

Generative Images

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Article analysis: Neural Optimal Transport

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Overview

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- μ, ν probability distributions on \mathcal{X}, \mathcal{Y} .
- Cost function: $c : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$.
- Problem: finding a **transport map** $T^* : \mathcal{X} \rightarrow \mathcal{Y}$ such that:

$$T^* \in \operatorname{Argmin}_{T\#\mu=\nu} \int_{\mathcal{X}} c(x, T(x)) d\mu(x) \quad (1)$$

where $(T\#\mu)(A) = \mu(T^{-1}(A))$ is the pushforward measure.
Hence, one can define:

$$\text{Cost}(\mu, \nu) = \int_{\mathcal{X}} c(x, T^*(x)) d\mu(x) \quad (2)$$

Kantorovich formulation: a relaxed OT problem

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- Let $\Pi(\mu, \nu)$ the set of distributions on $\mathcal{X} \times \mathcal{Y}$ with marginals μ and ν .
- Problem: find a **transport plan** $\pi^* \in \Pi(\mu, \nu)$ such that:

$$\pi^* \in \operatorname{Argmin}_{\pi \in \Pi(\mu, \nu)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\pi(x, y) \quad (3)$$

and we can define:

$$\text{Cost}(\mu, \nu) = \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\pi^*(x, y) \quad (4)$$

Weak OT Duality

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For weak OT cost C and a sufficiently regular function f ,

$$f^C(x) = \inf_{\rho \in \mathcal{P}(\mathcal{Y})} \left\{ C(x, \rho) - \int_{\mathcal{Y}} f(y) d\rho(y) \right\} \quad (5)$$

where $\mathcal{P}(\mathcal{Y})$ denotes the set of probability distributions on \mathcal{Y} .
Then, the dual form of the weak OT problem writes:

$$f^* \in \operatorname{Argmax}_f \int_{\mathcal{X}} f^C(x) d\mu(x) + \int_{\mathcal{Y}} f(y) d\nu(y) \quad (6)$$

and the cost can be defined as follows

$$\text{Cost}(\mu, \nu) = \int_{\mathcal{X}} f^{*C}(x) d\mu(x) + \int_{\mathcal{Y}} f^*(y) d\nu(y) \quad (7)$$

Weak dual OT reformulation

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- $\mathcal{X} \subset \mathbb{R}^n$, $\mathcal{Y} \subset \mathbb{R}^m$ and $\mathcal{Y} \subset \mathbb{R}^d$.
- Let $\rho \in \mathcal{P}(\mathcal{Z})$ with some basic assumptions.

Then, we have:

$$f^C(x) = \inf_t \left\{ C(x, T\#\rho) - \int_{\mathcal{Z}} f(t(z)) d\rho(z) \right\} \quad (8)$$

which leads to the maximin problem:

$$\text{Cost}(\mu, \nu) = \sup_f \inf_T \mathcal{L}(f, T) \quad (9)$$

where $\mathcal{L}(f, T) =$

$$\int_{\mathcal{Y}} f d\nu + \int_{\mathcal{X}} (C(x, T(x, \cdot)\#\rho) - \int_{\mathcal{Z}} f(T(x, z)) d\rho(z)) d\mu(x)$$

The trick: noise outsourcing

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- Here, they introduce $T : \mathcal{X} \times \mathcal{Z} \rightarrow \mathcal{Y}$.
- Trick known as **noise outsourcing**:

Theorem

If X and Y are random variables in suitable spaces \mathcal{X} and \mathcal{Y} , then there exists $\eta \sim \mathcal{U}([0, 1])$ with $\eta \perp\!\!\!\perp X$ and a function $h : [0, 1] \times \mathcal{X} \longrightarrow \mathcal{Y}$ such that $(X, Y) = (X, h(\eta, X))$ almost surely.

Weak OT: A summary

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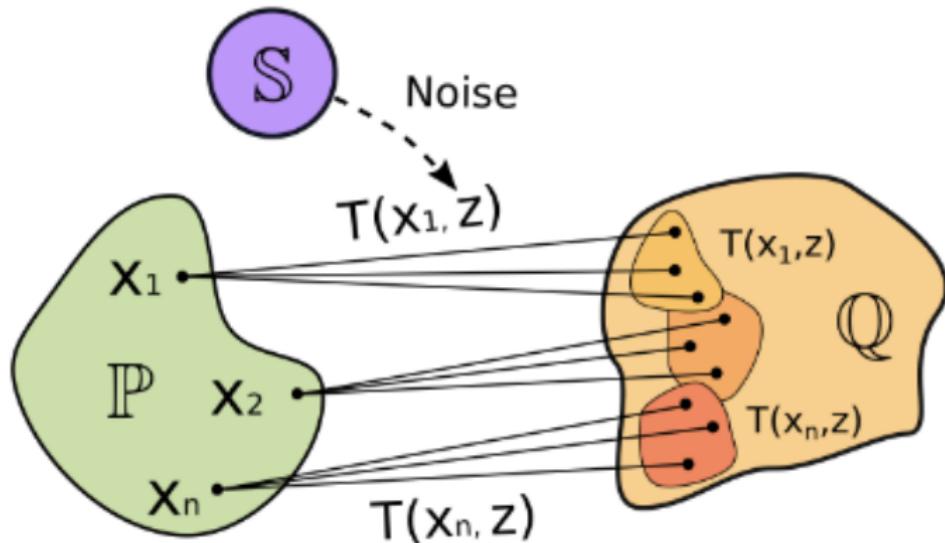


Figure: Transportation map with outsourced noise z (taken from [KSB22])

Stochastic Gradient Ascent Descent (SGAD)

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TODO: Need to add the algorithm, couldn't do it easily with a rescalebox.

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- 2D standard normal distribution for \mathcal{X} .
- Moon distribution for \mathcal{Y} .
- Weak OT cost for $\gamma = 1$:

$$C(x, \mu) = \int_{\mathcal{Y}} \frac{1}{2} \|x - y\|^2 d\mu(y) - \frac{1}{2} \text{Var}(\mu) = \frac{1}{2} \|x - \int_{\mathcal{Y}} y d\mu(y)\|^2 \quad (10)$$

The parameters:

- simple feedforward model.
 - 2 hidden layers (100 units each).
 - ReLU activation.
- Adam optimizer.

Results: the fitted distribution

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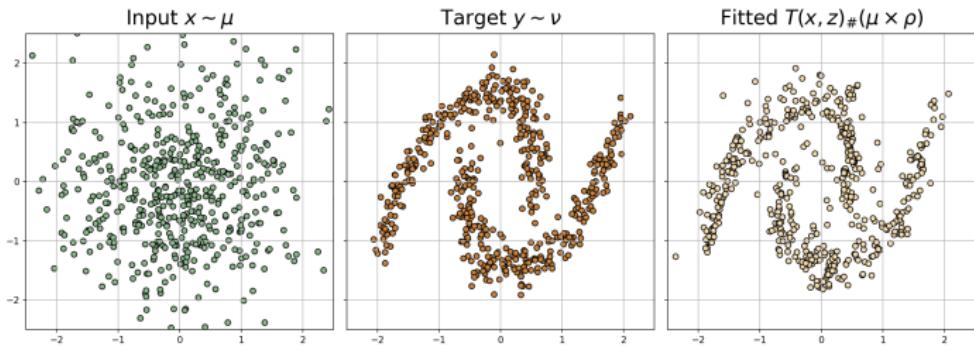


Figure: Synthetic data experiment. Left: input gaussian distribution. Middle: target distribution. Right: learned transport of the input distribution to the target distribution.

Results: a closer look at the map

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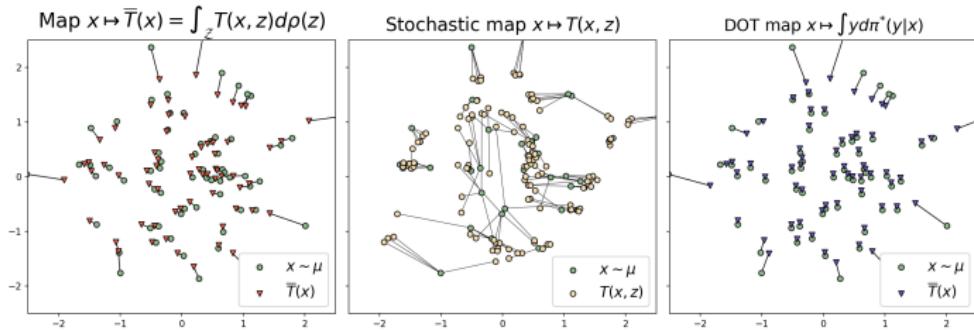


Figure: Synthetic data experiment. Left: average of the learned transport for different points. Middle: learned transport for a batch of points. Right: optimal transport plan obtained with the POT library.

Large-scale dataset

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- CelebA dataset with 200k celebrity face images.
- CartoonSet with 100k avatar 2D generated images.



Figure: Images samples from CartoonSet100K

Large-scale experiment: the parameters

- Resnet to parametrise f .
- U-Net to parametrise the map T .
- image size: 128×128 .
- Batch size: 128.
- Adam optimizer.
- $\text{lr} = 1 \times 10^{-4}$.
- $k_T = 10$.

Results: it works!

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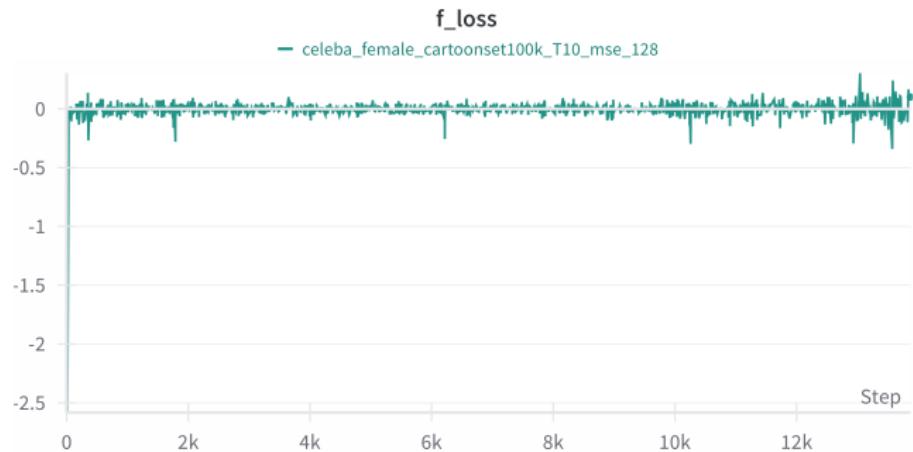


Figure: \mathcal{L}_f during training

Results: some generated avatars

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Figure: Iteration 1

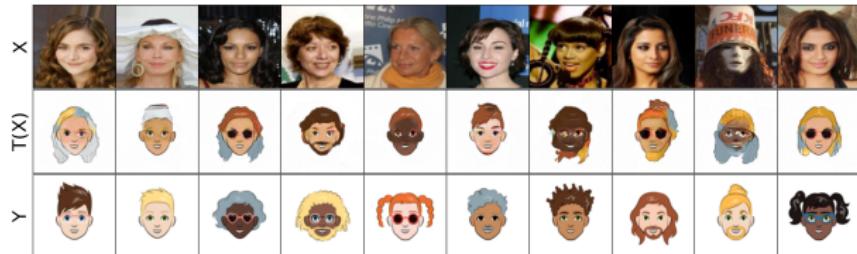


Figure: Iteration 5000

Results: an issue

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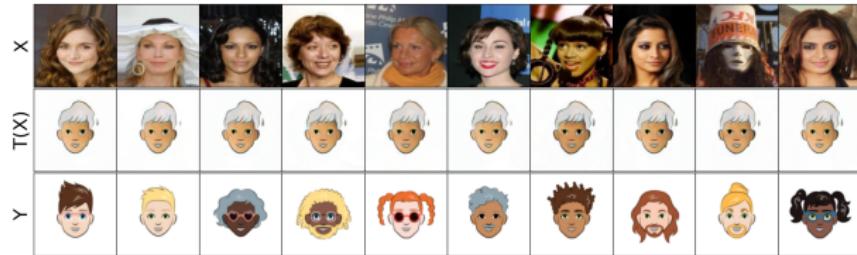


Figure: Iteration 13800

■ Mode collapse!

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- An algorithm to learn optimal transport maps.
- New approach to incorporate OT in ML.
- With good results on large-scale datasets!
- Good perspectives for generative models.

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Alexander Korotin, Daniil Selikhanovich, and Evgeny Burnaev, *Neural optimal transport*, arXiv (Cornell University) (2022).