

CYCLICALLY MONOTONE NON-OPTIMAL N -MARGINAL TRANSPORT PLANS AND SMIRNOV-TYPE DECOMPOSITIONS FOR N -FLOWS*

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Abstract. In the setting of optimal transport with $N \geq 2$ marginals, a necessary condition for transport plans to be optimal is that they are c -cyclically monotone. For $N = 2$ there exist several proofs that in very general settings c -cyclical monotonicity is also sufficient for optimality, while for $N \geq 3$ this is only known under strong conditions on c . Here we give a counterexample which shows that c -cyclical monotonicity is in general not sufficient for optimality if $N \geq 3$. Comparison with the $N = 2$ case shows how the main proof strategies valid for the case $N = 2$ might fail for $N \geq 3$. We leave open the question of what is the optimal condition on c under which c -cyclical monotonicity is sufficient for optimality. The new concept of an N -flow seems to be helpful for understanding the counterexample: our construction is based on the absence of finite-support closed N -flows in the set where our counterexample cost c is finite. To follow this idea we formulate a Smirnov-type decomposition for N -flows.

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1. INTRODUCTION, BASIC DEFINITIONS AND SETTING

Let $c : \vec{X} := X_1 \times X_2 \times \dots \times X_N \rightarrow Y$ be a cost, where $N \geq 2$, X_1, \dots, X_N are Polish spaces, and $Y = (Y, +, \geq)$ is an ordered semigroup (usually we take $Y = \mathbb{R}$ or $Y = (-\infty, +\infty]$). If μ_1, \dots, μ_N are probability measures with $\mu_j \in \mathcal{P}(X_k)$ and π_j is the canonical projection of \vec{X} onto X_k , then the possible ways to couple the N measures $\mu_k, 1 \leq k \leq N$ are encoded by the space of so-called *transport plans* defined as

$$\Pi(\mu_1, \dots, \mu_N) := \left\{ \gamma \in \mathcal{P}(\vec{X}) : (\pi_k)_\# \gamma = \mu_k \text{ for } 1 \leq k \leq N \right\}.$$

The N -marginal optimal transport problem with cost c as above with marginals $\mu_k, 1 \leq k \leq N$, is the following minimization problem:

$$\min \{ \langle c, \gamma \rangle : \gamma \in \Pi(\mu_1, \dots, \mu_N) \}, \quad \text{where } \langle c, \gamma \rangle := \int_{\vec{X}} c(\vec{x}) d\gamma(\vec{x}). \quad (1.1)$$

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Existence of minimizers can be ensured *e.g.* by assuming that c is lower semicontinuous and bounded below, by the direct method of the calculus of variations and via Prokhorov's theorem. We do not focus on existence and uniqueness in the present work, and for our purposes, when needed, we can just assume that minimizers exist. Both in the theoretical development and in algorithmic implementations, it becomes important to limit the class of plans γ that we are required to test in the minimization above (see [8] and the references therein).

One important property which in many cases ensures optimality of γ , and which is the main focus of the present paper, is c -monotonicity. This condition was introduced in the case of $N = 2$ marginals as a natural extension valid in the case $c(x, y) = \langle x, y \rangle$ for $x, y \in \mathbb{R}^d$, and makes a natural connection to convex analysis (see [15] and [12]). For a recent treatment of the case of general N from the point of view of the analogy with convex geometry, see [1], [2] and the references therein. We now pass to give the precise definition for general N .

A set $A \subset \vec{X}$ is c -monotone (or c -cyclically monotone) if for all $\ell \in \mathbb{N}$ and every N -ple of permutations $\vec{\sigma} = (\sigma_1, \dots, \sigma_N) \in (S_\ell)^N$, for every ℓ -ple $\vec{x} = (\vec{x}_1, \dots, \vec{x}_\ell) \in (\vec{X})^\ell$ with $\vec{x}_j = (x_j^1, \dots, x_j^N) \in A$ for each index $j = 1, \dots, \ell$ there holds

$$\sum_{j=1}^{\ell} c(\vec{x}_j) \leq \sum_{j=1}^{\ell} c((\vec{\sigma} \cdot \vec{x})_j), \quad \text{where } (\vec{\sigma} \cdot \vec{x})_j := (x_{\sigma_1(j)}^1, x_{\sigma_2(j)}^2, \dots, x_{\sigma_N(j)}^N) \in \vec{X}. \quad (1.2)$$

As pointed out for example in [9], this is equivalent to requiring that for any finitely supported measure $\alpha \in \mathcal{P}(\vec{X})$ with support contained in A , the plan α has minimal cost amongst plans with the same marginals as α and finite support contained in A . To verify this, it suffices to concentrate on the case of $\alpha \in \mathcal{P}(\vec{X})$ of the form

$$\alpha := \frac{1}{\ell} \sum_{j=1}^{\ell} \delta_{\vec{x}_j}, \quad \text{which has marginals } \pi_k(\alpha) = \frac{1}{\ell} \sum_{j=1}^{\ell} \delta_{x_j^k} \quad \text{and cost } \langle c, \alpha \rangle = \frac{1}{\ell} \sum_{j=1}^{\ell} c(\vec{x}_j).$$

Then we can compare α with the plan $\alpha' := \vec{\sigma}(\alpha)$ where the action of $\vec{\sigma} \in (S_\ell)^N$ on atomic probability measures with ℓ equal atoms $\mathcal{P}_\ell(\vec{X})$ is inherited from the action on $(\vec{X})^\ell$ by composing with the surjective ‘‘empirical measure’’ map

$$(\vec{X})^\ell \ni (\vec{x}_1, \dots, \vec{x}_\ell) \mapsto \frac{1}{\ell} \sum_{j=1}^{\ell} \delta_{\vec{x}_j} \in \mathcal{P}_\ell(\vec{X}). \quad (1.3)$$

Explicitly, take

$$\alpha' := \frac{1}{\ell} \sum_{j=1}^{\ell} \delta_{(\vec{\sigma} \cdot \vec{x})_j} \quad \text{and thus } \pi_k(\alpha') = \frac{1}{\ell} \sum_{j=1}^{\ell} \delta_{x_{\sigma_k(j)}^k} = \pi_k(\alpha) \quad \text{and } \langle c, \alpha' \rangle = \frac{1}{\ell} \sum_{j=1}^{\ell} c((\vec{\sigma} \cdot \vec{x})_j).$$

As is well known (see [8] and the references therein), the above measures are the extremals of the set of probabilities with marginals equal to those of α , and thus the linear optimization problem (1.1) achieves its minimum on this set. Therefore (1.2) implies that α has cost lower or equal than any competitor $\alpha' = \vec{\sigma}(\alpha)$ in this case.

In the case $N = 2$ the link between c -monotonicity of the support of transport plans and their optimality is well understood, see [3, 4, 11, 13] and the references therein. Recent progress has been made in [2, 7, 9] for the case of general N , with special focus on the case of costs c coming from potential theory and mathematical physics.

However a result at the same level of generality as *e.g.* [11] or [3] is missing for $N \geq 3$. The result [11] proves that c -monotonicity is equivalent to optimality for the case of general c in the case of atomic marginals,

with the only requirement being that there exists a finite-cost plan. A consequence of the counterexample from the present work is that such general result is simply false for any $N \geq 3$, due to phenomena absent in the case $N = 2$. This makes the characterization of optimality even more interesting, and a possible source of new mathematics, for $N \geq 3$. Note that $\#(S_\ell)^N = (\ell!)^N$ is of exponential growth in both N and ℓ , thus even in the case of measures with finitely many atoms, condition (1.2) is prohibitively hard to test in practice. It is even prohibitive to efficiently store on a computer all the competitors appearing in (1.2). The later problem is addressed in [8], to which we refer for further references in this direction.

2. THE COUNTEREXAMPLE

It has been proved in [11] that for $N = 2$ marginals, c -cyclical monotonicity is equivalent to optimality of transport plans. The same has been proved under stronger conditions for a general number of marginals, but the question remained open, of whether or not for $N > 2$ marginals the no-hypothesis theorem from [11] about the case of atomic measures also holds or if the ergodic approach [3] can be adapted. On a space X , we find:

$$\left\{ \begin{array}{l} \text{a cost } c : X^N \rightarrow (0, +\infty], \\ \text{a measure } \mu \in \mathcal{P}(X) \\ \text{a finite-cost plan } \gamma \in \mathcal{P}_{\text{sym}}(X^N) \end{array} \right. \text{ such that } \left\{ \begin{array}{l} \gamma \text{ is } c\text{-cyclically monotone,} \\ \text{the marginal of } \gamma \text{ is } \mu \\ \gamma \text{ is not } c\text{-optimal.} \end{array} \right. \quad (2.1)$$

2.1. A simple construction for c taking the value $+\infty$

Proposition 2.1. *There exist (c, μ, γ) satisfying (2.1) with $X = \mathbb{N}$ and $N = 3$.*

Remark 2.2.

- (Other $N \geq 3$) The case of more than three marginals follows from the above, *e.g.* by defining a cost c which only depends on three coordinates.
- (Same result on other metric spaces) The counterexample construction which we will do works on the space $X = \mathbb{N}$, however \mathbb{N} can be embedded injectively into another space Y of at least countable cardinality, such as $Y = \mathbb{R}$, in several ways: any sequence $(a_k)_{k \in \mathbb{N}}$ such that $a_k \in Y$ are distinct is such an embedding. In our proof only the value of c over the image $A_Y := \{a_k : k \in \mathbb{N}\}$ of such embedding is used, and thus c could be extended arbitrarily outside A_Y . Therefore one can generate a series of counterexamples in any such Y as well.
- (The fact that X is infinite is crucial) For finite X , monotonicity implies optimality of finite- c -cost plans, for any c and any $N \geq 2$. This follows by direct verification from the $\ell = \#X$ case of the monotonicity condition (1.2).
- (Growth requirements on the cost and atomicity of the measure) The proof becomes clearer if we allow $c = +\infty$ on a large subset and the measure μ is atomic. Note that [11] shows that such an example would not be possible for $N = 2$, and this is why the example shows a new phenomenon available only for $N \geq 3$. Relaxation of the above special properties of c, μ should be possible at the cost of a more technical proof. So we provide the proof in this case, and leave the finite- c , non-atomic μ cases open. On the other hand, we cannot have Proposition 2.1 to hold for c too tame. Indeed Griessler [9] showed that for $N = 3$, if $c(a, b, c) \leq f(a) + f(b) + f(c)$ holds μ -almost everywhere for some $f \in L^1(\mu)$, then c -cyclical monotonicity implies optimality. The positive result also holds for general N and can be extended by the De Pascale method [6] to more singular c , see also [7].

Proof of Proposition 2.1:

A cost taking the value $+\infty$. The cost c will be defined in terms of an auxiliary bounded function $f : \mathbb{N} \rightarrow (0, 1]$ as follows:

- $c(a, b, c)$ is symmetric with respect to permutations of the triple a, b, c .

- $c(1, 1, 1) := 1$.
- $c(a, a, a + 1) := f(a)$ for $a \geq 1$.
- $c(a, b, c) := +\infty$ for all the triples $\{a, b, c\}$ not described in the previous two cases.

Required properties of the function f . We don't need to fully specify the values of f but we require that

$$\sum_{k=1}^{\infty} 4^{-k} (f(2k-1) - f(2k)) > \frac{1}{6}. \quad (2.2)$$

(This is achieved, for example, if $f(1) > f(2) + \frac{2}{3}$ and f is decreasing.)

Two plans and their common marginal. We define

$$\mu := \sum_{k=1}^{\infty} 2^{-k} \delta_k, \quad (2.3)$$

$$\gamma := \sum_{k=1}^{\infty} 4^{-k} (\delta_{2k-1, 2k-1, 2k} + \delta_{2k-1, 2k, 2k-1} + \delta_{2k, 2k-1, 2k-1}), \quad (2.4)$$

$$\bar{\gamma} := \frac{1}{2} \delta_{1,1,1} + \frac{1}{2} \sum_{k=1}^{\infty} 4^{-k} (\delta_{2k, 2k, 2k+1} + \delta_{2k, 2k+1, 2k} + \delta_{2k+1, 2k, 2k}). \quad (2.5)$$

It is easy to check that $\gamma, \bar{\gamma} \in \mathcal{P}_{\text{sym}}(\mathbb{N}^3)$ and that μ is the first marginal of γ and of $\bar{\gamma}$. The two plans γ and $\bar{\gamma}$ have equal marginals because the plans are symmetric.

The plan γ is non-optimal. The c -cost of $\bar{\gamma}$ is lower than the c -cost of γ due to the properties of c, f :

$$\begin{aligned} \langle c, \gamma \rangle - \langle c, \bar{\gamma} \rangle &= 3 \sum_{k=1}^{\infty} 4^{-k} f(2k-1) - \frac{1}{2} - 3 \sum_{k=1}^{\infty} 4^{-k} f(2k) \\ &= 3 \sum_{k=1}^{\infty} 4^{-k} (f(2k-1) - f(2k)) - \frac{1}{2} \\ &\stackrel{(2.2)}{>} 0. \end{aligned}$$

The plan γ is c -cyclically monotone. To prove the above, we first note that, due to the symmetry of the problem, without loss of generality we may restrict to symmetric measures with atoms corresponding to integers smaller or equal to M :

$$\alpha = \sum_{k=1}^M \alpha_k (\delta_{2k-1, 2k-1, 2k})^{\text{sym}}, \quad \text{with } \alpha_k \geq 0, \quad \sum_{j=1}^M \alpha_k = 1. \quad (2.6)$$

The marginals of the above α are all equal to

$$\mu_{\alpha} := \sum_{k=1}^M \alpha_k \left(\frac{2}{3} \delta_{2k-1} + \frac{1}{3} \delta_{2k} \right).$$

We need to show that if $\alpha' \in \mathcal{P}_{\text{sym}}(\mathbb{N}^3)$ is another plan with the same marginals then $\langle c, \alpha' \rangle \geq \langle c, \alpha \rangle$.

If $\langle c, \alpha' \rangle = +\infty$ then the desired inequality holds, so we are left with the case $\langle c, \alpha' \rangle < +\infty$. In this case α' can be written in the form

$$\alpha' = \bar{a} \delta_{1,1,1} + \sum_{k=1}^M [a_k (\delta_{2k-1,2k-1,2k})^{\text{sym}} + b_k (\delta_{2k,2k,2k+1})^{\text{sym}}], \quad \bar{a}, a_k, b_k \geq 0, \quad \bar{a} + \sum_{k=1}^M (a_k + b_k) = 1,$$

and the marginal condition on α' translates into

$$\begin{aligned} 2\alpha_1 &= 3\bar{a} + 2a_1 \\ 2\alpha_k &= 2a_k + b_{k-1}, \quad \text{for } k \geq 2, \\ \alpha_k &= a_k + 2b_k, \quad \text{for } k \geq 1. \end{aligned} \tag{2.7}$$

Note that the equations (2.7) imply that

$$a_k + 2b_k = \alpha_k = a_k + \frac{b_{k-1}}{2}, \quad \text{for } k \geq 2,$$

This means that $b_{k+1} = \frac{1}{4}b_k$ for $k \geq 1$. For $k > M$ we have $b_k = 0$ thus we find $b_k = 0$ for all $k \geq 1$, and by (2.7) we get $\alpha_k = a_k$ for all k , which inserted in (2.7) gives $\bar{a} = 0$. Thus $\alpha' = \alpha$ is the only symmetric plan with marginals equal to α and finite cost. As this is true for every $\alpha \ll \gamma$ with finitely many atoms, we have that γ is c -cyclically monotone, as desired. \square

2.2. About the existence of everywhere finite c

In the search for a counterexample c which is now everywhere finite, we first consider the problem abstractly, in a very general setting.

Assume that there exist $\gamma, \bar{\gamma}$ finite-cost transport plans, such that γ is non-optimal and cyclically monotone, and $\bar{\gamma}$ is optimal. Then we consider the following sets of measures:

$$\begin{aligned} \mathcal{F}_\gamma &:= \left\{ \alpha \in \mathcal{P}(\vec{X}), \#(\text{spt}(\alpha)) < \infty, \alpha \ll \gamma \right\}, \\ \overline{\mathcal{F}}_\gamma &:= \left\{ \alpha' - \alpha : \alpha \in \mathcal{F}_\gamma, \alpha' \in \mathcal{P}(\vec{X}), (\pi_j)_\# \alpha = (\pi_j)_\# \alpha' \text{ for } j = 1, \dots, N \right\}. \end{aligned}$$

Note that \mathcal{F}_γ is composed of measures with finite-cardinality support by definition, and $\overline{\mathcal{F}}_\gamma$ is also composed of measures of finite support, because $\# \text{spt}((\pi_j)_\# \alpha) \leq \# \text{spt}(\alpha)$ for all j and $\# \text{spt}(\alpha') \leq \prod_j \# \text{spt}((\pi_j)_\# \alpha)$. Then the set of ‘‘counterexample’’ costs for which γ is cyclically monotone, but $\bar{\gamma}$ has better cost than γ , is given by

$$\mathcal{C}_{\text{cex}} := \left\{ \tilde{c} : \vec{X} \rightarrow [0, +\infty] : \langle \tilde{c}, \gamma - \bar{\gamma} \rangle > 0, \quad \forall \alpha' - \alpha \in \overline{\mathcal{F}}_\gamma, \quad \langle \tilde{c}, \alpha' - \alpha \rangle \geq 0 \right\}.$$

Our assumption that a counterexample cost exists (which we showed for $\vec{X} = \mathbb{N}^N, N \geq 3$), means that $\mathcal{C}_{\text{cex}} \neq \emptyset$, and we now consider the question of whether or not

$$\mathcal{C}_{\text{cex}} \cap \{ \tilde{c} : \vec{X} \rightarrow [0, +\infty] : \forall \vec{x} \in \vec{X}, c(\vec{x}) < +\infty \} \neq \emptyset$$

as well. Note that \mathcal{F}_γ and $\overline{\mathcal{F}}_\gamma$ are convex, but not closed under weak-* convergence of measures since γ belongs to the closure of \mathcal{F}_γ but not to \mathcal{F}_γ , and $-(\gamma - \bar{\gamma})$ is in the closure of $\overline{\mathcal{F}}_\gamma$ but not in $\overline{\mathcal{F}}_\gamma$. As \mathcal{C}_{cex} is composed on functionals of the form $\langle \tilde{c}, \cdot \rangle$ which are required to be nonpositive on $\overline{\mathcal{F}}_\gamma$ and negative on $-(\gamma - \bar{\gamma})$, this directly shows that all $\tilde{c} \in \mathcal{C}_{\text{cex}}$ are not continuous under weak-* convergence:

Lemma 2.3. *Let $\vec{X} = X_1 \times \cdots \times X_N$ and X_1, \dots, X_N be Polish spaces, and assume that $c : \vec{X} \rightarrow (-\infty, +\infty]$ is a cost for which there exist $\gamma \in \mathcal{P}(\vec{X})$ of finite cost, which is cyclically monotone and not optimal. Then the assignment $\tilde{\gamma} \mapsto \langle c, \tilde{\gamma} \rangle$ defined on $\{\gamma \in \mathcal{P}(\vec{X}) : \langle c, \gamma \rangle \in (-\infty, +\infty]\}$ is not continuous with respect to weak-* convergence.*

Nevertheless, we cannot exclude that there exist counterexamples c which are everywhere finite:

Open questions.

- (1) Do there exist Polish spaces X_1, \dots, X_N and a cost function $c : \vec{X} \rightarrow \mathbb{R}$ for which there exists a c -cyclically monotone non-optimal transport plan $\gamma \in \mathcal{P}(\vec{X})$?
- (2) Does such monotone non-optimal plan exist for finite c , for $X_1 = \cdots = X_N = \mathbb{R}^d$ and for marginal of γ equal to a measure μ which is absolutely continuous with respect to Lebesgue measure?

3. CYCLICAL MONOTONICITY AND N -FLOWS

3.1. Definition of N -graphs and N -flows

We give here a principle which allows to construct more complicated counterexamples with c taking the value $+\infty$. The idea is that we can interpret X^N as a (continuous or discrete) directed hypergraph and $c : X^N \rightarrow (-\infty, +\infty]$ as a weight on X^N .

The case $N = 2$. The simplest case $N = 2$ gives usual graphs: We then associate to $c : X^2 \rightarrow (-\infty, +\infty]$ the weighted directed graph

$$G = (V, E, w) \quad \text{where} \quad \begin{cases} V := X, \\ E := \{(x, y) : x, y \in X, c(x, y) < +\infty\}, \\ w : E \rightarrow \mathbb{R} \text{ is given by } w(x, y) := c(x, y). \end{cases}$$

Here we obtain usual (countable) weighted graphs if X is countable, and a generalization thereof otherwise. We will mostly concern ourselves with atomic measures and discrete spaces X for the time being.

The 3-graph associated to our counterexample. Weighted directed hypergraphs are defined analogously with directed edges replaced by N -ples of points in X . For example, the construction from the previous section gives a 3-graph with vertex set given by three copies of \mathbb{N}

$$V := \mathbb{N} \times \{1, 2, 3\}.$$

A 3-edge $\{(k, 1), (l, 2), (m, 3)\} \subset V$ can be identified with an ordered 3-ple (k, l, m) . Then the hypergraph relevant to the previous section has 3-edge set (see Fig. 1)

$$E := \{(1, 1, 1)\} \cup \{(k, k, k+1), (k, k+1, k), (k+1, k, k) : k \in \mathbb{N}\}.$$

Anytime we study optimal transport with the cost c from the previous section, the only edges which matter to our problem are the edges in E , due to c being infinite on couplings outside E . This is why we can say that the 3-graph (V, E) with weight given by c encodes our problem.

Definition of N -graphs and N -flows. More generally, considering N -marginal optimal transport on the set X , we proceed to the following definitions. Given X we define an N -vertex set $\tilde{X}_N := X \times \{1, \dots, N\}$. Then an N -edge over X is a subset of \tilde{X}_N of the form $\{(x_1, 1), \dots, (x_N, N)\}$, which can be identified with the ordered N -ple (x_1, \dots, x_N) . We denote by $E_N(X)$ the set of all N -edges over X , and the above identification of N -edges

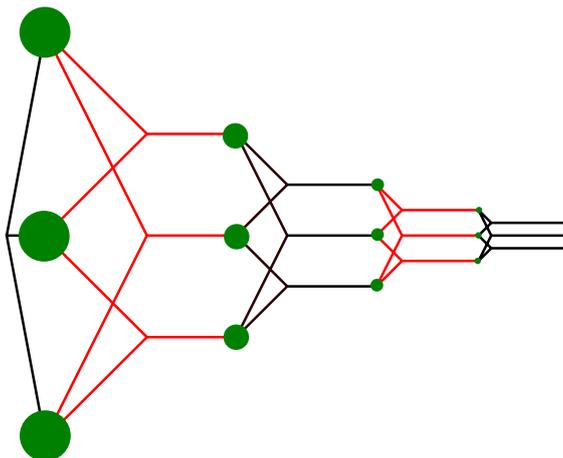


FIGURE 1. We depict here part of the 3-graph associated to the cost c from the counterexample we constructed in Proposition 2.1. Here each triple (a, b, c) such that $c(a, b, c) < +\infty$ (which gives an edge of the 3-graph) is denoted by a triod, and the green points correspond to elements in V . The black triods correspond to the support of the transport plan $\bar{\gamma}$ and the red ones correspond to the support of γ . The vertical diameter of triods and circles are roughly representing the weights that corresponding points are given in $\mu, \bar{\gamma}$ and γ .

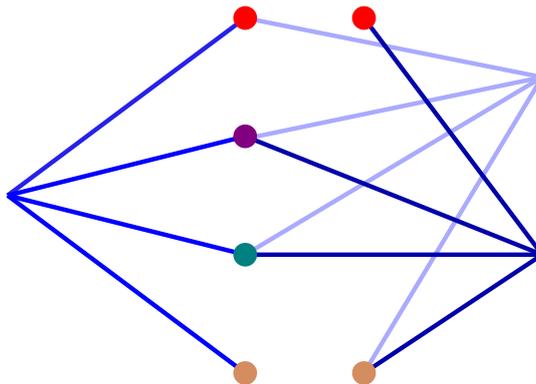


FIGURE 2. We show here a 4-graph with three 4-edges. We indicate the points belonging to X_1, X_2, X_3, X_4 by different colors (red, purple, green, orange), and the 4-edges of the graph are encoded by “spider graphs” with 4 legs, in different shades of blue.

with N -ples gives a bijection $E_N(X) \simeq X^N$. An N -graph over X is the datum of a subset of N -vertices $V \subset \tilde{X}_N$ and a subset of N -edges $\{(x_i, i), i = 1, \dots, N\}$ which are subsets of V . See Figure 2 for an example of 4-graph.

To a signed weight $m : E_N(X) \rightarrow \mathbb{R}$ and a subset of edges $A \subset E_N(X)$ we can associate an N -flow, which is the formal sum

$$[A] := \sum_{a \in A} m(a)[a].$$

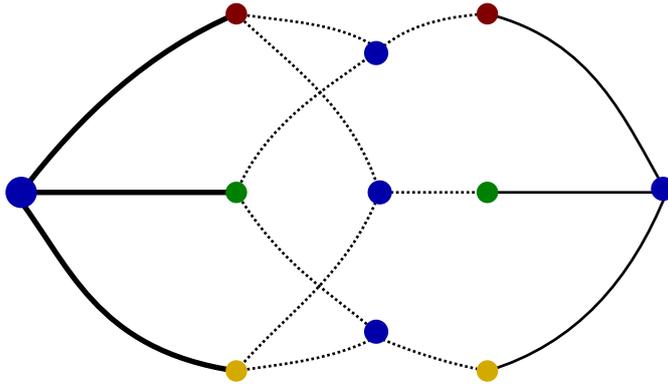


FIGURE 3. We show here an example of a closed 3-flow over a 3-graph with 5 edges. The 3-edges are represented by 3-legged spider graphs similarly to Figure 2. To visually encode the weights on the 3-graph, we use thickness to represent the absolute value of the weights, and dashed edges correspond to negative weights while non-dashed ones correspond to positive weights. Here the thick 3-spider has weight 1, the dashed thin ones have weights $-1/2$ and the non-dashed thin one has weight $1/2$. Again the color blue is reserved to 3-edges, while the other colors (dark red, green and yellow) encode to which one of X_1, X_2, X_3 the different endpoints of the 3-edges belong.

It will be useful later to also introduce the *mass of the N -flow* $[A]$ above, defined as

$$|[A]| := \sum_{a \in A} |m(a)|.$$

To an N -flow $[A]$ as above we associate its N -boundary, which is an N -ple of atomic measures given by

$$\partial^{(N)}[A] := (\mu_1, \dots, \mu_N), \quad \mu_i := \sum_{a=(a_1, \dots, a_N) \in A} m(a) \delta_{a_i},$$

whenever the sum is defined (in particular it is, if A is finite). If $[A]$ has $\partial^{(N)}[A] = 0$ then we say that $[A]$ is *closed* (see Fig. 3 for an example).

Composing with the bijection $X^N \simeq E_N(X)$ and by abuse of notation, we also identify a cost $c : X^N \rightarrow (-\infty, +\infty]$ with a weight function on N -edges, which we also denote by abuse of notation $c : E_N(X) \rightarrow (-\infty, +\infty]$. We denote by $\tilde{E}_N(X, c)$ the set of N -edges on which c takes finite values. We then call $(\tilde{X}_N, \tilde{E}_N(X, c), c)$, or also simply $(\tilde{X}_N, \tilde{E}_N, c)$, the N -graph associated to the transport cost c . Note that this graph could possibly be uncountable.

Given a finite N -edge set A with associated N -flow $[A]$, we can *integrate c on $[A]$* (the integral is set to be $+\infty$ if c takes the value $+\infty$ on A):

$$\langle c, [A] \rangle := \sum_{a \in A} m(a) c(a).$$

Remark 3.1. We could easily generalize and adapt the above definitions to the case that m is a measure over \tilde{E}_N , in case the latter is infinite, replacing the sums in our definitions by suitable integrals. However, defining c -cyclical monotonicity does not *per se* require us to talk about measures, as the definition (1.2) is formulated in purely combinatorial terms. Indeed, it turns out that the case in which the support A of $[A]$ is at most

countable is all we need, and this allows us to avoid discussing measurability issues which would make the discussion superfluously complicated.

3.2. Reformulating c -cyclical monotonicity in terms of N -flows

We are now in the position to give, using the definitions from the previous section, a combinatorial reformulation of the monotonicity condition (1.2), which allows us to describe more complicated counterexamples. It says that a set is c -monotone if and only if its flows are cost-minimizers at fixed boundary.

Proposition 3.2. *A set $A \subset \tilde{X}$ is c -monotone if and only if whenever $[F]$ and $[F']$ are finite, finite-mass N -flows with positive coefficients in the N -graph associated to c such that $[F]$ has support contained in A and $\partial^{(N)}([F] - [F']) = 0$, then there also holds $\langle c, [F] - [F'] \rangle \leq 0$.*

Proof. The proof is an easy verification, based on the following fact proved in the introduction: an equivalent condition for A to be c -monotone is that for any positive measure α supported on a finite subset $F \subset A$ and any finite positive measure α' with marginals equal to those of α , there holds $\langle c, \alpha - \alpha' \rangle \leq 0$. The support of α being included in the finite set F implies that $\alpha = \sum_{f \in F} \alpha(\{f\})\delta_f$. We can thus associate the N -flow $[F] := \sum_{f \in F} \alpha(\{f\})[f]$ to α . Similarly, since α' has atomic marginals it is itself atomic too and we can associate another N -flow $[F']$ to α' as above. The condition that α' and α share the same marginals is equivalent to requiring $\partial^{(N)}([F] - [F']) = 0$ as can be easily verified, and the condition $\langle c, \alpha - \alpha' \rangle \leq 0$ is equivalent to $\langle c, [F] - [F'] \rangle \leq 0$. \square

The counterexample from the previous section is generalized by the following.

Corollary 3.3. *If the N -graph associated to c supports no finite closed N -flows then all transport plans of finite c -cost are c -monotone.*

Proof. Let γ be a transport plan of finite c -cost, thus $\gamma(\{c < +\infty\}) = 1$. We are now applying Proposition 3.2 with A equal to the support of γ , in particular $A \subset \{c < +\infty\}$. However, if there existed $[F], [F']$ finite N -flows of finite mass in $(\tilde{X}_N, \tilde{E}_N, c)$, such that $[F]$ is supported on $\{c < +\infty\}$, such that $\partial^{(N)}([F] - [F']) = 0$, then $[F] - [F']$ would be a closed N -flow supported on the graph associated to c , contradicting the hypothesis. Thus the set of $[F], [F']$ for which we have to check the property $\langle c, [F] - [F'] \rangle \leq 0$ as in Proposition 3.2 is vacuous, and thus γ is c -monotone. \square

3.3. Special properties available for the case $N = 2$

It is instructive to consider the case $N = 2$, reinterpreting the proof methods [11] and [3].

We define a 2 -flow-path to be any 2 -flow of the form

$$[A] = \sum_{j=0}^k \left(\left[\left(a_1^{(j)}, a_2^{(j)} \right) \right] - \left[\left(a_1^{(j+1)}, a_2^{(j)} \right) \right] \right) \quad \text{or} \quad [A] = \sum_{j=0}^k \left(\left[\left(a_1^{(j)}, a_2^{(j)} \right) \right] - \left[\left(a_1^{(j)}, a_2^{(j+1)} \right) \right] \right),$$

where $k \in \mathbb{N}$ and $a_1^{(j)} \in X_1$ and $a_2^{(j)} \in X_2$ for $j = 0, \dots, k$. If $a_1^{(k+1)} = a_1^{(0)}$ or respectively $a_2^{(k+1)} = a_2^{(0)}$ in the above but no other pair of points coincide, then we call $[A]$ a 2 -flow-loop.

For the next definition, let $[A], [A_1], [A_2]$ be three 2 -flows such that $[A] = [A_1] + [A_2]$. In general we have $\|[A]\| \leq \|[A_1]\| + \|[A_2]\|$. If the equality sign holds in the latter inequality, we say that $[A_1], [A_2]$ form a *decomposition of $[A]$ without cancellations*.

It is easy to see that if a closed 2 -flow has the same support as $[A]$ above, then automatically it is a nonzero multiple of $[A]$. The principle that “mass is conserved along 2 -flow-loops” (which lacks an easy analogue for N -flows if $N > 2$, as a consequence of the counterexample in the proof of Prop. 2.1) helps us to prove the following:

Lemma 3.4. *A finite 2-flow $[A]$ closed if and only if $[A]$ is a finite sum of weighted 2-flow-loops without cancellations.*

Proof. The “if” part of the implication is obvious, as a sum of closed 2-flows is closed. The proof of the other implication is an adaptation of a folklore result on weighted directed graphs satisfying the Kirchhoff balance equation at each vertex, so we only sketch it for the convenience of the reader. The basic idea is to start with an edge of the 2-graph which is assigned lowest weight in absolute value, and use the Kirchhoff law to find a path of edges which is locally satisfying Kirchhoff law. When such path first self-intersects, we find one 2-flow-loop $[A']$ such that $[A'], [A] - [A']$ forms a decomposition of $[A]$ without cancellations. By repeating the procedure with $[A]$ replaced by $[A] - [A']$ we can keep diminishing the mass of the part not yet decomposed into loops, while diminishing the total number of loops in the graph corresponding to A . When the remaining graph is one single loop, the procedure ends.

In order to describe how we single out one loop in the above sketch of proof, consider the nontrivial case $[A] \neq 0$ and assume (as we can do up to change of sign symmetry) that for some $(a_1, a_2) \in A$ there holds $m := m(a_1, a_2) = \min\{|m(a'_1, a'_2)| : (a'_1, a'_2) \in A\}$. We start building a “2-path-flow” by defining $\gamma_1 := m[(a_1, a_2)]$. By considering the δ_{a_2} -coefficient in the expression for $\partial^{(2)}[A] = 0$, and due to the fact that $m = m(a_1, a_2) > 0$ is minimal by definition, we find that there exists $a'_1 \neq a_1 \in X_1$ such that (a'_1, a_2) belongs to the support of $[A]$ and $m(a'_1, a_2) \leq -m$. We add this edge with coefficient $-m$ to γ_1 and obtain $\gamma_2 := m([(a_1, a_2)] - [(a'_1, a_2)])$. By focusing now on the $\delta_{a'_1}$ -coefficient in the expression for $\partial^{(2)}[A] = 0$ we find $a'_2 \in X_2$ such that $(a'_1, a'_2) \in A$ and this edge has weight $m(a'_1, a'_2) \geq m$, and we define $\gamma_3 := m([(a_1, a_2)] - [(a'_1, a_2)] + [(a'_1, a'_2)])$. The procedure continues this way till we visit one point which was already visited before, and in this case a subpath of the 2-flow-path we reached is a 2-flow-loop. The procedure ends before step $k \leq |[A]|/m$ because $[A]$ is of finite mass, we have that $\gamma_k, [A] - \gamma_k$ is a decomposition of $[A]$ without cancellations for every k , and $|\gamma_k| = km$ for every k . \square

The above proof strategy also gives the following countable version of Lemma 3.4:

Lemma 3.5. *A finite-mass closed 2-flow over a countable set X is a superposition of 2-flow-loops without cancellations.*

If X is countable, $N = 2$, and c is arbitrary, Lemma 3.5 can be applied to optimal transport as follows. Given two distinct plans $\gamma, \bar{\gamma}$ with finite cost and with the same marginal, they define flows $[G_\gamma]$ and $[G_{\bar{\gamma}}]$ such that $[G_\gamma] - [G_{\bar{\gamma}}]$ is a closed 2-flow. So it is a superposition of finite loops. If we use c -monotonicity assumption on γ for each such loop, we find by linearity that $\langle c, [G_\gamma] \rangle \leq \langle c, [G_{\bar{\gamma}}] \rangle$, which due to the arbitrariness of $\bar{\gamma}$ implies the optimality of γ . This is basically the strategy of [11]. The failure of the above lemmas for $N \geq 3$ shows that such strategy does not extend for general c due to the higher combinatorial complexity of this case.

4. GENERALIZED SMIRNOV DECOMPOSITION FOR N -FLOWS

It would be useful to consider the classification of N -flows depending on the type of closed subflows they contain. Here we concentrate more on such properties for the model-case of N -graphs, in order to avoid measurability issues, as before. As a first basic step in a classification for N -flows based on their structure, we mention a decomposition result in Proposition 4.1, similar to [10, 14], and follow it up by a challenging open problem.

The properties emerging in this context have been studied for the decomposition of currents/flows into closed and acyclic parts from [10, 14]. The use of Smirnov decomposition in Optimal Transport type problems is not new, it has appeared in another setting in [5].

We introduce some terminology from [10, 14], which can be useful for the reader interested in exploring this direction further:

- An N -flow $[A]$ is a *subflow* of the N -flow $[B]$ if there exists an N -flow $[C]$ such that

$$[A] + [C] = [B] \quad \text{and} \quad |[A]| + |[C]| = |[B]|.$$

- If $[A] = 0$ or $[A] = [B]$ then $[A]$ is a *trivial subflow* of $[B]$.
- An N -flow $[A]$ is called *indecomposable* if its only subflows are scalar multiples of $[A]$.
- An N -flow is called *acyclic* if it has no nonzero closed subflows.
- Closed subflows would be called *cyclic* subflows in the literature on, but we stick to the term “closed” below, in continuity with the previous sections.
- An N -flow is called *solenoidal* if it is closed and has no finite closed subflows.

Proposition 4.1. *If $[A]$ is an N -flow with countable support such that $|[A]| < \infty$ then there exist unique subflows $[A_1], [A_2], [A_3]$ of $[A]$ such that $[A_1]$ is acyclic, $[A_2]$ is solenoidal and $[A_3]$ is a superposition of finite closed N -flows, such that $[A] = [A_1] + [A_2] + [A_3]$.*

A similar result holds with measurability assumptions for more general $[A]$, a case in which transport plans correspond to general measures. As the method for the case of currents in the above papers is quite similar, we leave the proof of the proposition to the reader.

In order to make Corollary 3.3 more concretely useful, we would need to consider the following.

Open problem. Find necessary conditions and sufficient conditions for an N -graph G to support no finite closed N -flows. Equivalently, find necessary conditions and sufficient conditions such that G supports only acyclic and solenoidal flows.

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