Regularized Optimal Transport is Ground Cost Adversarial

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Abstract

Regularizing Wasserstein distances has proved to be the key in the recent advances of optimal transport (OT) in machine learning. Most prominent is the entropic regularization of OT, which not only allows for fast computations and differentiation using Sinkhorn algorithm, but also improves stability with respect to data and accuracy in many numerical experiments. Theoretical understanding of these benefits remains unclear, although recent statistical works have shown that entropy-regularized OT mitigates classical OT’s curse of dimensionality. In this paper, we adopt a more geometrical point of view, and show using Fenchel duality that any convex regularization of OT can be interpreted as ground cost adversarial. This incidentally gives access to a robust dissimilarity measure on the ground space, which can in turn be used in other applications. We propose algorithms to compute this robust cost, and illustrate the interest of this approach empirically.

1. Introduction

Optimal transport (OT) has become a generic tool in machine learning, with applications in various domains such as supervised machine learning (Frogner et al., 2015; Abadeh et al., 2015; Courty et al., 2016), graphics (Solomon et al., 2015; Bonneel et al., 2016), imaging (Rabin & Papadakis, 2015; Cuturi & Peyré, 2016), generative models (Arjovsky et al., 2017; Salimans et al., 2018), biology (Hashimoto et al., 2016; Schiebinger et al., 2019) or NLP (Grave et al., 2019; Alaux et al., 2019). The key to using OT in these applications lies in the different forms of regularization of the original OT problem studied in the renowned books of (Villani, 2009; Santambrogio, 2015). Adding a small convex regularization to the classical linear cost not only helps on the algorithmic side, by convexifying the objective and allowing for faster solvers, but also add some stability with respect to the input measures, improving numerical results.

Regularizing OT Although entropy-regularized OT appears as the most studied regularization of OT, due to its algorithmic advantages (Cuturi, 2013), several other convex regularizations of the transport plan have been proposed in the community: quadratically-regularized OT (Essid & Solomon, 2017), OT with capacity constraints (Korman & McCann, 2015), Group-Lasso regularized OT (Courty et al., 2016), OT with Laplacian regularization (Flamary et al., 2014), among others. On the other hand, regularizing the dual Kantorovich problem was shown in (Liero et al., 2018) to be equivalent to unbalanced OT, that is optimal transport with relaxed marginal constraints.

Understanding why regularization helps The question of understanding why regularizing OT proves critical has triggered several approaches. One particularly active is the statistical study of entropic regularization: although classical OT suffers from the curse of dimensionality, as its empirical version converges at a rate of order $(1/n)^{1/d}$ (Dudley, 1969; Fournier & Guillin, 2015; Weed et al., 2019), Sinkhorn divergences have a sample complexity of $O(1/\sqrt{n})$ (Genevay et al., 2018; Mena & Niles-Weed, 2019). Entropic OT was also shown to perform maximum likelihood estimation in the Gaussian deconvolution model (Rigollet & Weed, 2018). Taking another approach, (Dessein et al., 2018; Blondel et al., 2018) have considered general classes of convex regularizations and characterized them from a more geometrical perspective. Recently, several papers (Flamary et al., 2018; Deshpande et al., 2019; Kolouri et al., 2019; Niles-Weed & Rigollet, 2019; Paty & Cuturi, 2019) proposed to maximize OT with respect to the ground cost, which can in turn be interpreted in light of ground metric learning (Cuturi & Avis, 2014). Continuing along these lines, we make a connection between regularizing and maximizing OT.

Contributions Our main goal is to provide a novel interpretation of regularized optimal transport in terms of ground cost robustness: regularizing OT amounts to maximizing unregularized OT with respect to the ground cost. Our contributions are:

1. We show that any convex regularization of the transport plan corresponds to ground-cost robustness (section 3);
2. We reinterpret classical regularizations of OT in the ground-cost adversarial setting (section 3.3);
3. We prove, under some technical assumption, a duality theorem for regularized OT, which we use to show that under the same assumption, there exists an optimal adversarial ground-cost that is separable (section 4);

4. We propose to extend the notion of ground-cost robustness to more than two measures, and focus on the case where the measures are time-varying (section 5);

5. We give some algorithms to solve the above-mentioned problems (section 6) and illustrate them on data (section 7).

2. Background on Optimal Transport and Notations

Let $\mathcal{X}$ be a compact Hausdorff space, and define $\mathcal{P}(\mathcal{X})$ the set of Borel probability measures over $\mathcal{X}$. We write $\mathcal{C}(\mathcal{X})$ for the set of continuous functions from $\mathcal{X}$ to $\mathbb{R}$, endowed with the supremum norm. For $\phi, \psi \in \mathcal{C}(\mathcal{X})$, we write $\phi \oplus \psi \in \mathcal{C}(\mathcal{X}^2)$ for the function $(x, y) \mapsto \phi(x) + \psi(y)$.

For $n \in \mathbb{N}$, we write $[n] = \{1, \ldots, n\}$. All vectors will be denoted with bold symbols. For a Boolean assertion $A$, we write $\iota(A)$ for its indicator function $\iota(A) = 0$ if $A$ is true and $\iota(A) = +\infty$ otherwise.

Kantorovich Formulation of OT For $\mu, \nu \in \mathcal{P}(\mathcal{X})$, we write $\Pi(\mu, \nu)$ for the set of couplings

$$\Pi(\mu, \nu) = \{\pi \in \mathcal{P}(\mathcal{X}^2) \text{ s.t. } \forall A, B \subset \mathcal{X} \text{ Borel, } \pi(A \times \mathcal{X}) = \mu(A), \pi(\mathcal{X} \times B) = \nu(B)\}.$$ 

For a real-valued continuous function $c \in \mathcal{C}(\mathcal{X}^2)$, the optimal transport cost between $\mu$ and $\nu$ is defined as

$$\mathcal{C}_c(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathcal{X}^2} c(x, y) \, d\pi(x, y).$$  \tag{1}

Since $c$ is continuous and $\mathcal{X}$ is compact, the infimum in (1) is attained, see Theorem 1.4 in (Santambrogio, 2015). Problem (1) admits the following dual formulation, see Proposition 1.11 and Theorem 1.39 in (Santambrogio, 2015):

$$\mathcal{C}_c(\mu, \nu) = \max_{\phi, \psi \in \mathcal{C}(\mathcal{X})} \int \phi \, d\mu + \int \psi \, d\nu.$$  \tag{2}

Space of Measures Since $\mathcal{X}$ is compact, the dual space of $\mathcal{C}(\mathcal{X}^2)$ is the set $\mathcal{M}(\mathcal{X}^2)$ of Borel finite signed measures over $\mathcal{X}^2$. For $F : \mathcal{M}(\mathcal{X}^2) \to \mathbb{R}$, we recall that $F$ is Fréchet-differentiable at $\pi$ if there exists $\nabla F(\pi) \in \mathcal{C}(\mathcal{X}^2)$ such that for any $h \in \mathcal{M}(\mathcal{X}^2)$, as $t \to 0$

$$F(\pi + th) = F(\pi) + t \int \nabla F(\pi) \, dh + o(t).$$ 

Similarly, $G : \mathcal{C}(\mathcal{X}^2) \to \mathbb{R}$ is Fréchet-differentiable at $c$ if there exists $\nabla G(c) \in \mathcal{M}(\mathcal{X}^2)$ such that for any $h \in \mathcal{C}(\mathcal{X}^2)$, as $t \to 0$

$$G(c + th) = G(c) + t \int h \, d\nabla G(c) + o(t).$$

Legendre–Fenchel Transformation For any functional $F : \mathcal{M}(\mathcal{X}^2) \to \mathbb{R} \cup \{+\infty\}$, we can define its convex conjugate $F^* : \mathcal{C}(\mathcal{X}^2) \to \mathbb{R} \cup \{+\infty\}$ and biconjugate $F^{**} : \mathcal{M}(\mathcal{X}^2) \to \mathbb{R} \cup \{+\infty\}$ as

$$F^*(c) := \sup_{\pi \in \mathcal{M}(\mathcal{X}^2)} \int c \, d\pi - F(\pi),$$

$$F^{**}(\pi) := \sup_{c \in \mathcal{C}(\mathcal{X}^2)} \int c \, d\pi - F^*(c).$$

$F^*$ is always lower semi-continuous (lsc) and convex as the supremum of continuous linear functions.

Specific notations For $F : \mathcal{M}(\mathcal{X}^2) \to \mathbb{R} \cup \{+\infty\}$, we write $\text{dom}(F) = \{\pi \in \mathcal{M}(\mathcal{X}^2) \mid F(\pi) < +\infty\}$ for its domain and will say $F$ is proper if $\text{dom}(F) \neq \emptyset$.

We will denote by $\mathcal{F}$ the set of proper lsc convex functions $F : \mathcal{M}(\mathcal{X}^2) \to \mathbb{R} \cup \{+\infty\}$, and for $\mu, \nu \in \mathcal{P}(\mathcal{X})$, we define the set $\mathcal{F}(\mu, \nu)$ of lsc convex functions that are proper on $\Pi(\mu, \nu)$:

$$\mathcal{F}(\mu, \nu) = \{F \in \mathcal{F} \mid \exists \pi \in \Pi(\mu, \nu), F(\pi) < +\infty\}.$$ 

3. Ground Cost Adversarial Optimal Transport

3.1. Definition

Instead of considering the classical linear formulation of optimal transport (1), we will consider the following more general nonlinear formulation:

Definition 1. Let $F \in \mathcal{F}$. For $\mu, \nu \in \mathcal{P}(\mathcal{X})$, we define:

$$\mathcal{W}_F(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} F(\pi).$$  \tag{3}

Lemma 1. The infimum in (3) is attained. Moreover, if $F \in \mathcal{F}(\mu, \nu)$, $\mathcal{W}_F(\mu, \nu) < +\infty$.

Proof. We can apply Weierstrass’s theorem since $\Pi(\mu, \nu)$ is compact and $F$ is lsc by definition.

For $F \in \mathcal{F}(\mu, \nu)$, there exists $\pi_0 \in \Pi(\mu, \nu)$ such that $F(\pi_0) < +\infty$, so $\mathcal{W}_F(\mu, \nu) \leq F(\pi_0) < +\infty$. \hfill \Box

The main result of this paper is the following interpretation of problem (3) as a ground-cost adversarial OT problem:
Theorem 1. For $\mu, \nu \in \mathcal{P}(X)$ and $F \in \mathcal{F}(\mu, \nu)$, minimizing $F$ over $\Pi(\mu, \nu)$ is equivalent to the following concave problem:

$$\mathcal{H}_F(\mu, \nu) = \sup_{c \in C(X^2)} \mathcal{T}(\mu, \nu) - F^*(c).$$

(4)

Proof. Since $F$ is proper, lsc and convex, Fenchel-Moreau theorem ensures that it is equal to its convex biconjugate $F^{**}$, so:

$$\min_{\pi \in \Pi(\mu, \nu)} F(\pi) = \min_{\pi \in \Pi(\mu, \nu)} F^{**}(\pi)$$

$$= \min_{\pi \in \Pi(\mu, \nu)} \sup_{c \in C(X^2)} \int c \, d\pi - F^*(c).$$

Define the objective $l(\pi, c) := \int c \, d\pi - F^*(c)$. Since $F^*$ is lsc as the convex conjugate of $F$, for any $\pi \in \Pi(\mu, \nu)$, $l(\pi, c)$ is usc. It is also concave as the sum of concave functions. Likewise, for any $c \in C(X^2)$, $l(c, \pi)$ is continuous and convex (in fact linear). Since $\Pi(\mu, \nu)$ and $C(X^2)$ are convex, and $\Pi(\mu, \nu)$ is compact, we can use Sion’s minimax theorem to swap the min and the sup:

$$\min_{\pi \in \Pi(\mu, \nu)} F(\pi) = \sup_{c \in C(X^2)} \min_{\pi \in \Pi(\mu, \nu)} \int c \, d\pi - F^*(c).$$

Remark 1. Note that the inequality

$$\mathcal{H}_F(\mu, \nu) \geq \sup_{c \in C(X^2)} \mathcal{T}(\mu, \nu) - F^*(c)$$

is in fact verified for any $F : \mathcal{M}(X^2) \to \mathbb{R} \cup \{+\infty\}$ since $F \geq F^{**}$ is always verified.

The supremum in equation (4) is not necessarily attained. Under some regularity assumption on $F$, we show that the supremum is attained and relate the optimal couplings and the optimal ground costs:

Proposition 1. Let $\mu, \nu \in \mathcal{P}(X)$ and $F \in \mathcal{F}(\mu, \nu)$. Suppose that $F$ is Fréchet-differentiable on $\Pi(\mu, \nu)$. Then the supremum in (4) is attained at $c_* = \nabla F(\pi_*)$ where $\pi_*$ is any minimizer of (3). Conversely, suppose $F^*$ is Fréchet-differentiable everywhere. If $c_*$ is the unique maximizer in (4), then $\pi_* = \nabla F^*(c_*)$ is a minimizer of (3).

In section 4, we will further characterize $c_*$ for a class of functions $F \in \mathcal{F}$. See a proof in appendix.

One interesting particular case of Theorem 1 is when the convex cost $\pi \rightarrow F(\pi)$ is a convex regularization of the classical linear optimal transport:

Corollary 1. Let $c_0 \in C(X^2)$, $\mu, \nu \in \mathcal{P}(X)$. Let $\varepsilon > 0$ and $R \in \mathcal{F}(\mu, \nu)$. Then:

$$\min_{\pi \in \Pi(\mu, \nu)} \int c_0 \, d\pi + \varepsilon R(\pi)$$

$$= \sup_{c \in C(X^2)} \mathcal{T}(\mu, \nu) - \varepsilon R^*(\frac{c - c_0}{\varepsilon}).$$

(5)

Proof. We apply theorem 1 with $F(\pi) = \int c_0 \, d\pi + \varepsilon R(\pi)$, for which we only need to compute the convex conjugate:

$$F^*(c) = \sup_{\pi \in \mathcal{M}(X^2)} \int c - c_0 \, d\pi - \varepsilon R(\pi)$$

$$= \varepsilon \sup_{\pi \in \mathcal{M}(X^2)} \int \frac{c - c_0}{\varepsilon} \, d\pi - R(\pi)$$

$$= \varepsilon R^*\left(\frac{c - c_0}{\varepsilon}\right).$$

3.2. Discrete Separable Case

In this subsection, we will focus on the discrete case where the space $X = \{1\}$ for some $n \in \mathbb{N}$. A probability measure $\mu \in \mathcal{P}(X)$ is then a histogram of size $n$ that we will represent by a vector $\mu \in \mathbb{R}^n_+$ such that $\sum_{i=1}^n \mu_i = 1$. Cost functions $c \in C(X^2)$ and transport plans $\pi \in \Pi(\mu, \nu)$ are now matrices $c, \pi \in \mathbb{R}^{n \times n}$.

We focus on regularization functions $R$ that are separable, i.e. of the form

$$R(\pi) = \sum_{i=1}^n \sum_{j=1}^n R_{ij}(\pi_{ij})$$

for some differentiable convex proper lsc $R_{ij} : \mathbb{R} \rightarrow \mathbb{R}$.

In applications, it may be natural to ask that the ground cost $c \in \mathbb{R}^{n \times n}$ has nonnegative entries. Adding this constraint on the adversarial cost corresponds to linearizing “at short range” the regularization $R$ for “small transport values”:

Proposition 2. Let $\varepsilon > 0$. For $\mu, \nu \in \mathcal{P}(X)$, it holds:

$$\sup_{c \in \mathbb{R}^{n \times n}_+} \mathcal{T}(\mu, \nu) - \varepsilon \sum_{ij} R_{ij}^*\left(\frac{c_{ij} - c_{0ij}}{\varepsilon}\right)$$

$$= \min_{\pi \in \Pi(\mu, \nu)} \langle c_0, \pi \rangle + \varepsilon \sum_{ij} \tilde{R}_{ij}(\pi_{ij})$$

(6)

where $\tilde{R}_{ij} : \mathbb{R} \rightarrow \mathbb{R}$ is the continuous convex function defined as

$$\tilde{R}_{ij}(x) := \begin{cases} R_{ij}(x) & \text{if } x \geq R_{ij}^*\left(\frac{c_{0ij}}{\varepsilon}\right) \\ & \text{otherwise} \end{cases}$$

Moreover, if $R_{ij}$ is of class $C^1$, then $\tilde{R}_{ij}$ is also $C^1$.

We give a proof in the appendix.

3.3. Examples

As presented in the introduction, several convex regularizations $R$ have been proposed. We give the ground cost adversarial counterpart for some of them: two examples in the continuous setting, and three $p$-norm based regularizations in the discrete case.
Figure 1. The entropy regularization \( R(x) = x \log(x) \) and its linearized version \( \tilde{R}(x) \) for small transport values.

Example 1 (Entropic Regularization). Let \( \mu, \nu \in \mathcal{P}(\mathcal{X}) \). For \( \pi \in \Pi(\mu, \nu) \), we define its relative entropy as \( \text{KL}(\pi | \mu \otimes \nu) = \int \log \frac{d\pi}{d\mu \otimes \nu} \, d\pi \). Then for \( c_0 \in \mathcal{C}(\mathcal{X}^2) \) and \( \varepsilon > 0 \), it holds:

\[
\min_{\pi \in \Pi(\mu, \nu)} \int c_0 \, d\pi + \varepsilon \text{KL}(\pi | \mu \otimes \nu) = \sup_{c \in \mathcal{C}(\mathcal{X}^2)} T_c(\mu, \nu) - \varepsilon \int \exp \left( \frac{c - c_0}{\varepsilon} \right) \, d\mu \otimes \nu + \varepsilon.
\]

Proof. Let \( \pi \in \mathcal{M}(\mathcal{X}^2) \), then:

\[
R(\pi) = \begin{cases} \int \log \frac{d\pi}{d\mu \otimes \nu} \, d\pi - \int d\pi + 1 & \text{if } \pi \ll \mu \otimes \nu \\ +\infty & \text{otherwise.} \end{cases}
\]

Applying corollary 1 concludes the proof.

Another case of interest is the so-called Subspace Robust Wasserstein distance recently proposed by (Paty & Cuturi, 2019). Here, the set of adversarial metrics is parameterized by a finite-dimensional parameter \( \Omega \), which allows to recover an adversarial metric defined on the whole space even when the measures are finitely supported.

Example 2 (Subspace Robust Wasserstein). Let \( d \in \mathbb{N}, k \in [d] \) and \( \mu, \nu \in \mathcal{P}(\mathbb{R}^d) \) with a finite second-order moment. For \( \pi \in \Pi(\mu, \nu) \), define \( V_\pi = \int (x - y) (x - y)^\top d\pi(x, y) \) and \( \lambda_1(V_\pi) \geq \ldots \geq \lambda_d(V_\pi) \) its ordered eigenvalues.

Then \( F : \pi \mapsto \sum_{i=1}^k \lambda_i(V_\pi) \) is convex, and

\[
\mathcal{S}_k(\mu, \nu) := \min_{\pi \in \Pi(\mu, \nu)} \sum_{i=1}^k \lambda_i(V_\pi) = \max_{0 \leq \Omega \leq I} \frac{\text{Tr}(\Omega)}{\text{Tr}(\Omega) - k} \mathcal{R} \Theta^2_k(\mu, \nu)
\]

where \( d^2_\Theta(x, y) = (x - y)^\top \Omega(x - y) \) is the squared Mahalanobis distance.

Proof. See Theorem 1 in (Paty & Cuturi, 2019). Note that in this case, \( \mathcal{X} = \mathbb{R}^d \) is not compact. This actually poses no problem since \( F^* \equiv +\infty \) outside a compact set, i.e. the set on metrics on which the maximization takes place is compact. Indeed, one can show that:

\[
F^*(c) = \iota(\exists \Omega \leq I \text{ with } \text{Tr}(\Omega) = k \text{ s.t. } c = d^2_\Theta). \quad \square
\]

Let us now consider \( p \)-norm based examples, which will subsume quadratically-regularized \((p = 2)\) OT studied in (Essid & Solomon, 2017; Lorenz et al., 2019) and capacity-constrained \((p = +\infty)\) OT proposed by (Korman & McCann, 2015).

For a matrix \( w \in \mathbb{R}_{++}^{n \times n} \) with \( \sum_{i,j} w_{ij} = n^2 \) and \( \pi \in \mathbb{R}^{n \times n} \), we will denote by \( \| \pi \|_{w,p} = \sum_{i,j} w_{ij} |\pi_{ij}|^p \) the \( w \)-weighted (powered) \( p \)-norm of \( \pi \). We also write \( 1/w \) for the matrix defined by \( (1/w)_{ij} = 1/w_{ij} \). In the following, we take \( p, q \in [1, +\infty] \) such that \( 1/p + 1/q = 1 \).

Example 3 (\( \| \cdot \|_{w,p} \) Regularization).

\[
\min_{\pi \in \Pi(\mu, \nu)} (c_0, \pi) + \frac{1}{p} \| \pi \|_{w,p}^p = \sup_{c \in \mathbb{R}^{n \times n}} \mathcal{T}_c(\mu, \nu) - \varepsilon \| \pi - c_0 \|_{w,q}^q \cdot \frac{1}{q} \| c - c_0 \| \| c - c_0 \|_{w,q}^q.
\]

In particular when \( p = 2 \) and \( w = 1 \), this corresponds to quadratically-regularized OT studied in (Essid & Solomon, 2017; Lorenz et al., 2019).

We give the details of the (straightforward) computations in the appendix.

Example 4 (\( \| \cdot \|_{w,p} \) Penalization).

\[
\min_{\pi \in \Pi(\mu, \nu)} (c_0, \pi) + \varepsilon \| \pi \|_{w,p} = \sup_{c \in \mathbb{R}^{n \times n}} \mathcal{T}_c(\mu, \nu).
\]

Proof. We apply Corollary 1 with \( R : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}^{n \times n} \) defined as \( R(\pi) = \| \pi \|_{w,p} \), for which we need to compute its convex conjugate. We know that the dual of \( \| \cdot \|_p \) is \( \iota(\| \cdot \|_q \leq 1) \), and using classical results about convex conjugates, \( \| \cdot \|_{w,p}^* = \iota(\| \cdot \|_1/w,q \leq 1) \).

Example 5 (\( \| \cdot \|_{w,p} \) Regularization).

\[
\min_{\pi \in \Pi(\mu, \nu)} (c_0, \pi) = \sup_{c \in \mathbb{R}^{n \times n}} \mathcal{T}_c(\mu, \nu) - \varepsilon \| c - c_0 \|_{w,q}.
\]

In particular when \( p = +\infty \) and \( w = 1 \), this coincides with capacity-constrained OT proposed by (Korman & McCann, 2015).

Proof. We apply Corollary 1 with \( R : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}^{n \times n} \) defined as \( R(\pi) = \| \pi \|_{w,p} \), for which we need to compute its convex conjugate. We know that the dual of \( \iota(\| \cdot \|_p \leq 1) \) is \( \| \cdot \|_q \), and using classical results about convex conjugates, \( \iota(\| \cdot \|_{w,p}) = \| \cdot \|_{1/w,q} \).

\( \square \)
4. Properties of the Adversarial Cost

Theorem 1 shows that regularizing OT is equivalent to maximizing unregularized OT with respect to the ground cost. This gives access to a robustly computed cost $c_*$ on the ground space, which we characterize in this section. We have already seen in proposition 1 that we can get $c_*$ if we have solved the primal problem $\mathcal{W}_F$. Under some technical assumption of $F$, we can show that there exists an optimal adversarial cost which is separable, that is of the form $c_*(x, y) = \phi(x) + \psi(y)$ for some functions $\phi, \psi \in C(X)$.

**Definition 2.** Let $F \in \mathcal{F}$. We will say that $F$ is separably $*$-increasing if for any $\phi, \psi \in C(X)$ and any $c \in C(X^2)$:

$$\phi + \psi \leq c \Rightarrow F^*(\phi + \psi) \leq F^*(c). \quad (7)$$

This definition, albeit not always verified e.g. in the classical linear case $F(\pi) = \int c \, d\pi$, is verified in various cases of interest, e.g. for the entropic or $\| \cdot \|_p$ regularizations:

**Example 6.** For $\mu, \nu \in \mathcal{P}(X)$, $c_0 \in C(X^2)$ and $\varepsilon > 0$, the entropy-regularized OT function

$$F : \pi \mapsto \int c_0 \, d\pi + \varepsilon \text{KL}(\pi || \mu \otimes \nu)$$

is separably $*$-increasing.

**Proof.** As in the proof of example 1,

$$F^*(c) = \varepsilon \int \exp \left( \frac{c - c_0}{\varepsilon} \right) - 1 \, d\mu \otimes \nu$$

which clearly verifies condition (7).

**Example 7.** In the discrete setting $X = [n]$, let $\mu, \nu \in \mathcal{P}(X)$, $c_0 \in \mathbb{R}^{n^2}$, $w \in \mathbb{R}^{n^2}$ summing to $n^2$. Take $p > 1$ and $\varepsilon > 0$. With $\varphi_{p}(x) = x^p$ if $x \geq 0$ and $\varphi_{p}(x) = +\infty$ if $x < 0$, the $\| \cdot \|_{w,p}$-regularized OT function

$$F : \pi \mapsto \langle c_0, \pi \rangle + \varepsilon \sum_{i,j} w_{ij} \varphi_{p}(c_{ij})$$

is separably $*$-increasing.

**Proof.** Note that minimizing $F$ over $\Pi(\mu, \nu) \subset \mathbb{R}^{n^2}$ is equivalent to minimizing $\tilde{F} : \pi \mapsto \langle c_0, \pi \rangle + \varepsilon \sum_{i,j} w_{ij} \varphi_{p}(c_{ij})$. One can show that, with $q > 1$ such that $1/p + 1/q = 1$ and $(x)_+ := \max\{0, x\}$:

$$F^*(c) = \frac{1}{q} \left\| \frac{c - c_0}{\varepsilon} \right\|_{1/q}^q$$

which clearly verifies condition (7).

When $F$ is separably $*$-increasing, we can easily prove a duality theorem for problem (3):

**Theorem 2 ($\mathcal{W}_F$ duality).** Let $\mu, \nu \in \mathcal{P}(X)$ and $F \in \mathcal{F}(\mu, \nu)$ a separably $*$-increasing function. Then:

$$\mathcal{W}_F(\mu, \nu) = \max_{\phi, \psi \in C(X)} \int \phi \, d\mu + \int \psi \, d\nu - F^*(\phi + \psi). \quad (8)$$

**Proof.** The main idea is to use Kantorovich duality (2) in the cost-adversarial formulation of $\mathcal{W}_F(\mu, \nu)$. Then the $*$-increasing property appears naturally as a condition for duality to hold. See the details in the appendix.

**Corollary 2.** If $\phi_*, \psi_*$ are optimal solutions in (8), the cost $\phi_* + \psi_* \in C(X^2)$ is an optimal adversarial cost in (4).

**Proof.** For $\phi, \psi \in C(X)$, note that

$$\mathcal{F}_{\phi,\psi}(\mu, \nu) = \int \phi \, d\mu + \int \psi \, d\nu.$$

Then using $\mathcal{W}_F$ duality:

$$\mathcal{W}_F(\mu, \nu) = \max_{\phi, \psi \in C(X)} \int \phi \, d\mu + \int \psi \, d\nu - F^*(\phi + \psi)$$

$$= \max_{\phi, \psi \in C(X)} \mathcal{F}_{\phi,\psi}(\mu, \nu) - F^*(\phi + \psi)$$

$$\leq \sup_{c \in C(X^2)} \mathcal{F}_{(\mu, \nu)} - F^*(c)$$

$$= \mathcal{W}_F(\mu, \nu)$$

where we have used Theorem 1 in the last line. This shows that the inequality is in fact an equality, so if $\phi_*, \psi_*$ are optimal dual potentials in (8), $\phi_* + \psi_*$ is an optimal adversarial cost in (4).

5. Adversarial Ground-Cost Sequence for Time-varying Measures

For two measures $\mu, \nu \in \mathcal{P}(X)$ and a separably $*$-increasing function $F \in \mathcal{F}(\mu, \nu)$, corollary 2 shows that there exists an optimal adversarial ground cost $c_*$ that is separable. This separability, which is verified e.g. in the entropic or quadratic case, means that the OT problem for $c_*$ is degenerate in the sense that any transport plan is optimal for the cost $c_*$. From a metric learning point of view, $c_*$ is not a suitable dissimilarity measure on $X$. But why limit ourselves to two measures? If we observe $N \in \mathbb{N}$ measures $\mu_1, \ldots, \mu_N \in \mathcal{P}(X)$, we could look for a ground cost $c \in C(X^2)$ that is adversarial to (part of) all the pairs:

$$\mathcal{P}_{F^*}(\mu_1, \ldots, \mu_N) := \sup_{c \in C(X^2)} \sum_{i \neq j} \mathcal{F}_c(\mu_i, \mu_j) - F^*(c) \quad (9)$$

for some convex regularization $F^* : C(X^2) \to \mathbb{R} \cup \{+\infty\}$. Although interesting from an application point of view, problem (9) does not correspond to any regularization of a transport plan. We thus study a slightly different problem.
5.1. Definition

For a sequence of measures \(\mu_{1:T} := \mu_1, \ldots, \mu_T \in \mathcal{P}(\mathcal{X})\), \(T \geq 2\), e.g. when we observe time-evolving data, we can look for a sequence of adversarial costs \(c_{t:T-1} := c_1, \ldots, c_{T-1} \in C(\mathcal{X}^2)\) which is globally adversarial:

**Definition 3.** For \(\eta > 0\), \(D : \mathcal{C}(\mathcal{X}^2) \times \mathcal{C}(\mathcal{X}^2) \to \mathbb{R} \cup \{+\infty\}\) and for \(t \in [T-1]\), \(F_t \in \mathcal{F}(\mu_t, \mu_{t+1})\), we define:

\[
W_{\eta,D,F}(\mu_{1:T}) := \sup_{c_t_{1:T-1}} \sum_{t=1}^{T-1} \mathcal{T}_{\epsilon_t}(\mu_t, \mu_{t+1}) - \eta D(c_t, \epsilon_{t+1}) - F_t^*(c_t)
\]

with the convention \(D(c_{T-1}, \epsilon_{T}) = 0\).

As we show in the two following propositions, \(W_{\eta,D,F}\) interpolates between two different behaviours: as \(\eta \to 0\), \(W_{\eta,D,F}\) will solve independently the successive \(T-1\) regularized OT problems, while as \(\eta \to \infty\), \(W_{\eta,D,F}\) enforces the uniqueness of a joint adversarial cost. Then \(W_{\eta,D,F}\) can be reinterpreted as a regularized multimarginal OT problem.

**Proposition 3.** With the notations of definition 3, for \(\eta = 0\):

\[
W_{0,D,F}(\mu_{1:T}) = \sum_{t=1}^{T-1} \mathcal{W}_{F_t}(\mu_t, \mu_{t+1}).
\]

**Proof.** Since the optimization problem is separable, it holds:

\[
W_{0,D,F}(\mu_{1:T}) = \sup_{c_1_{1:T-1}} \sum_{t=1}^{T-1} \mathcal{T}_{\epsilon_t}(\mu_t, \mu_{t+1}) - F_t^*(c_t)
\]

\[= \sum_{t=1}^{T-1} \sup_{c_t \in C(\mathcal{X}^2)} \mathcal{T}_{\epsilon_t}(\mu_t, \mu_{t+1}) - F_t^*(c_t)
\]

which gives the result using Theorem 1. \(\square\)

**Proposition 4 (Multimarginal interpretation).** With the notations of definition 3, suppose that:

1. \(D\) is continuous,
2. \(D\) is a divergence, i.e. \(D(c_1, c_2) = 0 \iff c_1 = c_2\) and \(D \geq 0\),
3. there exists a compact set \(K \subset C(\mathcal{X}^2)\) such that for all \(t \in [T-1]\), \(F_t \equiv +\infty\) outside of \(K\).

Then:

\[
\lim_{\eta \to +\infty} W_{\eta,D,F}(\mu_{1:T}) = \max_{c \in C(\mathcal{X}^2)} \sum_{t=1}^{T-1} \mathcal{T}_{\epsilon_t}(\mu_t, \mu_{t+1}) - F_t^*(c)
\]

\[= \min_{\pi \in \Pi(\mu_{1:T})} (F_1 \square \cdots \square F_{T-1}) \left( \sum_{t=1}^{T-1} (\text{proj}_{t,t+1})_t \pi \right)
\]

where \(\Pi(\mu_{1:T})\) is the set of probability measures in \(\mathcal{P}(\mathcal{X}^2)\) with marginals \(\mu_1, \ldots, \mu_T\), where for \(t \in [T-1]\)

\[
\text{proj}_{t,t+1} : \mathcal{X}^2 \ni (x_1, \ldots, x_T) \mapsto (x_t, x_{t+1}) \in \mathcal{X}^2
\]

and \(F_1 \square \cdots \square F_{T-1}\) is the infimal convolution:

\[
F_1 \square \cdots \square F_{T-1} : \mathcal{P}(\mathcal{X}^2) \to \mathbb{R} \cup \{+\infty\}
\]

\[
\pi \mapsto \inf \left\{ \sum_{t=1}^{T-1} F_t(\gamma_t) \left| \gamma_{1:T-1} \in \mathcal{M}(\mathcal{X}^2), \sum_{t=1}^{T-1} \gamma_t = \pi \right. \right\}
\]

We give a proof in appendix.

5.2. Time-varying Subspace Robust Wasserstein

Taking inspiration from the Subspace Robust Wasserstein (SRW) distance, we propose as a particular case of definition 3 a generalization of SRW to the case of a sequence of measures \(\mu_1, \ldots, \mu_T, T \geq 2\):

**Definition 4.** Let \(d \in \mathbb{N}\) and \(k \in \mathbb{N}[d]\). Define \(R_k = \{ \Omega \in \mathbb{R}^{d \times d} \mid 0 \preceq \Omega \preceq I, \text{Tr}(\Omega) = k \}\). We define the time-varying SRW between \(\mu_1, \ldots, \mu_T \in \mathcal{P}(\mathcal{X}^d)\) as:

\[
\mathcal{T}S_{k,\eta}(\mu_{1:T}) := \sup_{\Omega_1, \ldots, \Omega_{T-1} \in R_k} \sum_{t=1}^{T-1} \mathcal{J}_{\eta}(\mu_t, \mu_{t+1})
\]

\[= \sum_{t=1}^{T-1} \eta B^2(\Omega_t, \Omega_{t+1})
\]

where \(B^2(A, B) = \text{Tr}(A + B - 2(A^{1/2}BA^{1/2})^{1/2})\) is the squared Bures metric on the SDP cone.

Note that problem (11) is convex and verifies the hypothesis of proposition 4. If \(T = 2\), the time-varying SRW is equal to the classical SRW distance: \(\mathcal{T}S_{k,\eta}(\mu_1, \mu_2) = S_k(\mu_1, \mu_2)\).

6. Algorithms

From now on, we only consider the discrete case \(\mathcal{X} = \{1\}\).

6.1. Projected (Sub)gradient Ascent Solves Nonnegative Adversarial Cost OT

In the setting of subsection 3.2, we propose to run a projected subgradient ascent on the ground cost \(c \in \mathbb{R}^n\) to solve problem (6). Note that in this case, \(\mathcal{F}(\pi) := \langle c_0, \pi \rangle + \varepsilon \sum_{ij} \hat{R}_{ij}^* \left( \frac{c_{ij} - c_{0,ij}}{\varepsilon} \right)\) is not separably \(\ast\)-increasing, so we can hope that the optimal adversarial ground cost will not be separable.

At each iteration of the ascent, we need to compute a subgradient of \(g : c \mapsto \mathcal{J}_{c}(\mu, \nu) - \varepsilon R^* \left( \frac{c - c_0}{\varepsilon} \right)\) given by Danskin’s theorem:

\[
\partial g(c) = \left\{ \pi_* - \nabla R^* \left( \frac{c - c_0}{\varepsilon} \right) \left| \pi_* \in \arg \min_{\pi \in \Pi(\mu, \nu)} \langle c, \pi \rangle \right. \right\}
\]
Although projected subgradient ascent does converge, having access to gradients instead of subgradients, hence regularity, helps the convergence. We therefore propose to replace \( \mathcal{J}_c(\mu, \nu) \) by its entropy-regularized version

\[
\mathcal{J}_c^\eta(\mu, \nu) = \min_{\pi \in \Pi(\mu, \nu)} \langle c, \pi \rangle + \eta \sum_{ij} \pi_{ij}(\log \pi_{ij} - 1)
\]

in the definition of the objective \( g \). Then \( g \) is differentiable, because there exists a unique solution \( \pi_* \) in the entropic case. This will also speed up the computations of the gradient at each iteration using Sinkhorn algorithm. We can interpret this addition of a small entropy term in the adversarial cost formulation as a further regularization of the primal:

**Corollary 3.** Using the same notations as in Theorem 1, for \( \eta \geq 0 \):

\[
\sup_{c \in \mathbb{R}^{n \times n}} \mathcal{J}_c(\mu, \nu) - F^*(c) = \min_{\pi \in \Pi(\mu, \nu)} \sum_{ij} \pi_{ij}(\log \pi_{ij} - 1).
\]

### 6.2. Sinkhorn-like Algorithm for \( \ast \)-increasing \( F \in \mathcal{F} \)

If the function \( F \in \mathcal{F} \) is separably \( \ast \)-increasing, we can directly write the optimality conditions for the concave dual problem (8):

\[
\mu = \nabla F^*(\phi_\ast \otimes \psi_\ast) \mathbb{1}
\]

\[
\nu = \nabla F^*(\phi_\ast \otimes \psi_\ast)^\top \mathbb{1}
\]

where \( \mathbb{1} \) is the vector of all ones. We can then alternate between fixing \( \psi \) and solving for \( \phi \) in (12) and fixing \( \phi \) and solving for \( \psi \) in (13). In the case of entropy-regularized OT, this is equivalent to Sinkhorn algorithm. In quadratically-regularized OT, this is equivalent to the alternate minimization proposed by (Blondel et al., 2018). We give the detailed derivation of these facts in the appendix.

### 6.3. Coordinate Ascent for Time-varying SRW

Problem (11) is a globally convex problem of \( \Omega_1, \ldots, \Omega_{T-1} \). We propose to run a randomized coordinate ascent on the concave objective, i.e. to select \( \tau \in \mathbb{N} \) randomly at each iteration and doing a gradient step for \( \Omega_\tau \). We need to compute a subgradient of the objective \( h : \Omega_\tau \mapsto \sum_{t=1}^{T-1} \mathcal{J}_c(\mu_t, \mu_{t+1}) - \eta \mathbb{B}^2(\Omega_t, \Omega_{t+1}) \), given by:

\[
\nabla h(\Omega_\tau) = V(\pi_\tau) - \eta \partial_1 \mathbb{B}^2(\Omega_\tau, \Omega_{\tau+1}) - \eta \partial_2 \mathbb{B}^2(\Omega_{\tau-1}, \Omega_\tau)
\]

where \( \pi \mapsto V(\pi) \) is defined in example 2, \( \pi_\tau \in \mathbb{R}^{n \times n} \) is any optimal transport plan between \( \mu_\tau, \mu_{\tau+1} \) for cost \( d_{\Omega_{\tau}}^2 \), and \( \partial_1 \mathbb{B}^2, \partial_2 \mathbb{B}^2 \) are the gradients of the squared Bures metric with respect to the first and second arguments, computed e.g. in (Muzellec & Cuturi, 2018).

**Algorithm 2 Randomized (Block) Coordinate Ascent for Time-varying SRW**

**Input:** Measures \( \mu_1, \ldots, \mu_T \in \mathcal{P}(\mathbb{R}^d) \), dimension \( k \), learning rate \( lr \)

Initialize \( \Omega_1, \ldots, \Omega_{T-1} \in \mathbb{R}^{d \times d} \)

**for** \( i = 0 \) to \( \text{MAXITER} \) **do**

- Draw \( \tau \in \mathbb{N} \)
- \( \pi_\tau \leftarrow \text{OT}(\mu_\tau, \mu_{\tau+1}, \text{cost} = d_{\Omega_{\tau}}^2) \)
- \( \Omega_\tau \leftarrow \text{Proj}_{\mathcal{R}_k}[\Omega_\tau + lr \nabla h(\Omega_\tau)] \) using (14)

**end for**

### 7. Experiments

#### 7.1. Linearized Entropy-Regularized OT

We consider the entropy-regularized OT problem in the discrete setting:

\[
\mathcal{J}_c(\mu, \nu) = \min_{\pi \in \Pi(\mu, \nu)} \langle c_0, \pi \rangle + \varepsilon R(\pi)
\]

where \( c_0 \in \mathbb{R}^{n \times n} \) and \( R : \pi \mapsto \sum_{ij} \pi_{ij}(\log \pi_{ij} - 1) \). Since \( R \) is separable, we can constrain the associated adversarial cost to be nonnegative by linearizing the entropic regularization. By proposition 2, this amounts to solve

\[
\sup_{c \in \mathbb{R}^{n \times n}} \mathcal{J}_c(\mu, \nu) - \varepsilon \sum_{ij} \exp \left( \frac{c_{ij} - c_{0ij}}{\varepsilon} \right)
\]

\[
= \min_{\pi \in \Pi(\mu, \nu)} \langle c_0, \pi \rangle + \varepsilon \sum_{ij} \tilde{R}_{ij}(\pi_{ij})
\]

where \( \tilde{R}_{ij} : \mathbb{R} \rightarrow \mathbb{R} \) is defined as

\[
\tilde{R}_{ij}(x) := \begin{cases} x(\log x - 1) & \text{if } x \geq \exp \left( -\frac{c_{0ij}}{\varepsilon} \right) \\ -\frac{c_{0ij}}{\varepsilon} & \text{otherwise.} \end{cases}
\]

We first consider \( N = 100 \) couples of measures \( (\mu_i, \nu_i) \) in dimension \( d = 1000 \), each measure being a uniform measure on \( n = 100 \) samples from a Gaussian distribution with covariance matrix drawn from a Wishart distribution with \( k = d \) degrees of freedom. For each coupled,
we run Algorithm 1 to solve problem (15). This gives an adversarial cost $c^*_\varepsilon$. We plot in Figure 2 the mean value of $\|\hat{W}_\varepsilon - \tilde{\mathcal{J}}_\varepsilon(\mu_i, \nu_j)\|$ depending on $\varepsilon$, for $\hat{W}_\varepsilon$ equal to $\tilde{\mathcal{J}}_\varepsilon(\mu_i, \nu_j)$, $\mathcal{J}_\varepsilon(\mu_i, \nu_j)$ and the value of (15). For small values of $\varepsilon$, all three values converge to the real Wasserstein distance. For large $\varepsilon$, Sinkhorn stabilizes to the MMD (Genevay et al., 2016) while the robust cost goes to 0 (for the adversarial cost goes to 0).

In Figure 3, we visualize the effect of the regularization $\varepsilon$ on the ground cost $c^*_\varepsilon$ itself, for measures $\mu, \nu$ plotted in Figure 3a. We use multidimensional scaling on the adversarial cost matrix $c^*_\varepsilon$ (with distances between points from the same measures unchanged) to recover points in $\mathbb{R}^2$. For large values of $\varepsilon$, the adversarial cost goes to 0, which corresponds in the primal to a fully diffusive transport plan $\pi = \mu \nu^\top$.

**Figure 3.** Effect of the regularization strength on the metric: as $\varepsilon$ grows, the associated adversarial cost shrinks the distances.

**7.2. Learning a Metric on the Color Space**

We consider 20 measures $(\mu_i)_{i=1, \ldots, 10}, (\nu_j)_{j=1, \ldots, 10}$ on the red-green-blue color space identified with $\mathcal{X} = [0, 1]^3$. Each measure is a point cloud corresponding to the colors used in a painting, divided into two types: ten portraits by Modigliani ($\mu_i, i \in M$) and ten by Schiele ($\nu_j, j \in S$), see the appendix for the 20 pictures. As in SRW and time-varying SRW formulations, we learn a metric $c_{\Omega} \in C(\mathcal{X}^2)$ parameterized by a matrix $0 \leq \Omega \leq 1$ such that $\text{Tr} \Omega = 1$ that best separates the Modiglianis and the Schieses:

$$\Omega_* \in \arg\max_{\Omega \in \mathcal{X}_1} \sum_{i \in M} \sum_{j \in S} \mathcal{J}_\varepsilon(\mu_i, \nu_j).$$

We compute $\Omega_*$ using projected SGD, see the computational details in the appendix. We then use this one-dimensional metric $d^2_\Omega$, as a ground metric for OT-based color transfer (Rabin et al., 2014): an optimal transport plan $\pi$ between two color palettes $\mu_i, \nu_j$ gives a way to transfer colors from one painting to the other. Visually, transferring the colors using the classical quadratic cost $\|\cdot\|_2$ or the adversarially-learnt one-dimensional metric $d^2_\Omega$, makes no major difference, showing that when regularized, OT can extract sufficient information from lower dimensional representations.

**Figure 4.** Color transfer, best zoomed in. (a) and (b): Original paintings. (c): Schiele’s painting with Modigliani’s colors, using the learn adversarial one-dimensional metric $d^2_\Omega$. (d): Schiele’s painting with Modigliani’s colors, using the Euclidean metric $\|\cdot\|_2$.

**8. Conclusion**

In this paper, we have shown that any convex regularization of optimal transport can be recast as a ground cost adversarial problem. Under some technical assumption, we characterized the optimal ground cost as a separate function of its two arguments. In order to overcome this degeneration, we proposed a framework to learn an adversarial sequence of ground costs which is adversarial to a time-varying sequence of measures. Future work includes learning a continuous adversarial cost $c_{\Omega}$ parameterized by a neural network, under some regularity constraints (e.g. $c_{\Omega}$ is Lipschitz). On the application side, learning low-dimensional representations of time-evolving data could be applied in biology as a refinement of the methodology of (Schiebinger et al., 2019).

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References

Abadeh, S. S., Esfahani, P. M. M., and Kuhn, D. Distributionally robust logistic regression. In Advances in Neural Information Processing Systems, pp. 1576–1584, 2015.

Alaux, J., Grave, E., Cuturi, M., and Joulin, A. Unsupervised hyper-alignment for multilingual word embeddings. In International Conference on Learning Representations, 2019.

Arjovsky, M., Chintala, S., and Bottou, L. Wasserstein generative adversarial networks. Proceedings of the 34th International Conference on Machine Learning, 70:214–223, 2017.

Blondel, M., Seguy, V., and Rolet, A. Smooth and sparse optimal transport. In Storkey, A. and Perez-Cruz, F. (eds.), Proceedings of the Twenty-First International Conference on Artificial Intelligence and Statistics, volume 84 of Proceedings of Machine Learning Research, pp. 880–889, Playa Blanca, Lanzarote, Canary Islands, 09–11 Apr 2018. PMLR. URL http://proceedings.mlr.press/v84/blondel18a.html.

Bonneel, N., Peyré, G., and Cuturi, M. Wasserstein barycentric coordinates: histogram regression using optimal transport. ACM Transactions on Graphics, 35(4):71:1–71:10, 2016.

Courty, N., Flamary, R., Tuia, D., and Rakotomamonjy, A. Optimal transport for domain adaptation. IEEE transactions on pattern analysis and machine intelligence, 39(9):1853–1865, 2016.

Cuturi, M. Sinkhorn distances: lightspeed computation of optimal transport. In Advances in Neural Information Processing Systems 26, pp. 2292–2300, 2013.

Cuturi, M. and Avis, D. Ground metric learning. Journal of Machine Learning Research, 15:533–564, 2014.

Cuturi, M. and Peyré, G. A smoothed dual approach for variational Wasserstein problems. SIAM Journal on Imaging Sciences, 9(1):320–343, 2016.

Deshpande, I., Hu, Y.-T., Sun, R., Pyrros, A., Siddiqui, N., Koyejo, S., Zhao, Z., Forsyth, D., and Schwing, A. G. Max-sliced wasserstein distance and its use for gans. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pp. 10648–10656, 2019.

Dessein, A., Papadakis, N., and Rouas, J.-L. Regularized optimal transport and the rot mover’s distance. The Journal of Machine Learning Research, 19(1):590–642, 2018.

Dudley, R. M. The speed of mean Glivenko-Cantelli convergence. Annals of Mathematical Statistics, 40(1):40–50, 1969.

Essid, M. and Solomon, J. Quadratically-regularized optimal transport on graphs. arXiv preprint arXiv:1704.08200, 2017.

Feydy, J., Séjourné, T., Vialard, F.-X., Amari, S.-i., Trouve, A., and Peyré, G. Interpolating between optimal transport and mmd using sinkhorn divergences. In Chaudhuri, K. and Sugiyama, M. (eds.), Proceedings of Machine Learning Research, volume 89 of Proceedings of Machine Learning Research, pp. 2681–2690, PMLR, 16–18 Apr 2019. URL http://proceedings.mlr.press/v89/feydy19a.html.

Flamary, R., Courty, N., Rakotomamonjy, A., and Tuia, D. Optimal transport with laplacian regularization. In NIPS 2014, Workshop on Optimal Transport and Machine Learning, 2014.

Flamary, R., Cuturi, M., Courty, N., and Rakotomamonjy, A. Wasserstein discriminant analysis. Machine Learning, 107(12):1923–1945, 2018.

Fournier, N. and Guillin, A. On the rate of convergence in Wasserstein distance of the empirical measure. Probability Theory and Related Fields, 162(3-4):707–738, 2015.

Frogner, C., Zhang, C., Mobahi, H., Araya, M., and Poggio, T. A. Learning with a Wasserstein loss. In Advances in Neural Information Processing Systems, pp. 2053–2061, 2015.

Genevay, A., Cuturi, M., Peyré, G., and Bach, F. Stochastic optimization for large-scale optimal transport. In Advances in Neural Information Processing Systems, pp. 3440–3448, 2016.

Genevay, A., Chizat, L., Bach, F., Cuturi, M., and Peyré, G. Sample complexity of sinkhorn divergences. arXiv preprint arXiv:1810.02733, 2018.

Grave, E., Joulin, A., and Berthet, Q. Unsupervised alignment of embeddings with wasserstein procrustes. 2019.

Hashimoto, T., Gifford, D., and Jaakkola, T. Learning population-level diffusions with generative RNNs. In International Conference on Machine Learning, pp. 2417–2426, 2016.

Kolouri, S., Nadjahi, K., Simsekli, U., Badeau, R., and Rohde, G. Generalized sliced wasserstein distances. In Advances in Neural Information Processing Systems, pp. 261–272, 2019.

Korman, J. and McCann, R. Optimal transportation with capacity constraints. Transactions of the American Mathematical Society, 367(3):1501–1521, 2015.
Liero, M., Mielke, A., and Savaré, G. Optimal entropy-transport problems and a new hellinger–kantorovich distance between positive measures. *Inventiones Mathematicae*, 211(3):969–1117, 2018.

Lorenz, D. A., Manns, P., and Meyer, C. Quadratically regularized optimal transport. *arXiv preprint arXiv:1903.01112*, 2019.

Mena, G. and Niles-Weed, J. Statistical bounds for entropic optimal transport: sample complexity and the central limit theorem. In *Advances in Neural Information Processing Systems*, pp. 4543–4553, 2019.

Muzellec, B. and Cuturi, M. Generalizing point embeddings using the wasserstein space of elliptical distributions. In Bengio, S., Wallach, H., Larochelle, H., Grauman, K., Cesa-Bianchi, N., and Garnett, R. (eds.), *Advances in Neural Information Processing Systems 31*, pp. 10258–10269. Curran Associates, Inc., 2018.

Niles-Weed, J. and Rigollet, P. Estimation of wasserstein distances in the spiked transport model. *arXiv preprint arXiv:1909.07513*, 2019.

Paty, F.-P. and Cuturi, M. Subspace robust Wasserstein distances. In Chaudhuri, K. and Salakhutdinov, R. (eds.), *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pp. 5072–5081, Long Beach, California, USA, 09–15 Jun 2019. PMLR. URL http://proceedings.mlr.press/v97/paty19a.html.

Rabin, J. and Papadakis, N. Convex color image segmentation with optimal transport distances. In *International Conference on Scale Space and Variational Methods in Computer Vision*, pp. 256–269. Springer, 2015.

Rabin, J., Ferradans, S., and Papadakis, N. Adaptive color transfer with relaxed optimal transport. In *2014 IEEE International Conference on Image Processing (ICIP)*, pp. 4852–4856. IEEE, 2014.

Rigollet, P. and Weed, J. Entropic optimal transport is maximum-likelihood deconvolution. *Comptes Rendus Mathematique*, 356(11-12):1228–1235, 2018.

Salimans, T., Zhang, H., Radford, A., and Metaxas, D. Improving GANs using optimal transport. In *International Conference on Learning Representations*, 2018. URL https://openreview.net/forum?id=rkQkBNJAb.

Santambrogio, F. *Optimal transport for applied mathematicians*. Birkhauser, 2015.

Schiebinger, G., Shu, J., Tabaka, M., Cleary, B., Subramanian, V., Solomon, A., Gould, J., Liu, S., Lin, S., Berube, P., et al. Optimal-transport analysis of single-cell gene expression identifies developmental trajectories in reprogramming. *Cell*, 176(4):928–943, 2019.

Solomon, J., De Goes, F., Peyré, G., Cuturi, M., Butscher, A., Nguyen, A., Du, T., and Guibas, L. Convolutional Wasserstein distances: efficient optimal transportation on geometric domains. *ACM Transactions on Graphics*, 34(4):66:1–66:11, 2015.

Villani, C. *Optimal Transport: Old and New*, volume 338. Springer Verlag, 2009.

Weed, J., Bach, F., et al. Sharp asymptotic and finite-sample rates of convergence of empirical measures in wasserstein distance. *Bernoulli*, 25(4A):2620–2648, 2019.
A. Proofs

A.1. Proof for Proposition 1

Proof. Let $\pi_*$ be a minimizer of (3). Then using the optimality condition for $\sup_{c \in \mathbb{R}^{+\times n}} \int c \, d\pi - F^*(c)$, any $c$ such that $\pi_* \in \partial F^*(c)$ is a best response to $\pi_*$. But by Fenchel-Young inequality, such $c$ are exactly those in $\partial F(\pi_*) = \{\nabla F(\pi_*)\}$. Since $\nabla F(\pi_*)$ is the unique best response to $\pi_*$, it is necessarily optimal in (4). Conversely, if there is a unique maximizer $c_*$, then as a result of the above, $c_* = \nabla F(\pi_*)$ for some minimizer $\pi_*$ of the primal. Then $\nabla F^*(c_*)$ is optimal in the primal. \hfill \Box

A.2. Proof for Proposition 2

Proof. As in the proof of Theorem 1, we use Sion’s minimax theorem to get

$$\sup_{c \in \mathbb{R}^{+\times n}} \min_{\pi \in \Pi(\mu, \nu)} \left\langle c, \pi \right\rangle - \varepsilon \sum_{i,j} R^*_i (c_{ij} - c_{0ij}) \right.$$  

$$= \min_{\pi \in \Pi(\mu, \nu)} \sup_{c \in \mathbb{R}^{+\times n}} \left\langle c, \pi \right\rangle - \varepsilon \sum_{i,j} R^*_i (c_{ij} - c_{0ij}) \right.$$  

Since the optimization in $c \in \mathbb{R}^{+\times n}$ is separable, we only need to consider this optimization coordinate by coordinate, i.e., we only need to compute $\sup_{c_{ij} \in \mathbb{R}^+} \pi_i c_{ij} - f^*_i(c_{ij})$ for all $i, j \in [n]$, where $f^*_i(c_{ij}) = \varepsilon R^*_i c_{ij} - c_{0ij}$. Fix $\pi \in \Pi(\mu, \nu)$ and $i, j \in [n]$, and define $g_{ij} : \mathbb{R} \ni c_{ij} \mapsto \pi_i c_{ij} - f^*_i(c_{ij})$. Suppose that $z_{ij} = f^*_i(\pi_{ij}) \geq 0$. Then  

$$f_i(\pi_{ij}) = f^*_i(\pi_{ij}) = g_{ij}(z_{ij}) = \sup_{c_{ij} \in \mathbb{R}} g_{ij}(c_{ij}),$$  

and since $z_{ij} \geq 0$, $\sup_{c_{ij} \in \mathbb{R}^+} g_{ij}(c_{ij}) = f^*_i(\pi_{ij})$. This means that $R_i(\pi_{ij}) = R^*_i(\pi_{ij})$.

Suppose now that $z_{ij} = f^*_i(\pi_{ij}) < 0$. This means that  

$$\sup_{c_{ij} \in \mathbb{R}^+} g_{ij}(c_{ij}) < \sup_{c_{ij} \in \mathbb{R}} g_{ij}(c_{ij}).$$  

Since $g_{ij}$ is concave, this shows that $\sup_{c_{ij} \in \mathbb{R}^+} g_{ij}(c_{ij}) = g_{ij}(0) = -f^*_i(0)$, i.e., $R_i(\pi_{ij}) = -\frac{c_{0ij}}{\varepsilon} \pi_{ij} - R^*_i (-\frac{c_{0ij}}{\varepsilon}).$

Since $R_i$ is convex, $R^*_i$ is increasing with pseudo-inverse $R^*_i$. Furthermore, the optimality condition in the convex conjugate problem gives, for any $\alpha \in \mathbb{R}$:  

$$R^*_i(\alpha) = \alpha \times R^*_i(\alpha) - R^*_i \circ R^*_i(\alpha).$$  

So if $R_i$ is of class $C^1$, taking $\alpha = -\frac{c_{0ij}}{\varepsilon}$, as $x$ increases to $R^*_i(\alpha) \Rightarrow R_i(\pi_{ij}) = \tilde{R}_i(\pi_{ij}) = \tilde{R}_i(\pi_{ij})$, meaning that $\tilde{R}_{ij}$ is of class $C^1$. \hfill \Box

A.3. Proof of Example 3

Proof. We denote by $\text{sgn}(x)$ the set $\{+1\} if x > 0, \{-1\} if x < 0 and \{-1, 1\} if x = 0$. We apply Corollary 1 with $R : \mathbb{R}^{+\times n} \to \mathbb{R}^{+\times n}$ defined as $R(\pi) = \frac{1}{p} \|\pi\|^p_{w,p}$, for which we need to compute its convex conjugate:

$$R^*(c) = \sup_{\pi \in \mathbb{R}^{+\times n}} \langle \pi, c \rangle - \frac{1}{p} \sum_{ij} w_{ij} |\pi_{ij}|^p.$$  

Subdifferentiating with respect to $\pi_{ij}$:

$$c_{ij} \in \frac{1}{p} w_{ij} \frac{\partial}{\partial \pi_{ij}} |\pi_{ij}|^p = w_{ij} \text{sgn}(\pi_{ij}) |\pi_{ij}|^{p-1}.$$  

This implies that $\text{sgn}(\pi_{ij}) = \text{sgn}(c_{ij})$, so:

$$\pi_{ij} = \text{sgn}(c_{ij}) c_{ij} \left\| \frac{c_{ij}}{w_{ij}} \right\|^{q-1}.$$  

Finally,

$$R^*(c) = \sum_{ij} c_{ij} \text{sgn}(c_{ij}) \left\| \frac{c_{ij}}{w_{ij}} \right\|^{q-1} - \frac{1}{p} \sum_{ij} w_{ij} \left\| \frac{c_{ij}}{w_{ij}} \right\|^q$$  

$$= \frac{1}{q} \sum_{ij} \left\| \frac{c_{ij}}{w_{ij}} \right\|^{q}.$$  

\hfill \Box

A.4. Proof for Theorem 2

Proof. Using Theorem 1 and Kantorovich duality (2):

$$\mathcal{W}_F(\mu, \nu) = \sup_{c \in C(X)} \mathcal{J}_c(\mu, \nu) - F^*(c)$$  

$$= \sup_{c \in C(X)} \max_{\phi, \psi \in C(X)} \int \phi d\mu + \int \psi d\nu - F^*(c)$$  

$$= \sup_{c \in C(X)} \max_{\phi, \psi \in C(X)} \int \phi d\mu + \int \psi d\nu - F^*(c)$$  

$$= \max_{\phi, \psi \in C(X)} \int \phi d\mu + \int \psi d\nu - \sup_{c \in C(X)} F^*(c).$$  

\hfill \Box
Since $F$ is separably $*$-increasing, for any $\phi, \psi \in C(\mathcal{X})$,
\[
\inf_{c \in C(\mathcal{X}^2)} F^*(c) = F^*(\phi \oplus \psi),
\]
which shows the desired duality result.

\section*{A.5. Proof of Proposition 4}

\textbf{Proof}. We drop the dependence in $\mu_1, \ldots, \mu_T$ to ease the notation.

\textbf{Limit when $\eta \to +\infty$.}

Existence of the limit. Note that $\eta \to W_{\eta D,F}$ is decreasing because $D \geq 0$. It is also bounded from below, since for any $\eta \geq 0$, using the fact that $D(c, c) = 0$ for any $c \in C(\mathcal{X}^2)$:
\[
W_{\eta D,F} \geq \sup_{c \in C(\mathcal{X}^2)} \frac{1}{\eta} \sum_{t=1}^{T-1} \mathcal{J}_t(\mu_t, \mu_{t+1}) - F_t^*(c) > -\infty.
\]
So $W_{\eta D,F}$ admits a limit as $\eta \to +\infty$.

\textbf{Value of the limit.} Fix $\eta > 0$. Let $c_1^\eta, \ldots, c_{T-1}^\eta \in C(\mathcal{X}^2)$ such that
\[
\frac{1}{\eta} \sum_{t=1}^{T-1} \mathcal{J}_t^\eta(\mu_t, \mu_{t+1}) - F_t^*(c_t^\eta) - \eta D(c_t^\eta, c_{t+1}^\eta) \geq W_{\eta D,F} - \frac{1}{\eta}.
\]
Then:
\[
\frac{1}{T-1} \sum_{t=1}^{T-1} D(c_t^\eta, c_{t+1}^\eta) \leq \frac{1}{\eta} \left[ \frac{1}{\eta} - W_{\eta D,F} \right] + \frac{1}{T-1} \sum_{t=1}^{T-1} \mathcal{J}_t^\eta(\mu_t, \mu_{t+1}) - F_t^*(c_t^\eta).
\]
Note that $\frac{1}{T-1} \sum_{t=1}^{T-1} \mathcal{J}_t^\eta(\mu_t, \mu_{t+1}) - F_t^*(c_t^\eta)$ is upper-bounded by
\[
A := \sup_{c \in C(\mathcal{X}^2)} \frac{1}{T-1} \sum_{t=1}^{T-1} \mathcal{J}_t(c_t, \mu_{t+1}^\eta) - F_t^*(c_t),
\]
which is finite using hypothesis 3. Since $-W_{\eta D,F} \leq -A$, for any $t \in [T - 1]$,
\[
D(c_t^\eta, c_{t+1}^\eta) \leq \frac{1}{\eta} + \frac{(T - 2)A}{\eta}.
\]
On the other hand, by hypothesis 3 there exists a compact set $K \subset C(\mathcal{X}^2)$ such that for any $t \in [T]$, $F_t^* \equiv +\infty$ outside of $K$. Then up to a subsequence, for any $t \in [T - 1]$, $c_t^\eta \to c_t^\infty$ as $\eta \to \infty$ for some $c_t^\infty \in C(\mathcal{X}^2)$.

Taking the limit as $\eta \to +\infty$ in (16), and using the fact that $D$ is a continuous divergence gives $c_1^\infty = \ldots = c_{T-1}^\infty$, hence the result.

\textbf{Multimarginal interpretation.} It holds:
\[
\sup_{c \in C(\mathcal{X}^2)} \sum_{t=1}^{T-1} \mathcal{J}_t(\mu_t, \mu_{t+1}) - F_t^*(c) = \sup_{c \in C(\mathcal{X}^2)} \min_{\pi_1 \in \Pi(\mu_1, \mu_2)} \ldots \min_{\pi_{T-1} \in \Pi(\mu_{T-1}, \mu_T)} \int c d \left( \sum_{i=1}^{T-1} \pi_t \right) - \sum_{t=1}^{T-1} F_t^*(c).
\]
where we have glued $\pi_1, \ldots, \pi_{T-1}$ into $\pi \in \Pi(\mu_1; \mu_T)$ using the gluing lemma (Lemma 5.5 in (Santambrogio, 2015)) in line 4, swapped the min and the sup using Sion’s minimax theorem as in the proof of Theorem 1 in line 5 and used the fact that the convex conjugate of $\sum_{i=1}^{T-1} F_t^*$ is $F_1 \square \ldots \square F_{T-1}$ in the last line.

\section*{A.6. Proof for Subsection 6.2}

\textbf{Entropic OT} In the case of entropic OT,
\[
F(\pi) = (\pi, c_0) + \varepsilon \sum_{ij} \pi_{ij} \log \pi_{ij} - 1,
\]
so
\[
F^*(c) = \varepsilon \sum_{ij} \exp \left( \frac{c_{ij} - c_{0ij}}{\varepsilon} \right)
\]
and
\[
\nabla F^*(c) = \left[ \exp \left( \frac{c_{ij} - c_{0ij}}{\varepsilon} \right) \right]_{ij}.
\]
Then the system of equations (12) (13) is:
\[
\forall i, \mu_i = \sum_j \exp \left( \frac{\phi_{*i} + \psi_{*j} - c_{0ij}}{\varepsilon} \right) = \exp(\phi_{*i}/\varepsilon) [K \exp(\psi_{*i}/\varepsilon)]_i
\]
\[
\forall j, \nu_j = \sum_i \exp \left( \frac{\phi_{*i} + \psi_{*j} - c_{0ij}}{\varepsilon} \right) = \exp(\psi_{*j}/\varepsilon) [K^T \exp(\phi_{*i}/\varepsilon)]_j
\]
where $K = \exp(-c_0/\varepsilon) \in \mathbb{R}^{n \times n}$ and $\exp$ is taken elementwise. Then solving alternatively for $\phi$ and $\psi$ is exactly Sinkhorn algorithm.
Regularized Optimal Transport is Ground Cost Adversarial

Quadratic OT In the case of quadratic OT, using the notations and results from example 7:

\[ F(\pi) = \langle \pi, c_0 \rangle + \varepsilon \varphi_2(\pi_{ij}), \]

and

\[ F^*(c) = \frac{1}{2\varepsilon} \sum_{ij} \left[(c_{ij} - c_{0ij})^+\right]^2. \]

Then:

\[ \nabla F^*(c) = \frac{1}{\varepsilon} (c - c_0)^+. \]

The system of equations (12) (13) is:

\[ \forall i, \varepsilon \mu_i = \sum_j \left( \phi_{si} + \psi_{sj} - c_{0ij} \right)^+, \]

\[ \forall j, \varepsilon \nu_j = \sum_i \left( \phi_{si} + \psi_{sj} - c_{0ij} \right)^+. \]

which is what (Blondel et al., 2018) solve in their appendix B.

A.7. Proof for Corollary 3

Proof. Let \( R(\pi) := \sum_{ij} \pi_{ij} (\log \pi_{ij} - 1) \). Then:

\[
\sup_{c \in \mathbb{R}^{n \times n}} \mathscr{S}_\varepsilon^0(\mu, \nu) - F^*(c) \\
= \sup_{c \in \mathbb{R}^{n \times n}} \min_{\pi \in \Pi(\mu, \nu)} \langle \pi, c \rangle + \eta R(\pi) - F^*(c) \\
= \min_{\pi \in \Pi(\mu, \nu)} \eta R(\pi) + \sup_{c \in \mathbb{R}^{n \times n}} \langle \pi, c \rangle - F^*(c) \\
= \min_{\pi \in \Pi(\mu, \nu)} \eta R(\pi) + F(\pi)
\]

where we have used Sion’s minimax theorem as in the proof of Theorem 1 to swap the min and the sup, and used as well the fact that \( F = F^{**} \) given by Fenchel-Moreau theorem.

\[ \square \]

B. Experiments Details

B.1. Color Transfer

We first run a preprocessing on the pictures to downscale them. For each picture, we run a k-means clustering to quantize the colors, producing \( K = 1000 \) centroids \( x_1, \ldots, x_K \in [0, 1]^3 \). For each centroid \( x_k \), we give it a weight \( a_k \) corresponding to the proportion of original pixels that were assigned to \( x_k \). This outputs a measure \( \mu = \sum_k a_k \delta_{x_k} \in \mathcal{P}([0, 1]^3) \) with a support of size \( K = 1000 \).

In order to optimize over \( \Omega \in \mathcal{R}_1 \), we run SGD: at each iteration \( t \), we randomly select a pair \((i, j) \in M \times S \) of portraits, one \( \mu_i \) by Modigliani and the other \( \nu_j \) by Schiele, among the then portraits of Figures 5 and 6 (see next page). We then compute the optimal transport plan \( \pi_{i,j}^* \) between \( \mu_i \) and \( \nu_j \) with cost \( d_{ij}^2 \) and entropic regularization set to \( \varepsilon = 0.01 \), where \( \Omega_t \) is the current value for \( \Omega \). This gives the gradient \( \nabla \mathcal{L}_{\pi_{i,j}}^* \) for the pair \((i, j)\).

Given a portrait \( \mu_i, i \in M \) by Modigliani and a portrait \( \nu_j, j \in S \) by Schiele, we can transfer the color in \( \mu_i \) to Schiele’s portrait by computing an optimal transport plan \( \pi_{i,j} \) with a certain cost. Indeed, write \( \mu_i = \sum_k a_k \delta_{x_k} \) and \( \nu_j = \sum_l b_l \delta_{y_l} \). Then a color \( x_k \in [0, 1]^2 \) in the support of \( \mu_i \) can be sent to its barycentric projection \( \sum_{kl} \pi_{kl}^* a_k y_l \). For each color in the original portrait by Modigliani, we transfer its color to the one its corresponding centroid was sent to.
Figure 5. Portraits from Amedeo Modigliani

Figure 6. Portraits from Egon Schiele