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A Characterization of Random Variables with Minimum L^2-Distance

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A complete characterization of multivariate random variables with minimum L^2 Wasserstein-distance is proved by means of duality theory and convex analysis. This characterization allows to determine explicitly the optimal couplings for several multivariate distributions. A partial solution of this problem has been found in recent papers by Knott and Smith.

1. INTRODUCTION

For probability measures $P, Q \in M^1(\mathbb{R}^k, \mathbb{B}^k)$ let

$$\sigma(P, Q) = \inf\left\{\int |x-y|^2 \, d\mu(x, y); \mu \in M(P, Q)\right\} \tag{1}$$

denote the L^2 Wasserstein-distance, where $M(P, Q)$ is the set of all distribution functions with given marginals P, Q. The problem to find explicit solutions of (1) for $k \geqq 2$ or to determine $\sigma(P, Q)$ has been an open problem for long time (see, e.g., the discussion in [10, p. 654; 12]), while for $k=1$ the solution of (1) goes back to the classical papers of Frechét [2] and Hoeffding [5].

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If X, Y are square integrable random variables, $X \sim P$, $Y \sim Q$ ($X \sim P$ denoting that X has distribution P) then

$$E|X-Y|^2 = |EX-EY|^2 + \operatorname{tr} \Sigma_p + \operatorname{tr} \Sigma_Q - 2 \operatorname{tr} \operatorname{Cov}(X, Y), \tag{2}$$

where $\Sigma_p = \operatorname{Cov}(X)$, $\Sigma_Q = \operatorname{Cov}(Y)$. Therefore, problem (1) is equivalent to:

$$\text{Find } \sup\{\operatorname{tr}(\psi);\, \psi \in \operatorname{Cov}(P, Q)\}, \tag{3}$$

where $\operatorname{Cov}(P, Q) = \{\psi \in \mathbb{R}^{k \times k};\, \exists X \sim P,\ Y \sim Q \text{ with } \psi = \operatorname{Cov}(X, Y)\}$, and also equivalent to:

$$\text{Find } \sup\{E\langle X, Y\rangle;\, X \sim P,\ Y \sim Q\}. \tag{4}$$

For $P = N(a, \Sigma_1)$, $Q = N(b, \Sigma_2)$ one has

$$\operatorname{Cov}(P, Q) = \left\{\psi \in \mathbb{R}^{k \times k};\, \begin{pmatrix} \Sigma_1 & \psi \\ \psi^{\mathrm{T}} & \Sigma_2 \end{pmatrix} \geqq 0\right\} =: K \tag{5}$$

($\geqq 0$ denoting positive semidefiniteness) and in this case problem (1) was solved by Dowson and Landau [1] and Olkin and Pukelsheim [9] (cf. also [4, 3]). Obviously, for any $P, Q \in M^1(\mathbb{R}^k, \mathbb{B}^k)$ with means a, b and covariances Σ_1, Σ_2, respectively, one has

$$\operatorname{Cov}(P, Q) \subset K \tag{6}$$

and, therefore,

$$\sigma(P, Q) \geqq \sigma(N(a, \Sigma), N(b, \Sigma))$$

(cf. also Theorems 2.1 and 2.5 of [3]).

Some general results for problem (1) have been obtained recently in two papers of Knott and Smith [8, 13]. In [8] Knott and Smith consider the existence and description of solutions of the form $(X, \phi(X))$ with regular, invertible functions ϕ. In [13] they introduce the related notions of weak and strong optimality in the context of transportation problems for multivalued functions and obtain in this context sufficient conditions for strong optimality which under additional compactness assumptions are also necessary for weak optimality. Their results imply in particular sufficient conditions for problem (1).

We take up the idea of Knott and Smith and establish for problem (1) a necessary and sufficient condition. Some examples show the applicability of this characterization. We also give an extension of this result to distributions on general locally convex topological vector spaces.

2. Characterization of Solutions

For a closed convex function f on $\mathbb{R}^k$ (closed = lower semicontinuous) let f^* denote the conjugate function

$$f^*(y) = \sup_{x = \mathbb{R}^k} \{\langle x, y\rangle - f(x)\} \tag{8}$$

and denote the subdifferential of f in x by

$$\partial f(x) = \{y \in \mathbb{R}^k; f(z) - f(x) \geqq \langle z - x, y\rangle, z \in \mathbb{R}^k\} \tag{9}$$

(cf. Rockafellar [11]). The elements of $\partial f(x)$ are called subgradients of f at x. Then it holds that for all x, y,

$$f(x) + f^*(y) \geqq \langle x, y\rangle \tag{10}$$

with equality if and only if $y \in \partial f(x)$.

Theorem 1. *Let $P, Q \in M^1(\mathbb{R}^k, \mathbb{B}^k)$ with $\int |x|^2 \, dP(x) < \infty$, $\int |x|^2 \, dQ(x) < \infty$.*

(a) *There exists a solution μ of (1); equivalently, there exist rv's $X \sim P$, $Y \sim Q$ with $E|X - Y|^2 = \sigma(P, Q)$.*

(b) *Let $X \sim P$, $Y \sim Q$; then (X, Y) is a solution of (1) if and only if*

$$Y \in \partial f(X) \qquad \text{a.s. for some closed convex function } f. \tag{11}$$

Proof. (a) The existence of a solution of (1) is well known, cf. [10; 7, Theorem 2.19; 4].

(b) We shall make use of the following special case of duality theorems established by Kellerer [7, Theorem 2.6],

$$\begin{aligned} C(P, Q) &:= \sup\left\{\int \langle x, y\rangle \, d\mu(x, y); \mu \in M(P, Q)\right\} \\ &= \inf\left\{\int g \, dP + \int h \, dQ; g \in L^1(P), h \in L^1(Q)\right. \\ &\qquad \left.\langle x, y\rangle \leqq g(x) + h(y), \forall x, y\right\} =: I(P, Q). \end{aligned} \tag{12}$$

Let $X \sim P$, $Y \sim Q$ and assume that $Y \in \partial f(X)$ a.s. for a closed convex function f. Then for any other rv's $\tilde{X} \sim P$, $\tilde{Y} \sim Q$ holds by (10),

$$E\langle \tilde{X}, \tilde{Y}\rangle \leqq E(f(\tilde{X}) + f^*(\tilde{Y})) = E(f(X) + f^*(Y)) = E\langle X, Y\rangle. \tag{13}$$

Therefore, by (2), (4) the pair (X, Y) is an optimal coupling.

Let, conversely, (X, Y) be a solution of (1) and assume w.l.o.g. that $C(P, Q) = I(P, Q) < \infty$, then by Theorem 2.21 of [7] there exists a solution $g \in L^1(P)$, $h \in L^1(Q)$ of the right-hand side of (12). Defining $f = g^{**}$ we obtain that f is closed, convex, and $\langle x, y \rangle \leqq f(x) + f^*(y) \leqq g(x) + h(y)$; i.e., also the pair (f, f^*) is a solution of the right-hand side of (12). This implies that

$$\langle X, Y \rangle = f(X) + f^*(Y) \qquad \text{a.s.} \tag{14}$$

and, therefore, by (10) that $Y \in \partial f(X)$ a.s. ∎

EXAMPLES. (a) Note that the proof of the sufficient condition in Theorem 1(b) does not need the assumption of square integrability. The square integrability assumption is made in order to ensure the existence of integrable functions $f(x)$, $g(y)$ with $f(x) + g(y) \leqq \langle x, y \rangle$ which is needed for the existence of solutions for $I(P, Q)$.

(b) For a positive semidefinite matrix $T \in \mathbb{R}^{k \times k}$, let T^- denote the Moore Penrose inverse and define $f(x) = \frac{1}{2}(x, Tx)$, $g(y) = \frac{1}{2}(y, T^- y)$, then $f(x) + g(Tx) = \frac{1}{2}(x, Tx) + \frac{1}{2}(Tx, T^- Tx) = (x, Tx)$ and, moreover, $g = f^*$ on $\{x: Tx = 0\}^\perp$ (cf. [11, p. 108]). Therefore, if $Q = P^T$ denotes the image of P under T and if $X \sim P$, then the pair (X, TX) is an optimal coupling. With $\Sigma_2 := T \Sigma_1 T^T = \mathrm{Cov}(TX)$ this corresponds to the case that $rg(\Sigma_2) \subset rg(\Sigma_1)$. In the normal case we obtain in this way the solution of Dowson and Landau [1] and Olkin and Pukelsheim [9]. Especially, if $\sigma = (\sigma_1, ..., \sigma_k)$, $\sigma_i > 0$, then the scalings $(X, \sigma X)$, $\sigma X = (\sigma_1 X_1, ..., \sigma_k X_k)$ are optimal couplings. So we can easily calculate explicit distances in scale families like, e.g., isotropic Cauchy densities

$$f_\sigma(x_1, x_2) = \frac{\sigma}{2\pi(x_1^2 + x_2^2 + \sigma^2)^{3/2}}, \qquad \sigma > 0.$$

(c) An interesting consequence of Theorem 1 (b) is that for any P, $Q \in M^1(\mathbb{R}^k, \mathbb{B}^k)$, square integrable, one can find a closed convex function f and $X \sim P$, $Y \sim Q$ such that $Y \in \partial f(X)$ a.s. Especially, if $A \subset \mathbb{R}^k$, $B \subset \mathbb{R}^k$, $0 < \lambda^k(A) < \infty$, $0 < \lambda^k(B) < \infty$, then there exist rv's X, Y uniformly distributed on A, B with $Y \in \partial f(X)$. Of practical interest is to find smooth (polynomial) mappings $F: A \to B$ with $\partial F / \partial x \geqq 0$ (the Jacobi matrix of convex functions is positive semidefinite) such that $Y = TX$ is uniformly distributed on B. This problem leads to a Monge–Ampère partial differential equation. Some examples of this type are discussed by Knott and Smith [8].

(d) From Rockafellar [11, p. 238], holds: $T(x) \in \partial f(x)$ for some closed convex function if and only if T is cyclically monotone, i.e.,

$$\sum_{i=0}^{m-1} \langle x_{i+1} - x_i, Tx_i \rangle \leqq 0 \qquad \text{for } x_0, ..., x_{m-1}, x_m = x_0 \in \mathbb{R}^k. \tag{15}$$

(e) Let $\mathfrak{U} \in \mathbb{B}^k$, $T: U \to \mathbb{R}^k$ injective, measurable with $\partial T/\partial \chi$ positive definite. If $P \in M^1(\mathbb{R}^k, \mathbb{B}^k)$ with support $S(P) \subset \mathfrak{U}$ and density f, then $Q := P^T$ has the density $g := f \circ T^{-1} |\partial T^{-1}|$ on $V = T(U)$ (∂T^{-1} the Jacobi matrix). If $X \sim P$, then $(X, T(X))$ is an optimal coupling. This allows us to give many examples of solutions of (1), especially in exponential families.

(f) If $k = 1$ and F, G are the df's of P, Q, then, as is well known, a solution of (1) is given by $X = F^{-1}(U)$, $Y = G^{-1}(U)$, where U is uniform on (0, 1). Defining $\phi(x) := G^{-1} \circ F(x)$ and $f(x) := \int_0^x \phi(y)\, dy$, f is convex and $Y := G^{-1}(U) \in \partial f(F^{-1}(U))$. So the classical result is a consequence of Theorem 1.

(g) If $x_1, ..., x_n \in \mathbb{R}^k$, $y_1, ..., y_n \in \mathbb{R}^k$, $P := (1/n) \sum_{i=1}^n \varepsilon_{x_i}$, $Q := (1/n) \sum_{i=1}^n \varepsilon_{y_i}$, then any $\mu \in M(P, Q)$ is of the form $\mu = \Sigma\, s_{ij}\, \varepsilon_{(x_i, y_j)}$, where $S = (s_{ij})$ is a doubly stochastic matrix and the solution of (1) is attained by an extreme point of $M(P, Q)$. Therefore, (1) is equivalent to the rearrangement problem

$$\sum_{i=1}^n |x_i - y_{\pi(i)}|^2 = \inf_{\pi \in \gamma_n}, \tag{16}$$

where γ_n is the set of permutations of 1, ..., n.

If $y_i = Tx_i$, $1 \leqq i \leqq n$, T positive definite, then the identical permutation is a solution. In general it seems to be difficult to construct a mapping f as in Theorem 1. Approximative solutions may be based on (15). Assume that $\pi = id$ is our starting approximation. Then by (15) for $m = 2$ and any pairs i, j it should hold that

$$\langle x_i, y_i \rangle + \langle x_j, y_j \rangle \leqq \langle x_i, y_j \rangle + \langle x_j, y_i \rangle. \tag{17}$$

If for some pair i, j (17) is not satisfied then exchange y_i with y_j. This is repeated until all pairs satisfy (17). In the next step in (15) with $m = 3$ we consider all triples i, j, l and it should hold that

$$\langle x_i, y_i \rangle + \langle x_j, y_j \rangle + \langle x_l, z_l \rangle \geqq \langle x_i, y_j \rangle + \langle x_j, z_l \rangle + \langle x_l, z_i \rangle. \tag{18}$$

Repeat this procedure with $m = 2, 3, 4, ...$ until the objective function does not change essentially.

3. Maximal Correlation

The proof of Theorem 1 extends to a more general situation. Let E be a separable, locally convex topological vector space (lctvs) with dual space E^* supplied by the E-topology. Then

$$c: E \times E^* \to \mathbb{R}^1$$
$$(x, y) \to y(x) = : \langle x, y \rangle$$

is continuous w.r.t. the product topology on E, E^* and, therefore, c is measurable w.r.t. the Borel σ-algebra on $E \times E^*$ which is identical to the product σ-algebra. For tight probability measures P, Q on E, E^* let $M(P, Q)$ denote the set of all tight probability measures on $E \times E^*$ with marginals P, Q. Motivated by (4) we denote

$$C(P, Q) := \sup \left\{ \int C(x, y)\, d\mu(x, y);\, \mu \in M(P, Q) \right\} \tag{19}$$

the maximal "correlation" between rv's X, Y with $X \sim P$, $Y \sim Q$.

From Ioffe and Tichomirov [6] we use the following notations and results from convex analysis. Let for a closed convex function f on X and $x \in X$

$$\partial f(x) = \{ y \in E^*; f(z) \geqq (z - x, y), \forall z \} \tag{20}$$

denote the subdifferential of f at x (we admit that $f(x) = \infty$ and so in (20) we also can restrict to $z \in \operatorname{dom} f$). Furthermore, define the conjugate function

$$f^*(y) = \sup_x (\langle x, y \rangle - f(x)), \qquad y \in E^* \tag{21}$$

and, similarly, $f^{**} = (f^*)^*: E \to \bar{\mathbb{R}}^1$ (cf. [6, p. 159]). Then

$$f(x) + f^*(y) \geqq \langle x, y \rangle, \qquad \forall x \in E, y \in E^* \tag{22}$$

and

$$y \in \partial f(x) \qquad \text{iff} \quad f(x) + f^*(y) = \langle x, y \rangle. \tag{23}$$

For the application of Theorem 2.21 of [7], we need an additional assumption.

Theorem 2. *Let P, Q be tight probability measures on E, E^*, respectively, then*:

(a) *There exist rv's* $X \sim P$, $Y \sim Q$ *with* $E\langle X, Y\rangle = C(P, Q) = \inf\{\int f\,dP + \int f^*\,dQ; f \text{ convex, closed}\} = I(P, Q)$.

(b) *If* $C(P, Q) < \infty$, $c(x, y) \geqq f(x) + g(y)$ *for some* $f \in L^1(P)$, $y \in L^1(Q)$ *finite, and* $X \sim P$, $Y \sim Q$, *then it holds*: (X, Y) *is a solution of* (19) *if and only if* $Y \in \partial f(X)$ *for some closed convex* f.

From Theorem 2 one can infer as in Example 1(a) optimal couplings for Gaussian measures in Hilbert spaces (cf. also Theorem 3.5 of [3]).

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