



# On the existence of Monge maps for the Gromov–Wasserstein problem

Joint work with T. DUMONT (Mines Paristech/MVA), T. LACOMBE (LIGM).

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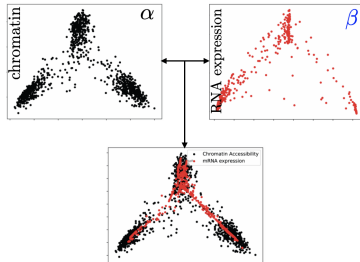
# 1. Introduction

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# One exciting motivation/application in computational biology

How to align clouds of points from different spaces?

1. Given a large population of cells.
2. Two or more experiences in which cells are killed (you cannot reuse it).
3. Observe results: collections of points in  $\mathbb{R}^{d_1}, \mathbb{R}^{d_2}$ .



**Figure 1:** "Gromov-Wasserstein optimal transport to align single-cell multi-omics data", (Demetci et al.)

## Comparing metric-measure spaces

Let  $\mathcal{X} = \{(X, d, \mu), (X, d) \text{ polish space}, \mu \text{ probability measure}\}$ .

How to compare such spaces ?

Isometric mm-spaces:  $\varphi : X \mapsto Y, \varphi_*(\mu) = \nu$  and  $\varphi$  isometric:  $\varphi^* d_Y = d_X$ .

- Memoli's proposal: quadratic optimization problem.
- Sturm's proposal: finding a common embedding in a metric space.

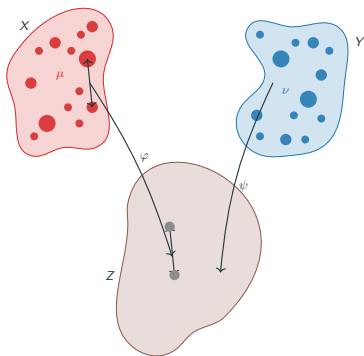
## Two different distances

$D^2$  distance: infimum on the set of embeddings, Sturm, 2006

$$D^2(X, Y) := \inf_{\psi, \varphi} \left\{ \inf_{\pi} \langle \pi, d_Z^2(\psi(x), \varphi(y)) \rangle ; (\psi, \varphi) : (X, Y) \mapsto Z \text{ and } \pi \in C_{\mu_X, \mu_Y} \right\},$$

$\psi, \varphi$  being **isometric embeddings**.

1. Reformulation on minimising a coupling pseudo-metric on  $X \times Y$ .
2. Non-convex optimization problem.

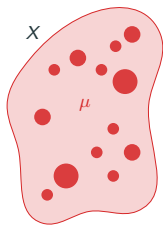


## Two different distances

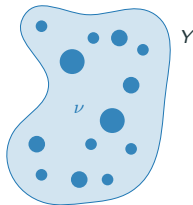
**GW<sup>2</sup> distance (Memoli): comparison of pairwise distances (distortion distances)**

$$GW^2(X, Y) := \inf_{\pi} \{ \langle \pi(x, y) \otimes \pi(x', y'), |d_X(x, x') - d_Y(y, y')|^2 \rangle; \pi \in C_{\mu_X, \mu_Y} \}.$$

1. Non-convex optimization problem.
2. Entropic regularization applies directly.



$$\Rightarrow (X \times X, \mu \otimes \mu)$$



$$\Rightarrow (Y \times Y, \nu \otimes \nu)$$

$$GW = \inf_{\tilde{\pi}} \int |d_X - d_Y|^2 d\tilde{\pi}$$

under the *non-convex* constraint  $\tilde{\pi} = \pi \otimes \pi$

## Properties of $D$ and $GW$

1. Same topology (on compact spaces with uniformly bounded diameters).
2.  $D$  gives complete metric space, not  $GW$ .
3. Both are length spaces. E.g.  $(X \times Y, (td_Y^2 + (1-t)d_X^2)^{1/2}, \pi)$  for  $GW$ .
4.  $GW$  has non-negative Alexandrov curvature.



## What is this talk about?

Two contributions on the Gromov-Wasserstein problem.

1. (First part) A mathematical study of the structure of the optimizers.
2. (Second part) A generalization relevant in practice to an unbalanced setting (e.g. the two point clouds do not have the same total mass).

What are the tools for that?

GW is a quadratic optimization problem on probability measures. Its linearization belongs to optimal transport.

1. Known and new technics in optimal transport.
2. Extension of part of my work on unbalanced optimal transport.

## **1. Introduction**

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### **1.1. Map solutions of OT**

**Brenier's theorem [?]**

Let  $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$  and  $c(x, y) = |x - y|^2$ . If  $\mu \ll \mathcal{L}^n$ , then there exists a unique solution to ?? induced by a **map**  $T = \nabla f$ , with  $f$  convex.

- Recall that linear optimization (whatever the cost) over the simplex  $\implies$  permutation.
- *Interest: structure on the minimizers.*
- generalized for Riemannian manifolds  $\mathcal{X}$  and  $\mathcal{Y}$  and for other cost functions  $c$ .

**Twist condition** Gangbo's PhD, [?, ?]

We say that  $c$  satisfies the **twist condition** if

for all  $x_0 \in \mathcal{X}$ ,  $y \mapsto \nabla_x c(x_0, y) \in T_{x_0} \mathcal{X}$  is injective. (Twist)

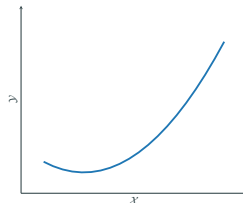
Suppose that  $c$  satisfies (Twist) and assume that any  $c$ -concave function is differentiable  $\mu$ -a.e. on its domain (e.g.  $\mu \ll \mathcal{L}^n$ ). If  $\mu$  and  $\nu$  have finite transport cost, *then ??* admits a **unique optimal transport plan**  $\pi^*$  induced by **a map** which is the gradient of a  $c$ -convex function  $f : \mathcal{X} \rightarrow \mathbb{R}$ :

$$\pi^* = (\text{id}, c\text{-exp}_x(\nabla f))_{\#} \mu.$$

- $c\text{-exp}_x(p)$  is the unique  $y$  such that  $\nabla_x c(x, y) + p = 0$ :

$$c\text{-exp}_x(p) = (\nabla_x c)^{-1}(x, -p).$$

- usual Riemannian exp when  $c(x, y) = d(x, y)^2/2$



**Twist condition** Gangbo's PhD, [?, ?]

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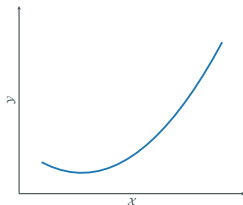
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$$\pi^* = (\text{id}, c\text{-exp}_x(\nabla f))_{\#} \mu.$$

examples:	twist
$ x - y ^2$ in $\mathbb{R}^n$	✓
$\langle x, y \rangle$ in $\mathbb{R}^n$	✓
$\langle x, y \rangle$ on $\mathbb{S}^{n-1}$	.

- other formulation:

$\forall y_1 \neq y_2, \quad x \mapsto c(x, y_1) - c(x, y_2)$  has no critical point.



**Subtwist condition** [?, ?]

We say that  $c$  satisfies the **subtwist condition** if

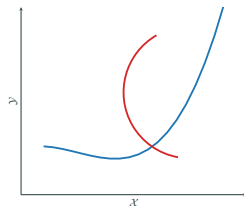
$\forall y_1 \neq y_2, \quad x \mapsto c(x, y_1) - c(x, y_2)$  has at most 2 critical points. (Subtwist)

Suppose that  $c$  satisfies (Subtwist). Under the *same assumptions than before*, ?? admits a unique optimal transport plan  $\pi^*$  induced by the **union of a map and an anti-map**:

$$\pi^* = (\text{id}, G)_\# \bar{\mu} + (H, \text{id})_\# (\nu - G_\# \bar{\mu})$$

for  $G : \mathcal{X} \rightarrow \mathcal{Y}$ ,  $H : \mathcal{Y} \rightarrow \mathcal{X}$  and  $0 \leq \bar{\mu} \leq \mu$  s.t.  $\nu - G_\# \bar{\mu}$  vanishes on the range of  $G$ .

	twist	subtwist
$\langle x, y \rangle$ on $\mathbb{S}^{n-1}$	.	✓



**m-twist condition** [?]

We say that  $c$  satisfies a  **$m$ -twist condition** if

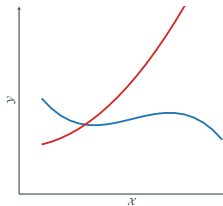
$$\forall x_0 \in \mathcal{X}, y_0 \in \mathcal{Y}, \quad \text{card} \{y \mid \nabla_x c(x_0, y) = \nabla_x c(x_0, y_0)\} \leq m. \quad (m\text{-twist})$$

Suppose that  $c$  satisfies ( $m$ -twist) and is **bounded**. Under the **same assumptions than before**, each optimal plan  $\pi^*$  of ?? is supported on the **graphs of  $k \leq m$  measurable maps  $T_i : \mathcal{X} \rightarrow \mathcal{Y}$** :

$$\pi^* = \sum_{i=1}^k \alpha_i (\text{id}, T_i)_\# \mu,$$

in the sense  $\pi^*(S) = \sum_{i=1}^k \int_{\mathcal{X}} \alpha_i(x) \mathbb{1}_S(x, T_i(x)) d\mu$  for any Borel  $S \subset \mathcal{X} \times \mathcal{Y}$ .

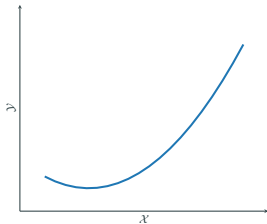
		twist	subtwist	2-twist
$1 - \cos(x - y)$	on $[0, 2\pi)$	·	✓	✓
our cost!	in $\mathbb{R}^n$	·	·	✓



*Twist*



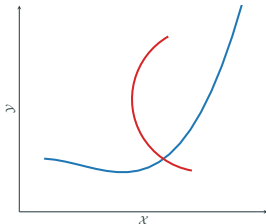
map



*Subwist*



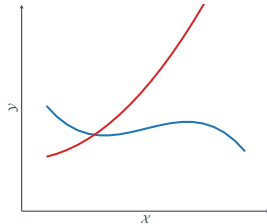
map/anti-map



*2-twist*



bimap



- all assumptions needed to apply them are satisfied when  $\mu$  and  $\nu$  have compact support and  $\mu$  has a density



# 1. Introduction

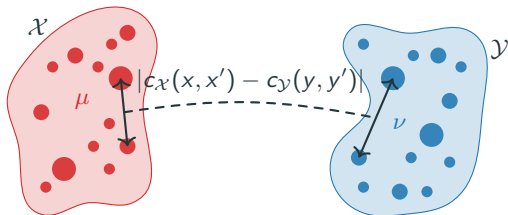
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## 1.2. Gromov–Wasserstein

## Gromov–Wasserstein problem

We consider the following quadratic minimization problem:

$$\inf_{\pi \in \Pi(\mu, \nu)} \iint_{\mathcal{X} \times \mathcal{Y}} |c_{\mathcal{X}}(x, x') - c_{\mathcal{Y}}(y, y')|^p d\pi(x, y) d\pi(x', y'). \quad (\text{GW})$$



- quadratic in  $\pi$  + non-convex  $\implies$  much harder than OT
- distance between mm-spaces, i.e.  $\text{GW}(\mathbb{X}, \mathbb{Y}) = 0$  iff  $\mathbb{X} = (\mathcal{X}, d_{\mathcal{X}}^q, \mu)$  and  $\mathbb{Y} = (\mathcal{Y}, d_{\mathcal{Y}}^q, \nu)$  are *strongly isomorphic* [?]

### Question

What can be said on the existence of Monge maps for the Gromov–Wasserstein problem?

## 1. Introduction

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### 1.3. Existing results

## Context

Let  $n \geq d$ . We consider the GW problem for  $\mu, \nu \in \mathbb{R}^n \times \mathbb{R}^d$  in 2 different settings:

1. the *inner product case*, where  $c_X = c_Y = \langle \cdot, \cdot \rangle$ :

$$\min_{\pi \in \Pi(\mu, \nu)} \iint_{\mathcal{X} \times \mathcal{Y}} |\langle x, x' \rangle - \langle y, y' \rangle|^2 d\pi(x, y) d\pi(x', y'),$$

(GW inner prod)

- e.g. on a  $d$ -dimensional sphere  $\mathbb{S}^{d-1}$

2. the *quadratic case*, where  $c_X = c_Y = |\cdot|^2$ :

$$\min_{\pi \in \Pi(\mu, \nu)} \iint_{\mathcal{X} \times \mathcal{Y}} \left| |x - x'|^2 - |y - y'|^2 \right|^2 d\pi(x, y) d\pi(x', y'),$$

(GW quadratic)

- standard choice for  $c_X$  and  $c_Y$

→ both studied in the literature [?, ?]

In the following,  $n = d$ .

## Existing results

1. the *inner product case*, where  $c_{\mathcal{X}} = c_{\mathcal{Y}} = \langle \cdot, \cdot \rangle$ :

[?]

Let  $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$  of finite second order moment with  $\mu \ll \mathcal{L}^n$ . Suppose that there exists a solution  $\pi^*$  such that  $M^* = \int y \otimes x \, d\pi^*(x, y)$  is of *full rank*. Then there exists an optimal map  $T = \nabla f \circ M^*$  with  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  convex.

2. the *quadratic case*, where  $c_{\mathcal{X}} = c_{\mathcal{Y}} = |\cdot|^2$ :

[?]

Let  $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$  with *density, rotationally invariant* around their barycenter. Then optimal transport plans are *induced by a map* which is the monotone increasing rearrangement between the radial distributions of  $\mu$  and  $\nu$ .

[?]

Let  $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$  with compact support. Assume that  $\mu \ll \mathcal{L}^n$  and that both  $\mu$  and  $\nu$  are centered. *Suppose* that there exists  $\pi^*$  such that  $M^* = \int y \otimes x \, d\pi^*(x, y)$  is of *full rank* and that *there exists a differentiable convex  $F : \mathbb{R} \rightarrow \mathbb{R}$  such that  $|T(x)|_2^2 = F'(|x|_2^2)$* , *then there exists an optimal map  $T = \nabla f \circ M^*$  with  $f$  convex.*

Let  $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$  with compact supports. Suppose  $\mu \ll \mathcal{L}^n$ .

1. **Theorem:** The (GW inner prod) problem admits a *map* as a solution.
2. **Theorem:** The (GW quadratic) problem either admits a *map*, a *bimap* or a *map/anti-map* as a solution.
3. **Conjecture:** The second claim is *tight*: there exists cases where optimal solutions of (GW quadratic) are *not maps*.

Bonus: complementary study of (GW quadratic) in dimension one.

## 2. Monge maps for GW

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## Preliminary: bilinear relaxation

Denote  $(GW) = \min_{\pi} F(\pi, \pi)$ ,  $F$  bilinear.

Possible relaxation:  $(GW) \geq \min_{\pi, \gamma} F(\pi, \gamma)$  with  $\pi, \gamma \in \Pi(\mu, \nu)$ .

### Tightness

If  $c_Y$  and  $c_X$  are both conditionally positive (or both conditionally negative), then the relaxation of  $GW_2^2$  *is tight*.

If  $(\pi_*, \gamma_*)$  minimizer of relaxation, then  $(\pi_*, \pi_*)$  and  $(\gamma_*, \gamma_*)$  also.

### Definition

A function  $c_X : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  is a conditionally negative kernel if for every  $n \geq 1$ ,  $x_1, \dots, x_n \in \mathcal{X}$  and every  $\alpha_1, \dots, \alpha_n$  such that  $\sum_i \alpha_i = 0$  then  $\sum_{ij} \alpha_i \alpha_j c_X(x_i, x_j) \leq 0$ .

### Proof.

Problem is *maximization* of a positive quadratic form + elementary computation. □

Examples: inner product cost, quadratic cost.

**First-order optimality condition** Linearization is an OT problem.

- $(\text{GW}) = \min_{\pi} F(\pi, \pi)$  with  $F$  symmetric bilinear
- $\pi^*$  minimizes  $(\text{GW}) \implies$  minimizes  $\pi \mapsto 2F(\pi, \pi^*)$ :

$$\min_{\pi \in \Pi(\mu, \nu)} \int C_{\pi^*}(x, y) d\pi(x, y), \quad \text{with } C_{\pi^*}(x, y) = \int |c_X(x, x') - c_Y(y, y')|^p d\pi^*$$

I will prove something on *one* of the minimizers of the linearization.  
Tightness of relaxation implies these are also minimizers of GW.

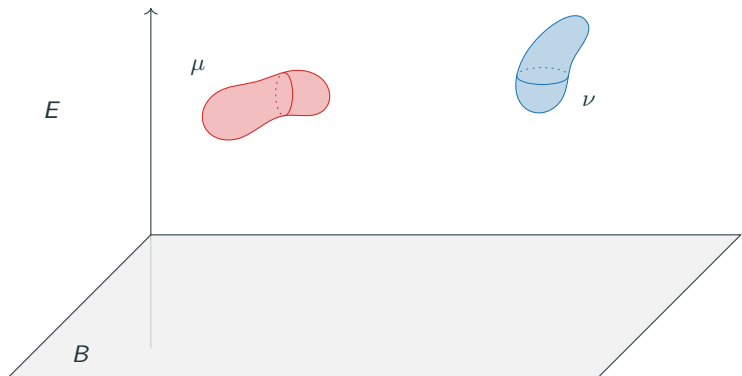
- twist conditions for our linearized costs?  $\implies$  not always, need something a bit more general.

## 2. Monge maps for GW

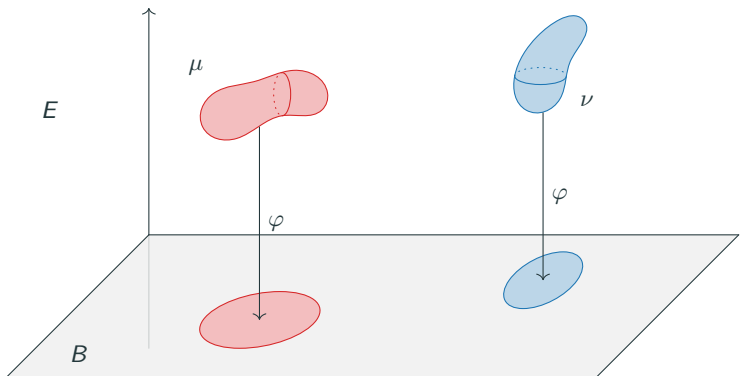
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### 2.1. A key lemma

“Let  $\mu, \nu \in \mathcal{P}(E)$ .”



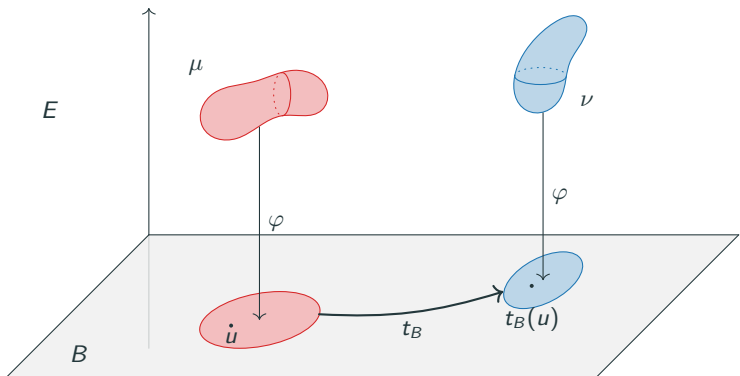
“Let  $\mu, \nu \in \mathcal{P}(E)$ . If we can send  $\mu$  and  $\nu$  in a space  $B$  by a function  $\varphi$ ,



“Let  $\mu, \nu \in \mathcal{P}(E)$ . If we can send  $\mu$  and  $\nu$  in a space  $B$  by a function  $\varphi$ , s.t.

$$c(x, y) = \tilde{c}(\varphi(x), \varphi(y)) \quad \text{for all } x, y \in E$$

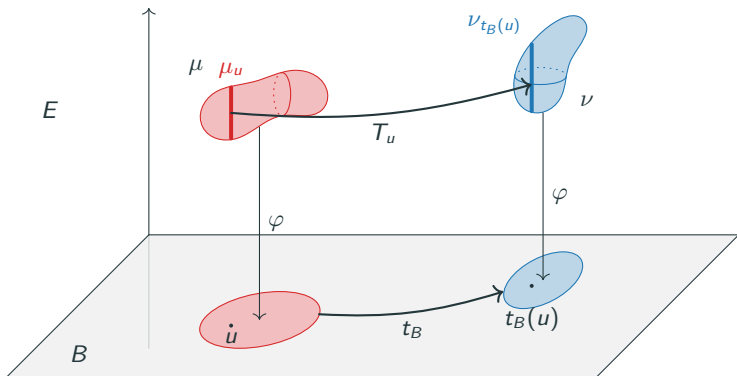
with  $\tilde{c}$  a *twisted* cost on  $B$ ,



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with  $\tilde{c}$  a *twisted* cost on  $B$ , then *we can construct an optimal map between  $\mu$  and  $\nu$ .*”



**Theorem: existence of a Monge map, inner product cost**

Let  $E_0$  be a measurable space and  $B_0$  and  $F$  be complete Riemannian manifolds. Let  $\mu, \nu \in \mathcal{P}(E_0)$  with *compact support*. Assume that there exists a set  $E \subset E_0$  s.t.  $\mu(E) = 1$  and that there exists a measurable map  $\Phi : E \rightarrow B_0 \times F$  that is injective and whose inverse on its image is measurable as well. Let  $\varphi \triangleq p_B \circ \Phi : E \rightarrow B_0$ . Let  $c : E_0 \times E_0 \rightarrow \mathbb{R}$  and suppose that there exists a *twisted*  $\tilde{c} : B_0 \times B_0 \rightarrow \mathbb{R}$  s.t.

$$c(x, y) = \tilde{c}(\varphi(x), \varphi(y)) \quad \text{for all } x, y \in E_0.$$

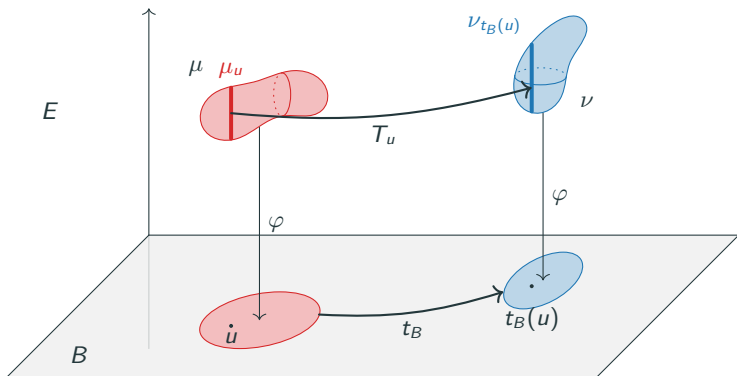
Assume that  $\varphi_{\#}\mu \ll \mathcal{L}_{B_0}$  and let thus  $t_B$  denote the unique Monge map between  $\varphi_{\#}\mu$  and  $\varphi_{\#}\nu$  for this cost. Suppose that there exists a disintegration  $((\Phi_{\#}\mu)_u)_u$  of  $\Phi_{\#}\mu$  by  $p_B$  s.t. for  $\varphi_{\#}\mu$ -a.e.  $u$ ,  $(\Phi_{\#}\mu)_u \ll \text{vol}_F$ .

Then *there exists an optimal map*  $T$  between  $\mu$  and  $\nu$  for the cost  $c$  that can be decomposed as

$$\Phi \circ T \circ \Phi^{-1}(u, v) = (t_B(u), t_F(u, v)) = \left( \underbrace{\tilde{c} - \exp_u(\nabla f(u))}_{\in B}, \underbrace{\exp_v(\nabla g_u(v))}_{\in \text{fiber}} \right),$$

with  $f : B_0 \rightarrow \mathbb{R}$   $\tilde{c}$ -convex and  $g_u : F \rightarrow \mathbb{R}$   $d_F^2/2$ -convex for  $\varphi_{\#}\mu$ -a.e.  $u$ .





1. *transport in B*:  $\tilde{c}$  satisfies (Twist) on  $B$ ;
2. *transport the fibers*: choose a map for each couple of fibers  $(\mu_u, \nu_{t_B(u)})$
3. is  $T(u, x) = T_u(x)$  *measurable*? need theorem! adaptation of [?] to the manifold setting

**Take-home message:**  $c(x, y) = \tilde{c}(\varphi(x), \varphi(y))$  with  $\tilde{c}$  twisted  $\implies$  map

## 2. Monge maps for GW

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### 2.2. Application: inner product cost

Let's work on (GW inner prod):

$$\min_{\pi \in \Pi(\mu, \nu)} \iint |\langle x, x' \rangle - \langle y, y' \rangle|^2 d\pi(x, y) d\pi(x', y') \quad (\text{GW inner prod})$$

$$\iff \min_{\pi \in \Pi(\mu, \nu)} \iint -\langle x, x' \rangle \langle y, y' \rangle d\pi(x, y) d\pi(x', y')$$

$\implies$  OT problem with

$$c(x, y) = - \int \langle x, x' \rangle \langle y, y' \rangle d\pi^*(x', y') = \dots = -\langle M^* x, y \rangle$$

$$\text{where } M^* \triangleq \int y' x'^T d\pi^*(x', y') \in \mathbb{R}^{n \times n}$$

rk $M^*$	$= n$	$\leq n - 1$
twist	✓	·
subtwist	✓	·
$m$ -twist, $m \geq 2$	✓	·

1. *a simplification*: up to SVD, suppose  $M^*$  is a diagonal matrix of singular values:

$$M^* = \begin{pmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_h & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix}$$

2. *rephrase the cost*:

$$\begin{aligned} c(x, y) &= -\langle M^* x, y \rangle \\ &= -\sum_{i=1}^h \sigma_i x_i y_i \\ &\triangleq \tilde{c}(p(x), p(y)) \quad \text{with } p \text{ the orthogonal projection on } \mathbb{R}^h. \end{aligned}$$

3. *apply key lemma!*

- $B$  is  $\mathbb{R}^h$
- fibers are  $\mathbb{R}^{n-h}$
- $\tilde{c}$  is twisted on  $\mathbb{R}^h$

$\Rightarrow$  optimal map + structure!

$$\text{for } x = (u, v) \in \mathbb{R}^h \times \mathbb{R}^{n-h}, \quad T(u, v) = (\nabla f \circ M^*(u), \nabla g_u(v)).$$

## 2. Monge maps for GW

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### 2.3. Application: quadratic cost

Similarly, we work on (GW quadratic) and relax to a classical OT problem with

$$c(x, y) = -|x|^2|y|^2 - 4\langle M^*x, y \rangle.$$

rk $M^*$	$= n$	$= n - 1$	$\leq n - 2$
twist	·	·	·
subtwist	✓	·	·
2-twist	✓	✓	·

Similarly, we work on (GW quadratic) and relax to a classical OT problem with

$$c(x, y) = -|x|^2|y|^2 - 4\langle M^*x, y \rangle.$$

rk $M^*$	$= n$	$= n - 1$	$\leq n - 2$
twist	·	·	·
subtwist	✓	·	·
2-twist	✓	✓	·
	⇓	⇓	⇓
	map/anti-map and bimap	bimap	...

### Theorem: quadratic cost

Let  $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$  of compact support. Suppose that  $\mu$  has a density. Let  $\pi^*$  be an optimal plan and  $M^* \triangleq \int y'x'^T d\pi^*(x', y')$ . Then:

- ✓ if  $\text{rk } M^* = n$ , there is an optimal *map/anti-map*,
- ✓ if  $\text{rk } M^* = n - 1$ , there is an optimal *bimap*,
- (!!) if  $\text{rk } M^* \leq n - 2$ , *there is an optimal map!*



1. *a simplification*: up to SVD,  $M^*$  is diagonal:

$$M^* = \begin{pmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_h & \\ & & & 0 \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix}. \quad \text{We note } x = \underbrace{(x_1, \dots, x_h)}_{x_H} \underbrace{(x_{h+1}, \dots, x_n)}_{x_\perp}.$$

2. *rephrase the cost*:

$$\begin{aligned} -c(x, y) &= |x|^2|y|^2 + 4\langle M^*x, y \rangle \\ &= |x_H|^2|y_H|^2 + |x_H|^2|y_\perp|^2 + |x_\perp|^2|y_H|^2 + |x_\perp|^2|y_\perp|^2 + 4\langle \tilde{M}x_H, y_H \rangle \\ &= |x_H|^2|y_H|^2 + |x_H|^2n(y) + n(x)|y_H|^2 + n(x)n(y) + 4\langle \tilde{M}x_H, y_H \rangle \\ &\triangleq -\tilde{c}(\varphi(x), \varphi(y)), \end{aligned}$$

with  $n : x \mapsto |x_\perp|^2$  and  $\varphi : x \mapsto (x_H, |x_\perp|^2)$ .

3. *apply key lemma!*

- $B$  is  $\mathbb{R}^h \times \mathbb{R}^+$
- the fibers are spheres  $\mathbb{S}^{n-h-1}$
- $\tilde{c}$  is twisted on  $\mathbb{R}^h \times \mathbb{R}^+$

$\Rightarrow$  optimal map + structure!

$$\text{for } x \approx (u, v) \in \mathbb{R}^h \times \mathbb{R}^+ \times \mathbb{S}^{n-h-1}, \quad T(u, v) = (\tilde{c} - \exp_u(\nabla f(u)), \exp_v(\nabla g_u(v))).$$

### **3. Summary & discussion**

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### Contributions

1. **Thm:** always a *map* for (GW inner prod)
2. **Thm:** a *map*, *bimap* or *map/anti-map* for (GW quadratic)
3. **Numerical Conj:** this second claim is *tight*
4. (**Thm:** monotone rearrangement optimal for (GW quadratic) between measures composed of *two distant parts*): global dominates the local.

### Some questions:

- quadratic cost:
  - better understanding of the 1d case.
- A (motivated) cost with tractable GW and structured maps?