 1$. The other direction follows from Theorem 3.1. ■

Thus we proved the following result.

Theorem 3.9. In arbitrary metric spaces (\mathcal{M}, ρ) the earth mover’s correlation $\Delta(X, Y) = e\text{Cor}(X, Y)$ satisfies axioms (a), (b*), (c*), and (d).

It is easy to see that for an arbitrary metric space (\mathcal{M}, δ) it cannot be true that $e\text{Cor}(X, Y) = 1$ always implies $Y = f(X)$ where f is a similarity. A counterexample is the following. Let \mathcal{M} be the set of points of the Euclidean plane with the usual Euclidean metric. Suppose that here $e\text{Cor}(X, Y) = 1$ implies $Y = f(X)$ where f is a similarity. If the random variables X and Y

are supported on the x line then we know that the similarity is $Y = aX + b$. Now define a new metric on the plane as follows: $\delta(x, y) = |x - y|$ if both x and y are on the x coordinate axis (the second coordinate is 0), otherwise for all $x \neq y$ define $\delta(x, y) = |x - y| + 1$. This does not change $\text{eCor}(X, Y) = 1$ because X and Y are supported on the x but $y = ax + b$ cannot be extended to the whole plane as a similarity with respect to the new metric.

Conjecture 3. *For Banach space valued random variables we have the iff statement in axiom (c): $\text{eCor}(X, f(X)) = 1$ if and only if $Y = f(X)$ with probability 1, where f is a similarity transformation of the Banach space.*

Although we could not prove this conjecture it is interesting to note that by a theorem of [24], any bijective similarity f of any Banach space (or of any normed linear space) is affine, that is, $f(x) - f(0)$ is linear. Thus similarities in Banach spaces must have a very simple structure.

By the way, it is interesting to note that we can always embed every metric space (\mathcal{M}, δ) into the Banach space $C_b(\mathcal{M})$ of bounded continuous functions on (\mathcal{M}, δ) , just take the function

$$f(x)(y) := \delta(x, y) - \delta(x_0, y),$$

where x_0 is an arbitrary element of \mathcal{M} .

We note that one can easily define the earth mover's correlation for more than two variables. The population version of eCov for three variables is as follows:

$$\text{eCov}(X, Y, Z) = \inf_{(X', Y', Z')} \mathbb{E}d[(X, Y, Z), (X', Y', Z')].$$

Here in distribution $X = X'$, $Y = Y'$, $Z = Z'$, and X', Y', Z' are independent, and we take the inf over all joint distributions of (X, Y, Z) and (X', Y', Z') .

The population version of the three-variate earth mover's correlation is

$$\text{eCor}(X, Y, Z) = \frac{\text{eCov}(X, Y, Z)}{\min \{ \text{eVar}(X), \text{eVar}(Y), \text{eVar}(Z) \}}.$$

Thus we have a natural measure for mutual dependence of more than two random variables.

4. Empirical earth mover's correlation

The earth mover's metric suggests the following earth mover's distance definition between two sequences $x := (x_1, x_2, \dots, x_n)$ and $y := (y_1, y_2, \dots, y_n)$:

$$\mathcal{E}(x, y) := \inf_{\pi} \sum_{i=1}^n \delta(x_i, y_{\pi(i)}),$$

where the infimum is taken for all permutation π on the integers $1, 2, \dots, n$. One can easily see that for real valued data, if the ordered sample is denoted by subscripts in brackets, then

$$\mathcal{E}(x, y) := \sum_{i=1}^n |x_{(i)} - y_{(i)}|.$$

The empirical version of eCov is the minimum transportation cost between the following two mass distributions or probability distributions:

(Q_1) $1/n$ mass at each point (x_i, y_i) , $i = 1, 2, \dots, n$

and

(Q_2) $1/n^2$ mass at each point (x_i, y_j) , $i, j = 1, 2, \dots, n$.

It is easy to see that the empirical eVar is the arithmetic average of the distances $\delta(x_i, x_j)$ because the cost to transport $1/n^2$ mass from the point (x_i, x_j) to the main diagonal (x, x) is at least $\delta(x_i, x_j)/n^2$ and we can achieve this via “horizontal” transportation only. This is not the case if we want to transport to n general points, not necessarily on the main diagonal. The “naive” computational complexity of the empirical eVar which is essentially Gini’s mean difference is $O(n^2)$ but for real valued random variables we can decrease it to $O(n \log n)$.

The complexity of the computation of the empirical eCov is less obvious.

Our transportation problem can be reduced to an assignment problem between two sets of n^2 points thus according to the “Hungarian algorithm” [19] this optimization can be solved in polynomial time. It was shown by [13] and [37] that the algorithmic complexity of assignment problem for two sets of n points is $O(n^3)$ thus in our case the complexity can be reduced to $O(n^6)$.

This is not very encouraging. A better complexity, namely $O(n^3 \log^2 n)$, is in [18]. Here the authors show that for the (linear) transportation problem with m supply nodes, n demand nodes and k feasible arcs there is an algorithm which runs in time proportional to $m \log m(k + n \log n)$ assuming w.l.o.g. that $m \geq n$, still at least one order of magnitude worse than the algorithmic complexity, $O(n^2)$, of computing the distance covariance or the distance correlation. This is the price we need to pay for the generality of eCov and eCor. The AMPL (A Mathematical Programming Language) code is easy to apply for computing empirical eCov and then eCor. In [2] it was shown that given n random blue and n random red points on the unit square, the transportation cost between them is typically $\sqrt{n \log n}$. Our problem is to find the optimal transportation costs when the distance is the Manhattan distance and the number of red points is different from the number of blue points (the total mass is the same). A recent paper [1] suggests that our task of computing the earth mover’s distance between two sets of size n^2 can be done with the first algorithm in the cited

paper with $O(\log^2(1/\varepsilon))$ approximation error bound in $O(n^{2+\varepsilon})$ steps, for any $\varepsilon > 0$. On related algorithmic optimizations see [3] and [4].

5. Conclusion

For Hilbert space valued random variables in [26] we proved that distance correlation is a good measure of dependence in the sense that distance correlation satisfies our axioms (i)–(iv). For general metric space valued random variables, however, this is not true. The earth mover's correlation (eCor) introduced in this paper works for general metric spaces in the sense that eCor satisfies axioms (a), (b*), (c*), (d), and we conjecture that under general conditions, e.g. for Banach space valued random variables, eCor satisfies (a), (b), (c), (d), too. These are counterparts of axioms (i)–(iv). Our main result is Theorem 3.1, the earth mover's version of the Cauchy–Bunyakovsky–Schwarz inequality. Conjectures 1 and 2 are challenges for further research aiming easier computations of eCor. If all we want is to test independence then we do not really need the empirical eCor, it is simpler to work with the empirical earth mover's covariance. For similar statistical tests see [11, 14].

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T. F. Móri

Alfréd Rényi Institute of Mathematics
Reáltanoda u. 13–15.
H-1053 Budapest
Hungary
mori.tamas@renyi.hu

G. J. Székely

National Science Foundation
2415 Eisenhower Avenue
Alexandria, VA 22314
USA
gszekely@nsf.gov