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ON c -CYCLICAL MONOTONICITY FOR OPTIMAL TRANSPORT PROBLEM WITH COULOMB COST

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ABSTRACT. It is proved that c -cyclical monotonicity is a sufficient condition for optimality in the multi-marginal optimal transport problem with Coulomb repulsive cost. The notion of c -splitting set and some mild regularity property are the tools. The result may be extended to Coulomb like costs.

1. INTRODUCTION AND STATEMENT OF THE MAIN RESULT

The following variational problem is the multi-marginal version of the relaxation, proposed by Kantorovich, for the Monge optimal transport problem. Let X_1, \dots, X_N be Polish spaces and let ρ_1, \dots, ρ_N be probability measures on the corresponding spaces, i.e. $\rho_i \in \mathcal{P}(X_i)$. Denote by $\Pi(\rho_1, \dots, \rho_N) = \{P \in \mathcal{P}(X_1 \times \dots \times X_N) : \pi_{\#}^i P = \rho_i, \forall i\}$ where π^i denotes the projection on the i -th factor of the Cartesian product and $f_{\#}\mu$ denotes the push-forward of the measure μ via the map f . Let $c : X_1 \times \dots \times X_N \rightarrow \mathbb{R} \cup \{-\infty, +\infty\}$. The variational problem of interest is

$$\min_{P \in \Pi(\rho_1, \dots, \rho_N)} \int c(x_1, \dots, x_N) dP. \quad (1.1)$$

The elements of $\Pi(\rho_1, \dots, \rho_N)$ are called **transport plans**. Existence of minimizers follows by the Direct Method of the Calculus of Variations under the assumptions that c is lower semi-continuous and bounded from below. Compactness is given by Prokhorov's theorem (and the assumption that X_i Polish space is related to this).

The two marginal case (i.e. $N = 2$) is the most studied. The name *multi-marginal* refers to the case $N > 2$. In the multi-marginal case, most of the structure of the two marginal case is lost since that structure is related to the connection between convexity and invertibility of the gradient.

The literature on the two marginal case is extensive and we refer the interested reader to [33, 39, 40], less is known on the multi-marginal case, which however has

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several applications. Some general results are available in [6, 25, 30, 29, 32], results for special costs are available, for example in [18] for the quadratic cost with some generalization in [23], and in [8] for the determinant. More applications are emerging in [19]. Applications to economics of the multi-marginal optimal transportation problems include, for example, the problem of team-matching which is a generalization of the classical marriage problem [7, 9]. Applications to physics are related to quantum chemistry and the strong interacting regime for particles which are described in [35, 37, 36]. By now there are several papers on the transport theory for the Coulomb cost and some more general repulsive cost, a selection is given by [5, 11, 10, 14, 17, 16].

Inspired by the saying “*Less is more*”¹, in this paper we will focus on the Coulomb cost, however this cost can be used as a model cost for more general situations.

We consider the case $X_i = \mathbb{R}^d$ for all i and $\rho_1 = \dots = \rho_N = \rho$, c will be the Coulomb repulsive cost

$$c(x_1, \dots, x_n) = \sum_{1 \leq i < j \leq n} \frac{1}{|x_i - x_j|}.$$

Then, we will study some properties of the minimizers of

$$\min_{P \in \Pi(\rho)} \int \sum_{1 \leq i < j \leq n} \frac{1}{|x_i - x_j|} dP(x_1, \dots, x_n), \quad (1.2)$$

which will be called **optimal transport plans**. The property that we will study here is the c -cyclical monotonicity.

Definition 1.1. A set $\Gamma \subset \mathbb{R}^{Nd}$ is c -cyclically monotone if for all $n \in \mathbb{N}$ and points $(x_1^1, \dots, x_N^1), \dots, (x_1^n, \dots, x_N^n) \in \Gamma$ and all permutation $\sigma_2, \dots, \sigma_N \in \mathcal{S}_n$

$$\sum_{i=1}^n c(x_1^i, \dots, x_N^i) \leq \sum_{i=1}^n c(x_1^i, x_2^{\sigma_2(i)}, \dots, x_N^{\sigma_N(i)}).$$

A transport plan $P \in \Pi(\rho)$ is c -cyclically monotone if it is concentrated on a c -cyclically monotone set.

Remark 1.2. Notice that if c is continuous (even with values in $[0, +\infty]$ as in this paper) then a transport plan P is c -cyclically monotone if and only if the support $\text{spt}P$ is c -cyclically monotone.

Under little assumptions the c -cyclical monotonicity is a necessary condition for optimality in problem (1.1) above. Sufficiency happens most of the time and here we will prove that this is also the case of Coulomb type multi-marginal repulsive costs. But let us take this occasion to recall some known results.

¹“*Well, less is more, Lucrezia: I am judged.*”, from *Andrea Del Sarto* by *Robert Browning*

For the two marginal case the necessity of the condition may be proved under the assumptions that the negative part of c is integrable with respect to any transport plan, c is lower semi-continuous, real valued and of finite cost (see [40]) or under the assumption that c is lower semi-continuous with values in $[0, +\infty]$ (see [33]).

In [31] a lower semi-continuous cost c with values in $[0, +\infty]$ is considered and it is proved that c -cyclical monotonicity is sufficient if ρ_1 and ρ_2 are purely atomic or if c is continuous (possibly with value $+\infty$). The result above is complemented by the results of [34] where it is proved that c lower semi-continuous is enough if c takes only finite values in $[0, +\infty)$. Finally, in Th. 2.4 of [3], the authors give a measure theoretic criterion to assess the optimality of a c -cyclically monotone transport plan followed by Cor. 2.5 which contains a practical way to check the condition of the Theorem.

In the multi-marginal case sufficiency of c -cyclical monotonicity is proved in [22] under the assumptions that c is continuous, bounded from below and with finite values (or $c \in [0, +\infty)$) and such that there exist functions $f_i \in L^1_{\rho_i}$ for which

$$c(x_1, \dots, x_N) \leq f_1(x_1) + \dots + f_N(x_N).$$

The last assumption can not be satisfied by Coulomb-like costs.

For transport costs which tend to $+\infty$ when $|x_i - x_j| \rightarrow 0$ the concentration of the datum ρ plays an important role in the finiteness and the continuity of the cost and in properties of optimal transport plans [2, 4, 12, 38]. For $\rho \in \mathcal{P}(\mathbb{R}^d)$ we introduce a measure of the concentration of ρ at the scale r

$$\mu_\rho(r) = \sup_{x \in \mathbb{R}^d} \rho(B(x, r)).$$

The main theorem in this paper is the following

Theorem 1.3. *Let ρ be such that $\lim_{r \rightarrow 0} \mu_\rho(r) < 1/N$. Let $P \in \Pi(\rho)$ be a plan with finite cost and c -cyclically monotone. Then P is an optimal transport plan.*

Remark 1.4. The condition $\lim_{r \rightarrow 0} \mu_\rho(r) < 1/N$ is equivalent to saying that ρ has atoms of weight strictly smaller than $1/N$. However the condition expressed by the limit is more practical for some proof and may be useful to work in more general settings.

2. c-SPLITTING SETS AND N-UPLES AND ESTIMATES

The notion of c -splitting set appeared first in [26] in an accurate analysis of the problem of existence of optimal transport maps. Then in [22] it has been used in relation to c -cyclical monotonicity for multi-marginal optimal transport problems. One advantage of this notion which is illustrated in Lemma 2.5 in [22], is that useful notions of topology and set theory allow the passage from an easier situation (finite sets) to a more complicate one (infinite sets).

Definition 2.1. A set $\Gamma \subset \mathbb{R}^{Nd}$ is c -splitting if there exists a N -tuple (u_1, \dots, u_N) with $u_i : \mathbb{R}^d \rightarrow [-\infty, +\infty)$ such that $u_1(x_1) + \dots + u_N(x_N) \leq c(x_1, \dots, x_N)$ everywhere in \mathbb{R}^{Nd} with equality on Γ . The functions (u_1, \dots, u_N) will be called a c -splitting N -tuple for Γ and will be denoted by $(u_i)_i$.

As proved in [22] the splitting N -tuple can be taken measurable. This is also one of the consequences of the next lemma.

Lemma 2.2. *Let $(u_i)_i$ be a c -splitting N -tuple for Γ ; then there exists a c -splitting N -tuple $(\tilde{u}_i)_i$ which satisfies*

$$u_i \leq \tilde{u}_i,$$

and

$$\tilde{u}_i(x) = \inf \left\{ c(y_1, \dots, x, y_{i+1}, \dots, y_N) - \sum_{j \neq i} \tilde{u}_j(y_j) : y_j \in \mathbb{R}^d \right\} \quad \forall x \in \mathbb{R}^d. \quad (2.1)$$

In particular \tilde{u}_i is measurable for every i .

Proof. We first define

$$\bar{u}_1(x) := \inf \left\{ c(x, y_2, \dots, y_N) - \sum_{j \geq 2} u_j(y_j) : y_j \in \mathbb{R}^d \right\};$$

and

$$\bar{u}_i(x) := \inf \left\{ c(x, y_2, \dots, y_N) - \sum_{j < i} \bar{u}_j(y_j) - \sum_{i < j} u_j(y_j) : y_j \in \mathbb{R}^d \right\}.$$

From $u_1(x_1) + \dots + u_N(x_N) \leq c(x_1, \dots, x_N)$ we obtain that $u_1(x) \leq \bar{u}_1(x)$, from the definition of \bar{u}_1 it follows that $\bar{u}_1(x_1) + \dots + u_N(x_N) \leq c(x_1, \dots, x_N)$ which, in turns implies $u_2(x) \leq \bar{u}_2(x)$ and so we have $u_i(x) \leq \bar{u}_i(x)$.

We then consider

$$\mathcal{A}(u) = \left\{ (v_i)_i : u_i \leq v_i \text{ and } v_1(x_1) + \dots + v_N(x_N) \leq c(x_1, \dots, x_N) \right\}$$

with the partial ordering $(v_i^A)_i \leq (v_i^B)_i$ if $v_i^A(x) \leq v_i^B(x)$ for all i and x . With this partial ordering, every chain (totally ordered subset) of \mathcal{A} admits an upper bound, given by the pointwise sup. As in the proof of Theorem 1.4 in [28], we conclude from Zorn's Lemma that \mathcal{A} contains at least one maximal element $(\tilde{u}_i)_i$, which satisfies all the required properties. In fact, by the maximality and the construction above, we have

$$\tilde{u}_i \leq \overline{\tilde{u}_i} \leq \tilde{u}_i.$$

Moreover, since $(\tilde{u}_i)_i \in \mathcal{A}(u)$, it satisfies

$$\tilde{u}_1(x_1) + \dots + \tilde{u}_N(x_N) \leq c(x_1, \dots, x_N), \text{ in } \mathbb{R}^{Nd},$$

and on Γ the equality holds since the two extremes of

$$u_1(x_1) + \cdots + u_N(x_N) \leq \tilde{u}_1(x_1) + \cdots + \tilde{u}_N(x_N) \leq c(x_1, \dots, x_N)$$

coincide. \square

Remark 2.3. Taking some constant $\alpha_1, \dots, \alpha_N$ such that $\sum \alpha_i = 0$ we may then redefine $u_i(x) = \tilde{u}_i(x) + \alpha_i$ and we still obtain a c -splitting N -tuple which satisfies

$$u_i(x) = \inf \left\{ c(y_1, \dots, y_{i-1}, x, y_{i-1}, \dots, y_N) - \sum_{j \neq i} u_j(y_j) : y_j \in \mathbb{R}^d \right\}.$$

The choice of the constants α_i can be made so that the functions u_i take specific and admissible values at some points.

For $\alpha \geq 0$ we consider

$$D_\alpha = \{(x_1, \dots, x_N) : |x_i - x_j| \leq \alpha \text{ for some } i \neq j\}.$$

and we introduce the notation

$$C(P) := \int c(x_1, \dots, x_N) dP.$$

The following proposition is a variation of Prop. 3.8 in [15] and Th. 2.4 in [4] according to the quantitative improvement given in [12] which also appears in [38].

Proposition 2.4. *Let ρ be such that $\lim_{r \rightarrow 0} \mu_\rho(r) < 1/N$. Let $P \in \Pi(\rho)$ be a plan with finite cost and c -cyclically monotone. Let r be such that $\mu_\rho(r) < 1/N$ and let α and β be such that $\beta/2 < r$,*

$$\frac{1}{\alpha} > \frac{4(N-1)}{\beta}, \quad \frac{1}{\beta} > \frac{C(P)}{1 - N\mu_\rho(r)}. \quad (2.2)$$

Then

$$spt(P) \cap D_\alpha = \emptyset$$

so that $P(D_\alpha) = 0$.

Proof. First, by the permutation invariance of the Coulomb cost, we may assume that P is symmetric (permutation invariant), otherwise we may replace P by

$$\tilde{P} := \frac{1}{N!} \sum_{\sigma \in \mathcal{S}_N} \sigma_\# P,$$

which has same cost, the same marginals and it is still c -cyclically monotone. Since the diagonal strips are symmetric $P(D_\alpha) = \tilde{P}(D_\alpha)$.

Assume, by contradiction, that $\mathbf{x} = (x_1, \dots, x_N) \in D_\alpha \cap spt P$ and, without loss of generality, that $|x_1 - x_2| \leq \alpha$. We will later show that there exists

$$\mathbf{y} \in (spt P \setminus D_\beta) \cap \left((B(x_1, \frac{\beta}{2}))^c \right)^N.$$

For such \mathbf{y} at least one of the coordinates y_i does not belongs to $\bigcup_{j=2}^N B(x_j, \frac{\beta}{2})$ otherwise, since there are $N - 1$ balls of diameter β and N coordinates y_i , two of the coordinates would belong to the same ball and then, since the balls have radius $\beta/2$, $\mathbf{y} \in D_\beta$ which we excluded ². By symmetry of P we may assume that the *good* coordinate is y_1 . The existence of \mathbf{y} with the properties above violates the c -cyclical monotonicity property, in fact

$$\begin{aligned} c(x_1, \dots, x_N) + c(y_1, \dots, y_N) &= \sum_{j=2}^N \frac{1}{|x_1 - x_j|} + \sum_{2 \leq i < j \leq N} \frac{1}{|x_i - x_j|} + \sum_{j=2}^N \frac{1}{|y_1 - y_j|} + \\ &\quad + \sum_{2 \leq i < j \leq N} \frac{1}{|y_i - y_j|} \\ &\geq \frac{1}{\alpha} + \sum_{2 \leq i < j \leq N} \frac{1}{|x_i - x_j|} + \sum_{2 \leq i < j \leq N} \frac{1}{|y_i - y_j|}, \end{aligned}$$

on the other hand

$$\begin{aligned} c(y_1, \dots, x_N) + c(x_1, \dots, y_N) &= \sum_{j=2}^N \frac{1}{|y_1 - x_j|} + \sum_{2 \leq i < j \leq N} \frac{1}{|x_i - x_j|} + \sum_{j=2}^N \frac{1}{|x_1 - y_j|} + \\ &\quad + \sum_{2 \leq i < j \leq N} \frac{1}{|y_i - y_j|} \\ &\leq 2\left(\frac{2(N-1)}{\beta}\right) + \sum_{2 \leq i < j \leq N} \frac{1}{|x_i - x_j|} + \sum_{2 \leq i < j \leq N} \frac{1}{|y_i - y_j|}, \end{aligned}$$

and this, by (2.2) above, contradict the c -cyclical monotonicity.

²this is an important part of the idea which allowed [12] to obtain optimal constants.

To prove the existence of \mathbf{y} we estimate the measure of the complementary set

$$\begin{aligned}
 & P(D_\beta \cup \bigcup_{i=1}^N \mathbb{R}^d \times \cdots \times \overbrace{B(x_1, \frac{\beta}{2})}^i \times \cdots \times \mathbb{R}^d) \\
 & \leq P(D_\beta) + \sum_{i=1}^N P(\mathbb{R}^d \times \cdots \times \overbrace{B(x_1, \frac{\beta}{2})}^i \times \cdots \times \mathbb{R}^d) \\
 & \leq \beta C(P) + N\rho(B(x_1, \frac{\beta}{2})) \\
 & < 1 - N\mu_\rho(r) + N\rho(B(x_1, \frac{\beta}{2})) \\
 & = 1 - N(\mu_\rho(r) - \rho(B(x_1, \frac{\beta}{2}))) \leq 1
 \end{aligned}$$

where the third inequality follows from (2.2) and, since P is a probability measure, the set where we need to find \mathbf{y} is non empty (is even of positive P measure). \square

Remark 2.5. Proposition 2.4 above holds for more general costs at the price of some technical complication in the proof. We refer the reader to [4, 12] for details.

Next we connect c -cyclical monotonicity with c -splitting. The basic idea is to use some topological ideas from Lemma 2.5 of [22] together with the ideas of Proposition 2.4 which allow to control the unboundedness of the cost.

Proposition 2.6. *Let ρ be such that $\lim_{r \rightarrow 0} \mu_\rho(r) < 1/N$. Let $P \in \Pi(\rho)$ be a plan with finite cost and c -cyclically monotone. Then $\Gamma = \text{spt}P$ is a c -splitting set and there exists a c -splitting N -tuple (u_1, \dots, u_N) for Γ and two positive constants r and k such that for ρ -a.e. x*

$$|u_i|(x) \leq \frac{2N(N-1)^2}{r} - (N-1)^2k := \mathbf{k}.$$

Proof. By Proposition 2.4 $\Gamma \subset \mathbb{R}^{Nd} \setminus D_\alpha$ and it is c -cyclically monotone. We begin by choosing $r < \frac{\alpha}{2}$ and we consider a point $(\bar{x}_1, \dots, \bar{x}_N) \in \text{spt}P$ (then, in particular, the point does not belongs to D_α). Then we take a, possibly smaller, r so that

$$\rho(B(\bar{x}_1, r)) + \cdots + \rho(B(\bar{x}_N, r)) < \varepsilon \ll \frac{1}{4}. \quad (2.3)$$

It follows that the set

$$\{(y_1, \dots, y_N) \in \text{spt}P \mid y_i \notin B(\bar{x}_j, r) \text{ for } i, j = 1, \dots, N\}$$

has positive P measure and we may take $(\bar{y}_1, \dots, \bar{y}_N)$ in this last set. Let $G \subset \Gamma$ be a c -splitting set with $(\bar{x}_1, \dots, \bar{x}_N), (\bar{y}_1, \dots, \bar{y}_N) \in G$. Since by Linear Programming finite sets are always c -splitting it is always possible to find many sets G with this property.

By Lemma 2.2 and Remark 2.3 we may choose a c -splitting N -tuple for G that satisfies

$$(1) \quad u_i(\bar{x}_i) = \frac{c(\bar{x}_1, \dots, \bar{x}_N)}{N} := k \text{ for all } i,$$

$$(2) \quad u_i(x) = \inf \{c(y_1, \dots, x, y_{i+1}, \dots, y_N) - \sum_{k \neq i} u_k(y_k)\}, \text{ for all } i \text{ and } x.$$

Since, at least, $r < \frac{\alpha}{2}$ we have the following estimate. If $x \notin \cup_{i=2}^N B(\bar{x}_i, r)$ then

$$\begin{aligned} u_1(x) &\leq c(x, \bar{x}_2, \dots, \bar{x}_N) - u_2(\bar{x}_2) - \dots - u_N(\bar{x}_N) \leq \\ &\leq c(x, \bar{x}_2, \dots, \bar{x}_N) - u_2(\bar{x}_2) - \dots - u_N(\bar{x}_N) \leq \\ &\leq \frac{N(N-1)}{r} - (N-1)k. \end{aligned} \quad (2.4)$$

And since, by construction, \bar{y}_1 does not belong to the balls centered at \bar{x}_i the estimate (2.4) above holds for $u_1(\bar{y}_1)$ and then

$$\begin{aligned} u_2(\bar{y}_2) + \dots + u_N(\bar{y}_N) &= c(\bar{y}_1, \dots, \bar{y}_N) - u_1(\bar{y}_1) \geq \\ &\geq -\left(\frac{N(N-1)}{r} - (N-1)k\right). \end{aligned}$$

Finally, up to a division by 2 of r we have that for all $x \in \cup_{i=2}^N B(\bar{x}_i, r)$

$$\begin{aligned} u_1(x) &\leq c(x, \bar{y}_2, \dots, \bar{y}_N) - u_2(\bar{y}_2) - \dots - u_N(\bar{y}_N) \leq \\ &\leq \frac{N(N-1)}{r} + \frac{N(N-1)}{r} - (N-1)k. \end{aligned} \quad (2.5)$$

This completes the estimate from above of u_1 . The same computation holds for the other u_i . The estimate from above of the u_i given by (2.4) and (2.5) translates in an estimates from below which holds ρ -a.e.. Indeed for ρ -a.e. x there holds

$$u_1(x) = \inf \{c(x, x_2, \dots, x_n) - u_2(x_2) - \dots - u_N(x_N)\} \geq (N-1)^2 k - \frac{2N(N-1)^2}{r}.$$

So that for every G there is a c -splitting N -tuple which is bounded by \mathbf{k} . Now, following an idea of [22], let us consider for every $G \subset \Gamma$ the set of splitting N -tuples bounded by \mathbf{k}

$$S_G = \{(u_1, \dots, u_N) : (u_i) \text{ is } c\text{-splitting for } G \text{ and } |u_i| \leq \mathbf{k}, \forall i\},$$

and

$$\mathcal{G} = \{S_G : G \subset \Gamma, \text{ finite and } (\bar{x}_1, \dots, \bar{x}_N), (\bar{y}_1, \dots, \bar{y}_N) \in G\}.$$

Each of the sets S_G is a closed subset (with respect to the pointwise convergence) of the compact set $(\mathbb{R}^d)^{[-\mathbf{k}, \mathbf{k}]} \times \dots \times (\mathbb{R}^d)^{[-\mathbf{k}, \mathbf{k}]}$ and the family \mathcal{G} satisfies the finite

intersection property since if G_1 and G_2 are admissible (i.e. finite and contain the two points above) then

$$S_{G_1 \cup G_2} \subset S_{G_1} \cap S_{G_2}.$$

It follows that

$$\bigcap_{G \text{ admissible}} S_G$$

is non empty and any element of such intersection is a c -splitting N -tuple for Γ . \square

Remark 2.7. The idea of using finite sets G in the proof above could be seen as the analogue of the discretization considered in [15] to prove the existence of solutions for the dual problem.

3. PROOF OF TH. 1.3 AND ONE APPLICATION

Proof. (of Th. 1.3) To conclude we just need to use the duality for the Kantorovich problem in an indirect way.

Let $P \in \Pi(\rho)$ be a plan with finite cost and c -cyclically monotone, and let $Q \in \Pi(\rho)$ be any transport plan. Let Γ be the c -splitting set on which P is concentrated and let (u_1, \dots, u_N) be the c -splitting N -uple for Γ given by Prop. 2.6, since each of the u_i is bounded we may write

$$\begin{aligned} \int cdP &= \int u_1(x_1) + \dots + u_N(x_N) dP \\ &= \int u_1(x_1) d\rho + \dots + \int u_N(x_N) d\rho \\ &\leq \int cdQ. \end{aligned}$$

where the second equality is allowed by the fact that the u_i s are bounded. \square

In Prop. 2.9 of [13] it is proved that for some special, radially symmetric ρ in the plane the transport plan associated to a radially symmetric map proposed in [36] is c -cyclically monotone. As a consequence of Th. 1.3 above this implies the optimality of the map which was conjectured in [36].

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