Convexity Regularizer for Neural Optimal Transport

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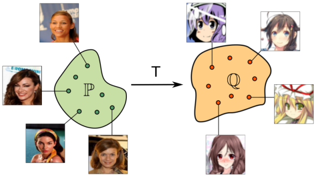
The research idea:

Let's consider the following Unpaired Image-to-Image Style Translation:



where we have:

$$\begin{cases} \textbf{Inputs: } \text{two unpaired dataset sample empirically from some p.d.f } \mathbb{P} \text{ and } \mathbb{Q} \\ \textbf{Output: } \text{a Style translation map } T : \mathcal{X} \longrightarrow \mathcal{Y} \text{ such that } T_{\#}\mathbb{P} = \mathbb{Q} \end{cases}$$

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The research idea (cont.):

- The method proposed in the research paper uses adversarial training (kind of GANs), which is not very stable to compute the optimal transport map T.
- From the theory , the method's optimal "discriminator" must be convex, and its gradient can be used for inverse mapping from the target distribution to the source distribution.
- Hence our goal is to add a convexity regularizer in the loss of neural optimal transport algorithm to improve its stability during transport training and the high-quality of the inverse target-to-input mapping.

General Notations

- $\mathcal{X}$ and $\mathcal{Y}$ are some polish spaces
- $\mathcal{P}(\mathcal{X})$ and $\mathcal{P}(\mathcal{Y})$ are sets of probability defined respectively on $\mathcal{X}$ and $\mathcal{Y}$
- For a measurable map $T : \mathcal{X} \longrightarrow \mathcal{Y}$ the operator $T_{\#}$ denotes the so called push-forward operator

Mathematical Background

- **Monge's Optimal Transport formulation**
  For $\mathbb{P} \in \mathcal{P}(\mathcal{X}), \mathbb{Q} \in \mathcal{P}(\mathcal{Y})$ and a cost function $c : \mathcal{X} \times \mathcal{Y} \longrightarrow \mathbb{R}$, Monge's primal formulation of the cost is

$$\textbf{Cost}(\mathbb{P}, \mathbb{Q}) \stackrel{\text{def}}{=} \inf_{T_{\#}\mathbb{P}=\mathbb{Q}} \int_{\mathcal{X}} c(x, T(x)) d\mathbb{P}(x) \tag{1}$$

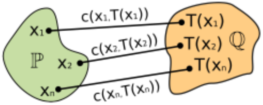

Figure: Monge's OT formulation.

Here the minimum is taken over the set of mesurables functions called transport maps $T : \mathcal{X} \longrightarrow \mathcal{Y}$ that maps the marginal distribution $\mathbb{P}$ to $\mathbb{Q}$. The optimal transport map T^* is called the OT map

Mathematical Background (cont.)

Note: The equation (1) is not symmetric and for some $\mathbb{P}, \mathbb{Q}$ it may happen that their is no T such that $T_{\#}\mathbb{P} = \mathbb{Q}$ (does not allow mass splitting)

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Mathematical Background (cont.)

- **Strong OT formulation**
  To overcome the mass splitting problem (Kantorovich, 1958) proposed the following reformulation

$$\textbf{Cost}(\mathbb{P},\mathbb{Q}) \stackrel{\text{def}}{=} \inf_{\pi\in\Pi(\mathbb{P},\mathbb{Q})} \int_{\mathcal{X}\times\mathcal{Y}} c(x, T(x))d\pi(x,y) \tag{2}$$

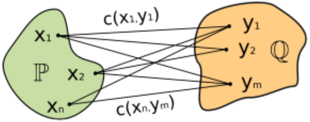

Figure: Strong OT formulation

and the minimum is taken over all the transport plan π which represent all distributions on $\mathcal{X}\times\mathcal{Y}$ whose marginals are $\mathbb{P}$ and $\mathbb{Q}$ and the optimal plan denoted by π^*

The two main important results of the research paper

- **Corollary:**

$$\textbf{Cost}(\mathbb{P}, \mathbb{Q}) = \underset{f}{\text{Sup}}\underset{T}{\text{Inf}}\mathcal{L}(f, T),$$

where $\mathcal{L}(f, T) = \int_{\mathcal{Y}} f(y)d\mathbb{Q}(y) + \int_{\mathcal{X}} \left(c(x, T(x, \dot{)}_{\#}\mathbb{S}) - \int_{\mathcal{Z}} f(T(x, z))d\mathbb{S} \right) \mathbb{P}(x)d$

- **Lemma:**
For any f^* that maximizes the dual form of the weak OT cost between $\mathbb{P}$ and $\mathbb{Q}$ and for any stochastic map T^* which realizes some optimal transport plan π^*, it holds that

$$T^* \in \underset{T}{\text{argInf}}\mathcal{L}(f^*, T).$$

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Algorithm to Learn the Optimal Transport Plans

Algorithm 1: Neural optimal transport (NOT)

Input :distributions $\mathbb{P}, \mathbb{Q}, \mathbb{S}$ accessible by samples; mapping network $T_\theta : \mathbb{R}^P \times \mathbb{R}^S \to \mathbb{R}^Q$; potential network $f_\omega : \mathbb{R}^Q \to \mathbb{R}$; number of inner iterations K_T; (weak) cost $C : \mathcal{X} \times \mathcal{P}(\mathcal{Y}) \to \mathbb{R}$; empirical estimator $\widehat{C}\big(x, T(x, Z)\big)$ for the cost;

Output :learned stochastic OT map T_θ representing an OT plan between distributions $\mathbb{P}, \mathbb{Q}$;

repeat

  Sample batches $Y \sim \mathbb{Q}$, $X \sim \mathbb{P}$; for each $x \in X$ sample batch $Z_x \sim \mathbb{S}$;

  $\mathcal{L}_f \leftarrow \frac{1}{|X|} \sum_{x \in X} \frac{1}{|Z_x|} \sum_{z \in Z_x} f_\omega\big(T_\theta(x, z)\big) - \frac{1}{|Y|} \sum_{y \in Y} f_\omega(y)$;

  Update ω by using $\frac{\partial \mathcal{L}_f}{\partial \omega}$;

  for $k_T = 1, 2, \ldots, K_T$ **do**

    Sample batch $X \sim \mathbb{P}$; for each $x \in X$ sample batch $Z_x \sim \mathbb{S}$;

    $\mathcal{L}_T \leftarrow \frac{1}{|X|} \sum_{x \in X} \Big[\widehat{C}\big(x, T_\theta(x, Z_x)\big) - \frac{1}{|Z_x|} \sum_{z \in Z_x} f_\omega\big(T_\theta(x, z)\big)\Big]$;

    Update θ by using $\frac{\partial \mathcal{L}_T}{\partial \theta}$;

until *not converged*;

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Convexity Regularization (theoretical)

- From the theory we have the potential $f(x) = f^*(x)\frac{|X|}{2}$
- By posing $f(x) = \frac{||x||^2}{2} - \psi(x)$ and equating with the above formula we obtain

$$\boxed{\psi(x) = -f^*\frac{|X|}{2} + \frac{||x||^2}{2}}$$

- We desire ψ to be a convex function which satisfies the Jensen's inequality

$$\psi(tx_1 + (1-t)x_2) - t\psi(x_1) - (1-t)\psi(x_2) \leq 0, \;\; t \in [0,1] \tag{3}$$

- Then, we define and penalize the loss function to hold Jensen's inequality

$$\mathcal{L}(X_1, X_2) = \psi(tX_1 + (1-t)X_2) - t\psi(X_1) - (1-t)\psi(X_2) \leq 0 \tag{4}$$

Convexity Regularization (cont.)

- To make loss positive we may apply the **ReLU** function; hence let define

$$\mathrm{R}(X_1, X_2) = \textbf{ReLU}(\mathcal{L}(X_1, X_2))$$

- Finally we uses the mean of $\mathrm{R}(X_1, X_2)$ as a regularization term which can be multiplied by a given learning rate, in this case we are using two learning rate, 0.01 and 0.001

Sample of our results

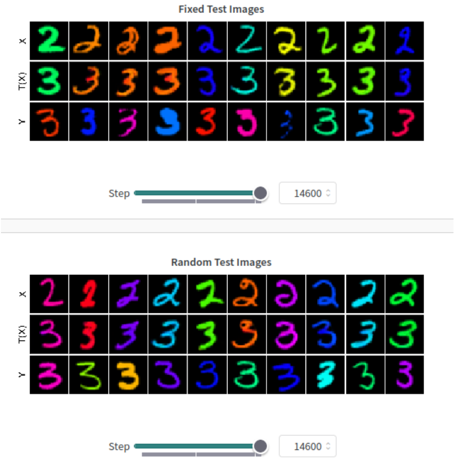

Figure: Regularized Model in Training with a learning rate of 0.01

Sample of our results(cont.)

Figure: Regularized Model in Training with a learning rate of 0.001