Multi-Marginal Optimal Transportation and Many-Electron Systems

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Abstract

In my Bachelor's thesis, I consider two special cases of the multi-marginal optimal transportation problem. In the first one, a special discrete marginal measure is considered. The Birkhoff- von Neumann theorem assures that in the classical two-marginal case, there exist optimizers of the so-called Monge-form. I give simple examples that show that for more than two marginals, optimizers are not always of this form, following [3]. The second special case treats cost-functions of a special form. As was shown in [1], the problem can then by reduced to a two-marginal problem with an additional constraint, called n-density representability. I give an explicit characterization of the discrete n-density representable measures.

Problem Formulation

The multi-marginal optimal transportation problem considered here has the following form. Given

- A marginal number $n \geq 2$
- A marginal measure $\mu \in P(\mathbb{R}^d)$
- A cost-function $c : (\mathbb{R}^d)^n \to [0, \infty]$

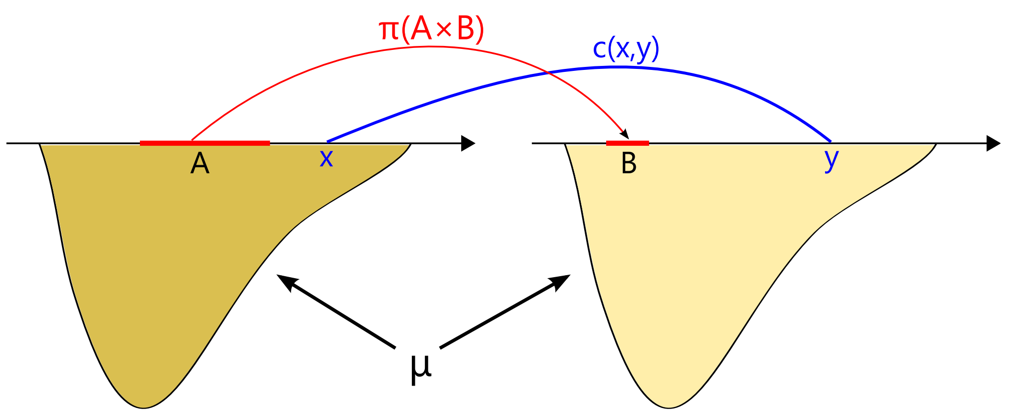
solve the minimization problem

$$\inf_{\substack{\pi \in P((\mathbb{R}^d)^n) \\ \pi \mapsto \mu}} \int_{(\mathbb{R}^d)^n} c(x_1, \ldots, x_n) d\pi$$

The so-called marginal condition $\pi \mapsto \mu$ means that each projection of π onto one of the n components is equal to the marginal measure μ. Formally, this means

$$\pi((\mathbb{R}^d)^{m-1} \times A \times (\mathbb{R}^d)^{n-m}) = \mu(A) \ \forall A \subset \mathbb{R}^d \text{ measurable } \forall m = 1, \ldots, n$$

In the classical two-marginal (i.e. $n = 2$) case, this can be interpreted as the problem of finding the cheapest way to transport mass from one hole, whose form is modelled by the measure μ, to another hole with the same form. $c(x, y)$ indicates the cost of transporting mass sitting at x to some point y.



A Discrete Case

Consider the special case

$$\mu = \frac{1}{l} \sum_{i=1}^{l} \delta_i$$

i.e. μ is contentrated on l points giving the same mass to each of them.

Definition (Monge-form). *A measures $\pi \in P(\{1, \ldots, l\}^n)$ is said to have Monge-form, if it is concentrated on the graph of a function $T : \{1, \ldots, l\} \to \{1, \ldots, l\}^{n-1}$, i.e.*

$$\pi(\text{graph}\, T) = 1$$

Question. *For which values of n and l is it true that for every cost-function c, there exists a Monge-form optimizer $\pi^* \in P(\{1, \ldots, l\}^n)$?*

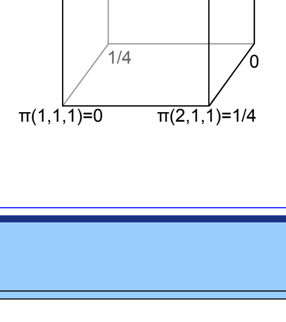
Motivation: A measure of Monge-form is uniquely determined by $T \Rightarrow$ reduction from the l^n unknowns $\pi(\{i_1, \ldots, i_n\})$ to the l unknowns $T(i)$.
Writing P_l^n for the set of measures $\pi \in P(\{1, \ldots, l\}^n)$ with $\pi \mapsto \mu$, we get a geometric reformulation of our question:

Question. *For which values of n and l does every extreme point of P_l^n have the Monge-form?*

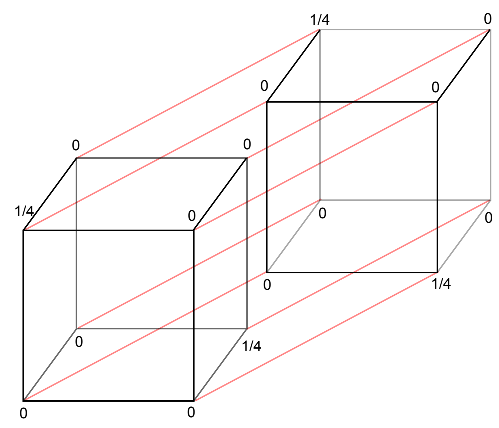
It is well-known [3], that unfortunately this only is the case if $n = 2$

Theorem. *For arbitrary $n > 2$ and $l > 1$, there exists an extreme point of P_l^n which does not have the Monge-form.*

In my thesis, I give a simple construction for such non-Monge extreme points for arbitrary $n > 2$ and $l > 1$. The most minimalistic example is in P_2^3:



Observation: The front side of the cube is a normalized 2×2 identity matrix, the back side is a permutation of it.
To construct examples for $n > 3$, find a suitable higher-dimensional analogue for identity matrices. This yields for example the non-Monge extreme point



in P_2^4.
Non-Monge points for $l > 2$ can be constructed by "glueing" such $l = 2$ points.

n-Density Representability

Consider another special case: Marginal number n and marginal measure μ are arbitrary, but c has a special form:

$$c(x_1, \ldots, x_n) = \sum_{1 \leq i < j \leq n} h(x_i, x_j)$$

with a symmetric function h. Such a cost-function appears for example in relation to the Kohn- Sham density functional theory [2]. As was shown in [1], symmetry porperties of c can be used to massively reduce the dimension of the transport problem:

Definition (n-density representability). *A measure $\nu \in P((\mathbb{R}^d)^2)$ is called n-density representable (n-d. r.), if there exists a symmetric measure $\pi \in P((\mathbb{R}^d)^n)$ such that μ is the projection of π onto the first two coordinates:*

$$\nu(V) = \pi(V \times (\mathbb{R}^d)^{n-2})$$

Theorem. *The n-marginal problem can be reduced to a two-marginal problem with an additional constraint:*

$$\inf_{\pi \mapsto \mu} \int_{X^n} c(x_1, \ldots, x_n) d\pi = \binom{n}{2} \inf_{\substack{\nu \mapsto \mu \\ \nu \text{ n-d. r.}}} \int_{X^2} d(x_1, x_2) d\nu$$

The problem that arises with the reformulated two-marginal problem is that there does not exist a convenient characterization of the set of n-density representable measures up to now. In my thesis, I give a characterization of the discrete n-density representable measures, i.e. of the set

$$P_{n-d.r.}(\{1, \ldots, l\}^2) := \{\nu \in P_{n-d.r.}(\{1, \ldots, l\}^2) : \nu \text{ n-d.r.}\}$$

This is a generalization of [1], where the special case $l = 2$ is considered.

Theorem. *The set $P_{n-d.r.}(\{1, \ldots, l\}^2)$ is equal to*

$$\text{conv}\left\{ \left(1 + \frac{1}{n-1}\right) \left(\sum_{k=1}^{l} \lambda_k \delta_k\right) \otimes \left(\sum_{k=1}^{l} \lambda_k \delta_k\right) - \frac{1}{n-1} (id \times id) \# \left(\sum_{k=1}^{l} \lambda_k \delta_k\right) : \sum \lambda_i = 1 \text{ and } \lambda_i \in \{0, 1/n, \ldots, (n-1)/n, 1\} \right\}$$

References

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2. Codina Cotar, Gero Friesecke and Claudia Klüppelberg. Density functional theory and optimal transportation with Coulomb cost. Communications on Pure and Applied Mathematics, 66(4) : 548 – 599, 2013.
3. Nathan Linial and Zur Luria. On the vertices of the d-dimensional Birkhoff polytope. Discrete & Computational Geometry, 51(1) : 161 – 170, 2014