1 Experiments

The explicit computations of the $(4, 2)$-Gromov-Wasserstein distance between Euclidean spheres provides a helpful tool for benchmarking common optimal transport packages. The authors are aware of two well-known and commonly used python implementations of optimal transport solvers: Python Optimal Transport (POT) CITE and Optimal Transport Tools (OTT) CITE. These package implement two of the common methods for computing the Gromov-Wasserstein distance–either with entropic regularization (as with OTT) or without (as implemented in POT).[1] All experiments and their results are available at the Github repository, CITE.

The goal of this section is to benchmark various sampling methods and the number of samples required to obtain accurate estimates of the Gromov-Wasserstein distance while also understanding the accuracy of the various solvers.

We run two sorts of experiments. First, we examine how the number of samples relates to the choice of a regularized or non-regularized solver. Second, we fix the number of samples and vary the dimensionality of the spheres.

1.1 Varied points experiment

In this experiment, we fix the dimensions of both spheres and vary the number of samples we draw from each one. For each number of points, we run 20 trials of each sampling method and Gromov-Wasserstein solver for each number of samples between 10 and 200 in increments of 10 (inclusive). The plotted lines are the mean values estimated from the 20 trials, while the shaded area includes the central 80% of samples.

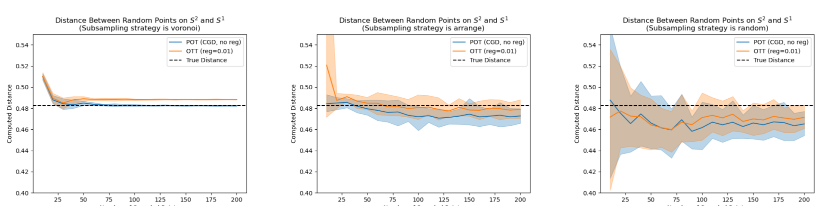

Figure 1: Estimating the Gromov-Wasserstein distance between $\mathbb{S}^2_E$ and $\mathbb{S}^1_E$.

1.2 Varied dimensions experiment

In this experiment, we fixed the number of samples taken at 100 and varied the dimensions of the two spheres, the solver method, and subsampling method.

[1]In fact, POT provides implementations of both solving techniques, but we include OTT, which only provides the regularized solver, since it is faster CITE because of its JAX implementation.

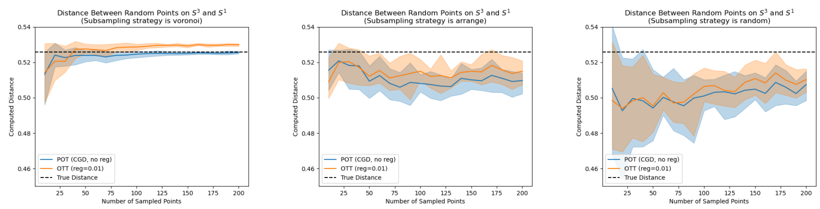

Figure 2: Estimating the Gromov-Wasserstein distance between $\mathbb{S}^3_E$ and $\mathbb{S}^1_E$.

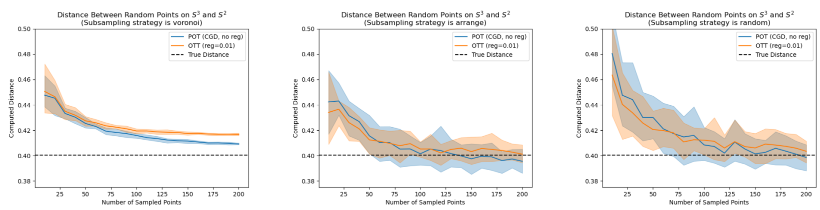

Figure 3: Estimating the Gromov-Wasserstein distance between $\mathbb{S}^3_E$ and $\mathbb{S}^2_E$.

Using the results of the trials for fixed sphere dimensions, m and n, $\hat{d}^i_{m,n}$, where $i = 1, \cdots, n_{\text{trials}}$, we estimated the true distance,

$$d_{m,n} \approx \hat{d}_{m,n} = \frac{1}{n_{\text{trials}}} \sum_{i=1}^{n_{\text{trials}}} \hat{d}^i_{m,n}.$$

We then recorded the relative error of this estimator: relative error$_{m,n}$ = $\frac{\hat{d}_{m,n} - d_{m,n}}{d_{m,n}}$. Each of these values is recorded in the corresponding entry of the heatmap.