TECHNICAL NOTE

Note on the Optimal Transportation of Distributions

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Abstract. We extend our work on the optimal mapping of distributions in three directions: (a) we consider any set-valued mapping, not just diffeomorphisms; (b) we distinguish between weak and strong optimality, and identify strong optimality with cyclic monotonicity; and (c) we prove that, under some restrictions, a weakly optimal mapping has the subgradient property.

Key Words. Marginal distributions, cyclic monotonicity, subgradient mappings.

1. Introduction

In the well-known transportation problem, we are given sources \( f_1, f_2, \ldots, f_p \) and sinks \( g_1, g_2, \ldots, g_q \), together with a \( p \times q \) matrix \( C \), whose \((i,j)\)th element is the cost of transporting one unit from the \( i \)th source to the \( j \)th sink, \( \sum f_i = \sum g_j \). We seek a \( p \times q \) matrix \( R \), whose \((i,j)\)th element is the amount transported from the \( i \)th source to the \( j \)th sink. The problem is then:

\[
\text{minimize } \sum \sum r_{ij}C_{ij},
\]

s.t. \( \sum_{j=1}^{q} r_{ij} = f_i, \quad i = 1, 2, \ldots, p, \)

\( \sum_{i=1}^{p} r_{ij} = g_j, \quad j = 1, 2, \ldots, q, \)

\( r_{ij} \geq 0. \)

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For some \( m \leq \min(p, q) \), we can find \( m \times 1 \) vectors \( x_1, x_2, \ldots, x_p \) and \( y_1, y_2, \ldots, y_q \), such that

\[
c_{ij} = \|x_i - y_j\|^2.
\]

The problem is then equivalent to:

\[
\text{maximize } \sum \sum r_{ij} x_i y_j, \text{ with the same constraints on } r_{ij}.
\]

If \( f_1 = f_2 = \cdots = f_p = 1/p \) and \( g_1 = g_2 = \cdots = g_q = 1/q \), we have the assignment problem, and the optimal \( r_{ij} \) are 0 or 1.

In Ref. 1, we gave a generalization of the assignment problem, in which the \( p \) sources are replaced by a d.f. \( F(x) \), defined on \( A \subset \mathbb{R}^m \), and the \( q \) sources by a d.f. \( G(y) \), defined on \( B \subset \mathbb{R}^m \). Then, we sought a one-to-one mapping \( \phi: A \rightarrow B \), such that, if \( X \) had d.f. \( F \), \( \phi(X) \) had d.f. \( G \), which maximized \( \mathbb{E}(X' \phi(X)) \). The symbol d.f. stands for distribution function.

In this paper, we effectively generalize the transportation problem, by considering multi-valued mappings, so that transfers to several sinks from the same source are allowed.

In Ref. 1, a one-to-one mapping \( \phi: A \rightarrow B \), \( A, B \subset \mathbb{R}^m \) was defined to be optimal if, for given distribution functions \( F, G \) on \( A, B \),

\[
\mathbb{E}(X' \phi(X)) \geq \mathbb{E}(X' Y), \tag{1}
\]

for any d.f. \( L \) on \( \mathbb{R}^{2m} \) with margins \( F(x), G(y) \), and if \( Y = \phi(X) \) has d.f. \( G \) when \( X \) has d.f. \( F \). We shall henceforth refer to this property as weak optimality. The criterion

\[
\mathbb{E}_F(\|X - \phi(X)\|^2) \leq \mathbb{E}_{L}(\|X - Y\|^2) \tag{2}
\]

is equivalent to (1).

The weak optimality introduced by (1) generalizes the problem, when \( n = 1 \), of finding a one-to-one mapping \( Y = \phi(X) \) which maximizes the correlation between \( X \) and \( Y \) for \( X, Y \) with given fixed marginal distributions \( F, G \). There are references to work on this problem in Ref. 1.

In Ref. 1, we proved that, if \( \phi \) is a diffeomorphism and \( \frac{\partial \phi(x)}{\partial x'} \) is a (symmetric) positive-semidefinite matrix for all \( x \in A \), then \( \phi \) is weakly optimal.

Now, if \( F, G \) are discrete distributions, there may not be such a weakly optimal \( \phi \). If \( F \) for instance gives all its probability to value 0, and \( G \) is continuous, then no one-to-one \( \phi \) can be weakly optimal. What is needed is a multivalued mapping \( \phi \) which allows more than one value of \( Y \) for each \( X \). We introduce a stronger form of optimality in order to show that