1. Introduction

We present a new method for solving the K-means clustering problem through optimal transportation.

We solve discrete optimal transportation from the variational principle and propose a clustering algorithm which can be considered as a generalization of Lloyd's.

Our variational optimal transportation deals with probability distribution in convex domains. Thus our formulation is convex and its optimization is tractable via Newton’s method. This is particularly useful in the Euclidean space.

We design an iterative clustering algorithm and apply it to domain adaptation, remeshing, and representation learning.

2. Motivation

The K-means clustering loss:

\[
\text{arg min}_Y \sum_i \sum_j \| y_i - y_j \|^2
\]

The Wasserstein distance: the minimum cost:

\[
\text{arg min}_Y \sum_i \sum_j \| y_i - y_j \|^2
\]

The Wasserstein distance is also known as the Kantorovich-Rubinstein duality. It is a natural generalization of the K-means clustering problem.

3. Variational Optimal Transportation

\[
E(h) = \int_{\mathbb{R}^d} \sum_{i,j} \mu_i(y) d(x-y)
\]

\[
\frac{\partial^2 E(h)}{\partial h_{ij}} = -\delta_{ij}
\]

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4. Experiments

5. Conclusions

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