VARIABILITY REDUCTION USING OPTIMAL TRANSPORT

Kai Hung, Andrew Lipnick, Ryan Shìjié Dù, Nina Mortensen, Esteban G. Tabak

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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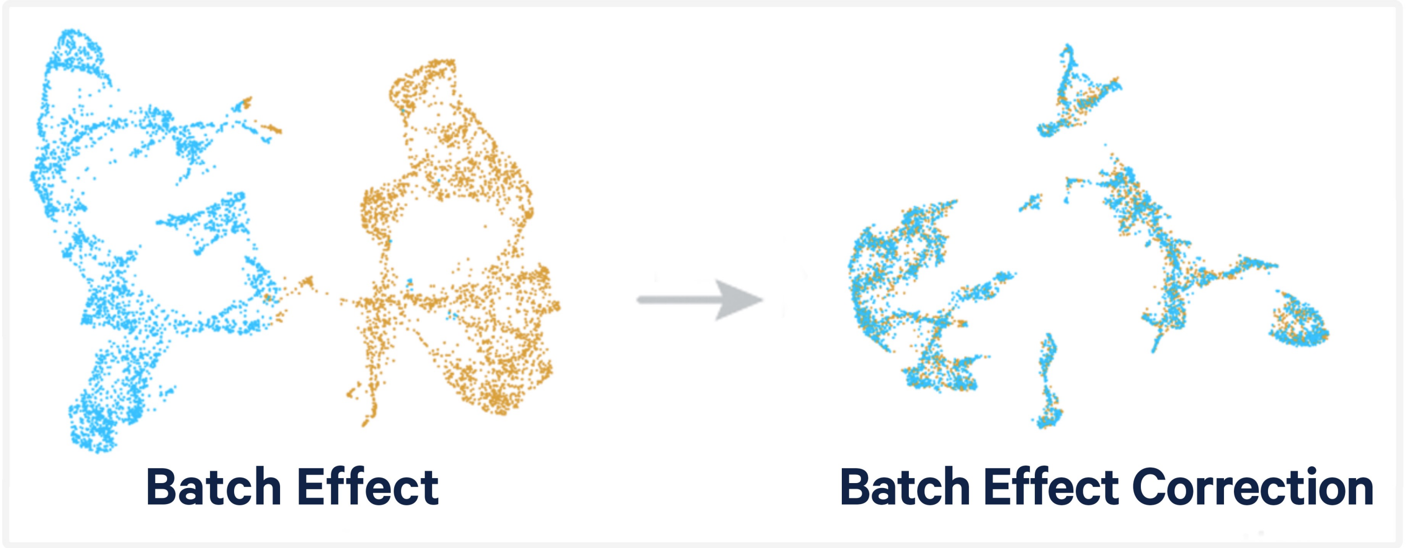

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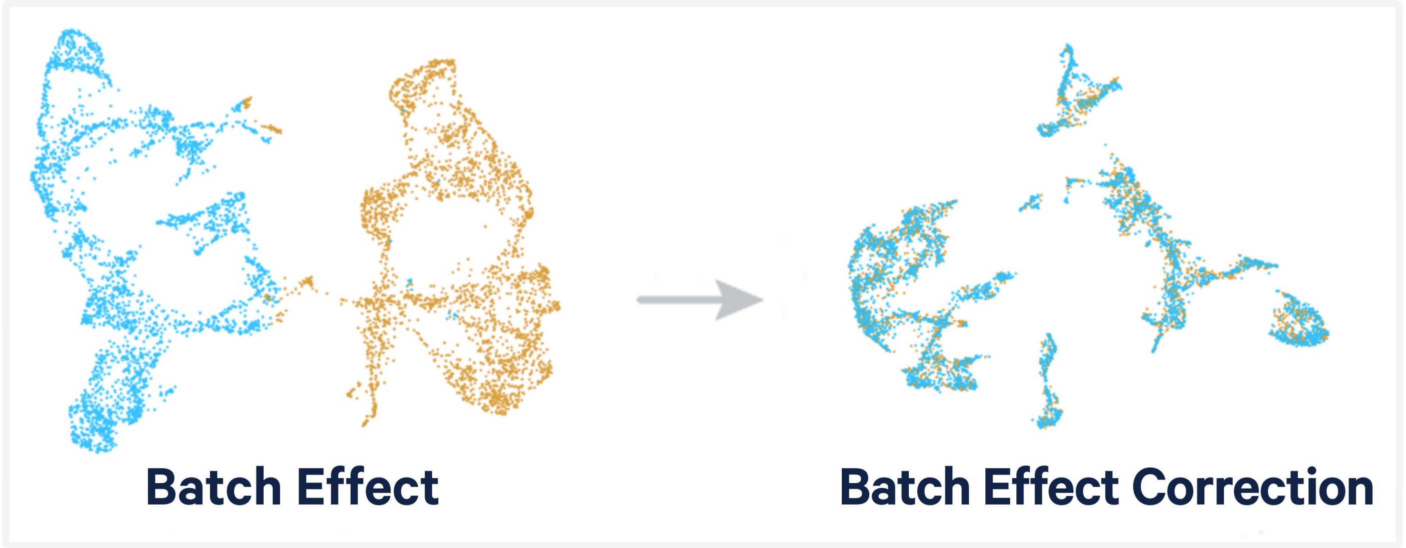

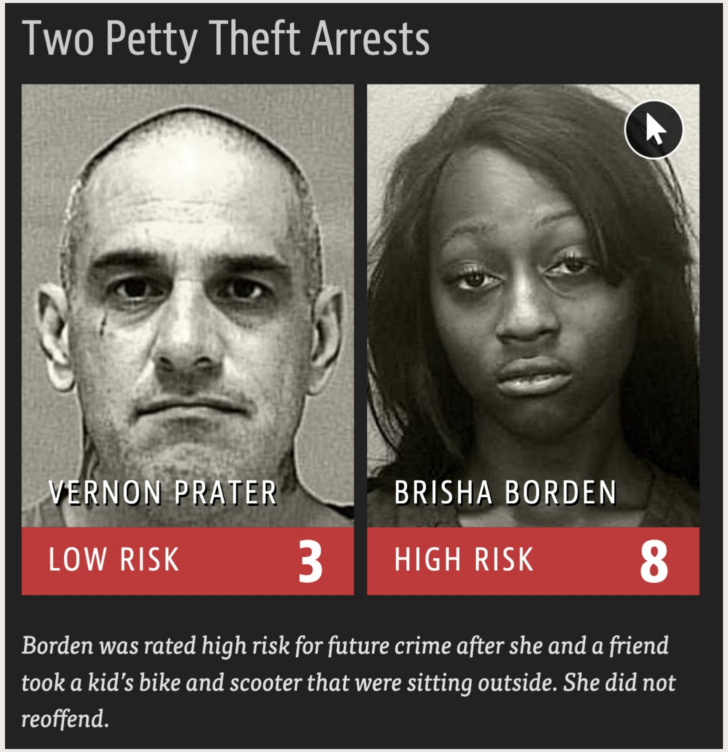

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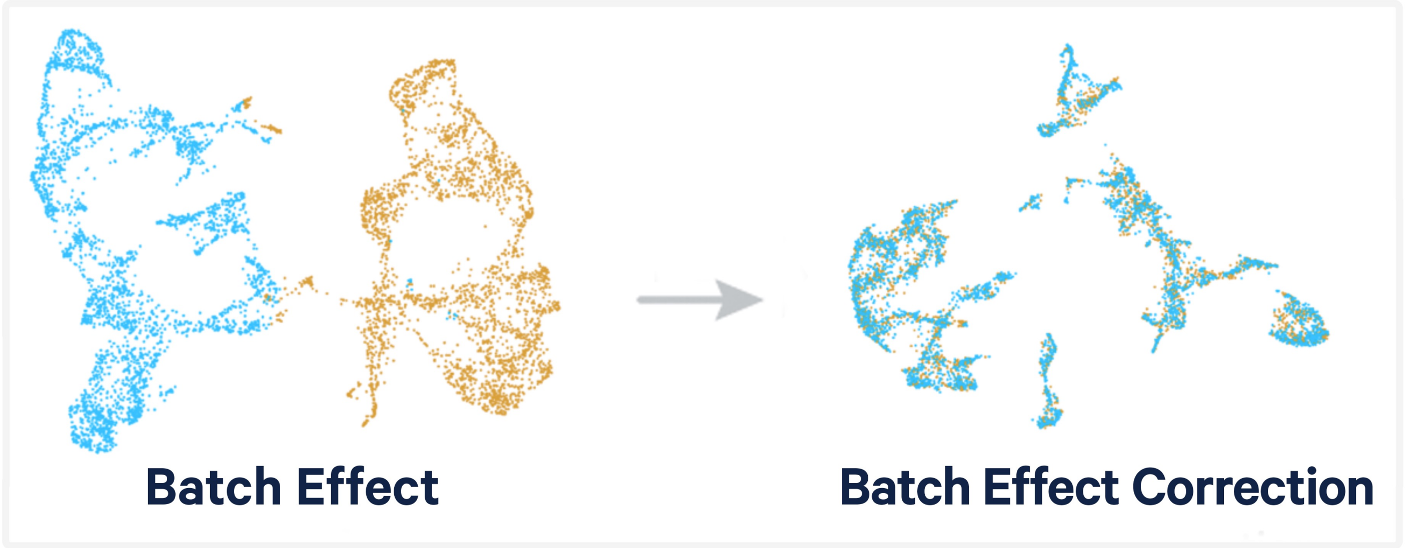

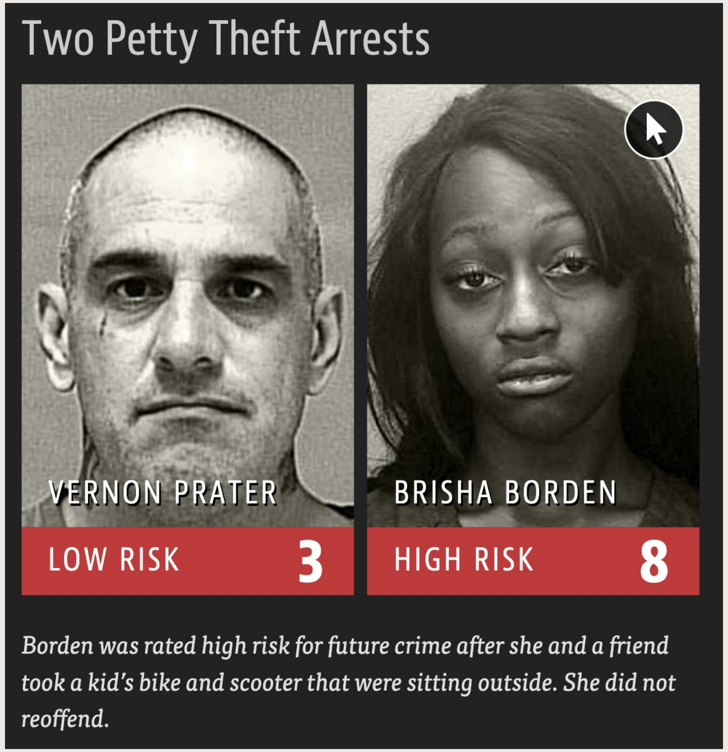

For more on batch effect correction, check out the resources curated by 10X Genomics.
Also, please refer to this article on machine learning bias in criminal sentencing.

Let X be the original data, Z be the "unwanted" factor, and Y be the "filtered" version of X.

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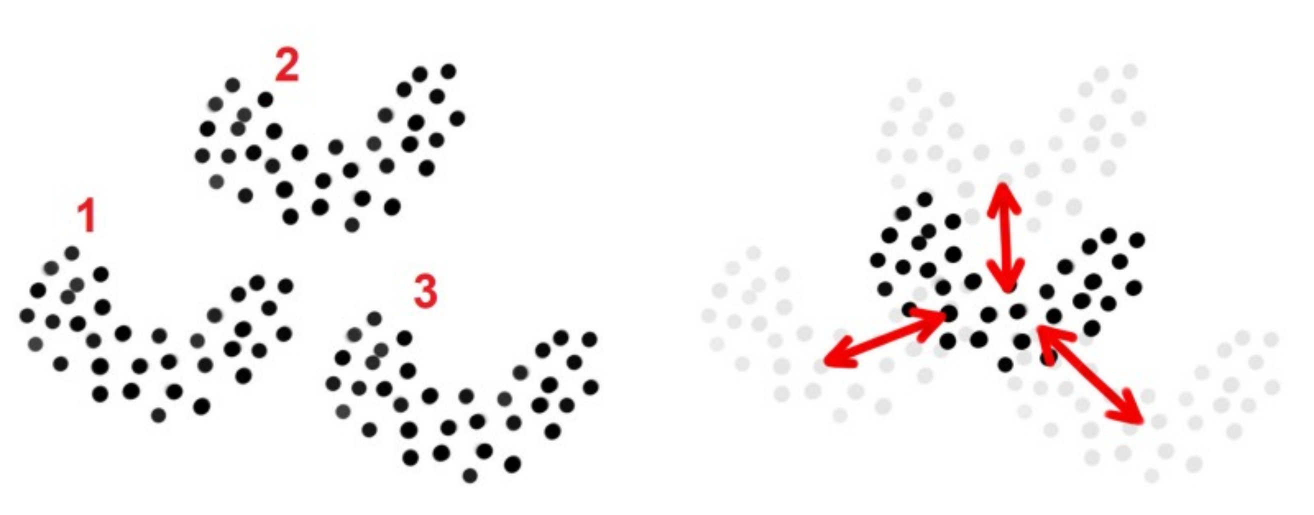

Figure 1: Each data point x is characterized by hidden factor $z \in \{1, 2, 3\}$. The filtration process is akin to computing the optimal transport barycenter of the conditional distributions $\rho(x \mid z)$ for all z.

Source: H. Yang, E. Tabak. *Conditional Density Estimation, Latent Variable Discovery, and Optimal Transport*. 2019.

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

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

Here, $c(x, y)$ is the cost function between x and y, $\rho(x|z)$ is the conditional probability distribution of x given z, and $\gamma(z)$ is the probability distribution of z.

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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.

$$D_{KL}(\pi(y,z)||\mu(y)\gamma(z))$$

Altogether, we have the following objective.

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

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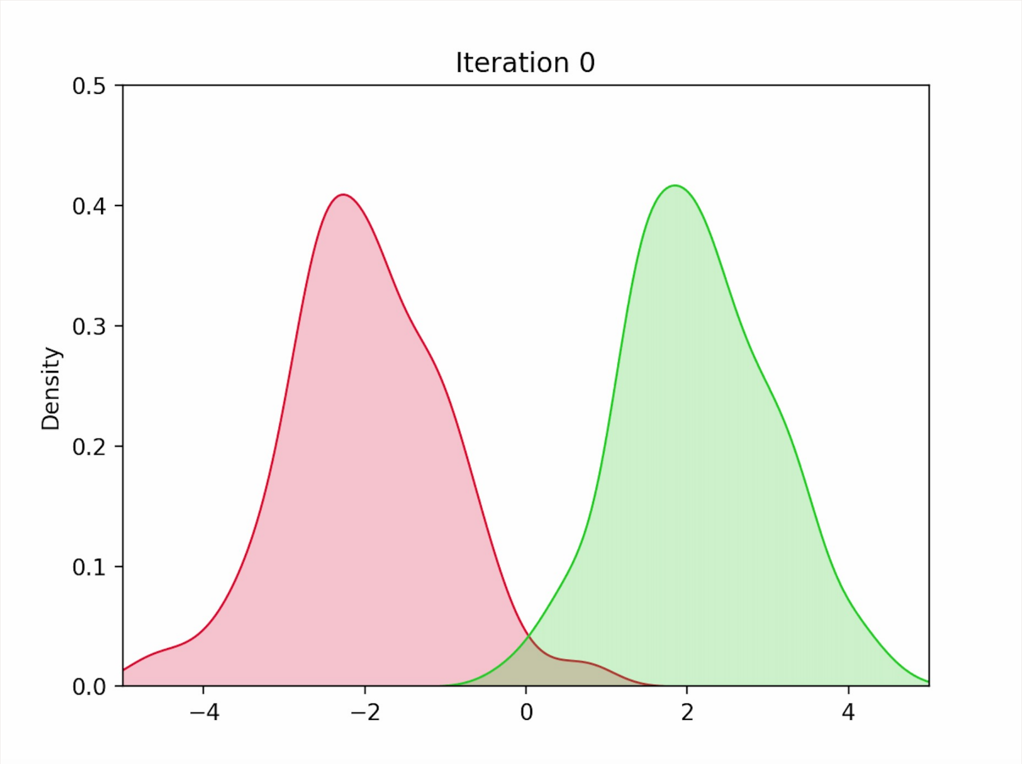
The data-based formulation using samples $\{x_i, z_i\}_i$ yield us

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

where $\pi(y_i, z_i)$, $\mu(y_i)$, and $\gamma(z_i)$ are approximated using KDE.

Simulation Results: Gaussian Experiment



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 $\mu(y)$.

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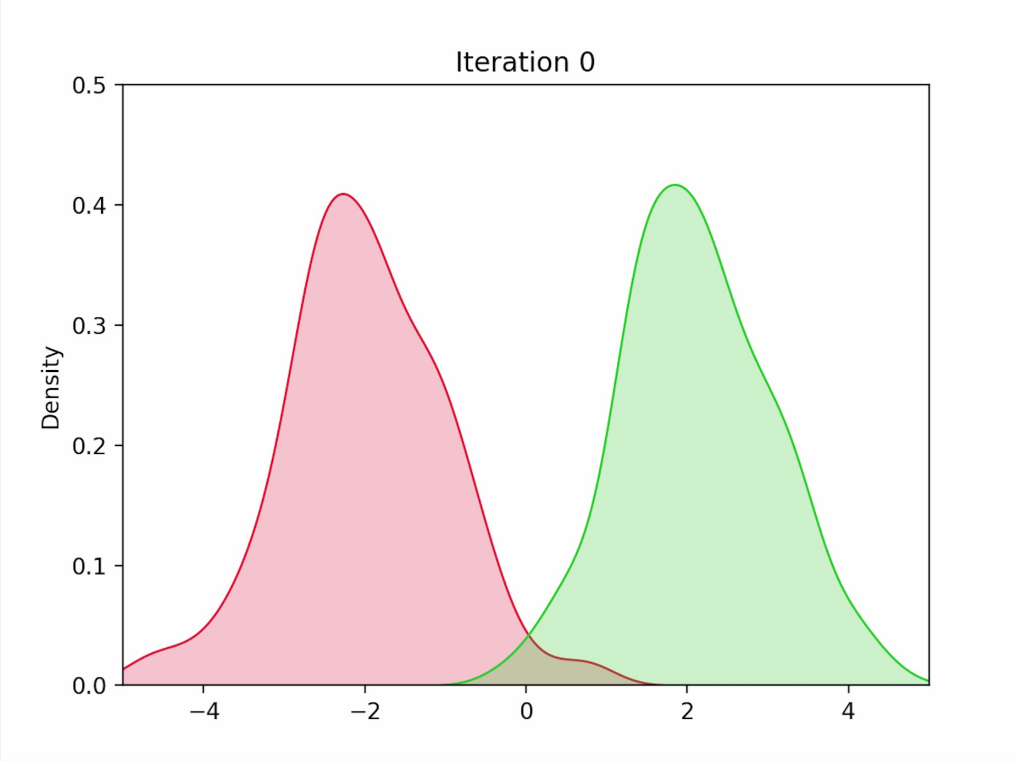

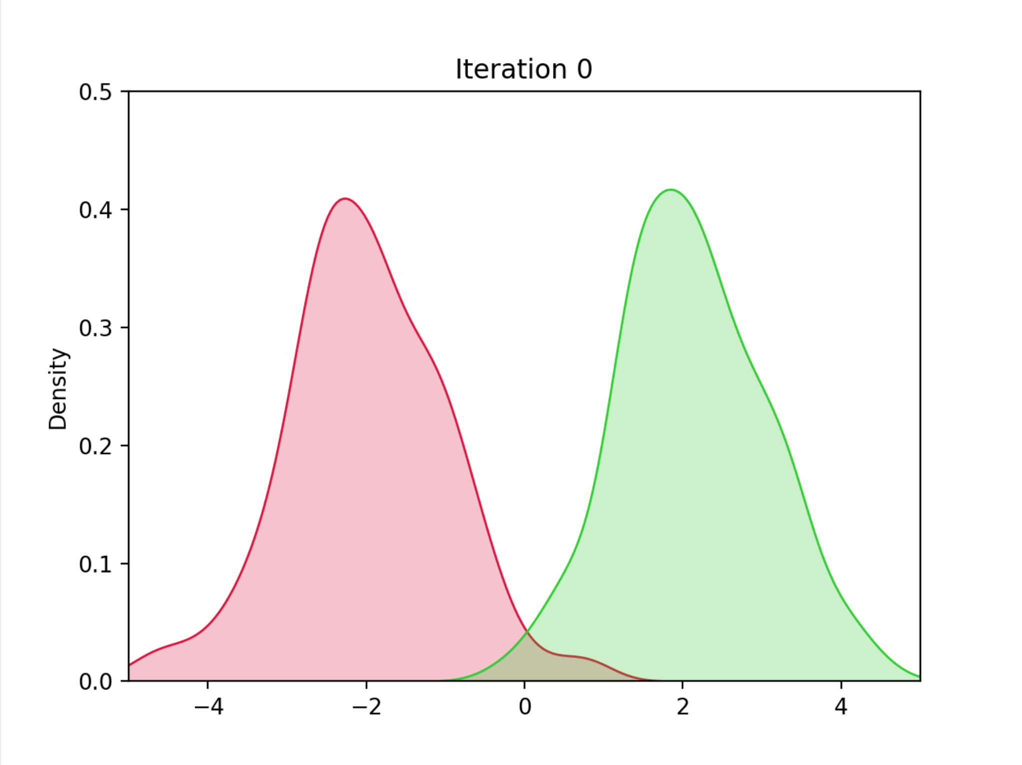

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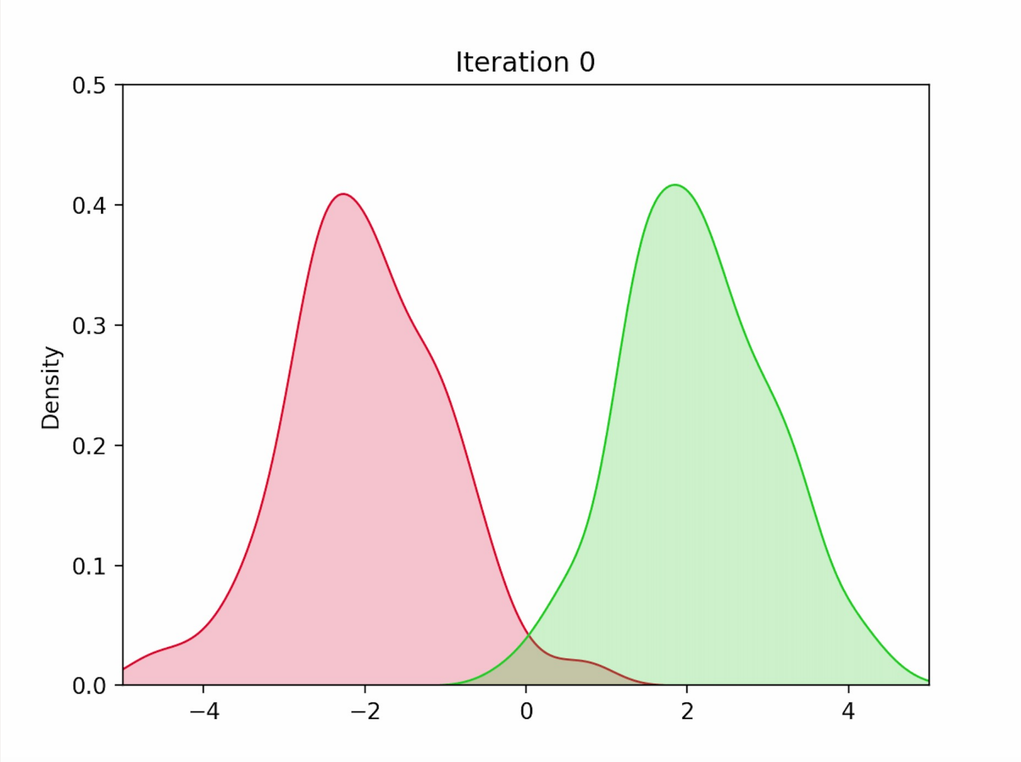
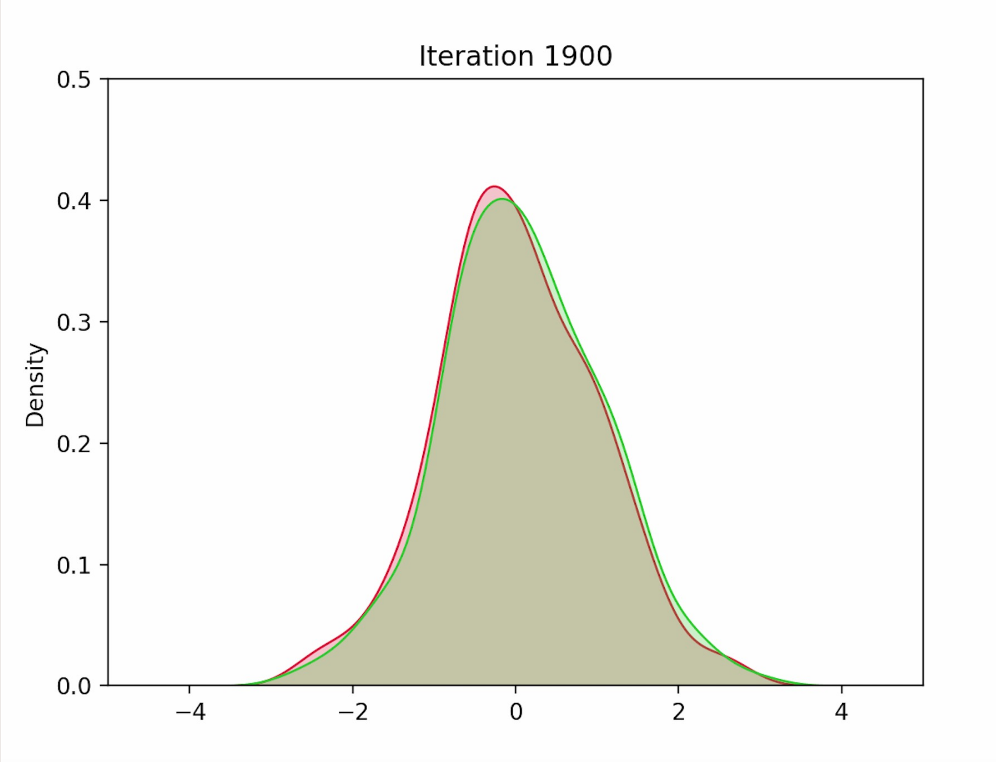
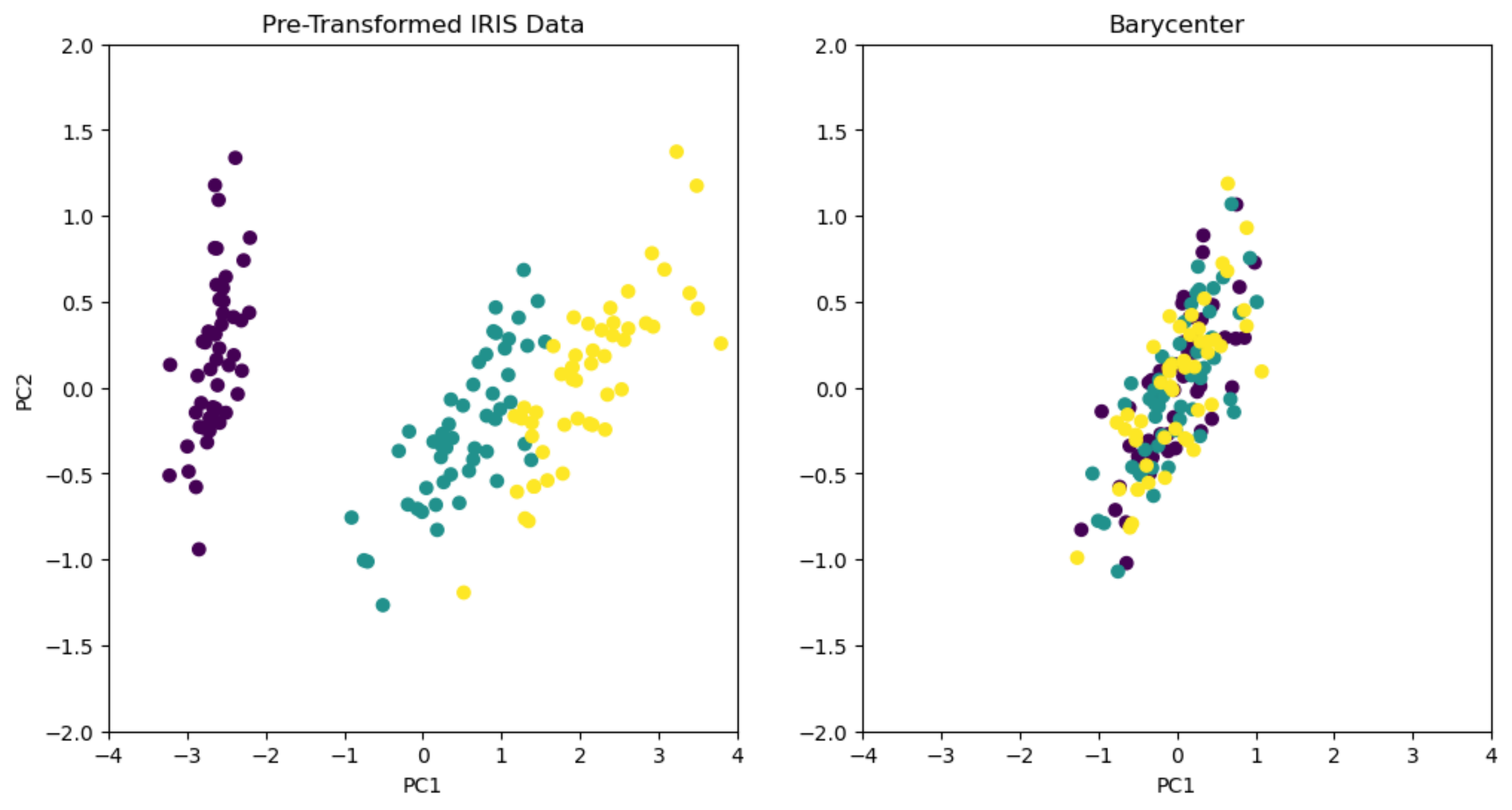




Simulation Results: Iris Dataset



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- **Factor discovery** through identifying the factor z that *maximizes the reduction in variability* among all factors.
- **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?