Minibatch Wasserstein distance

Asymptotic and gradients

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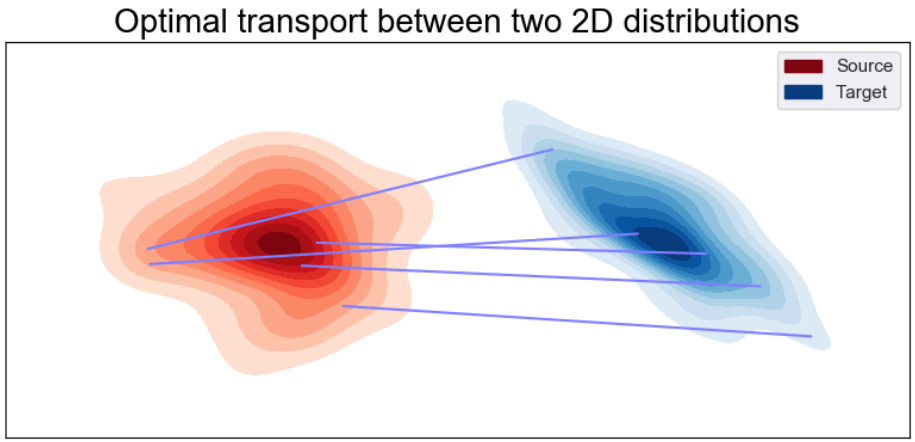
Wasserstein distance



Optimal Transport seeks a probability coupling $\pi \in \mathcal{P}(\mathcal{X} \times \mathcal{Y})$ between $\mathcal{X}$ and $\mathcal{Y}$ which minimizes a ground cost c.

$$\pi^* = \underset{\pi}{\operatorname{argmin}} \int_{\mathcal{X}\times\mathcal{Y}} c(\mathbf{x},\mathbf{y})\pi(\mathbf{x},\mathbf{y})d\mathbf{x}d\mathbf{y}$$

$$\text{s.t.} \quad \pi \in \mathcal{P} = \left\{\pi \geq \mathbf{0}, \int_{\mathcal{X}} \pi(\mathbf{x},\mathbf{y})\mathrm{d}\mathbf{y} = \mu_s, \int_{\mathcal{Y}} \pi(\mathbf{x},\mathbf{y})\mathrm{d}\mathbf{x} = \mu_t\right\}$$

π is a joint probability measure with marginals μ_s and μ_t

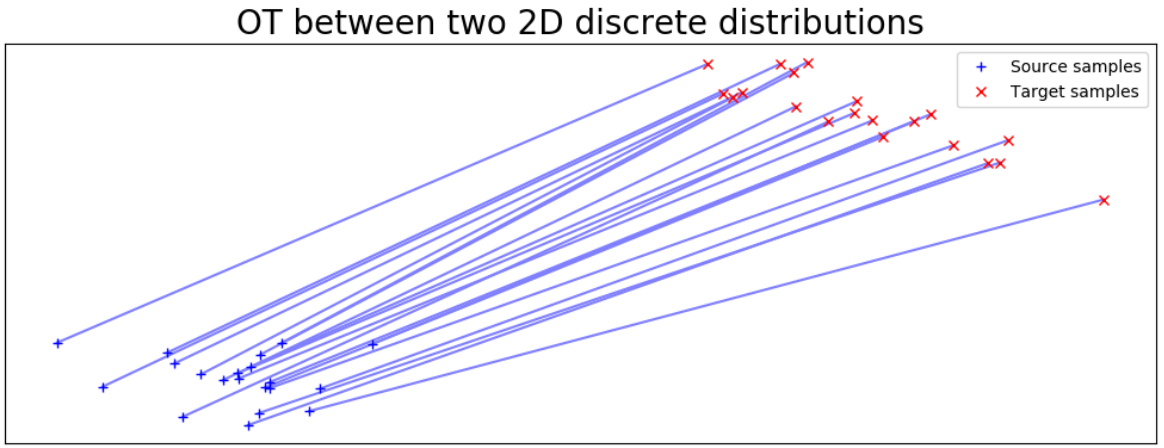
Discrete Optimal Transport

For discrete measures $\mu_s = \sum_{i=1}^{n} a_i \delta_{\mathbf{x}_i^s}$ and $\mu_t = \sum_{i=1}^{n} b_i \delta_{\mathbf{x}_i^t}$, OT becomes a linear program:

$$\pi^* = \underset{\pi \in \mathcal{U}(\mu_s, \mu_t)}{\operatorname{argmin}} \left\{ \langle \pi, \mathbf{C} \rangle_F = \sum_{i,j} \pi_{i,j} c_{i,j} \right\}$$

where $\mathbf{C}$ is a cost matrix with $c_{i,j} = c\left(\mathbf{x}_i^s, \mathbf{x}_j^t\right)$ and the marginals constraints are

$$\mathcal{U}(\mu_s, \mu_t) = \left\{ \pi \in \left(\mathbb{R}^+\right)^{\mathbf{n_s} \times \mathbf{n_t}} | \pi \mathbf{1_{n_t}} = \mathbf{a}, \pi^{\mathbf{T}} \mathbf{1_{n_s}} = \mathbf{b} \right\}$$



Wasserstein distance

Definition

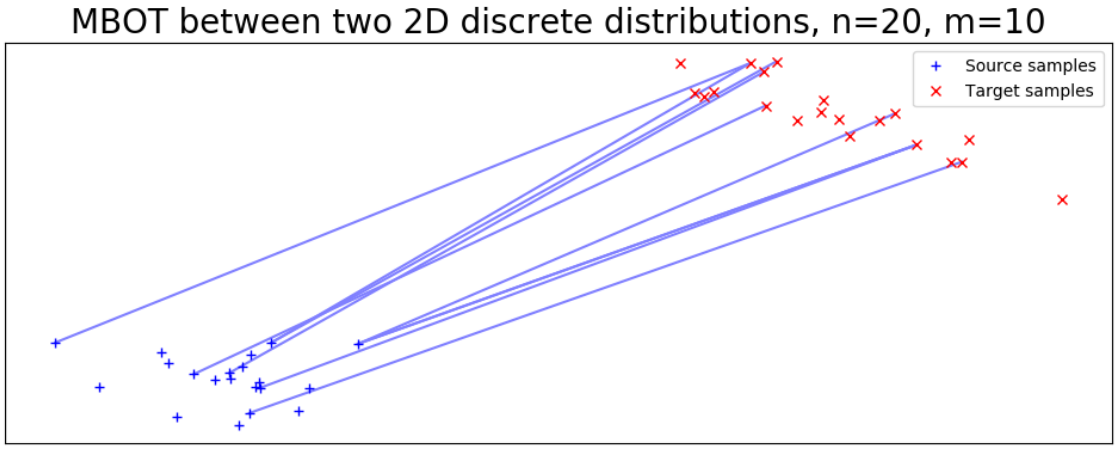
Optimal transport measures the distance between probablity distributions:

$$W_{\mathbf{C}} = \min_{\pi \in \mathcal{U}(\mu_s, \mu_t)} \langle \pi, \mathbf{C} \rangle_F$$

- If $\mathbf{C}$ is a metric then $W_{\mathbf{C}}$ becomes a metric
- A solution always exists
- Complexity of discrete OT is $\mathcal{O}(n^3)$

MBOT

Minibatch-Wasserstein distance



Let $m \leq n$, [Damodaran et al., 2018, Genevay et al., 2018] compute optimal transport between minibatch of sub-measures:

$$U_W(\alpha, \beta) := \mathbb{E}_{(X,Y)\sim\alpha^{\otimes m}\otimes\beta^{\otimes m}}[W(X, Y)]$$

- Complexity of discrete MBOT is $\mathcal{O}(m^3)$
- Left unjustified until now !

Estimate mini-batch Wasserstein distance

We define the following estimators:

Definition (Complete estimator)

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

where $\mathcal{P}_m(\alpha_n)$ is the set of all m-combination without replacement.

Definition (Incomplete estimator)

Pick an integer $k > 0$,

$$\widetilde{U}_W^k(\alpha_n, \beta_n) := k^{-1} \sum_{(A,B) \in D_k} W(A, B)$$

where D_k is a set of cardinality k whose elements are minibatches drawn at random.

Estimator properties

Proposition

The loss function $U_W(\alpha_n, \beta_n)$ *is:*

- *Unbiased estimator*
- *Strictly positive loss:* $U_W(\alpha_n, \alpha_n) > 0$
- *Not a metric*

Estimate mini-batch transportation plan

Similar estimator can be built for the mini-batch transportation plan π^*

Definition (Complete plan estimator)

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

and a subsample one:

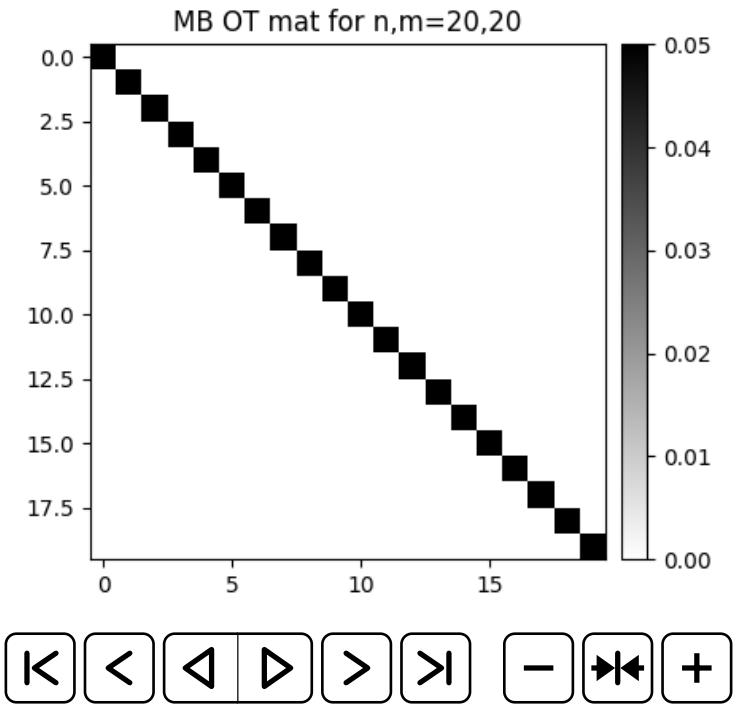
Definition (Incomplete plan estimator)

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

Proposition: Π_m is a transportation plan! (i.e. $\Pi_m \in \mathcal{U}(\mu_s, \mu_t)$)

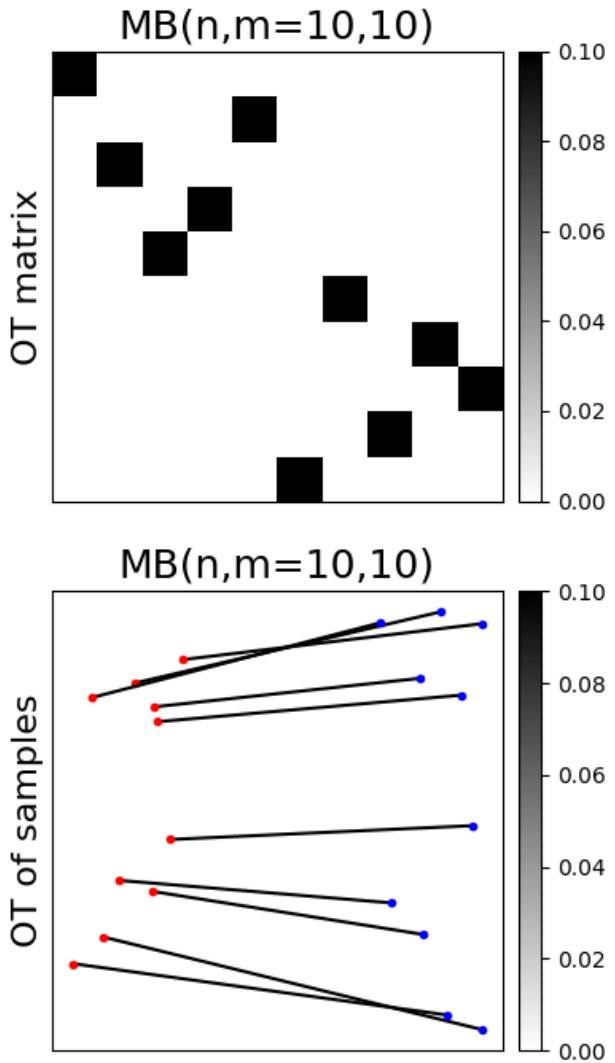
1D case

OT has a close form when measures lie in 1D space. Let us consider two 1D-measures with $n = 20$.



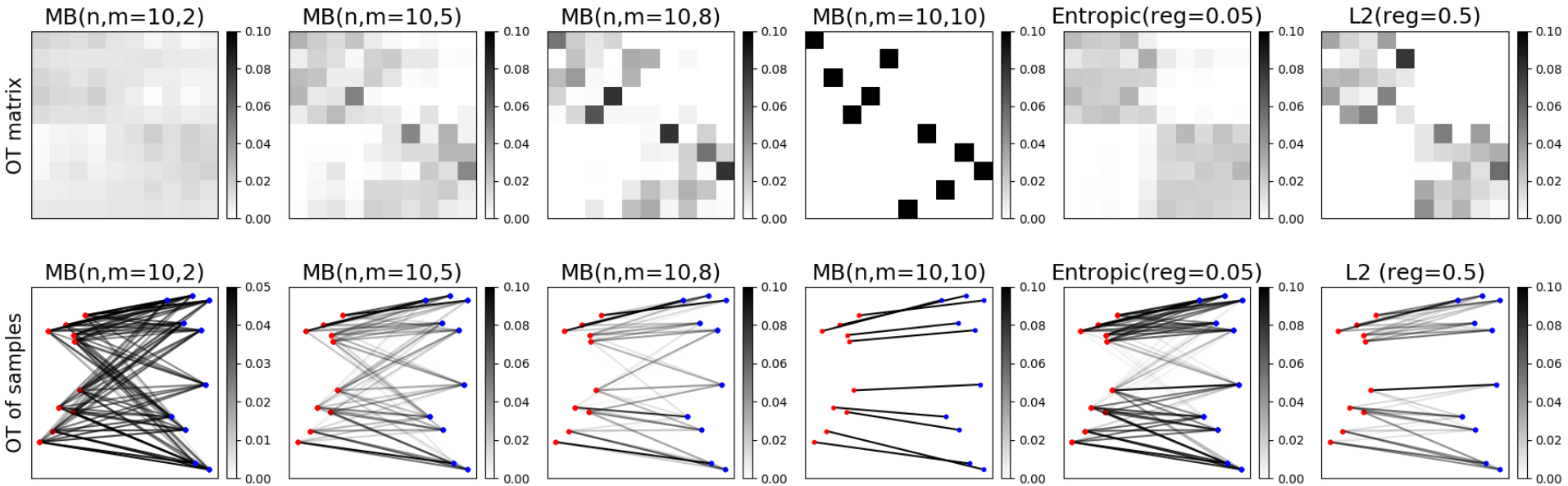
2D examples

Let us consider two 2D-measures with $n = 10$.



2D examples

Let us consider two 2D-measures with $n = 10$.



Learning properties

Asymptotic loss estimator

How far is our incomplete estimator $\widetilde{U}_h^k(\alpha_n, \beta_n)$ to the loss between full measures $U_h(\alpha, \beta)$?

Theorem (Maximal deviation bound)

Let $\delta \in (0, 1)$ and consider two compact distributions α, β. We have a deviation bound between $\widetilde{U}_h^k(\alpha_n, \beta_n)$ and $U_h(\alpha, \beta)$, with probability at least $1 - \delta$ on the draw of α_n, β_n and D_k:

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

where M_W is a constant.

Deviation transportation plan

How far is our incomplete estimator Π_k to the complete minibatch transportation plan Π_m?

Theorem (Distance to marginals)

Let $\delta \in (0,1)$, and consider two distributions α_n, β_n. For all $k \geqslant 1$, all $1 \leqslant i \leqslant n$, with probability at least $1-\delta$ on the draw of α_n, β_n and D_k we have:

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

Optimization

Can we optimize our loss with modern optimization methods such as SGD ?

Theorem (Exchange of Gradient and expectation)

Consider two distributions α and β on two bounded subsets $\mathcal{X}$ and $\mathcal{Y}$, a $\mathcal{C}^1$ 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:

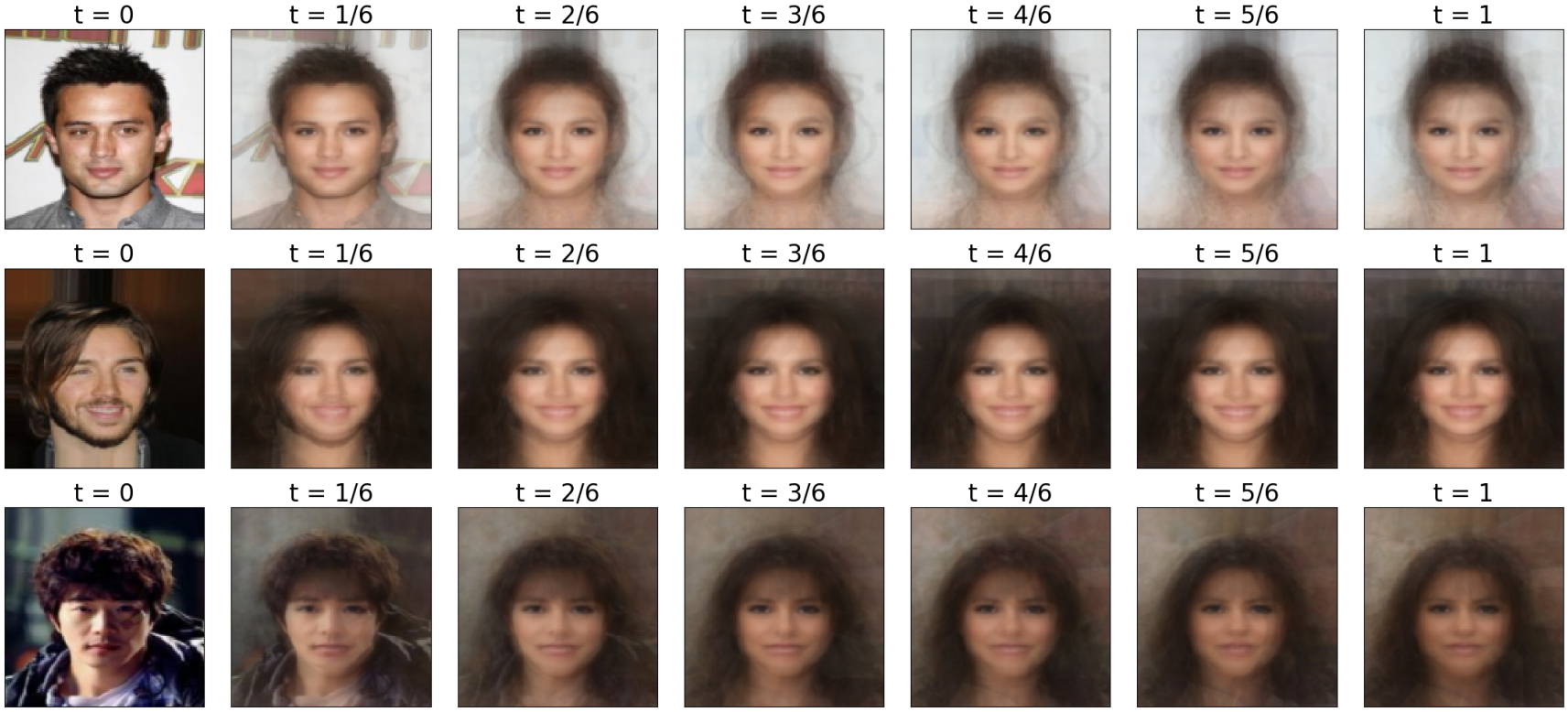
$$\nabla_\lambda \mathop{\mathbb{E}}_{Y_\lambda \sim \beta_\lambda^{\otimes m}} h(A, Y_\lambda) = \mathop{\mathbb{E}}_{Y_\lambda \sim \beta_\lambda^{\otimes m}} \nabla_\lambda h(A, Y_\lambda) \tag{2}$$

Experiments

Gradient flow

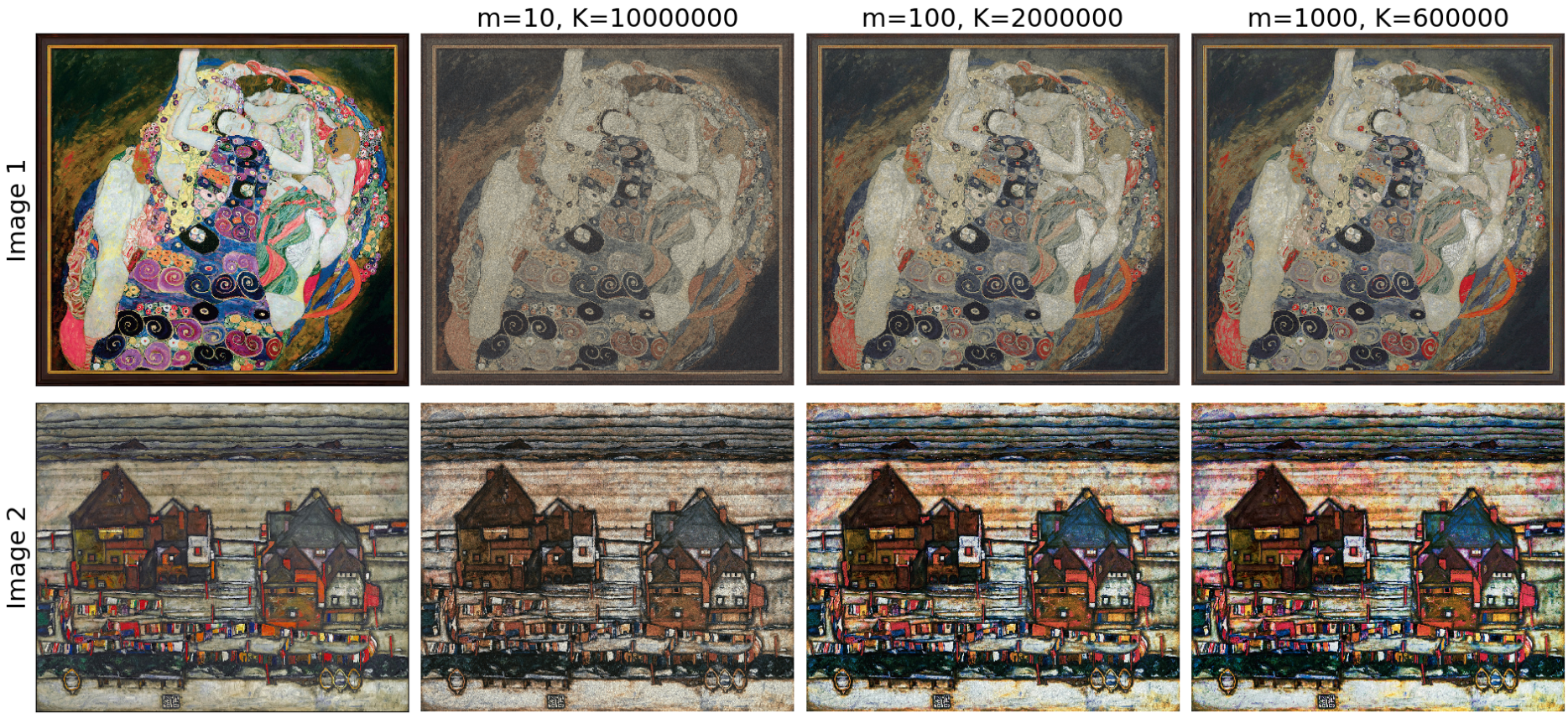
Minibatch Wasserstein gradient flow between male and female images.

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



Color transfer

Transfert of color between two input images (1M pixels) using Π_k.



Paper

Full details in our AISTATS 2020 paper !

Check it out : https://arxiv.org/abs/1910.04091

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