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On *c*-cyclical monotonicity for optimal transport problem with Coulomb cost

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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.

Key words: Multi-marginal optimal transportation, Monge–Kantorovich problem, optimality condition, *c*-cyclical monotonicity

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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 $\rho_1, \dots, \rho_N$ be probability measures on the corresponding spaces, i.e. $\rho_i \in \mathcal{P}(X_i)$. Denote by $\Pi(\rho_1, \dots, \rho_N) = \{P \in \mathcal{P}(X_1 \times \cdots \times X_N) \,:\, \pi^i_\sharp P = \rho_i,\ \forall i\}$ where π^i denotes the projection on the ith factor of the Cartesian product and $f_\sharp \mu$ denotes the push-forward of the measure μ via the map f. Let $c : X_1 \times \cdots \times X_N \to \mathbb{R} \cup \{-\infty,\ +\infty\}$. The variational problem of interest is

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

The elements of $\Pi(\rho_1, \dots, \rho_N)$ are called **transport plans**. Existence of minimisers follows from 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 (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 several applications. Some general results are available in [7, 25, 29, 30, 32], results for special costs are available, e.g., in [19] for the quadratic cost with some generalisation in [24], and in [9] for the determinant. More applications are emerging in [20]. Applications to economics of the multi-marginal optimal

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transportation problems include, e.g., the problem of team matching which is a generalisation of the classical marriage problem [8, 10]. Applications to physics are related to quantum chemistry and the strong interacting regime for particles which are described in [21, 22, 35–37]. 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, 13, 15, 17, 18, 28].

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 $\rho_1 = \cdots = \rho_N = \rho$; c will be the Coulomb repulsive cost:

$$c(x_1, \ldots, x_n) = \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|}.$$

Then, we will study some properties of the minimisers of

$$\min_{P \in \Pi(\rho)} \int \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} dP(x_1, \ldots, x_N), \tag{1.2}$$

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 $(x_1^1, \ldots, x_N^1), \ldots, (x_1^n, \ldots, x_N^n) \in \Gamma$ and all permutation $\sigma_2, \ldots, \sigma_N \in \mathcal{S}_n$:

$$\sum_{i=1}^{n} c\left(x_1^i, \ldots, x_N^i\right) \le \sum_{i=1}^{n} c\left(x_1^i, x_2^{\sigma_2(i)}, \ldots, x_N^{\sigma_N(i)}\right).$$

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 sptP 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.

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 above result is complemented by the results of [34] where it is proved that c is lower semi-continuous if c takes only finite values in $[0, +\infty)$. See also reference 1

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

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Finally, in Theorem 2.4 of [3], the authors give a measure theoretic criterion to assess the optimality of a c-cyclically monotone transport plan followed by Corollary 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 [23] 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

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

The last assumption cannot be satisfied by Coulomb-like costs.

For transport costs which tend to $+\infty$ when $|x_i - x_j| \to 0$, 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 [4, 6, 14, 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 $\lim_{r\to 0} \mu_\rho(r) < 1/N$. 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 $\lim_{r\to 0} \mu_\rho(r) < 1/N$ 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*-tuples 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 [23], 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 [23] 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 $u_i : \mathbb{R}^d \to [-\infty, +\infty)$ such that $u_1(x_1) + \cdots + u_N(x_N) \leq c(x_1, \dots, x_N)$ 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 [23], 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 $(\tilde{u})_i$ which satisfies*

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

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and

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

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

Proof We first define

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

and

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

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

We then consider

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

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

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

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. □

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

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

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and we introduce the notation

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

The following proposition is a variation of Proposition 3.8 in [16] and Theorem 2.4 in [6] according to the quantitative improvement given in [14] which also appears in [38].

Proposition 2.4 *Let ρ be such that $\lim_{r\to 0} \mu_\rho(r) < 1/N$. 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 $\beta/2 < r$,*

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

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

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

which has the same cost and 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 $\mathbf{x} = (x_1, \dots, x_N) \in D_\alpha \cap sptP$ and, without loss of generality, that $|x_1 - x_2| \le \alpha$. We will later show that there exists

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

For such $\mathbf{y}$, at least one of the coordinates y_i does not belong to $\bigcup_{j=2}^N B(x_i, \frac{\beta}{2})$ 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

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

on the other hand,

[2] This is an important part of the idea which allowed [14] to obtain optimal constants.

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

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

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

$$P\left(D_\beta\cup\cup_{i=1}^{N}\mathbb{R}^d\times\cdots\times\overbrace{B\left(x_1,\frac{\beta}{2}\right)}^{i}\times\cdots\times\mathbb{R}^d\right)$$
$$\le P(D_\beta)+\sum_{i=1}^{N}P\left(\mathbb{R}^d\times\cdots\times\overbrace{B\left(x_1,\frac{\beta}{2}\right)}^{i}\times\cdots\times\mathbb{R}^d\right)$$
$$\le\beta C(P)+N\rho\left(B\left(x_1,\frac{\beta}{2}\right)\right)$$
$$<1-N\mu_\rho(r)+N\rho\left(B\left(x_1,\frac{\beta}{2}\right)\right)$$
$$=1-N(\mu_\rho(r)-\rho\left(B\left(x_1,\frac{\beta}{2}\right)\right)\le 1,$$

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). □

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 [6, 14] 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 [23] 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 $\lim_{r\to 0}\mu_\rho(r)<1/N$. Let $P\in\Pi(\rho)$ be a plan with finite cost and c-cyclically monotone. Then $\Gamma=sptP$ 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*

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

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 $(\bar{x}_1,\dots,\bar{x}_N)\in sptP$ (then, in particular, the point does not belongs to D_α). Then we take a, possibly smaller, r, so that

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

It follows that the set

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

has positive P measure and we may take $(\bar{y}_1, \ldots, \bar{y}_N)$ in this last set. Let $G \subset \Gamma$ be a c-splitting set with $(\bar{x}_1, \ldots, \bar{x}_N)$, $(\bar{y}_1, \ldots, \bar{y}_N) \in G$. 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) $u_i(\bar{x}_i) = \frac{c(\bar{x}_1, \ldots, \bar{x}_N)}{N} := k$ for all i and
(2) $u_i(x) = \inf\{c(y_1, \ldots, x, y_{i+1} \ldots, y_N) - \sum_{k \neq i} u_k(y_k)\}$, for all i 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

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

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

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

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

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

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 estimate from below which holds ρ-a.e. Indeed, for ρ-a.e. x, there holds

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

So that for every G, there is a c-splitting N-tuple which is bounded by $\mathbf{k}$. Now, following an idea of [23], let us consider for every $G \subset \Gamma$, the set of splitting N-tuples bounded by $\mathbf{k}$

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

and

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

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

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

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. □

Remark 2.7 *The idea of using finite sets G in the proof above could be seen as the analogue of the discretisation considered in [16] to prove the existence of solutions for the dual problem.*

3 Proof of Theorem 1.3 and one application

Proof (of Theorem 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 Proposition 2.6, since each of the u_i is bounded, we may write

$$\begin{aligned} \int c dP &= \int u_1(x_1) + \cdots + u_N(x_N) dP \\ &= \int u_1(x_1) d\rho + \cdots + \int u_N(x_N) d\rho \\ &\leq \int c dQ. \end{aligned}$$

where the second equality is allowed by the fact that the u_is are bounded. □

In Proposition 2.9 of [12], it is proved that for some special, radially symmetric ρ in the plane, the transport plan associated with a radially symmetric map proposed in [37] is c-cyclically monotone. As a consequence of Theorem 1.3 above, this implies the optimality of the map which was conjectured in [37].

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Conflict of interest

None.

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