VARIABILITY REDUCTION USING OPTIMAL TRANSPORT

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AGENDA

- Problem Formulation
- Motivation
- Methods
  - Data-driven optimal transport barycenter
- Simulation Results
- Future Works
Often, we would like a method to filter out the effect of unwanted variables from a data distribution while preserving the original data as best as possible.
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For more on batch effect correction, check out the resources curated by 10X Genomics. Also, please refer to this article on machine learning bias in criminal sentencing.
Let $X$ be the original data, $Z$ be the “unwanted” factor, and $Y$ be the “filtered” version of $X$.

$$\min_{Y} \max_{\lambda} \text{data\_deformation}(X, Y) - \lambda \cdot \text{independence}(Y, Z).$$
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Figure 1: Each data point $x$ is characterized by hidden factor $z \in \{1, 2, 3\}$. The filtration process is akin to computing the optimal transport barycenter of the conditional distributions $\rho(x | z)$ for all $z$.

Formally, we can frame this problem in terms of **optimal transport**. Specifically, we quantify the **data deformation** using an optimal transport distance.

$$\min_{y = T(x, z)} \int c(x, y) \rho(x | z) \gamma(z) dx dz$$

Here, $c(x, y)$ is the cost function between $x$ and $y$, $ho(x | z)$ is the conditional probability distribution of $x$ given $z$, and $\gamma(z)$ is the probability distribution of $z$. 
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$$\min_{y=T(x,z)} \int c(x, y) \rho(x | z) \gamma(z) \, dx \, dz$$

And we measure the independence between $y$ and $z$ using their mutual information, which is the KL divergence between the joint and the product of their distributions.

$$D_{KL}(\pi(y, z) \parallel \mu(y) \gamma(z))$$
Altogether, we have the following objective.

$$\min_{y=T(x,z)} \max_\lambda \int c(x, y) \rho(x|z) \gamma(z) dx dz + \lambda \cdot D_{KL}(\pi(y, z) || \mu(y) \gamma(z))$$
Altogether, we have the following objective.

\[
\min_{y=T(x,z)} \max_{\lambda} \int c(x, y) \rho(x|z) \gamma(z) dx dz + \lambda \cdot D_{KL}(\pi(y, z)||\mu(y)\gamma(z))
\]

The data-based formulation using samples \(\{x_i, z_i\}_i\) yield us

\[
\min_{y_i} \max_{\lambda} \sum_i c(x_i, y_i) + \lambda \cdot \sum_i \log \left( \frac{\pi(y_i, z_i)}{\mu(y_i)\gamma(z_i)} \right)
\]

where \(\pi(y_i, z_i), \mu(y_i),\) and \(\gamma(z_i)\) are approximated using KDE.
Let \( \{x_i, z_i\}_i \) be a sample of points such that \( x_i \) is sampled from \( \mathcal{N}(-2, 1) \) if \( z_i = 0 \) and \( \mathcal{N}(2, 1) \) otherwise.

We wish to find the distribution \( \mu(y) \).
Simulation Results: Gaussian Experiment
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Simulation Results: Iris Dataset
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- Factor discovery through identifying the factor $z$ that maximizes the reduction in variability among all factors.
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- **Factor discovery** through identifying the factor $z$ that maximizes the reduction in variability among all factors.
- **Data augmentation** through reversal of the transformed data points to a specific factor $z^*$ that may have little samples otherwise.
The variability reduction problem paves the way to...

- **Factor discovery** through identifying the factor $z$ that maximizes the reduction in variability among all factors.
- **Data augmentation** through reversal of the transformed data points to a specific factor $z^*$ that may have little samples otherwise.
- **Semi-supervised classification** by solving the barycenter problem with observations with unknown factors.
That’s it! Questions?