On Scalable and Efficient Computation of Large Scale Optimal Transport

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Optimal Transport (OT)

The OT problem aims to **align** data from multiple sources.

**Resource Allocation**: We want to assign a set of assets to a set of receivers so that an optimal economic benefit is achieved.

**Domain Adaptation**: We collect multiple datasets from different domains, and we need to learn a model from a source dataset, which can be further adapted to target datasets.

Both applications can be formulated as OT problems.
Optimal Transport

**Formulation** OT aims to find an optimal joint distribution $\gamma^*$ of $\mu$ and $\nu$, which minimizes the expectation on some cost function $c$, i.e.,

$$
\gamma^* = \arg \min_{\gamma} \mathbb{E}_{(X,Y) \sim \gamma} [c(X,Y)],
$$

subject to $X \sim \mu, \ Y \sim \nu$.

$\gamma^*$ is referred as the **optimal transport plan**, suggesting the way to transport between $\mu$ and $\nu$ with minimum cost.

**Existing Methods** Discretization + Linear Programming
The number of grids needs to scale exponentially w.r.t. dimension
SPOT

- **OT**: $\gamma^* = \arg\min_{\gamma} \mathbb{E}_{(X,Y) \sim \gamma}[c(X,Y)]$, s.t. $X \sim \mu, Y \sim \nu$.

- Approximate $\gamma^*$ by an implicit generative model $G(Z)$,
  \[ G(Z) = \left[ \frac{G_X(Z)}{G_Y(Z)} \right] \approx \left[ \frac{X}{Y} \right], \]
  where $Z \sim \rho, X \sim \mu, Y \sim \nu$.

- Substitute $G(Z)$ into OT problem, we can rewrite the problem as
  \[ \arg\min_{G} \mathbb{E}_{Z \sim \rho}[c(G_X(Z), G_Y(Z))], \]
  subject to $\mathcal{W}_1(G_X(Z), \mu) = 0, \mathcal{W}_1(G_Y(Z), \nu) = 0$.
  where $\mathcal{W}_1(G_X(Z), \mu)$ denotes the standard Wasserstein metric between a random vector $G_X(Z)$ and a distribution $\mu$. Here we use the fact that $\mathcal{W}_1(G_X(Z), \mu) = 0$ indicates $G_X(Z) \sim \mu$. 

\[
\min_{G \in \mathcal{G}} \max_{\lambda_X \in \mathcal{F}_X^1, \lambda_Y \in \mathcal{F}_Y^1} \mathbb{E}_{Z \sim \rho} [c(G_X(Z), G_Y(Z))] \\
+ \eta (\lambda_X (G_X(Z), X) + \lambda_Y (G_Y(Z), Y))
\]
Computing Wasserstein Distance (WD)

**WD** is the expected cost of optimal transport plan,

\[ \mathcal{W} = \mathbb{E}_{(X,Y) \sim \gamma^*} [c(X, Y)]. \]

Here, ROT is the state-of-the-art method (Seguy, 2018).
Generate Paired Samples

$X$

$Y$

$G_X(Z)$

$G_Y(Z)$

Photos-Monet
Domain Adaptation (DA)

Setting:

\(\{x_i\} \quad \{y_j\} \)

\[
\begin{array}{cccccc}
4 & 7 & 9 & 5 & \ldots \\
\hline
4 & 7 & 9 & 5 & \ldots \\
\end{array}
\]

Goal: predict the labels of \(\{y_j\}\).

<table>
<thead>
<tr>
<th>Source</th>
<th>MNIST</th>
<th>USPS</th>
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<tr>
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Domain Adaptation (DA)

Setting:

\[
\{x_i\} = \begin{array}{cccc}
4 & 7 & 9 & 5 \\
\end{array} \\
\text{Labels} = \begin{array}{cccc}
4 & 7 & 9 & 5 \\
\end{array} \\
\{y_j\} = \begin{array}{cccc}
\end{array} \\
\text{Labels} = \begin{array}{cccc}
\end{array} \\
\]

Goal: predict the labels of \( \{y_j\} \).

New DA method – DASPOT

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Domain Adaptation (DA)

Setting:

\[ \{x_i\} \quad \{y_j\} \]

Labels: 4 7 9 5 \ldots

\[ \{x_i\} \quad \{y_j\} \]


Goal: predict the labels of \( \{y_j\} \).

New DA method – DASPOT

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