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► **To cite this version:**

Kilian Fatras, Younes Zine, Rémi Flamary, Rémi Gribonval, Nicolas Courty. Learning with minibatch Wasserstein : asymptotic and gradient properties. AISTATS 2020 - 23rd International Conference on Artificial Intelligence and Statistics, Jun 2020, Palermo, Italy. pp.1-20. hal-02502329

HAL Id: hal-02502329

<https://hal.science/hal-02502329v1>

Submitted on 9 Mar 2020

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Learning with minibatch Wasserstein : asymptotic and gradient properties

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Abstract

Optimal transport distances are powerful tools to compare probability distributions and have found many applications in machine learning. Yet their algorithmic complexity prevents their direct use on large scale datasets. To overcome this challenge, practitioners compute these distances on minibatches *i.e.* they average the outcome of several smaller optimal transport problems. We propose in this paper an analysis of this practice, which effects are not well understood so far. We notably argue that it is equivalent to an implicit regularization of the original problem, with appealing properties such as unbiased estimators, gradients and a concentration bound around the expectation, but also with defects such as loss of distance property. Along with this theoretical analysis, we also conduct empirical experiments on gradient flows, GANs or color transfer that highlight the practical interest of this strategy.

1 Introduction

Measuring distances between probability distributions is a key problem in machine learning. Considering the space of probability distributions $\mathcal{M}_1^+(\mathcal{X})$ over a space \mathcal{X} , and given an empirical probability distribution $\alpha \in \mathcal{M}_1^+(\mathcal{X})$, we want to find a parametrized distribution β_λ which approximates the distribution α . Measuring the distance between the distributions requires a function $L : \mathcal{M}_1^+(\mathcal{X}) \times \mathcal{M}_1^+(\mathcal{X}) \rightarrow \mathbb{R}$. The distribution β is parametrized by a vector λ and the goal is to find the best λ which minimizes the distance L between β_λ and

α , *i.e.* $L(\alpha, \beta_\lambda)$. As the distributions are empirical, we need a distance L with good statistical performance and which have optimization guarantees with modern optimization techniques. Optimal transport (OT) losses as distances have emerged recently as a competitive tool on this problem [Genevay et al., 2018, Arjovsky et al., 2017]. The corresponding estimator is usually found in the literature under the name of *Minimum Kantorovich Estimator* [Bassetti et al., 2006, Peyré and Cuturi, 2019]. Furthermore, OT losses have been widely used to transport samples from a source domain to a target domain using barycentric mappings [Ferradans et al., 2013, Courty et al., 2017, Seguy et al., 2018].

Several previous works challenged the heavy computational cost of optimal transport, as the Wasserstein distance comes with a complexity of $\mathcal{O}(n^3 \log(n))$, where n is the size of the probability distribution supports. Variants of optimal transport have been proposed to reduce its complexity. [Cuturi, 2013] used an entropic regularization term to get a strongly convex problem which is solvable using the Sinkhorn algorithm with a computational cost of $\mathcal{O}(n^2)$, both in time and space. However, despite some scalable solvers based on stochastic optimization [Genevay et al., 2016, Seguy et al., 2018], in the big data setting n is very large and still leads to bottleneck computation problems especially when trying to minimize the OT loss. That is why [Genevay et al., 2018, Damodaran et al., 2018] use a minibatch strategy in their implementations to reduce the cost per iteration. They propose to compute the averaged of several optimal transport terms between minibatches from the source and the target distributions. However, using this strategy leads to a different optimization problem that results in a “non optimal” transportation plan between the full original distributions. Recently, [Bernton et al., 2017] worked on minimizers and [Sommerfeld et al., 2019] on a bound between the true optimal transport and the minibatch optimal transport. However they did not study the asymptotic convergence, the loss properties and behavior of the minibatch loss.

In this paper we propose to study minibatch optimal transport by reviewing its relevance as a loss function. After defining the minibatch formalism, we will show which properties are inherited and which ones are lost. We describe the asymptotic behavior of the estimator and show that we can derive a concentration bound without dependence on the data space dimension. Then, we prove that the gradients of the minibatch OT losses are unbiased, which justifies its use with SGD in [Genevay et al., 2018]. Finally, we demonstrate the effectiveness of minibatches in large scale setting and show how to alleviate the memory issues for barycentric mapping. The paper is structured as follows: in Section 2, we propose a brief review of the different optimal transport losses. In Section 3, we give formal definitions of the minibatch strategy and illustrate their impacts on OT plans. Basic properties, asymptotic behaviors of the estimator and differentiability are then described. Finally in Section 4, we highlight the behavior of the minibatch OT losses on a number of experiments: gradient flows, generative networks and color transfer.

2 Wasserstein distance and regularization

Wasserstein distance The Optimal Transport metric measures a distance between two probability distributions $(\alpha, \beta) \in \mathcal{M}_+^1(\mathcal{X}) \times \mathcal{M}_+^1(\mathcal{Y})$ by considering a ground metric c on the space \mathcal{X} [Peyré and Cuturi, 2019]. Formally, the Wasserstein distance between two distributions can be expressed as

$$W_c(\alpha, \beta) = \min_{\pi \in U(\alpha, \beta)} \int_{\mathcal{X} \times \mathcal{Y}} c(\mathbf{x}, \mathbf{y}) d\pi(\mathbf{x}, \mathbf{y}), \quad (1)$$

where $U(\alpha, \beta)$ is the set of joint probability distribution with marginals α and β such that $U(\alpha, \beta) = \{\pi \in \mathcal{M}_+^1(\mathcal{X}, \mathcal{Y}) : \mathbf{P}_{\mathcal{X}}\#\pi = \alpha, \mathbf{P}_{\mathcal{Y}}\#\pi = \beta\}$. $\mathbf{P}_{\mathcal{X}}\#\pi$ (resp. $\mathbf{P}_{\mathcal{Y}}\#\pi$) is the marginalization of π over \mathcal{X} (resp. \mathcal{Y}). The ground cost $c(\mathbf{x}, \mathbf{y})$ is usually chosen as the Euclidean or squared Euclidean distance on \mathbb{R}^d , in this case W_c is a metric as well. Note that the optimization problem above is called the Kantorovitch formulation of OT and the optimal π is called an optimal transport plan. When the distributions are discrete, the problem becomes a discrete linear program that can be solved with a cubic complexity in the size of the distributions support. Also the convergence in population of the Wasserstein distance is known to be slow with a rate $O(n^{-1/d})$ depending on the dimensionality d of the space \mathcal{X} and the size of the population n [Weed and Bach, 2019]. [Gerber and Maggioni, 2017] used a multi-scale strategy in order to compute a fast approximation of the Wasserstein distance.

Entropic regularization Regularized entropic OT was proposed in [Cuturi, 2013] and leads to a more efficient $O(n^2)$ solver. We define the entropic loss as:

$$W_c^\varepsilon(\alpha, \beta) = \min_{\pi \in U(\alpha, \beta)} \int_{\mathcal{X} \times \mathcal{Y}} c(\mathbf{x}, \mathbf{y}) d\pi(\mathbf{x}, \mathbf{y}) + \varepsilon H(\pi|\xi),$$

with $H(\pi|\xi) = \int_{\mathcal{X} \times \mathcal{Y}} \log\left(\frac{d\pi(\mathbf{x}, \mathbf{y})}{d\alpha(\mathbf{x})d\beta(\mathbf{y})}\right) d\pi(\mathbf{x}, \mathbf{y})$ where $\xi = \alpha \otimes \beta$ and ε is the regularization coefficient. We call this function, the entropic OT loss. As we will see later, this entropic regularization also makes the problem strongly convex and differentiable with respect to the cost or the input distributions.

It is well known that adding an entropic regularization leads to sub-optimal solutions π on the original problem, and it is not a metric since $W_c^\varepsilon(\beta, \beta) \neq 0$. This motivated [Genevay et al., 2018] to introduce an unbiased loss which uses the entropic regularization and called it the Sinkhorn divergence. It is defined as:

$$S_c^\varepsilon(\alpha, \beta) = W_c^\varepsilon(\alpha, \beta) - \frac{1}{2}(W_c^\varepsilon(\alpha, \alpha) + W_c^\varepsilon(\beta, \beta))$$

It can still be computed with the same order of complexity as the entropic loss and has been proven to interpolate between OT and maximum mean discrepancy (MMD) [Feydy et al., 2019] with respect to the regularization coefficient. MMD are integral probability metrics over a reproducing kernel Hilbert space [Gretton et al.,]. When ε tends to 0, we get the OT solution back and when ε tends to ∞ , we get a solution closer to the MMD solution. Second, as proved by [Feydy et al., 2019], if the cost c is Lipschitz, then S_c^ε is a convex, symmetric, positive definite loss function. Hence the use of the Sinkhorn divergence instead of the regularized OT. The sample complexity of the Sinkhorn divergence, that is the convergence rate of a metric between a probability distribution and its empirical counterpart as a function of the number of samples, was proven in [Genevay et al., 2019] to be: $O\left(\frac{n}{\sqrt{n}} \left(1 + \frac{1}{\varepsilon^{\lfloor d/2 \rfloor}}\right)\right)$ where d is the dimension of \mathcal{X} . We see an interpolation between MMD and OT sample complexity depending on ε .

Minibatch Wasserstein While the entropic loss has better computational complexity than the original Wasserstein distance, it is still challenging to compute it for a large dataset. To overcome this issue, several papers rely on a minibatch computation [Genevay et al., 2018, Damodaran et al., 2018, Liutkus et al., 2019, Kolouri et al., 2016]. Instead of computing the OT problem between the full distributions, they compute an averaged of OT problems between batches of the source and the target domains. It differs from [Gerber and Maggioni, 2017] as the size of the minibatch remains constant. Several work came out to justify the minibatch paradigm. [Bernton et al., 2017] showed that for generative models, the minimizers of the minibatch loss converge to the true minimizer when the minibatch size increases. [Sommerfeld et al., 2019] considered another approach, where they approximate OT with the minibatch strategy and exhibit a deviation bound between the two quantities. We follow a different approach from the two previous work. We are interested in the behavior of using the minibatch strategy as a loss function. We study the asymptotic behavior of using minibatch, the

optimization procedure, the resulting transportation plan and the behavior of such a loss for data fitting problems.

3 Minibatch Wasserstein

In this section we first define the Minibatch Wasserstein and illustrate it on simple examples. Next we study its asymptotic properties and optimization behavior.

3.1 Notations and Definitions

Notations Let $\mathbf{X} = (X_1, \dots, X_n)$ (resp. $\mathbf{Y} = (Y_1, \dots, Y_n)$) be samples of n iid random variables drawn from a distribution α (resp. β) on the source (resp. target) domain. We denote by α_n and β_n the empirical distributions of support $\{X_1, \dots, X_n\}$ and $\{Y_1, \dots, Y_n\}$ respectively. The weights of X_i (resp. Y_i) are uniform, i.e equal to $1/n$. We further suppose that α and β have compact support, the ground cost is then bounded by a constant M . $\alpha^{\otimes m}$ denotes a sample of m random variables following α . In the rest of the paper, we will not make a difference between a batch A of cardinality m and its associated (uniform probability) distribution $\hat{A} := \frac{1}{m} \sum_{a \in A} \delta_a$. The number of possible mini-batches of size m on n distinct samples is the binomial coefficient $\binom{n}{m} = \frac{n!}{m!(n-m)!}$. For $1 \leq m \leq n$, we write $\mathcal{P}_m(\alpha_n)$ (resp. $\mathcal{P}_m(\beta_n)$) the collection of subsets of cardinality m of α_n (resp. of β_n). We will denote the integer part of the ratio n/m as $\lfloor n/m \rfloor$.

Definitions We will first give formal definitions of the different quantities that we will use in this paper. We start with minibatch Wasserstein losses for continuous, semi-discrete and discrete distributions.

Definition 1 (Minibatch Wasserstein definitions). *Given an OT loss h and an integer $m \leq n$, we define the following quantities:*

The continuous loss:

$$U_h(\alpha, \beta) := \mathbb{E}_{(X,Y) \sim \alpha \otimes \beta} [h(X, Y)] \quad (2)$$

The semi-discrete loss:

$$U_h(\alpha_n, \beta) := \binom{n}{m}^{-1} \sum_{A \in \mathcal{P}_m(\alpha_n)} \mathbb{E}_{Y \sim \beta} [h(A, Y)] \quad (3)$$

The discrete-discrete loss:

$$U_h(\alpha_n, \beta_n) := \binom{n}{m}^{-2} \sum_{A \in \mathcal{P}_m(\alpha_n)} \sum_{B \in \mathcal{P}_m(\beta_n)} h(A, B) \quad (4)$$

where h can be the Wasserstein distance W , the entropic loss W_ϵ or the sinkhorn divergence S_ϵ for a cost $c(\mathbf{x}, \mathbf{y})$.

Note that h is a U-statistic kernel. Note also that the minibatches elements are drawn without replacement. These

quantities represent an average of Wasserstein distance over minibatches of size m . Note that samples in A have uniform weights $1/m$ and that the ground cost can be computed between all pair of batches A and B . It is easy to see that (29) is an empirical estimator of (6). In real world applications, computing the average over all batches is too costly as we have a combinatorial number of batches, that is why we will rely on a subsampled quantity.

Definition 2 (Minibatch subsampling). *Pick an integer $k > 0$. We define:*

$$\tilde{U}_h^k(\alpha_n, \beta_n) := k^{-1} \sum_{(A,B) \in D_k} h(A, B) \quad (5)$$

where D_k is a set of cardinality k whose elements are drawn at random from the uniform distribution on $\Gamma := \mathcal{P}_m(\{X_1, \dots, X_n\}) \times \mathcal{P}_m(\{Y_1, \dots, Y_n\})$.

As the transportation plan might be of interest, let us now review the minibatch definition for the OT plan which can be built for all OT variants which have an OT plan. Formal definitions are provided in appendix.

Definition 3 (Mini-batch transport plan). *Consider α_n and β_n two discrete probability distributions. For each $A = \{a_1, \dots, a_m\} \in \mathcal{P}_m(\alpha_n)$ and $B = \{b_1, \dots, b_m\} \in \mathcal{P}_m(\beta_n)$ we denote by $\Pi_{A,B}$ the optimal plan between the random variables, considered as a $n \times n$ matrix where all entries are zero except those indexed in $A \times B$. We define the averaged mini-batch transport matrix:*

$$\Pi_m(\alpha_n, \beta_n) := \binom{n}{m}^{-2} \sum_{A \in \mathcal{P}_m(\alpha_n)} \sum_{B \in \mathcal{P}_m(\beta_n)} \Pi_{A,B}. \quad (6)$$

Following the subsampling idea, we define the subsampled minibatch transportation matrix for A and B :

$$\Pi_k(\alpha_n, \beta_n) := k^{-1} \sum_{(A,B) \in D_k} \Pi_{A,B} \quad (7)$$

where D_k is drawn as in Definition 2.

It is well known that the Wasserstein distance suffers from biased gradients [Bellemare et al., 2017]. We study if $U_h(\alpha_n, \beta_n)$ has a bias wrt $U_h(\alpha, \beta)$, and then the bias in $U_h(\alpha_n, \beta_n)$ gradients for first order optimization methods.

3.2 Illustration on simple examples

To illustrate the effect of the minibatch, we compute Π_m (6) on two simple examples.

Distributions in 1D The 1D case is an interesting problem because we have access to a closed-form of the optimal transport solution which allows us to calculate the closed-form of a minibatch paradigm. It is the foundation of the sliced Wasserstein distance [Bonnotte, 2013] which

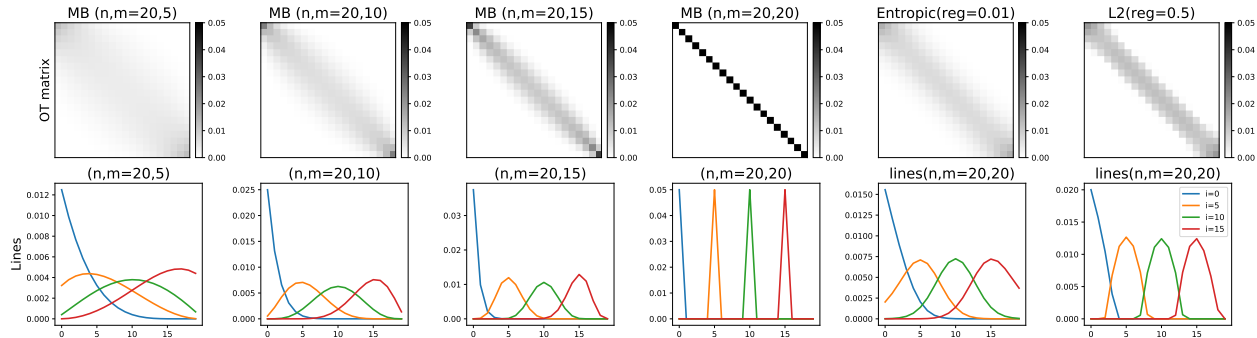


Figure 1: Several OT matrices between distributions with $n = 20$ samples in 1D. The first row shows the minibatch OT matrices Π_m for different values of m , the second row provides the shape of the distributions on the rows of Π_m . The two last columns correspond to classical entropic and quadratic regularized OT.

is widely used as an alternative to the Wasserstein distance [Liutkus et al., 2019, Kolouri et al., 2016].

We suppose that we have uniform empirical distributions α_n and β_n . We assume (without loss of generality) that the points are ordered in their own distribution. In such a case, we can compute the 1D Wasserstein 1 distance with cost $c(x, y) = |x - y|$ as: $W(\alpha_n, \beta_n) = \frac{1}{n} \sum_{i=1}^n |x_i - y_j|$ and the OT matrix is simply an identity matrix scaled by $\frac{1}{n}$ (see [Peyré and Cuturi, 2019] for more details). After a short combinatorial calculus (given in appendix A.5), the 1D minibatch transportation matrix coefficient $\pi_{j,k}$ can be computed as $\pi_{j,k} =$:

$$\frac{1}{m} \binom{n}{m}^{-2} \sum_{i=i_{\min}}^{i_{\max}} \binom{j-1}{i-1} \binom{k-1}{i-1} \binom{n-j}{m-i} \binom{n-k}{m-i}$$

where $i_{\min} = \max(0, m - n + j, m - n + k)$ and $i_{\max} = \min(j, k)$. i_{\min} and i_{\max} represent the sorting constraints.

We show on the first row Figure 1 the minibatch OT matrices Π_m with $n = 20$ samples for different value of the minibatch size m . We also provide on the second row of the figure a plot of the distributions in several rows of Π_m . We give the matrices for entropic and quadratic regularized OT for comparison purpose. It is clear from the figure that the OT matrix densifies when m decreases, which has a similar effect as entropic regularization. Note the more localized spread of mass of quadratic regularization that preserve sparsity as discussed in [Blondel et al., 2018]. While the entropic regularization spreads the mass in a similar manner for all samples, minibatch OT spreads less the mass on samples at the extremities. Note that the minibatch OT matrices solution is for ordered samples and do not depend on the position of the samples once ordered, as opposed to the regularized OT methods. This will be better illustrated in the next example.

Minibatch Wasserstein in 2D We illustrate the OT matrix between two empirical distributions of 10 samples each

in 2D in Figure 2. We use two 2D empirical distributions (point cloud) where the samples have a cluster structure and the samples are sorted *w.r.t.* their cluster. We can see from the OT matrices in the first row of the figure that the cluster structure is more or less recovered with the regularization effect of the minibatches (and also regularized OT). On the second row one can see the effect of the geometry of the samples on the spread of mass. Similarly to 1D, for Minibatch OT, samples on the border of the simplex cannot spread as much mass as those in the center and have darker rows. This effect is less visible on regularized OT.

3.3 Basic properties

We now state some basic properties for minibatch Wasserstein losses. All properties are proved in the appendix. The first property is about the transportation plan Π_m between the two initial distributions, defined in (6).

Proposition 1. *The transportation plan $\Pi_m(\alpha_n, \beta_n)$ is an admissible transportation plan between the full input distributions α_n, β_n , and we have : $U_h(\alpha_n, \beta_n) \geq W(\alpha_n, \beta_n)$.*

The fact that Π_m is an admissible transportation plan means that even though it is not optimal, we still do transportation similarly to regularized OT. Note that Π_k is not a transportation plan, in general, for a finite k but we study its asymptotic convergence to marginals in the next section. Regarding our empirical estimator, when we have *iid* data, it enjoys the following property:

Proposition 2 (Unbiased estimator). *$U_h(\alpha_n, \beta_n)$ is an unbiased estimator of $U_h(\alpha, \beta)$ for the continuous setting and of $U_h(\alpha_n, \beta)$ for the semi-discrete setting.*

As we use minibatch OT for loss function, it is of interest to see if it is still a distance on the distribution space such as the Wasserstein distance or the Sinkhorn divergence.

Proposition 3 (Positivity and symmetry). *The minibatch Wasserstein losses are positive and symmetric losses. However, they are not metrics since $U_h(\alpha, \alpha) > 0$.*

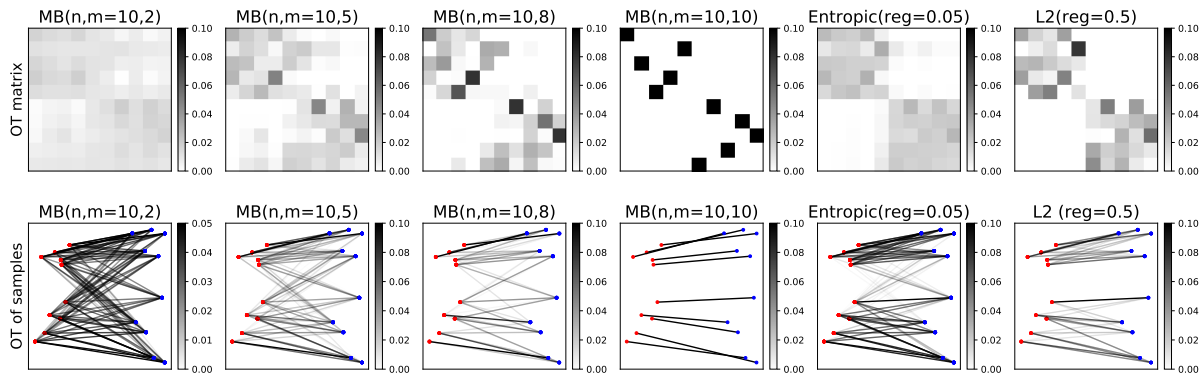


Figure 2: Several OT matrices between 2D distributions with $n = 10$ samples. The first row shows the minibatch OT matrices Π_m for different values of m , the second row provide the shape of the distributions on the rows of the OT matrices. The second row provide a 2D visualization of where the mass is transported between the 2D positions of the sample.

The minibatch Wasserstein losses inherits some properties from the Wasserstein distance but the minibatch procedure leads to a strictly positive loss even when starting from unbiased losses such as Sinkhorn divergence or Wasserstein distance. Remarkably, the Sinkhorn divergence was introduced in the literature to correct the bias from the entropic regularization, and interestingly it was performed in practice on GANs experiments with a minibatch strategy which reintroduced a bias. Whether removing the bias by following the same idea than the Sinkhorn divergence leads to a positive loss is an open question left to future work. Furthermore, given the definition of the minibatch losses it is natural to conjecture that they are convex. Informal ingredients towards a proof of this fact are given in the supplementary material.

An important parameter is the value of the minibatch size m . We remark that the minibatch procedure allows us to interpolate between OT, when $m = n$ and averaged pairwise distance, when $m = 1$. The value of m will also be important for the convergence of our estimator as we will see in the next section.

3.4 Asymptotic convergence

We are now interested in the asymptotic behavior of our estimator $\tilde{U}_h^k(\alpha_n, \beta_n)$ and its deviation to $U_h(\alpha, \beta)$. We will give a deviation bound between our subsampled estimator and the expectation (taken on both drawn minibatches and drawn empirical data) of our estimator. This result is given in the continuous setting but a similar result holds for the semi-discrete setting and it follows the same proof. We will give a bound with respect to both k and n .

Theorem 1 (Maximal deviation bound). *Let $\delta \in (0, 1)$, $k \geq 1$ and m be fixed, and consider two distributions α, β with bounded support and an OT loss $h \in \{W, W_\epsilon, S_\epsilon\}$. We have a deviation bound between $\tilde{U}_h^k(\alpha_n, \beta_n)$ and*

$U_h(\alpha, \beta)$ depending on the number of empirical data n and the number of batches k , with probability at least $1 - \delta$ on the draw of α_n, β_n and D_k we have:

$$|\tilde{U}_h^k(\alpha_n, \beta_n) - U_h(\alpha, \beta)| \leq M_h \left(\sqrt{\frac{\log(\frac{2}{\delta})}{2 \lfloor \frac{n}{m} \rfloor}} + \sqrt{\frac{2 \log(\frac{2}{\delta})}{k}} \right)$$

where M_h depends on h and scales at most as $\mathcal{O}(\log(m))$.

This result can be extended with a Bernstein bound (see appendix). The proof is based on two quantities gotten from the triangle inequality. The first quantity is the difference between $U_h(\alpha_n, \beta_n)$ and its expectation $U_h(\alpha, \beta)$. $U_h(\alpha_n, \beta_n)$ is a two-sample U-statistic and we can prove a bound between itself and its expectation in probability [Hoeffding, 1963]. The second quantity is the difference between $U_h(\alpha_n, \beta_n)$ and the expectation of $\tilde{U}_h^k(\alpha_n, \beta_n)$. We use the difference between the two quantities to obtain a new random variable quantity. From this new random variable, we use the Hoeffding inequality to obtain a dependence with respect to k .

This deviation bound shows that if we increase the number of data n and batches k while keeping the minibatch size m fixed, we get closer to the expectation. We will investigate the dependence on k and m in different scenarios in the numerical experiments. Remarkably, the bound does not depend on the dimension of \mathcal{X} , which is an appealing property when optimizing in high dimension.

As discussed before, an interesting output of Minibatch Wasserstein is the minibatch OT matrix Π_m . Since it is hard to compute in practice, we investigate the error on the marginal constraint of Π_k . In what follows, we denote by $\Pi_{(i)}$ the i -th row of matrix Π and by $\mathbf{1} \in \mathbb{R}^n$ the vector whose entries are all equal to 1.

Theorem 2 (Distance to marginals). *Let $\delta \in (0, 1)$, and consider two distributions α_n, β_n . For all $k \geq 1$, all $1 \leq$*

$i \leq n$, with probability at least $1 - \delta$ on the draw of α_n, β_n and D_k we have:

$$|\Pi_k(\alpha_n, \beta_n)_{(i)} \mathbf{1} - \frac{1}{n}| \leq \sqrt{\frac{2 \log(2/\delta)}{k}}. \quad (8)$$

The proof uses the convergence of Π_k to Π_m and the fact that Π_m is a transportation plan and respects the marginals.

3.5 Gradient and optimization

In this section we review the optimization properties of the minibatch OT losses to ensure the convergence of our loss functions with modern optimization frameworks. We study a standard parametric data fitting problem. Given some discrete samples $(x_i)_{i=1}^n \subset \mathcal{X}$ from some unknown distribution α , we want to fit a parametric model $\lambda \mapsto \beta_\lambda \in \mathcal{M}(\mathcal{X})$ to α using the mini-batch Wasserstein distance for a set Λ in an Euclidian space.

$$\min_{\lambda \in \Lambda} U_h(\alpha_n, \beta_\lambda) \quad (9)$$

Such problems are written as semi discrete OT problems because one of the distributions is continuous while the other one is discrete. For instance, generative models fall under the scope of such problems [Genevay et al., 2018] also known as minimal Wasserstein estimation. As we have an expectation over one of the distributions, we would like to use a stochastic gradient descent strategy to minimize the problem. By using SGD for their method, [Genevay et al., 2018] observed that it worked well in practice and they got meaningful results with minibatches. However it is well known that the empirical Wasserstein distance is a biased estimator of the Wasserstein distance over the true distributions and leads to biased gradients as discussed in [Bellemare et al., 2017], hence SGD might fail. The goal of this section is to prove that unlike the full Wasserstein distance, the minibatch strategy does not suffer from biased gradients.

As stated in Proposition 2, we enjoy an unbiased estimator. However, the original Wasserstein distance is not differentiable, hence we will, further on, only consider the entropic loss and the Sinkhorn divergence which are differentiable.

Theorem 3 (Exchange of Gradient and expectation). *Consider two distributions α and β on two bounded subsets \mathcal{X} and \mathcal{Y} , a C^1 cost. Assume $\lambda \mapsto Y_\lambda$ is differentiable. Then we are allowed to exchange gradients and expectation when h is the entropic loss or the Sinkhorn divergence:*

$$\nabla_\lambda \mathbb{E}_{Y_\lambda \sim \beta_\lambda^{\otimes m}} h(A, Y_\lambda) = \mathbb{E}_{Y_\lambda \sim \beta_\lambda^{\otimes m}} \nabla_\lambda h(A, Y_\lambda) \quad (10)$$

The proof relies on the differentiation lemma. Contrary to the full Wasserstein distance, we proved that the minibatch OT losses do not suffer from biased gradients and this justifies the use of SGD to optimize the problem.

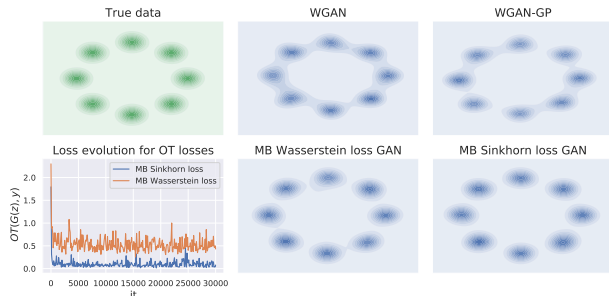


Figure 3: Generated data in 2D for gaussian modes for several generative models.

4 Experiments

In this section, we illustrate the behavior of minibatch Wasserstein. We use it as a loss function for generative models, use it for gradient flow and color transfer experiments. For our experiments, we relied on the POT package [Flamary and Courty, 2017] to compute the exact OT solver or the entropic OT loss and the Geomloss package [Feydy et al., 2019] for the Sinkhorn divergence. The generative model and gradient flow experiments were designed in PyTorch [Paszke et al., 2017] and all the code is released here *.

4.1 Minibatch Wasserstein generative networks

We illustrate the use of minibatch Wasserstein loss for generative modeling [Goodfellow et al., 2014]. The goal is to learn a generative model to generate data close to the target data. We draw 8000 points which follow 8 different gaussian modes (1000 points per mode) in 2D where the modes form a circle. After generating the data, we use a minibatch Wasserstein distance and minibatch Sinkhorn divergence as loss functions with a squared euclidian cost and compared them to WGAN [Arjovsky et al., 2017] and its variant with gradient penalty WGAN-GP [Gulrajani et al., 2017]. We give implementation details in supplementary.

We show the estimated 2D distributions in Figure 3. For the same architecture it seems that MB Wasserstein trains better generators than WGAN and WGAN-GP. This could come from the fact that MB Wasserstein minimize a complex but well posed objective function (with the squared euclidian cost) while WGAN still need to solve the minmax problem making convergence more difficult especially on this 2D problem.

4.2 Minibatch Wasserstein gradient flow

For a given target distribution α , the purpose of gradient flows is to model a distribution $\beta(t)$ which at each iter-

*https://github.com/kilianFatras/minibatch_Wasserstein

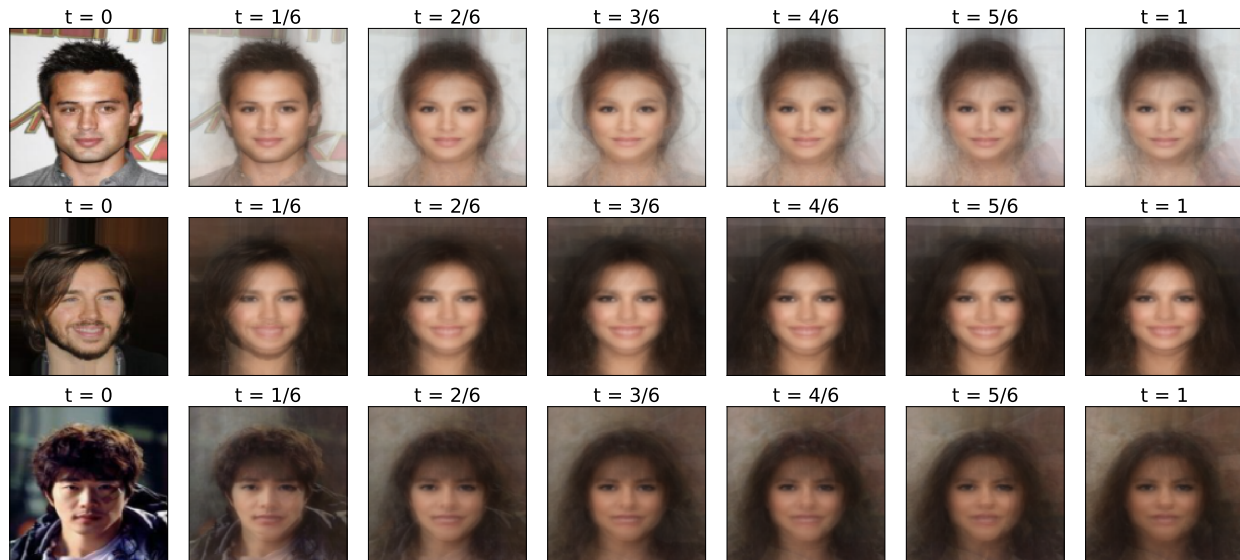


Figure 4: Gradient flow on the CelebA dataset. Source data are 5000 male images while target data are 5000 female images. The batch size m is set to 500 and the number of minibatch k is set to 10. The results were computed with the minibatch Wasserstein distance.

ation follows the gradient direction to minimize the loss $\beta_t \mapsto h(\alpha, \beta_t)$ [Peyré, 2015, Liutkus et al., 2019]. The gradient flow simulate the non parametric setting of data fitting problem. In this setting, the modeled distribution β is parametrized by a vector λ which is the vector position \mathbf{x} that encodes its support.

We follow the same procedure as in [Feydy et al., 2019]. The original gradient flow algorithm uses an Euler scheme. Formally, starting from an initial distribution at time $t = 0$, it means that at each iteration we integrate the ODE

$$\dot{\mathbf{x}}(t) = -\nabla_{\mathbf{x}} F(\mathbf{x}(t)).$$

In our case, we cannot compute the gradient directly from our minibatch OT losses. As the OT loss inputs are distributions, we have an inherent bias when we calculate the gradient from the weights $\frac{1}{m}$ of samples. To correct this bias, we multiply the gradient by the inverse weight m . Finally, for each data \mathbf{x} we integrate:

$$\dot{\mathbf{x}}(t) = -m \nabla_{\mathbf{x}} \left[\tilde{U}_h^k(\alpha_n, \beta_n) \right] (\mathbf{x}(t)) \quad (11)$$

We recall that the inherent bias from minibatch makes that the final solution can not be the target distribution.

The considered data are from the CelebA dataset [Liu et al., 2015]. We use 5000 male images as source data and 5000 female images as target data. We show the evolution of 3 samples in the source data in Figure 4. We use a squared euclidean cost, a batch size of 500, a learning rate of 0.05 and make 750 iterations. k did not need to be large and was set to 10 in order to stabilize the gradient flow. We see a natural evolution in the images along the gradient flow similar to results obtained in [Liutkus et al., 2019]. Interestingly the gradient flow with MB Wasserstein in Figure 4

leads to possibly more detailed backgrounds than with MB Sinkhorn (provided in supplementary) probably due to the two layers of regularization in the latter.

4.3 Large scale barycentric mapping for color transfer

The purpose of color transfer is to transform the color of a source image so that it follows the color of a target image. Optimal Transport is a well known method to solve this problem and has been studied before in [Ferradans et al., 2013, Blondel et al., 2018]. Images are represented by point clouds in the RGB color space identified with $[0, 1]$. Then by calculating the transportation plan between the two point clouds, we get a transfer color mapping by using a barycentric projection. As the number of pixels might be huge, previous work selected a subset of pixels using k-means clusters for each point cloud. This strategy allows to make the problem memory tractable but loses some information. With MB optimal transport, we can compute a barycentric mapping for all pixels in the image by incrementally updating the mapping at each minibatch. When one selects a source batch A and a target batch B, she just needs to update the transformed vector between the considered batches as $Y_s|_A = \sum_{B \in \mathcal{P}_m(\beta_n)} \Pi_{A,B} X_t|_B$. Indeed, to perform the color transfer when we have the full Π_k matrix, we compute the matrix product:

$$Y_s = n_s \Pi_k(\alpha_n, \beta_n) X_t \quad (12)$$

that can be computed incrementally by considering restriction to batches (the full algorithm is given in appendix). To the best of our knowledge, it is the first time that a barycentric mapping algorithm has been scaled up to 1M pixel

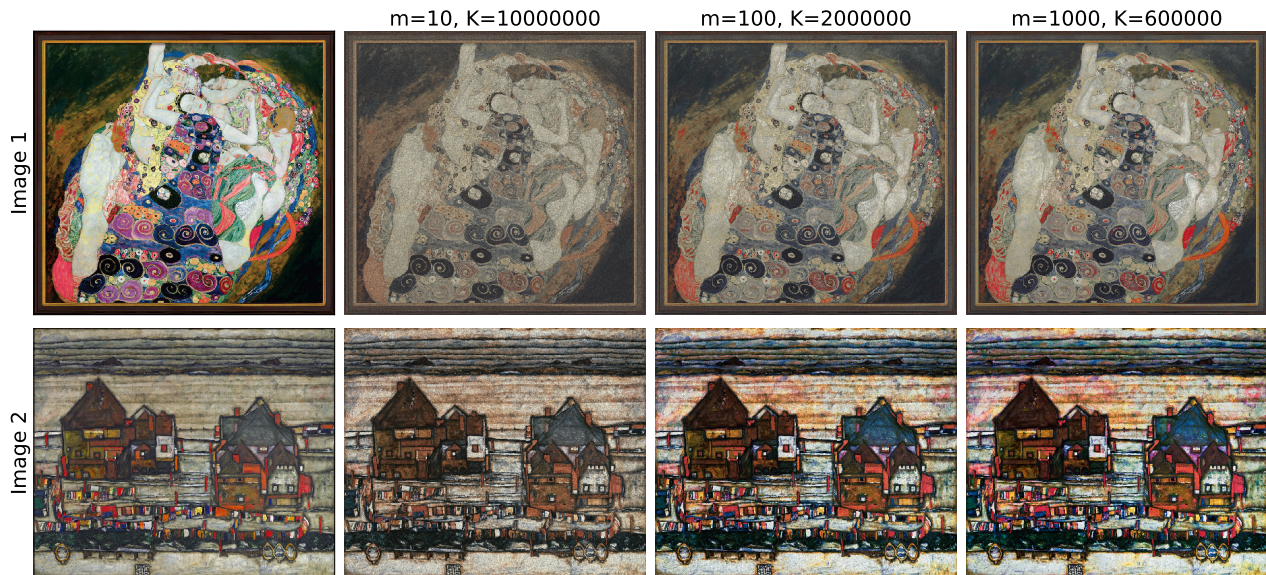


Figure 5: Color transfert between full images for different batch size and number of batches. (Top) color transfert from image 1 to image 2. (Bottom) color transfert from image 2 to image 1.

images. About the required memory for experiments, the memory cost to store data is $O(n)$. The minibatch OT calculus requires $O(m^2)$ because we need to store the ground cost and the OT plan. The marginal experiment requires $O(n)$, as we just need to average the marginals of the plan. Finally, the memory cost is $O(n)$ while OT is $O(n^2)$.

The source image has (943000, 3) RGB dimension and the target image has RGB dimension (933314, 3). For this experiments, we used the minibatch Wasserstein distance with squared euclidean ground cost for several m and k . We used batch of size 10, 100 and 1000. We selected k so as to obtain a good visual quality and observed that a smaller k was needed when using large minibatches. Further experiments which show the dependence on k can be found in appendix. Also note that performing MB optimal transport can be done in parallel and can be greatly speed-up on multi-CPU architectures. One can see in 5 the color transfer (in both directions) provided with our method. We can see that the diversity of colors falls when the batch size is too small as the entropic solver would do for a large regularization parameter. However, even for 1M pixels, a batch size of 1000 is enough to keep a good diversity of colors.

We also studied empirically the results of theorem 2, as shown in Figure 6 we recover the $O(k^{-1/2})$ convergence rate on the marginal with a constant depending on the batch size m . Furthermore, we also empirically studied the computational time and showed that our method is not affected by the number of points with a fixed complexity when an algorithm like Sinkhorn still has a $O(n^2)$ complexity. These experiments show that the minibatch Wasserstein losses are well suited for large scale problems where both memory and computational time are issues.

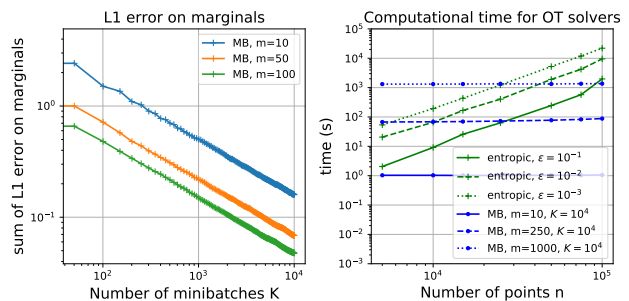


Figure 6: (left) L1 error on both marginals (loglog scale). We selected 1000 points from original images and computed the error on marginals for several m and k (loglog scale). (Right) Computation time for several OT solvers for several number of points in the input distributions, the computation time of the cost matrix is included.

5 Conclusion

In this paper, we studied the impact of using a minibatch strategy in order to reduce the Wasserstein distance complexity. We review the basic properties, and studied the asymptotic behavior of our estimator. We showed a deviation bound between our subsampled estimator and the expectation of our estimator. Furthermore, we studied the optimization procedure of our estimator and proved that it enjoys unbiased gradients. Finally, we demonstrated the effect of minibatch strategy with gradient flow experiments, color transfer and GAN experiments. Future works will focus on the geometry of minibatch Wasserstein (for instance on barycenters) and on investigating a debiasing approach similar to the one used for Sinkhorn Divergence.

Acknowledgements

Authors would like to thank Thibault Séjourné and Jean Feydy for fruitful discussions. This work is partially funded through the projects OATMIL ANR-17-CE23-0012 and 3IA Côte d’Azur Investments ANR-19-P3IA-0002 of the French National Research Agency (ANR).

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Learning with minibatch Wasserstein : asymptotic and gradient properties

Supplementary material

Outline. The supplementary material of this paper is organized as follows:

- In section A, we first review the formalism with definitions, basic property proofs, statistical proofs and optimization proofs. Then we give details about the 1D case.
- In section B, we give extra experiments for domain adaptation, minibatch Wasserstein gradient flow in 2D and on the celebA dataset and finally, color transfer.

A Formalism

In what follows, without any loss of generality and in order to simplify the notations we will work with the cost matrix $C = C(X, Y) = (|X_i - Y_j|)_{1 \leq i, j \leq n}$.

A.1 Definitions

We start giving the formal definitions for the transportation plan Π_m . We recall that the discrete entropy of a coupling matrix is defined as $H(P) = -\sum_{i,j} P_{i,j} (\log(P_{i,j}) - 1)$ [chapitre 4, [Peyré and Cuturi, 2019]]. The entropic regularization parameter $\varepsilon \in \mathbb{R}_+$.

Definition 4 (Mini-batch Transport). *Let $A \in \mathcal{P}_m(\alpha_n)$ and $B \in \mathcal{P}_m(\beta_n)$ be two sets. We denote by $\Pi_{A,B}^0(\alpha_n, \beta_n) = (\Pi_{A,B}^0(i, j))_{1 \leq i, j \leq m} \in \mathbb{R}^{m \times m}$ an optimizer of the optimal transport. Formally,*

$$\Pi_{A,B}^0 = \underset{\Pi \in U(A,B)}{\operatorname{argmin}} \langle \Pi, C_{|A,B} \rangle - \varepsilon H(\Pi) \quad (13)$$

where $C_{|A,B} \in \mathbb{R}^{m \times m}$ is the matrix extracted from C by considering elements of the lines (resp. columns) of C which belong to A (resp. B) and H the entropy term. ε is a positive real number that can be equal to 0 to get the original OT problem.

For two sets $A \in \mathcal{P}_m(\alpha_n)$ and $B \in \mathcal{P}_m(\beta_n)$ we denote by $\Pi_{A,B}(\alpha_n, \beta_n) \in \mathbb{R}^{n \times n}$ the matrix

$$\Pi_{A,B} = (\Pi_{A,B}^0(i, j) \mathbf{1}_A(i) \mathbf{1}_B(j))_{(i,j) \in \alpha_n \times \beta_n} \quad (14)$$

Definition 5 (Averaged mini-batch transport). *We define the empirical averaged mini-batch transport matrix $\Pi_m(\alpha_n, \beta_n)$ by the formula*

$$\Pi_m := \frac{1}{\binom{n}{m}^2} \sum_{A \in \mathcal{P}_m(\alpha_n)} \sum_{B \in \mathcal{P}_m(\beta_n)} \Pi_{A,B} \quad (15)$$

Moreover, we can define the averaged Wasserstein distance over all mini batches as :

$$U_W(\alpha_n, \beta_n) = \langle \Pi_m, C \rangle \quad (16)$$

Remark 1. *Note that this construction is consistent with $U_h(\alpha_n, \beta_n)$.*

A.2 Basic properties

Proposition 4. Π_m is a transportation plan between the empirical distributions α_n, β_n .

Proof. We need to verify that the marginals sum to one -e.g. that the sum over any row (resp. column) is equal to $\frac{1}{n}$. Without loss of generality, we will fix a source sample (or row): i_0 . A simple combinatorial argument gives that $\sum_{A \in \mathcal{P}_m(\alpha_n)} \mathbf{1}_A(i_0) = \binom{n-1}{m-1}$. Now we are ready to sum over the row i_0 .

$$\sum_{j=1}^n \Pi_m(i_0, j) = \frac{1}{\binom{n}{m} \binom{n}{m}} \sum_{j=1}^n \sum_{A \in \mathcal{P}_m(\alpha_n)} \sum_{B \in \mathcal{P}_m(\beta_n)} \Pi_{A,B}(i_0, j) \quad (17)$$

$$= \frac{1}{\binom{n}{m} \binom{n}{m}} \sum_{B \in \mathcal{P}_m(\beta_n)} \sum_{j=1}^n \Pi_{A,B}^0(i_0, j) \mathbf{1}_B(j) \sum_{A \in \mathcal{P}_m(\alpha_n)} \mathbf{1}_A(i_0) \quad (18)$$

$$= \frac{1}{\binom{n}{m} \binom{n}{m}} \sum_{B \in \mathcal{P}_m(\beta_n)} \underbrace{\sum_{j=1}^n \Pi_{A,B}^0(i_0, j) \mathbf{1}_B(j)}_{=1/m} \binom{n-1}{m-1} \quad (19)$$

$$= \frac{1}{\binom{n}{m} \binom{n}{m}} \binom{n}{m} \frac{1}{m} \binom{n-1}{m-1} \quad (20)$$

$$= \frac{1}{n} \quad (21)$$

The argument is similar for the summation over any column. □

Remark 2 (Positivity, symmetry and bias). *Let $m < n$, the quantity U_h is positive and symmetric but also strictly positive, i.e $U_h(\alpha_n, \alpha_n) > 0$. Indeed,*

$$U_h(\alpha_n, \alpha_n) := \frac{1}{\binom{n}{m}^2} \sum_{A \in \mathcal{P}_m(\alpha_n)} \sum_{A' \in \mathcal{P}_m(\alpha_n)} h(A, A') \quad (22)$$

$$= \frac{1}{\binom{n}{m}^2} \sum_{(A, A') \in \mathcal{P}_m(\alpha_n) \times \mathcal{P}_m(\beta_n), A \neq A'} h(A, A') > 0 \quad (23)$$

Convexity We introduce a few notations. Let $\mathcal{D}(\mathbb{R}^d)$ be the space defined by

$$\mathcal{D}(\mathbb{R}^d) := \left\{ \sum_{i=1}^p \gamma_i \delta_{x_i} : (\gamma_i)_{1 \leq i \leq p} \in (\mathbb{R}_+)^p, \sum_{i=1}^p \gamma_i = 1; p \in \mathbb{N}; (x_i)_{1 \leq i \leq p} \in (\mathbb{R}^d)^p \right\} \quad (24)$$

It is easy to see that $\mathcal{D}(\mathbb{R}^d)$ is convex. One can actually extend in a natural way the definition of U_h to the set $\mathcal{D}(\mathbb{R}^d) \times \mathcal{D}(\mathbb{R}^d)$. Assuming this can be done, the intuition for convexity is that U_h is an average of convex terms [(section 9.1 and prop 4.6, [Peyré and Cuturi, 2019]). We then claim the convexity of the following maps:

$$\begin{aligned} (\alpha_n, \beta_n) &\mapsto U_W(\alpha_n, \beta_n) \\ \mathcal{D}(\mathbb{R}^d) \times \mathcal{D}(\mathbb{R}^d) &\rightarrow \mathbb{R} \end{aligned}$$

and for $h = W_\epsilon$ or $h = S_\epsilon$:

$$\begin{aligned} \alpha_n &\mapsto U_h(\alpha_n, \beta_n) \\ \mathcal{D}(\mathbb{R}^d) &\rightarrow \mathbb{R} \\ \beta_n &\mapsto U_h(\alpha_n, \beta_n) \\ \mathcal{D}(\mathbb{R}^d) &\rightarrow \mathbb{R} \end{aligned}$$

A.3 Statistical proofs

Note that because the distributions α and β are compactly supported, there exists a constant $M > 0$ such that for any $1 \leq i, j \leq n$, $|X_i - Y_j| \leq M$ with $M := \text{diam}(\text{Supp}(\alpha) \cup \text{Supp}(\beta))$. We define the following quantity depending on the

OT loss h :

$$M_h = \begin{cases} \text{diam}(\text{Supp}(\alpha) \cup \text{Supp}(\beta)) & \text{if } h = W \\ \frac{3}{2} \{ \text{diam}(\text{Supp}(\alpha) \cup \text{Supp}(\beta)) + \varepsilon(2 \log_2(m) + 1) \} & \text{if } h = W_\varepsilon \text{ or } S_\varepsilon \end{cases} \quad (25)$$

Lemma 1 (Upper bounds). *Let $(A, B) \in \mathcal{P}_m(\alpha_n) \times \mathcal{P}_m(\beta_n)$. We have the following bound for each of the above considered OT losses h :*

$$|h(A, B)| \leq 2M_h \quad (26)$$

Proof. We start with the case $h = W$. Note that with our choice of cost matrix $C = (C_{i,j})$ one has $0 \leq C_{i,j} \leq M_W$. We have for a transport plan $\Pi = (\Pi_{i,j})$ between A and B (with respect to the cost matrix $C_{|A,B}$)

$$|\langle \Pi, C_{|A,B} \rangle| \leq \sum_{1 \leq i,j \leq m} (C_{|A,B})_{ij} \Pi_{i,j} \leq M_W \sum_{1 \leq i,j \leq m} \Pi_{i,j} = M_W$$

Hence, $h(A, B) \leq M_W$.

If $h = W_\varepsilon$ for an $\varepsilon > 0$. Let us denote by $E(q) = -\sum_{i=1}^r q_i \log(q_i)$ the Shannon entropy of the discrete probability distribution $q = (q_i)_{1 \leq i \leq r}$. Using the classical fact : $0 \leq E(q) \leq \log_2(r)$ one estimates for a transport plan Π :

$$|\langle \Pi, C_{|A,B} \rangle - \varepsilon H(\Pi)| \leq M_W + \varepsilon(E(\Pi) + 1) \leq M_W + \varepsilon(\log_2(m^2) + 1) \leq 2M_h$$

which gives the intended bound by definition of W_ε . Lastly, for $h = S_\varepsilon$, since it is basically the sum of three terms of the form W_ε one can conclude. \square

Proof of Theorem 1 We now give the details of the proof of theorem 1. We start by recalling the definitions of our losses.

Definition 6 (Minibatch Wasserstein definitions). *Given an OT loss h and an integer $m \leq n$, we define the following quantities:*

The continuous loss:

$$U_h(\alpha, \beta) := \mathbb{E}_{(X,Y) \sim \alpha \otimes \beta} [h(X, Y)] \quad (27)$$

The semi-discrete loss:

$$U_h(\alpha_n, \beta) := \binom{n}{m}^{-1} \sum_{A \in \mathcal{P}_m(\alpha_n)} \mathbb{E}_{Y \sim \beta \otimes m} [h(A, Y)] \quad (28)$$

The discrete-discrete loss:

$$U_h(\alpha_n, \beta_n) := \binom{n}{m}^{-2} \sum_{A \in \mathcal{P}_m(\alpha_n)} \sum_{B \in \mathcal{P}_m(\beta_n)} h(A, B) \quad (29)$$

The subsample discrete-discrete loss. Pick an integer $k > 0$. We define:

$$\tilde{U}_h^k(\alpha_n, \beta_n) := k^{-1} \sum_{(A,B) \in D_k} h(A, B) \quad (30)$$

where D_k is a set of cardinality k whose elements are drawn at random from the uniform distribution on $\Gamma := \mathcal{P}_m(\{X_1, \dots, X_n\}) \times \mathcal{P}_m(\{Y_1, \dots, Y_n\})$. Where h can be the Wasserstein distance W , the entropic loss W_ε or the sinkhorn divergence S_ε for a cost $c(\mathbf{x}, \mathbf{y})$.

Lemma 2 (U-statistics concentration bound). *Let $\delta \in (0, 1)$ and m be fixed, we have a concentration bound between $U_h(\alpha_n, \beta_n)$ and the expectation over minibatches $U_h(\alpha, \beta)$ depending on the number of empirical data n which follow α and β .*

$$|U_h(\alpha_n, \beta_n) - U_h(\alpha, \beta)| \leq M_h \sqrt{\frac{\log(2/\delta)}{2 \lfloor n/m \rfloor}} \quad (31)$$

with probability at least $1 - \delta$. Furthermore, a Bernstein concentration bound is available. Let us denote the variance of the OT loss h over the batches σ_h^2 , i.e., $\sigma_h^2 = \text{Var}(h(X_1, \dots, X_m, Y_1, \dots, Y_m))$. The variance is bounded by M_h^2 . Then we have with probability at least ε :

$$P(|U_h(\alpha_n, \beta_n) - U_h(\alpha, \beta)| \geq \varepsilon) \leq 2 \exp \left(\frac{-\lfloor n/m \rfloor \varepsilon^2}{2(\sigma_h^2 + \frac{M_h}{3} \varepsilon)} \right) \leq 2 \exp \left(\frac{-\lfloor n/m \rfloor \varepsilon^2}{2(M_h^2 + \frac{M_h}{3} \varepsilon)} \right) \quad (32)$$

Proof. $U_h(\alpha_n, \beta_n)$ is a two-sample U-statistic and $U_h(\alpha, \beta)$ is its expectation as α_n and β_n have *iid* random variables. $U_h(\alpha_n, \beta_n)$ is a sum of dependant variables and Hoeffding found a way to rewrite $U_h(\alpha_n, \beta_n)$ as a sum of independent random variables. As our data are *iid* and our OT loss is bounded, we can apply its third theorem to our U-statistic. The proof can be found in [Hoeffding, 1963, Section 5] (the two sample U-statistic case is discussed in 5.b). \square

Lemma 3 (Deviation bound). *Let α_n and β_n be empirical distributions of respectively α and β , let $\delta \in (0, 1)$ and $k \geq 1$. We have a deviation bound between $\tilde{U}_h^k(\alpha_n, \beta_n)$ and $U_h(\alpha_n, \beta_n)$ depending on the number of batches k .*

$$|\tilde{U}_h^k(\alpha_n, \beta_n) - U_h(\alpha_n, \beta_n)| \leq M_h \sqrt{\frac{2 \log(2/\delta)}{k}} \quad (33)$$

with probability at least $1 - \delta$.

Proof. First note that $\tilde{U}_h^k(\alpha_n, \beta_n)$ is an incomplete U-statistic of $U_h(\alpha_n, \beta_n)$. Let us consider the sequence of random variables $((\mathbf{1}_l(A, B))_{(A, B) \in \Gamma})_{1 \leq l \leq k}$ such that $\mathbf{1}_l(A, B)$ is equal to 1 if (A, B) has been selected at the l -th draw and 0 otherwise. By construction of \tilde{U}_h^k , the aforementioned sequence is an i.i.d sequence of random vectors and the $\mathbf{1}_l(A, B)$ are bernoulli random variables of parameter $1/|\Gamma|$. We then have

$$\tilde{U}_h^k(\alpha_n, \beta_n) - U_h(\alpha_n, \beta_n) = \frac{1}{k} \sum_{l=1}^k \omega_l \quad (34)$$

where $\omega_l = \sum_{(A, B) \in \Gamma} (\mathbf{1}_l(A, B) - \frac{1}{|\Gamma|}) h(A, B)$. Conditioned upon $X = (X_1, \dots, X_n)$ and $Y = (Y_1, \dots, Y_n)$, the variables ω_l are independent, centered and bounded by $2M_h$ thanks to lemma 1. Using Hoeffding's inequality yields

$$\mathbb{P}(|\tilde{U}_h^k(\alpha_n, \beta_n) - U_h(\alpha_n, \beta_n)| > \varepsilon) = \mathbb{E}[\mathbb{P}(|\tilde{U}_h^k(\alpha_n, \beta_n) - U_h(\alpha_n, \beta_n)| > \varepsilon | X, Y)] \quad (35)$$

$$= \mathbb{E}[\mathbb{P}(|\frac{1}{k} \sum_{l=1}^k \omega_l| > \varepsilon | X, Y)] \quad (36)$$

$$\leq \mathbb{E}[2e^{-\frac{k\varepsilon^2}{2M_h^2}}] = 2e^{-\frac{k\varepsilon^2}{2M_h^2}} \quad (37)$$

which concludes the proof. \square

Theorem 4 (Maximal deviation bound). *Let $\delta \in (0, 1)$, $k \geq 1$ and m be fixed, we have a maximal deviation bound between $\tilde{U}_h^k(\alpha_n, \beta_n)$ and the expectation over minibatches $U_h(\alpha, \beta)$ depending on the number of empirical data n which follow α and β and the number of batches k .*

$$|\tilde{U}_h^k(\alpha_n, \beta_n) - U_h(\alpha, \beta)| \leq M_h \sqrt{\frac{\log(2/\delta)}{2 \lfloor n/m \rfloor}} + M_h \sqrt{\frac{2 \log(2/\delta)}{k}} \quad (38)$$

with probability at least $1 - \delta$

Proof. Thanks to lemma 3 and A.3 we get

$$|\tilde{U}_h^k(\alpha_n, \beta_n) - U_h(\alpha, \beta)| \leq |\tilde{U}_h^k(\alpha_n, \beta_n) - U_h(\alpha_n, \beta_n)| + |U_h(\alpha_n, \beta_n) - U_h(\alpha, \beta)| \quad (39)$$

$$\leq M_h \sqrt{\frac{\log(2/\delta)}{2 \lfloor n/m \rfloor}} + M_h \sqrt{\frac{2 \log(2/\delta)}{k}} \quad (40)$$

with probability at least $1 - (\frac{\delta}{2} + \frac{\delta}{2}) = 1 - \delta$. We can get a sharper bound using the Bernstein inequality instead of the Hoeffding inequality as detailed in lemma . \square

Proof of Theorem 2 We now give the details of the proof of theorem 2. In what follows, we denote by $\Pi_{(i)}$ the i -th row of matrix Π . Let us denote by $\mathbf{1} \in \mathbb{R}^n$ the vector whose entries are all equal to 1.

Theorem 5 (Distance to marginals). *Let $\delta \in (0, 1)$, we have for all $k \geq 1$ and all $1 \leq j \leq n$:*

$$|\Pi_k(\alpha_n, \beta_n)_{(i)} \mathbf{1} - \frac{1}{n}| \leq \sqrt{\frac{2 \log(2/\delta)}{k}} \quad (41)$$

with probability at least $1 - \delta$.

Proof. We would like to remind that Π_m is a transportation plan between the full input distributions α_n and β_n and hence, it verifies the marginals, i.e $\Pi_m(\alpha_n, \beta_n)_i \times \mathbf{1} = \frac{1}{n}$. Let us consider the sequence of random variables $((\mathbf{1}_p(A, B)_{(A, B) \in \Gamma})_{1 \leq p \leq k})$ such that $\mathbf{1}_p(A, B)$ is equal to 1 if (A, B) has been selected at the p -th draw and 0 otherwise. By construction of $\Pi_k(\alpha_n, \beta_n)$, the aforementioned sequence is an i.i.d sequence of random vectors and the $\mathbf{1}_p(A, B)$ are bernoulli random variables of parameter $1/|\Gamma|$. We then have

$$\Pi_k(\alpha_n, \beta_n)_{(i)} \mathbf{1} = \frac{1}{k} \sum_{p=1}^k \omega_p \quad (42)$$

where $\omega_p = \sum_{(A, B) \in \Gamma} \sum_{j=1}^n (\Pi_{A, B})_{i, j} \mathbf{1}_p(A, B)$. Conditioned upon $X = (X_1, \dots, X_n)$ and $Y = (Y_1, \dots, Y_n)$, the random vectors ω_p are independent, and bounded by 1. Moreover, one can observe that $\mathbb{E}[\Pi_k(\alpha_n, \beta_n)_i \mathbf{1}] = \Pi_m(\alpha_n, \beta_n)_i \mathbf{1}$. Using Hoeffding's inequality yields

$$\mathbb{P}(|\Pi_k(\alpha_n, \beta_n)_i \mathbf{1} - \Pi_m(\alpha_n, \beta_n)_i \mathbf{1}| > \varepsilon) = \mathbb{E}[\mathbb{P}(|\frac{1}{k} \sum_{p=1}^k \omega_p - \mathbb{E}[\frac{1}{k} \sum_{p=1}^k \omega_p]| > \varepsilon | X, Y)] \quad (43)$$

$$\leq 2e^{-2k\varepsilon^2} \quad (44)$$

which concludes the proof. \square

A.4 Optimization

The main goal of this section is to give a justification of optimization for our minibatch OT losses by giving the **proof of theorem 3**. More precisely, we show that for the losses W_ε and S_ε , one can exchange the gradient symbol ∇ and the expectation \mathbb{E} . It shows for example that a stochastic gradient descent procedure is unbiased and as such legitimate.

Main hypothesis. We assume that the map $\lambda \mapsto C(A, Y_\lambda)$ is differentiable. For instance for GANs, it is verified when the neural network in the generator is differentiable -which is the case if the nonlinear activation functions are all differentiable- and when the cost chosen in the Wasserstein distance is also differentiable.

We introduce the map

$$g : (\Pi, C) \mapsto \langle \Pi, C \rangle - \varepsilon H(\Pi)$$

To prove this theorem, we first define a map we will use the "Differentiation Lemma".

Lemma 4 (Differentiation lemma). *Let V be a nontrivial open set in \mathbb{R}^p and let \mathcal{P} be a probability distribution on \mathbb{R}^d . Define a map $C : \mathbb{R}^d \times \mathbb{R}^d \times V \rightarrow \mathbb{R}$ with the following properties:*

- For any $\lambda \in V$, $\mathbb{E}_{\mathcal{P}}[|C(X, Y, \lambda)|] < \infty$
- For P -almost all $(X, Y) \in \mathbb{R}^d \times \mathbb{R}^d$, the map $V \rightarrow \mathbb{R}$, $\lambda \rightarrow C(X, Y, \lambda)$ is differentiable.
- There exists a P -integrable function $\varphi : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ such that $|\partial_\lambda C(X, Y, \lambda)| \leq g(x)$ for all $\lambda \in V$.

Then, for any $\lambda \in V$, $E_{\mathcal{P}}[|\partial_\lambda C(X, Y, \lambda)|] < \infty$ and the function $\lambda \rightarrow E_{\mathcal{P}}[C(X, Y, \lambda)]$ is differentiable with differential:

$$E_{\mathcal{P}} \partial_\lambda [C(X, Y, \lambda)] = \partial_\lambda E_{\mathcal{P}} [C(X, Y, \lambda)] \quad (45)$$

The following result will also be useful.

Lemma 5 (Danskin, Rockafellar). *Let $g : (z, w) \in \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ be a function. We define $\varphi : z \mapsto \max_{w \in W} g(z, w)$ where $W \subset \mathbb{R}^d$ is compact. We assume that for each $w \in W$, the function $g(\cdot, w)$ is differentiable and that $\nabla_z g$ depends continuously on (z, w) . If in addition, $g(z, w)$ is convex in z , and if \bar{z} is a point such that $\operatorname{argmax}_{w \in W} g(\bar{z}, w) = \{\bar{w}\}$, then φ is differentiable at \bar{z} and verifies*

$$\nabla \varphi(\bar{z}) = \nabla_z g(\bar{z}, \bar{w}) \quad (46)$$

The last theorem shows that the entropic loss is differentiable with respect to the cost matrix. Indeed, the theorem directly applies since the problem is strongly convex. This remark enables us to obtain the following result.

Theorem 6 (Exchange gradient and expectation). *Let us suppose that we have two distributions α and β on two bounded subsets \mathcal{X} and \mathcal{Y} , a C^1 cost. Assume $\lambda \mapsto Y_\lambda$ is differentiable. Then for the entropic loss and the Sinkhorn divergence:*

$$\nabla_\lambda \mathbb{E}_{Y_\lambda \sim \beta_\lambda^{\otimes m}} h(A, Y_\lambda) = \mathbb{E}_{Y_\lambda \sim \beta_\lambda^{\otimes m}} \nabla_\lambda h(A, Y_\lambda) \quad (47)$$

Proof. Regarding the Sinkhorn divergence, as it is the sum of three terms of the form W_ε , it suffices to show the theorem for $h = W_\varepsilon$

The first and the third conditions of the Differentiation Lemma are trivial as we have supposed that our distributions have compact supports. Hence, the minibatch Wasserstein exists and is bounded on a finite set. We can also build a measurable function φ which takes the biggest cost value $\|c\|_\infty$ inside \mathcal{X} and 0 outside. As \mathcal{X} is compact, the integral of the function over \mathbb{R}^d is finite.

The problem is in the second hypothesis where we need to prove that W_ε is differentiable almost everywhere. We have to show that the following function $\lambda \mapsto \varphi_A(\lambda)$ is differentiable:

$$\varphi_A : \lambda \mapsto \min_{\Pi \in U(a,b)} \langle \Pi, C(A, \lambda) \rangle - \varepsilon H(\Pi)$$

where $C(A, \lambda)$ is the cost computed using pairwise distances between A and Y_λ . Since $\lambda \mapsto C(A, \lambda)$ is differentiable almost everywhere by our hypothesis on $\lambda \mapsto y_\lambda$, it suffices, by composition, to show that $C \mapsto \min_{\Pi \in U(a,b)} \langle \Pi, C \rangle - \varepsilon H(\Pi)$ is differentiable in $C \in \mathbb{R}^{m \times m}$. We obtain this using lemma 5 and the fact that there is one unique solution to the entropically regularized optimal transport problem. □

A.5 1D case

We now give the full combinatorial calculus for the 1D case. We start by sorting all the data and give to each of them an index which represents their position after the sorting phase. Then we select and sort all the minibatches. x_j can not be at a position superior to its index j inside a batch. For a fixed x_j , a simple combinatorial arguments tells you that there are $C_{x_j}^i$ sets where x_j is at the i -th position:

$$C_{i,x_j}^{m,n} = \binom{j-1}{i-1} \binom{n-j}{m-i} \quad (48)$$

Suppose that x_j is transported to a y_k points in the target mini batch. Then, they both share the same positions i in their respective minibatch. As there are several i where x_j is transported to y_k , we sum over all those possible positions. Hence our current transportation matrix coefficient $\Pi_{j,k}$ can be calculated as :

$$\Pi_{j,k} = \sum_{i=i_{\min}}^{i_{\max}} C_{i,x_j}^{m,n} C_{i,y_k}^{m,n} \quad (49)$$

Where $i_{\min} = \max(0, m - n + j, m - n + k)$ and $i_{\max} = \min(j, k)$. i_{\min} and i_{\max} represent the sorting constraints. Furthermore, as we have uniform weight histograms, we will transport a mass of $\frac{1}{m}$ and averaged it by the total number of transportation. So finally, our transportation matrix coefficient $\Pi_{j,k}$ are:

$$\Pi_{j,k} = \frac{1}{m \binom{n}{m}^2} \sum_{i=i_{\min}}^{i_{\max}} C_{i,x_j}^{m,n} C_{i,y_k}^{m,n} \quad (50)$$

B Extra experiments

In this section, we present extra experiments on the utility of using minibatch Wasserstein loss for domain adaptation, gradient flow and color transfer. We also give the algorithm which computes the barycentric mapping incrementally.

B.1 Generative models

We give implementation details of our batch Wasserstein generative models. We use a normal Gaussian noise in a latent space of dimension 10 and the generator is designed as a simple multilayer perceptron with 2 hidden layers of respectively 128 and 32 units with ReLU activation functions, and one final layer with 2 output neurons. For the different OT losses, the generator is trained with the same learning rate equal to 0.05. The optimizer is the Adam optimizer with $\beta_1 = 0$ and $\beta_2 = 0.9$. For the Sinkhorn divergence we set ε to 0.01. For WGAN and WGAN-GP we train a discriminator with the same hidden layers than the generator. We update the discriminator 5 times before one update of the generator. WGAN is trained with RMSprop optimizer and WGAN-GP with Adam optimizer ($\beta_1 = 0$, $\beta_2 = 0.9$) as done in their original papers. The learning rate is set to 10^{-4} for both. WGAN-GP has a gradient penalty parameter set to 10. All models are trained for 30000 iterations with a batch size of 100. Our minibatch OT losses use $k = 1$, which means that we compute the stochastic gradient on only one minibatch, and larger k was not needed to get meaningful results.

B.2 Domain adaptation

Domain adaptation problems consist to transfer knowledge from a source domain to a target domain. The goal is to use the labeled data in the source domain in order to classify the unlabeled data in the target domain. [Courty et al., 2017] used optimal transport to transport the source data to the target data by computing an OT map. Then they used a barycentric mapping to transport the source data to the target domain with their label. Optimal transport has been successful on this problem and we now want to study the impact of the minibatch OT losses and different OT variants.

We consider two common datasets for domain adaptation problems : MNIST [LeCun and Cortes, 2010] and USPS [Hull, 1994]. The datasets are composed of hand written digits between 0 and 9. MNIST have 60000 training samples and USPS have 7291 training samples. We select 7000 samples from each dataset. The used cost for those experiments is a normalized squared euclidean cost. We want to study the number of samples which are transported on same labeled data from the source dataset to the target dataset. That is why we will study the proportion of mass between same labeled data in the transportation matrix.

The experiments use minibatch Wasserstein loss. We will use several k and m values, while for the entropic OT loss we will consider values of epsilon between 10^{-3} and 1. For each m and k , we conducted the experiments 10 times and we plot the mean and standard deviation for each m and k .

This experiment shows that considering a very small batch size hurts the number of images transported on correct labels and taking a large number of batches does not correct the performance. We also see that the number of batches k reduces the variance and should decrease when the batch size increases. Furthermore, we see that when m decreases, we have a similar performance than for the entropic OT loss with a large regularization parameter ε . We conjecture, that doing the minibatch entropic loss with a large ε parameter can lead to over regularization and can hurt the performance.

B.3 Minibatch Wasserstein gradient flow

We experimented the minibatch OT gradient flow to distributions in 2D. The purpose is to see the relevance of minibatch Wasserstein gradient flow for shape matching applications. We used the same experiments as in [Feydy et al., 2019] and relied on the geomloss package. In 2D we selected 500 data points following the image’s pixel distribution. The experiments were conducted with the minibatch Wasserstein loss. We observe that we are not able to recover the target distribution, it is expected as our loss is strictly positive. However, for large enough batch size, the final distribution fits almost perfectly the target distribution and our loss leads to a good approximation.

Nevertheless we can see that taking a batch size too small results in a loss of information and drives the data toward the high density area as pointed in the 2D experiments. Regarding the number of minibatches k , it does not influence the shape of the final distribution.

Regarding the gradient flow on the celebA dataset, we now show the results when we use the minibatch Sinkhorn divergence instead of the minibatch Wasserstein distance. The minibatch Sinkhorn divergence is slower in practice than the minibatch

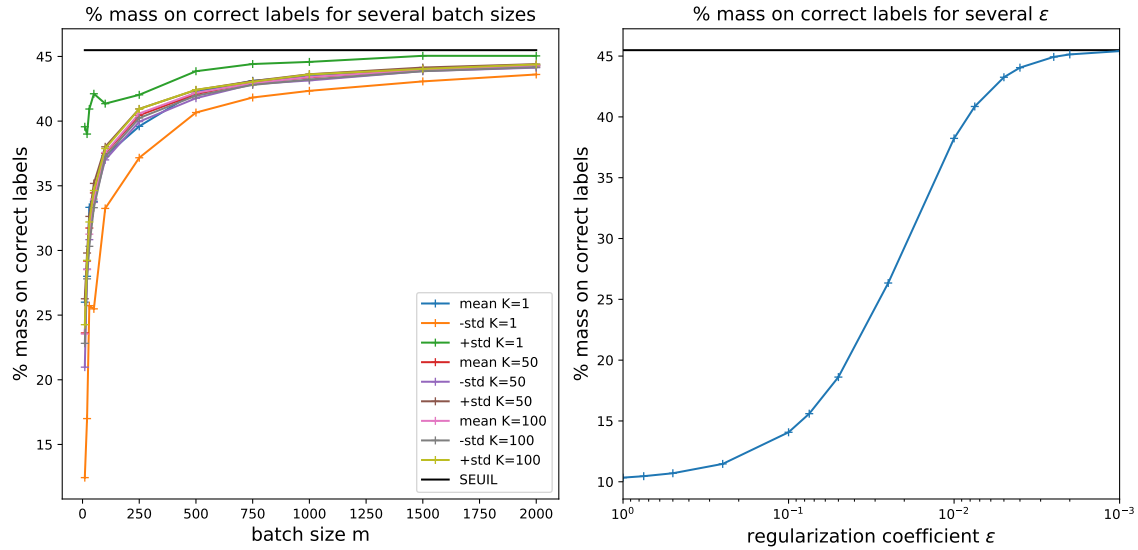


Figure 7: Proportion of correct transferred data between S/T domains for OT MB.

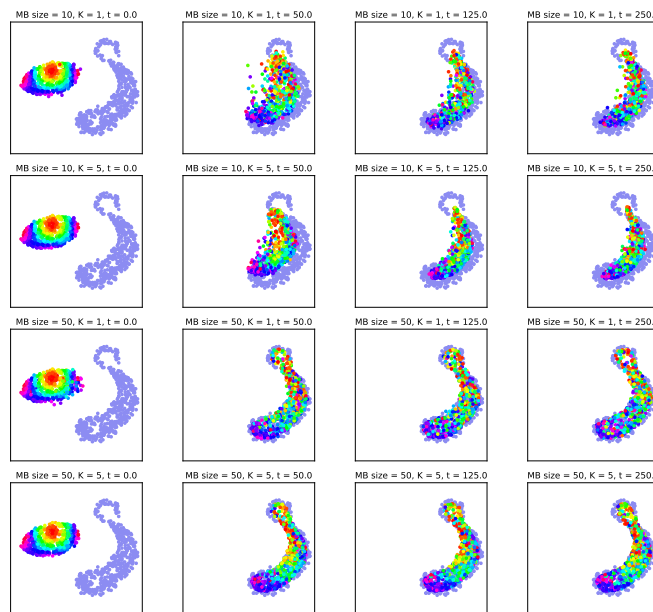


Figure 8: Gradient flow between 2D distributions for several batch sizes m and several number of batches k . The source and the target distributions have 500 samples each.

Wasserstein distance and the samples converge toward different pictures. However, we can still see a natural evolution in the images along the gradient flow.

B.4 Color transfer between subset of images

In order to present the influence of k for barycentric mapping, we present extra experiments for color transfer. We compute a k -means clustering with l clusters for each point cloud. For each image, we computed 1000 k -means clusters of the point clouds and applied the optimal transport algorithms between those subsets. We consider batch size of 10, 50 and 100. We show the color transfer for each image for $k = 5000$ and $k = 20000$ batches.

In what follows, we present the algorithm which computes the color transfer vectors incrementally without requiring the

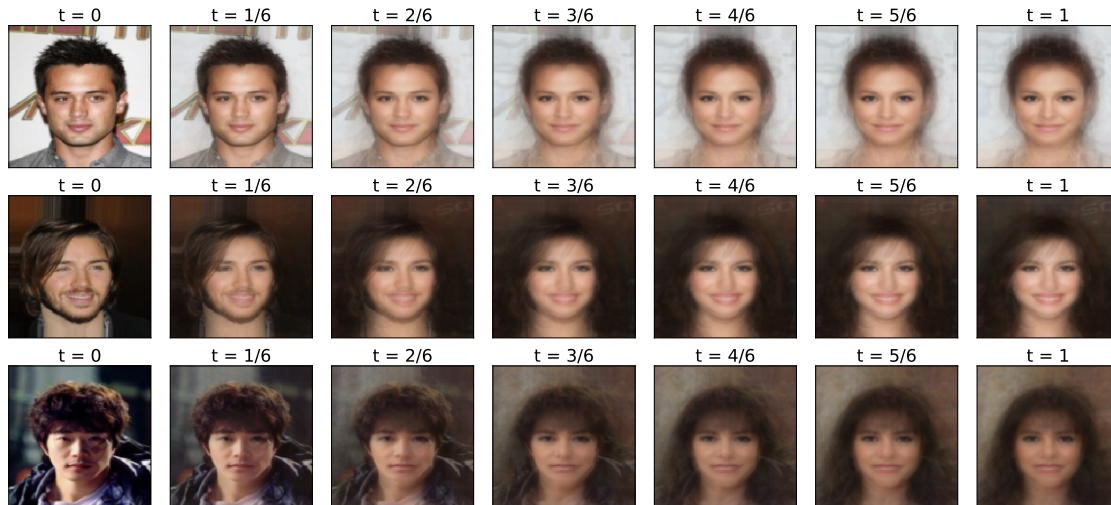


Figure 9: Gradient flow on the CelebA dataset. Source data are 5000 male images while target data are 5000 female images. The batch size m is set to 500 and the number of minibatch k is set to 10. The results were computed with the minibatch Sinkhorn divergence.

storage of the full cost matrix neither the full transportation matrix Π_k .

Algorithm 1: Computation of incremental color transfer

- 1 **Inputs:** m, k , source domain $\mathbf{X}_s \in \mathbb{R}^{n \times d}$, target domain $\mathbf{X}_t \in \mathbb{R}^{n \times d}$;
 - 2 **Results :** $\mathbf{Y}_s, \mathbf{Y}_t$;
 - 3 **Initialisation :** $\mathbf{Y}_s \in \mathbb{R}^{n \times d}, \mathbf{Y}_t \in \mathbb{R}^{n \times d}$;
 - 4 **for** $t=1, \dots, k$ **do**
 - 5 Select a set A of m samples in \mathbf{X}_s ;
 - 6 Select a set B of m samples in \mathbf{X}_t ;
 - 7 Compute the restricted cost $C_{A,B}$;
 - 8 $G \leftarrow \underset{\Pi \in \mathcal{U}(A,B)}{\operatorname{argmin}} \langle C_{A,B}, \Pi \rangle$;
 - 9 $\mathbf{Y}_s|_A \leftarrow \mathbf{Y}_s|_A + G \cdot \mathbf{X}_t|_B$;
 - 10 $\mathbf{Y}_t|_B \leftarrow \mathbf{Y}_t|_B + G^T \cdot \mathbf{X}_s|_A$;
 - 11 **end**
 - 12 **return** $\frac{n}{k} \mathbf{Y}_s, \frac{n}{k} \mathbf{Y}_t$
-

We see that for each batch size m , when the number of batches k increases, we get better resolution for our images. It is expected as our matrix Π_k gets closer to Π_m . However, when m is small, we will need to have a large k to get good resolutions for images. We can see this phenomenon for $m = 10$, where $k = 5000$ was not enough to have a good resolution. However, $k = 5000$ was enough to get good resolutions for $m = 1000$.

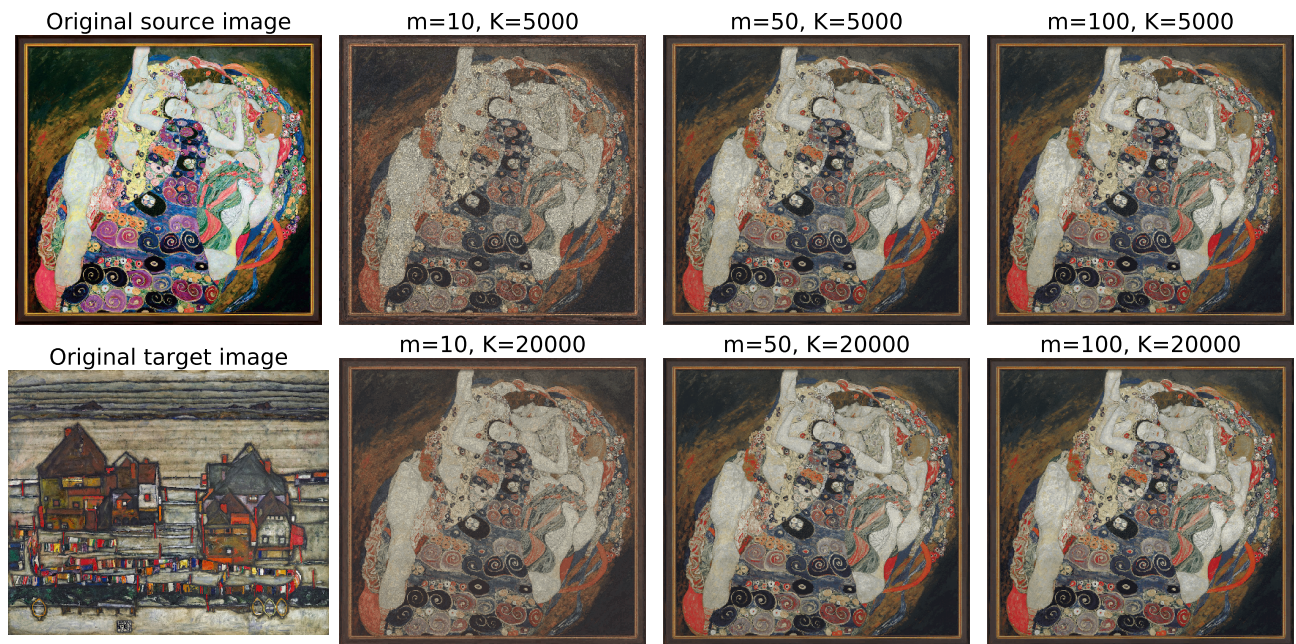


Figure 10: Color transfer from MB Wasserstein loss for several m and K . The minibatch Wasserstein distance is computed between subsets of original images.