Abstract

This article connects the theory of extremal doubly stochastic measures to the geometry and topology of optimal transportation.

We begin by reviewing an old question (# 111) of Birkhoff in probability and statistics [4], which is to give a necessary and sufficient condition on the support of a joint probability to guarantee extremality among all measures which share its marginals. Following work of Douglas, Lindenstrauss, and Beneš and Štěpán, Hestir and Williams [15] found a necessary condition which is nearly sufficient; we relax their subtle measurability hypotheses separating necessity from sufficiency slightly, yet demonstrate by example that to be sufficient certainly requires some measurability. Their condition amounts to the vanishing of $\gamma$ outside a countable alternating sequence of graphs and antigraphs in which no two graphs (or two antigraphs) have domains that overlap, and where the domain of each graph / antigraph in the sequence contains the range of the succeeding antigraph (respectively, graph). Such sequences are called numbered limb systems. Surprisingly, this characterization can be used to resolve the uniqueness question for optimal transportation on manifolds with the topology of the sphere.
Extremal doubly stochastic measures and optimal transportation*

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1 Introduction

An $n \times n$ doubly stochastic matrix refers to a matrix of non-negative entries whose columns and rows each sum to 1. The doubly stochastic matrices form a convex subset of all $n \times n$ matrices — in fact a convex polytope, whose extreme points are in bijective correspondence with the $n!$ permutations on $n$-letters, according to a theorem of Birkhoff [3] and von Neumann [32]. For example, the $3 \times 3$ doubly stochastic matrices,

$$
\begin{pmatrix}
s & t & 1 - s - t \\
u & v & 1 - u - v \\
1 - s - u & 1 - t - v & s + t + u + v - 1
\end{pmatrix}
$$

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form a 4-dimensional polytope with 6 vertices. Shortly after proving this characterization, Birkhoff [4, Problem 111] initiated the search for a infinite-dimensional generalization, thus stimulating a line of research which remains fruitful even today.

A doubly stochastic measure on the square refers to a non-negative Borel probability measure on $[0,1]^2$ whose horizontal and vertical marginals both coincide with Lebesgue measure $\lambda$ on $[0,1]$. The set of doubly stochastic measures forms a convex set we denote by $\Gamma(\lambda, \lambda)$ (which is weak-$\ast$ compact in the Banach space dual to continuous functions $C([0,1]^2)$ normed by their suprema $\|\cdot\|_\infty$). A measure is said to be extremal in $\Gamma(\lambda, \lambda)$ if it cannot be decomposed as a convex combination $\gamma = (1 - t)\gamma_0 + t\gamma_1$ with $0 < t < 1$ and $\gamma_0, \gamma_1 \in \Gamma(\lambda, \lambda)$, except trivially with $\gamma_0 = \gamma_1$. Since the Krein-Milman theorem asserts that convex combinations of extreme points are dense (in any compact convex subset of a topological vector space, Figure 1), it is natural to want to characterize the extreme points of $\Gamma(\lambda, \lambda)$. Another motivation for such a characterization is that every continuous linear functional on $\Gamma(\lambda, \lambda)$ is minimized at an extreme point. Whether or not this extremum is uniquely attained can be an interesting question: in Figure 1 the horizontal coordinate is minimized at a single point but maximized at two extreme points (and along the segment joining them).

![Figure 1: Krein-Milman asserts a compact convex set K can be reconstructed from its extreme points (denoted here by solid circles • and solid lines −).](image)

Motivated by applications like the optimization problem just mentioned,
we prefer to formulate the question in slightly greater generality, by replacing the two copies of $([0, 1], \lambda)$ with probability spaces $(X, \mu)$ and $(Y, \nu)$, where $X$ and $Y$ are each subsets of a complete separable metric space, and $\mu$ and $\nu$ are Borel probability measures on $X$ and $Y$ respectively. This widens applicability of the answer to this question without increasing its difficulty. Letting $\Gamma(\mu, \nu)$ denote the Borel probability measures on $X \times Y$ having $\mu$ and $\nu$ for marginals, we wish to characterize the extreme points of the convex set $\Gamma(\mu, \nu)$. Ideally, as in the finite-dimensional case, this characterization would be given in terms of some geometrical property of the support of the measure $\gamma$ in $X \times Y$. Indeed, if $\mu = \sum_{i=1}^{m} m_i \delta_{x_i}$ and $\nu = \sum_{j=1}^{n} n_j \delta_{y_j}$ are finite, our problem reduces to characterizing the extreme points of the convex set $A$ of $m \times n$ matrices with prescribed column and row sums:

$$A = \{a_{ij} \geq 0 \mid m_i = \sum_{j=1}^{n} a_{ij}, \sum_{i=1}^{m} a_{ij} = n_j \}.$$ 

A matrix $(a_{ij})$ is well-known to be extremal in $A$ if and only if it is *acyclic*, meaning for every sequence $a_{i_1j_1}, \ldots, a_{i_kj_k}$ of non-zero entries occupying $k \geq 2$ distinct columns and $k$ distinct rows, the product $a_{i_1j_2} \cdots a_{i_{k-1}j_k}a_{i_kj_1}$ must vanish — see Figure 2 or Denny [9], where the terminology *aperiodic* is used. Similarly, a set $S \subset X \times Y$ is acyclic if for every $k \geq 2$ distinct points $\{x_1, \ldots, x_k\} \subset X$ and $\{y_1, \ldots, y_k\} \subset Y$, at least one of the pairs $(x_1y_1), (x_1, y_2), (x_2, y_2), \ldots, (x_{k-1}, y_k), (x_k, y_k), (x_k, y_1)$ lies outside of $S$.

Figure 2: In an *acyclic* matrix the product of $x$'s and $o$'s must vanish
A functional analytic characterization of extremality was supplied by Douglas [10] and by Lindenstrauss [21]: it asserts that $\gamma$ is extremal in $\Gamma(\mu, \nu)$ if and only if $L^1(X, d\mu) \oplus L^1(Y, d\nu)$ is dense in $L^1(X \times Y, d\gamma)$. Although this result is a useful starting point, it is not quite the characterization we desire for applications, since it is not easily expressed in terms of the geometry of the support of $\gamma$. Significant further progress was made by Beneš and Štěpán, who showed every extremal doubly stochastic measure vanishes outside some acyclic subset $S \subset X \times Y$ [2]. Hestir and Williams refined this condition, showing that it becomes sufficient under an additional Borel measurability hypothesis which, unfortunately, is not always satisfied [15]. Some of the subtleties of the problem were indicated already by Losert’s counterexamples [22]. The difficulty of the problem resides partly in the fact that any geometrical characterization of optimality must be invariant under arbitrary measure-preserving transformations applied independently to the horizontal (abscissa) and vertical (ordinate) variables.

In this manuscript we review this line of research, clarifying the nature of the gap separating necessity from sufficiency and pointing out that it can be narrowed slightly by replacing the Borel $\sigma$-algebra with suitably adapted measure-completions. We conclude by describing an application to the question of uniqueness in optimal transportation, which is one of the original and most important examples of an infinite-dimensional program [16], and appears naturally in applications [27] [31]. It arises when one wants to use a continuum of sources to supply a continuum of sinks (modeled by $\mu$ and $\nu$ respectively) as efficiently as possible. The question addressed is to identify cost functions $c(x, y)$ on the product space $X \times Y$ whose minimum expected value against measures in $\Gamma(\mu, \nu)$ is uniquely attained. When $X$ and $Y$ are differentiable manifolds and $c \in C^1(X \times Y)$, to guarantee uniqueness it turns out to be sufficient that $y_1 \neq y_2$ imply $x \in X \rightarrow c(x, y_1) - c(x, y_2)$ has no critical points, except perhaps for a single global maximum and a single global minimum. This generalizes to some compact manifolds $X$ a criterion of Gangbo [12], Carlier [7], Levin [20] and Ma, Trudinger and Wang [23], which asserts that the absence of critical points implies uniqueness; (their condition further implies that almost every source supplies a single sink, thus solving another transportation problem first posed by Monge [25], which our condition does not do). When satisfied, our criterion implies that the manifold $X$, if compact, has the topology of the sphere. Uniqueness, however, remains an interesting open question for compact manifolds which are not topological spheres. This surprising application was first developed in an economic
context by Chiappori, McCann, and Nesheim [8].

2 Measures on graphs are push-forwards

Before recalling the characterization of interest, let us develop a bit of notation in a simpler setting, and a key argument that we shall require. Impatient or knowledgeable readers can skim the present section and proceed directly to the final sections below.

Let $X$ and $Y$ be subsets of complete separable metric spaces, and fix a non-negative Borel measure $\mu$ on $X$. Suppose $f : X \to Y$ is $\mu$-measurable, meaning $f^{-1}(B)$ is in the $\sigma$-algebra completion of the Borel subsets of $X$ with respect to the measure $\mu$, whenever $B$ is relatively Borel in $Y$. Then a Borel measure on $Y$ is induced, denoted $f_\# \mu$ and called the push-forward of $\mu$ through $f$, and given by

$$(f_\# \mu)[B] := \mu[f^{-1}(B)]$$

for each Borel $B \subset Y$. Defining the projections $\pi^X(x, y) = x$ and $\pi^Y(x, y) = y$ on $X \times Y$, this notation permits the horizontal and vertical marginals of a measure $\gamma \geq 0$ on $X \times Y$ to be expressed as $\pi^X_\# \gamma$ and $\pi^Y_\# \gamma$ respectively.

The next lemma shows that any measure supported on a graph can be deduced from its horizontal marginal. It improves on Lemma 2.4 of [14] and various other antecedents, by using an argument from Villani’s Theorem 5.28 [31] to extract $\mu$-measurability of $f$ as a conclusion rather that a hypothesis. As work of, e.g., Hestir and Williams [15] implies, although measures on graphs are extremal in $\Gamma(\mu, \nu)$, the converse is far from being true; this peculiarity is an inevitable consequence of the infinite divisibility of $(X, \mu)$.

**Lemma 2.1 (Measures on graphs are push-forwards)** Let $X$ and $Y$ be subsets of complete separable metric spaces, and $\gamma \geq 0$ a $\sigma$-finite Borel measure on the product space $X \times Y$. Denote the horizontal marginal of $\gamma$ by $\mu := \pi^X_\# \gamma$. If $\gamma$ vanishes outside the graph of $f : X \to Y$, meaning $\{(x, y) \in X \times Y \mid y \neq f(x)\}$ has zero outer measure, then $f$ is $\mu$-measurable and $\gamma = (id_X \times f)_\# \mu$.

**Proof.** Since outer-measure is subadditive, it costs no generality to assume the subsets $X$ and $Y$ are in fact complete and separable, by extending $\gamma$
in the obvious (minimal) way. Any \( \sigma \)-finite Borel measure \( \gamma \) is regular and \( \sigma \)-compact on a complete separable metric space; e.g. p. 255 of [11] or Theorem I-55 of [30]. Since \( \gamma \) vanishes outside \( \text{Graph}(f) := \{(x, f(x)) \mid x \in X\} \), there is an increasing sequence of compact sets \( K_i \subset K_{i+1} \subset \text{Graph}(f) \) whose union \( K_\infty = \lim_{i \to \infty} K_i \) contains the full mass of \( \gamma \). Compactness of \( K_i \subset \text{Graph}(f) \) implies continuity of \( f \) on the compact projection \( X_i := \pi^X(K_i) \). Thus the restriction \( f_\infty \) of \( f \) to \( X_\infty := \pi^X(K_\infty) \) is a Borel map whose graph \( K_\infty = \text{Graph}(f_\infty) \) is a \( \sigma \)-compact set of full measure for \( \gamma \). We now verify that \( \gamma \) and \((\text{id}_{X_\infty} \times f_\infty)\# \mu \) assign the same mass to each Borel rectangle \( U \times V \subset X \times Y \). Since \((U \times V) \cap \text{Graph}(f_\infty) = ((U \cap f_\infty^{-1}(V)) \times Y) \cap \text{Graph}(f_\infty) \) we find

\[
\gamma(U \times V) = \gamma((U \cap f_\infty^{-1}(V)) \times Y) = \mu(U \cap f_\infty^{-1}(V)),
\]

proving \( \gamma = (\text{id}_{X_\infty} \times f_\infty)\# \mu \). Taking \( U = X \setminus X_\infty \) and \( V = Y \) shows \( X \setminus X_\infty \) is \( \mu \)-negligible. Since \( \text{id}_X \times f \) differs from the Borel map \( \text{id}_{X_\infty} \times f_\infty \) only on the \( \mu \)-negligible complement of the \( \sigma \)-compact set \( X_\infty \), we conclude \( f \) is \( \mu \)-measurable and \( \gamma = (\text{id}_X \times f)\# \mu \) as desired. \( \blacksquare \)

The preceding lemma shows that any measure concentrated on a graph is uniquely determined by its marginals; \( \gamma \) is therefore extremal in \( \Gamma(\pi^X_\# \gamma, \pi^Y_\# \gamma) \). As the results of the next section show, the converse is far from being true.

### 3 Numbered limb systems and extremality

In this section we adapt Hestir and Williams [15] notion of a numbered limb system to \( X \times Y \). Using the axiom of choice, Hestir and Williams deduced from the acyclicity condition of Beneš and Štěpán [2] that each extremal doubly stochastic measure vanishes outside some numbered limb system. Conversely, they showed that vanishing outside a number limb system is sufficient to guarantee extremality of a doubly stochastic measure, provided the graphs (and antigraphs) comprising the system are Borel subsets of the square. Our main theorem gives a new proof of this converse in the more general setting of subsets \( X \times Y \) of complete separable metric spaces, and under a slightly weaker measurability hypothesis on the graphs and antigraphs. A simple example shows that some measurability hypothesis is nevertheless required. In the next section, we shall see how this converse is germane to the question of uniqueness in optimal transportation.
Given a map \( f : D \rightarrow Y \) on \( D \subset X \), we denote its graph, domain, range, and the graph of its (multivalued) inverse by

\[
\text{Graph}(f) := \{(x, f(x)) \mid x \in D\},
\]

\[
\text{Dom } f := \pi_X(\text{Graph}(f)) = D,
\]

\[
\text{Ran } f := \pi_Y(\text{Graph}(f)),
\]

\[
\text{Antigraph}(f) := \{(f(x), x) \mid x \in \text{Dom } f\} \subset Y \times X.
\]

More typically, we will be interested in the \( \text{Antigraph}(g) \subset X \times Y \) of a map \( g : D \subset Y \rightarrow X \).

![Diagram](image)

Figure 3: The subsets \( I_k \) need not be connected; in this numbered limb system they are represented as connected sets for visual convenience only.

**Definition 3.1 (Numbered limb system)** Let \( X \) and \( Y \) be Borel subsets of complete separable metric spaces. A relation \( S \subset X \times Y \) is a numbered limb system if there is a countable disjoint decomposition of \( X = \bigcup_{i=0}^{\infty} I_{2i+1} \) and of \( Y = \bigcup_{i=0}^{\infty} I_{2i} \) with a sequence of maps \( f_{2i} : \text{Dom}(f_{2i}) \subset Y \rightarrow X \) and \( f_{2i+1} : \text{Dom}(f_{2i+1}) \subset X \rightarrow Y \) such that \( S = \bigcup_{i=1}^{\infty} \text{Graph}(f_{2i-1}) \cup \text{Antigraph}(f_{2i}) \), with \( \text{Dom}(f_k) \cup \text{Ran}(f_{k+1}) \subset I_k \) for each \( k \geq 0 \). The system has (at most) \( N \) limbs if \( \text{Dom}(f_k) = \emptyset \) for all \( k > N \).

Notice the map \( f_0 \) is irrelevant to this definition though \( I_0 \) is not; we may always take \( \text{Dom}(f_0) = \emptyset \), but require \( \text{Ran}(f_1) \subset I_0 \). The point is
the following theorem and its corollary, which extends and relaxes the result proved by Hestir and Williams for Lebesgue measure \( \mu = \nu = \lambda \) on the interval \( X = Y = [0, 1] \). In it, \( \Gamma(\mu, \nu) \) denotes the set of non-negative Borel measures on \( X \times Y \) having \( \mu = \pi_X^X \gamma \) and \( \nu = \pi_Y^X \gamma \) for marginals. As in the preceding lemma, we say \( \gamma \) vanishes outside of \( S \subset X \times Y \) if \( \gamma \) assigns zero outer measure to the complement of \( S \) in \( X \times Y \).

**Theorem 3.2 (Numbered limb systems yield unique correlations)**

Let \( X \) and \( Y \) be subsets of complete separable metric spaces, equipped with \( \sigma \)-finite Borel measures \( \mu \) on \( X \) and \( \nu \) on \( Y \). Suppose there is a numbered limb system \( S = \bigcup_{i=1}^{\infty} \text{Graph}(f_{2i-1}) \cup \text{Antigraph}(f_{2i}) \) with the property that \( \text{Graph}(f_{2i-1}) \) and \( \text{Antigraph}(f_{2i}) \) are \( \gamma \)-measurable subsets of \( X \times Y \) for each \( i \geq 1 \) and for every \( \gamma \in \Gamma(\mu, \nu) \) vanishing outside of \( S \). If the system has finitely many limbs or \( \mu[X] < \infty \), then at most one \( \gamma \in \Gamma(\mu, \nu) \) vanishes outside of \( S \). If such a measure exists, it is given by \( \gamma = \sum_{k=1}^{\infty} \gamma_k \) where

\[
\gamma_{2i-1} = (id_X \times f_{2i-1})\gamma \eta_{2i-1}, \quad \gamma_{2i} = (f_{2i} \times id_Y)\gamma \eta_{2i}, \quad (2)
\]

\[
\eta_{2i-1} = \left( \mu - \pi_X^X \gamma_{2i} \right)|_{\text{Dom} f_{2i-1}}, \quad \eta_{2i} = \left( \nu - \pi_Y^Y \gamma_{2i} \right)|_{\text{Dom} f_{2i}}. \quad (3)
\]

Here \( f_k \) is measurable with respect to the \( \eta_k \) completion of the Borel \( \sigma \)-algebra. If the system has \( N < \infty \) limbs, \( \gamma_k = 0 \) for \( k > N \), and \( \eta_k \) and \( \gamma_k \) can be computed recursively from the formulae above starting from \( k = N \).

**Proof.** Let \( S = \bigcup_{i=1}^{\infty} \text{Graph}(f_{2i-1}) \cup \text{Antigraph}(f_{2i}) \) be a numbered limb system whose complement has zero outer measure for some \( \sigma \)-finite measure \( 0 \leq \gamma \in \Gamma(\mu, \nu) \). This means that \( I_k \supset \text{Dom} f_k \) gives a disjoint decomposition of \( X = \bigcup_{i=0}^{\infty} I_{2i+1} \) and of \( Y = \bigcup_{i=0}^{\infty} I_{2i} \), and that \( \text{Ran}(f_k) \subset I_{k-1} \) for each \( k \geq 1 \). Assume moreover, that \( \text{Graph}(f_{2i}) \) and \( \text{Antigraph}(f_{2i-1}) \) are \( \gamma \)-measurable for each \( i \geq 1 \). We wish to show \( \gamma \) is uniquely determined by \( \mu, \nu \) and \( S \).

The graphs \( \text{Graph}(f_{2i-1}) \) are disjoint since their domains \( I_{2i-1} \) are disjoint, and the antigraphs \( \text{Antigraph}(f_{2i}) \) are disjoint since their domains \( I_{2i} \) are. Moreover, \( \text{Graph}(f_{2i-1}) \) is disjoint from \( \text{Antigraph}(f_{2j}) \) for all \( i, j \geq 1 \): \( \text{Ran}(f_{2i-1}) \subset I_{2i-2} \) prevents \( \text{Graph}(f_{2i-1}) \) from intersecting \( \text{Antigraph}(f_{2j-2}) \) unless \( j = i \) since the domains \( I_{2j-2} \) are disjoint, and \( \text{Graph}(f_{2i-1}) \) cannot intersect \( \text{Antigraph}(f_{2i-2}) \) since \( \text{Dom}(f_{2i-1}) \subset I_{2i-1} \) and \( \text{Dom}(f_{2i-1}) \subset I_{2i-1} \) is disjoint from \( \text{Ran}(f_{2i-2}) \subset I_{2i-3} \).

Let \( \gamma_k \) denote the restriction of \( \gamma \) to \( \text{Antigraph}(f_k) \) for \( k \) even and to \( \text{Graph}(f_k) \) for \( k \) odd. Then \( \gamma = \sum \gamma_k \) by our measurability hypothesis,
and \( \gamma_k \) restricts to a Borel measure on \( X \times \text{Dom} f_k \) if \( k \) is even, and on \( \text{Dom} f_k \times Y \) if \( k \) odd. Defining the marginal projections \( \mu_k = \pi^X \gamma_k \) and \( \nu_k = \pi^Y \gamma_k \), setting \( \eta_k = \nu_k \) if \( k \) even and \( \eta_k = \mu_k \) if \( k \) odd yields \( \text{(2)} \) and the \( \eta_k \)-measurability of \( f_k \) immediately from Lemma 2.1. Since \( \nu_{2i} \) vanishes outside \( \text{Dom} f_{2i} \), from \( \nu = \sum_{k=1}^{\infty} \nu_k \) we derive \( \nu_{2i} = (\nu - \sum_{k \neq 2i} \nu_k)|_{\text{Dom} f_{2i}}. \) For \( k \) even, \( \nu_k \) vanishes outside \( \text{Dom} f_k \subset I_k \), while for \( k \) odd, \( \nu_k \) vanishes outside \( \text{Ran} f_k \subset I_{k-1} \), which is disjoint from \( \text{Dom} f_{2i} \) unless \( k = 2i + 1 \). Thus \( \eta_{2i} = (\nu - \nu_{2i+1})|_{\text{Dom} f_{2i}}. \) The formula \( \text{(3)} \) for \( \eta_{2i-1} \) follows from similar considerations.

It remains to show the representation \( \text{(2)}-\text{(3)} \) specifies \( (\gamma_k, \eta_k) \) uniquely for all \( k \geq 1 \), and hence determines \( \gamma = \sum \gamma_k \) uniquely. If the system has \( N < \infty \) limbs, \( I_k = \emptyset \) for \( k > N \) and hence \( \gamma_k = 0 \). We can compute \( \eta_k \) and \( \gamma_k \) starting with \( k = N \), and then recursively from the formulae above for \( k = N - 1, N - 2, \ldots, 1 \), so the formulae represent \( \gamma \) uniquely. If instead \( S \) has countably many limbs, suppose there are two finite Borel measures \( \gamma \) and \( \bar{\gamma} \) vanishing outside of \( S \) and having the same marginals \( \mu \) and \( \nu \). For each \( k \geq 1 \), recall that

\[
K_k := \begin{cases} 
\text{Graph}(f_k) & \text{k odd}, \\
\text{Antigraph}(f_k) & \text{k even},
\end{cases}
\]

is measurable with respect to both \( \gamma \) and \( \bar{\gamma} \). Given \( \epsilon > 0 \), take \( N \) large enough so that both \( \gamma \) and \( \bar{\gamma} \) assign mass less than \( \epsilon \) to \( \bigcup_{k=N}^{\infty} K_k \). Set \( \gamma_k = \gamma|_{K_k} \) and \( \bar{\gamma}_k = \bar{\gamma}|_{K_k} \) and denote their marginals by \( (\mu_k, \nu_k) = (\pi^X \gamma_k, \pi^Y \gamma_k) \) and \( (\bar{\mu}_k, \bar{\nu}_k) = (\pi^X \bar{\gamma}_k, \pi^Y \bar{\gamma}_k) \). Observe that both \( \gamma^e := \sum_{k=1}^{N} \gamma_k \) and \( \bar{\gamma}^e := \sum_{k=1}^{N} \bar{\gamma}_k \) are concentrated on the same numbered limb system; it has finitely many limbs, and the differences \( \delta \mu^e = \sum_{k=1}^{N} (\bar{\mu}_k - \mu_k) \) and \( \delta \nu^e = \sum_{k=1}^{N} (\bar{\nu}_k - \nu_k) \) between the marginals of \( \gamma^e \) and \( \bar{\gamma}^e \) have total variation at most \( 2\epsilon \). Since the \( \delta \mu_{2i-1} = \bar{\mu}_{2i-1} - \mu_{2i-1} \) are mutually singular, as are the \( \delta \nu_{2i} = \bar{\nu}_{2i} - \nu_{2i} \), we find the sum of the total variations of

\[
\delta \eta_k := \begin{cases} 
\bar{\mu}_k - \mu_k & \text{k odd}, \\
\bar{\nu}_k - \nu_k & \text{k even},
\end{cases}
\]

is bounded: \( \sum_{k=1}^{N} \| \delta \eta_k \|_{TV(\text{Dom} f_k)} < 4\epsilon \). Using \( \text{(2)} \) to derive

\[
\| \bar{\gamma}_k - \gamma_k \|_{TV(X \times Y)} = \begin{cases} 
\| (id_X \times f_k)_# \delta \eta_k \|_{TV(X \times Y)} & \text{k odd}, \\
\| (f_k \times id_Y)_# \delta \eta_k \|_{TV(X \times Y)} & \text{k even},
\end{cases}
\]

and

\[
= \| \delta \eta_k \|_{TV(\text{Dom} f_k)}
\]

10
and summing on \(k\) yields \(\|\tilde{\gamma}^\epsilon - \gamma^\epsilon\|_{TV(X \times Y)} < 4\epsilon\). Since \(\gamma^\epsilon \to \gamma\) and \(\tilde{\gamma}^\epsilon \to \tilde{\gamma}\) as \(\epsilon \to 0\), we conclude \(\tilde{\gamma} = \gamma\) to complete the uniqueness proof. □

As in Hestir and Williams [15], the uniqueness theorem above implies extremality as an immediate consequence.

**Corollary 3.3 (Sufficient condition for extremality)** Let \(X\) and \(Y\) be subsets of complete separable metric spaces, equipped with \(\sigma\)-finite Borel measures \(\mu\) on \(X\) and \(\nu\) on \(Y\). Suppose there is a numbered limb system \(S = \bigcup_{i=1}^\infty \text{Graph}(f_{2i-1}) \cup \text{Antigraph}(f_{2i})\) with the property that \(\text{Graph}(f_{2i-1})\) and \(\text{Antigraph}(f_{2i})\) are \(\gamma\)-measurable subsets of \(X \times Y\) for each \(i \geq 1\), for every \(\gamma \in \Gamma(\mu, \nu)\) vanishing outside of \(S\). If the system has finitely many limbs or \(\mu[X] < \infty\), then any measure \(\gamma \in \Gamma(\mu, \nu)\) vanishing outside of \(S\) is extremal in the convex set \(\Gamma(\mu, \nu)\).

**Proof.** Suppose a measure \(\gamma \in \Gamma(\mu, \nu)\) vanishes outside a numbered limb system \(S\) satisfying the hypotheses of the corollary. If \(\gamma = (1-t)\gamma_0 + t\gamma_1\) with \(\gamma_0, \gamma_1 \in \Gamma(\mu, \nu)\) and \(0 < t < 1\), then \(\gamma \geq \gamma_0\) and \(\gamma \geq \gamma_1\), so both \(\gamma_0\) and \(\gamma_1\) vanish outside of \(S\). According to Theorem 3.2, they are uniquely determined by \(S\) and their marginals, hence \(\gamma_0 = \gamma_1\) to establish the corollary. □

The following example confirms that a measurability gap still remains between the necessary and sufficient conditions for extremality. It is a close variation on the standard example of a non-Lebesgue measurable set from real analysis. Together with the lemma and theorem preceding, this example makes clear that measurability is required only to allow the graphs to be separated from each other and from the antigraphs in an additive way.

**Example 3.4 (An acyclic set supporting non-extremal measures)** Let \(\lambda\) denote Lebesgue measure and define the maps \(f_0(x) = x\) and \(f_1(x) = x + \sqrt{2} \mod 1\) on the unit interval \(X = Y = [0, 1]\). Notice \(\text{Graph}(f_i) \subset [0, 1]^2\) supports the doubly stochastic measure \(\gamma_i = (id \times f_i)_\# \lambda\) for \(i = 0\) and \(i = 1\); (both measures are extremal in \(\Gamma(\lambda, \lambda)\) by Corollary 3.3). Irrationality of \(\sqrt{2}\) implies \(S = \text{Graph}(f_0) \cup \text{Graph}(f_1)\) is an acyclic set, hence can be expressed as a numbered limb system according to Hestir and Williams [15]. On the other hand, there are doubly stochastic measures such as \(\gamma := \frac{1}{2}(\gamma_0 + \gamma_1)\) which vanish outside of \(S\) but which are manifestly not extremal.
4 Uniqueness of optimal transportation

In this section we illustrate the significance of the foregoing results by applying them to the uniqueness question for optimal transportation on manifolds. Given subsets $X$ and $Y$ of complete separable metric spaces equipped with Borel probability measures, representing the distributions $\mu$ of production on $X$ and $\nu$ of consumption on $Y$, the Kantorovich-Koopmans [16] [19] transportation problem is to find $\gamma \in \Gamma(\mu, \nu)$ correlating production with consumption so as to minimize the expected transportation cost

$$\inf_{\gamma \in \Gamma(\mu, \nu)} \int_{X \times Y} c(x, y) d\gamma(x, y)$$

against some continuous function $c \in C(X \times Y)$. Hereafter we shall be solely concerned with the case in which $X$ is a differentiable manifold, $\mu$ is absolutely continuous with respect to coordinates on $X$, and the cost function $c \in C^1(X \times Y)$ is differentiable with local control on the magnitude of its $x$-derivative $d_x c(x, y)$ uniformly in $y$; for convenience we also suppose $Y$ to be a differentiable manifold and $c$ is bounded, though though this is not really necessary: substantially weaker assumptions also suffice [8].

In this setting one immediately asks whether the infimum (4) is uniquely attained. Since attainment is evident, the question here is uniqueness. If $c$ satisfies a twist condition, meaning $x \in X \rightarrow c(x, y_1) - c(x, y_2)$ has no critical points for $y_1 \neq y_2 \in Y$, then not only is the minimizing $\gamma$ unique, but its mass concentrates entirely on the graph of a single map $f_1 : X \rightarrow Y$ (a numbered limb system with one limb), thus solving a form of the transportation problem posed earlier by Monge [25] [17]. This was proved in comparable generality by Gangbo [12], Carlier [7], Levin [20], and Ma, Trudinger and Wang [23], building on the more specific examples of strictly convex cost functions $c(x, y) = h(x - y)$ in $X = Y = \mathbb{R}^n$ analyzed by Caffarelli [6] and Gangbo and McCann [13], and in case $h(x) = |x|^2$ by Abdellaoui and Heinich, Brenier, Cuesta-Albertos, Matran, and Tuero-Diaz, Cullen and Purser, Knott and Smith, and Rüschendorf and Rachev; see [7] [13] [31]. Adding further restrictions beyond this twist hypothesis allowed Ma, Trudinger, Wang, and later Loeper, to develop a regularity theory for the map $f_1 : X \rightarrow Y$, embracing Delanoe, Caffarelli and Urbas’ results for the quadratic cost, Gangbo and McCann’s for its restriction to convex surfaces, and Wang’s reflector antenna design, which involves the restriction of $c(x, y) = -\log |x - y|$ to the sphere; references may be found in [18] [31]. Unfortunately, the twist
hypothesis, also known as a generalized Spence-Mirrlees condition in the economic literature, cannot be satisfied for smooth costs $c$ on compact manifolds $X \times Y$, and apart from the result we are about to discuss there are no general theorems which guarantee uniqueness of minimizer to (4) in this setting. With this in mind, let us state our main theorem, a version of which was established in a more complicated economic setting by Chiappori, Nesheim, and McCann [8]. We expect the simpler formulation and argument given below to prove more interesting and accessible to a mathematical readership.

**Theorem 4.1 (Uniqueness of optimal transport on manifolds)**

Let $X$ and $Y$ be complete separable manifolds equipped with Borel probability measures $\mu$ on $X$ and $\nu$ on $Y$. Let $c \in C^1(X \times Y)$ be a bounded cost function such that for each $y_1 \neq y_2 \in Y$, the map

$$x \in X \rightarrow c(x, y_1) - c(x, y_2)$$

has no critical points, save at most one global minimum and at most one global maximum. Assume $d_x c(x, y)$ is locally bounded in $x$, uniformly in $Y$. If $\mu$ is absolutely continuous with respect to coordinate measure on $X$, then the minimum (4) is uniquely attained; moreover, the minimizer $\gamma \in \Gamma(\mu, \nu)$ vanishes outside a numbered limb system having at most two limbs.

**Proof.** Here we give only the proof that there is a numbered limb system having at most two limbs, outside of which the mass of all minimizers $\gamma$ vanishes. A detailed argument confirming the plausible fact that the graphs of these limbs are Borel subsets of $X \times Y$ can be found in [8]. Uniqueness of $\gamma$ then follows from Theorem 3.2.

By linear programming duality due to Kantorovich and Koopmans in this context, it is well-known [31] that there exist potentials $q \in L^1(X, d\mu)$ and $r \in L^1(Y, d\nu)$ with

$$q(x) = \inf_{y \in Y} c(x, y) - r(y)$$

such that

$$\inf_{\gamma \in \Gamma(\mu, \nu)} \int_{X \times Y} c(x, y) d\gamma(x, y) = \int_X q(x) d\mu(x) + \int_Y r(y) d\nu(y).$$

From (6) we see

$$c(x, y) - q(x) - r(y) \geq 0,$$
while (7) implies any minimizer $\gamma \in \Gamma(\mu, \nu)$ vanishes outside the zero set $Z \subset X \times Y$ of the non-negative function appearing in (8). It remains to show this set $Z$ is contained in a numbered limb system consisting of at most two limbs (apart from a $\mu \otimes \nu$ negligible set).

From (6), $q$ is locally Lipschitz, since $d_x c(x, y)$ is controlled locally in $x$, independently of $y \in Y$. Rademacher’s theorem therefore combines with absolute continuity of $\mu$ to imply $q$ is differentiable $\mu$-almost everywhere; we can safely ignore any points in $X$ where differentiability of $q$ fails, since they constitute a set of zero volume: $\gamma[\text{Dom } Dq \times Y] = \mu[\text{Dom } Dq] = 1$. Taking $x_0 \in \text{Dom } Dq$, suppose $(x_0, y_1)$ and $(x_0, y_2)$ both lie in $Z$, hence saturate the inequality (5). Then $d_x c(x_0, y_1) = Dq(x_0) = d_x c(x_0, y_2)$. In case the cost is twisted, meaning (5) has no critical points, we conclude $y_1 = y_2$ hence $Z \cap (\text{Dom } Dq \times Y)$ is contained in a graph. This completes the proofs by Gangbo, Carlier, and Ma-Trudinger-Wang, of existence (and uniqueness) of a solution $y_1 = f_1(x_0)$ to Monge’s problem, pairing almost every $x_0 \in X$ with a single $y_1 \in Y$. Notice uniqueness follows from Lemma 2.1 without further measurability assumptions.

In the present setting, however, we only know that $x_0$ must be a global minimum or global maximum of the function (5). Exchanging $y_1$ with $y_2$ if necessary yields

$$q(x) \leq c(x, y_1) - r(y_1) \leq c(x, y_2) - r(y_2)$$  \hspace{1cm} \text{(9)}$$

for all $x \in X$, the second inequality being strict unless $x = x_0$, in which case both inequalities are saturated. Strictness of inequality (5) implies $(x, y_2) \not\in Z$ unless $x = x_0$. In other words, $(x, y_2) \in Z$ lies on the antigraph of a function $f_2(y_2) = x_0$ well-defined at $y_2$. There may or may not be a point $y_0 \in Y$ different from $y_1$ such that

$$q(x) \leq c(x, y_0) - r(y_0) \leq c(x, y_1) - r(y_1)$$

for all $x \in X$. If such a point $y_0$ exists, then $(x_0, y_1) \in \text{Antigraph}(f_2)$ as above. If no such $y_0$ exists, setting $f_1(x_0) := y_1$ yields $Z \cap (\text{Dom } Dq \times Y) \subset \text{Graph}(f_1) \cup \text{Antigraph}(f_2)$. Since the range of $f_1$ is disjoint from the domain of $f_2$, this completes the proof that — up to $\gamma$-negligible sets — $Z$ lies in a numbered limb system with at most two limbs, as desired. $lacksquare$

Let us conclude by recalling an example of an extremal doubly stochastic measure which does not lie on the graph of a single map, drawn from
work of Gangbo and McCann [14] and Ahmad [1] on optimal transportation, and developed in an economic context by Chiappori, McCann, and Nesheim [8]. Other examples may be found in the work of Seethoff and Shiflett [28], Losert [22], Hestir and Williams [15], Gangbo and McCann [13], Uckelmann [29], McCann [24], and Plakhov [26].

Imagine the periodic interval $X = Y = \mathbb{R}/2\pi \mathbb{Z} = [0, 2\pi]$ to parameterize a town built on the boundary of a circular lake, and let probability measures $\mu$ and $\nu$ represent the distribution of students and available places in schools, respectively. Suppose the distribution of students is smooth and non-vanishing but peaks sharply at the northern end of the lake, and the distribution of schools is smooth and non-vanishing but peaks sharply at the southern end of the lake. If the cost of transporting a student residing at location $\theta \in [0, 2\pi]$ to school at location $\phi \in [0, 2\pi]$ is presumed to be given in terms of the angle commuted by $c(\theta, \phi) = 1 - \cos(\theta - \phi)$, the most effective pairing of students with places in schools is given by the measure in $\Gamma(\mu, \nu)$ which attains the minimum:

$$\min_{\gamma \in \Gamma(\mu, \nu)} \int_{X \times Y} c(\theta, \phi) \, d\gamma(\theta, \phi).$$

According to results of Gangbo and McCann [14], this minimizer is unique, and its support is contained in the union of the graphs of two maps $t^\pm : X \to Y$. A schematic illustration is given in Figure 4, where the restriction of the support to the subsets marked by $\pm$ on the flat torus $X \times Y$ represent $\text{graph}(t^+)$ and $\text{graph}(t^-)$ respectively. The dotted lines mark $\phi - \theta = \pm \frac{\pi}{2}, \pm \frac{3\pi}{2}$. The necessary positivity of $\gamma|_{J_X \times J_{Y1}} > 0$ in this picture may be explained by observing that although it is cost-effective for all students to attend a school where they live, this is incompatible with the concentration of students at the north end of the lake, and of schools at the south end. Once this imbalance is corrected by sending a sufficient number of northern students to southern schools by the map $t^-$, the remaining students can be assigned to school near their home using the map $t^+$. Periodicity of graphs on the flat torus can be used to represent the support as a numbered limb system in more than one way; see Figure 5 which exploits the fact that the support of $\gamma$ in Figure 4 intersects $X \times J_{Y2}$ in a graph and $X \times (Y - J_{Y1})$ in an anti-graph.

Chiappori, Nesheim and McCann [8] called the uniqueness hypothesis limiting the number of critical points to at most one maximum and and at most one minimum in (5) the subtwist condition. Although it is satisfied
in the example above, it is an unfortunate fact that the subtwist condition cannot be satisfied by any smooth function $c(\theta, \phi)$ on a product of manifolds $X \times Y$ with more complicated Morse structures than the sphere. It is an interesting open problem to find a criterion on a smooth cost $c(\theta, \phi)$ on $X = Y = \mathbb{R}^2/\mathbb{Z}^2$ which guarantees uniqueness of the minimum (10) for all smooth densities $\mu$ and $\nu$ on the torus. Although we expect such costs to be generic, not a single example of such a cost is known to us. Hestir and Williams criteria for extremality seems likely to remain relevant to such questions, and it is natural to conjecture that the complexity of the Morse structure of the manifold $X$ plays a role in determining the required number of limbs in the system.

![Schematic support of the optimal measure from the example](image)

Figure 4: Schematic support of the optimal measure from the example
Figure 5: Two different numbered limb systems which represent Figure 4.

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