NEEMo: Neural Estimation of Energy Mover's Distance

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Geometric shape fitting based on Optimal Transport using Lipschitz Networks

Minimize $\theta \rightarrow \theta - \nabla_\theta \mathrm{EMD}_\phi$

Parametrized shape: θ

This is a parametrization of an arbitrary geometric shape, for instance, the radius and coordinates of the center of a circle. Many novel (and old) observables can be constructed as such.

N-subjet → N-points

Pile-up → Uniform rectangle

N-circliness, N-diskiness, Triangularness, etc.

Parametrized Distribution

This is a collection of m particles parametrized by θ: $\mathbb{P} = \{w_\theta^i, \mathbf{y}_\theta^i\}_{i=1}^m$

Examples: drawn from $\mathcal{N}(\mu, \sigma)$, uniform circles, disks, triangles, uniform rectangles, etc.

Target Distribution

The event to fit given by a collection of particles: $\mathbb{Q} = \{E^i, \mathbf{x}^i\}_{i=1}^n$

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EMD Estimation

Using the KR duality, a lower bound on the $\mathrm{EMD}_\phi(\mathbb{P}_\theta, \mathbb{Q})$ is estimated by the NN which is then minimized by the shape parameters in the following minimax optimization problem:

$$\mathcal{O}(\mathbb{Q}) = \min_\theta \max_\phi \left[\sum_{i=1}^{n} E^i f_\phi(\mathbf{x}^i) - \sum_{i=1}^{m} w_\theta^i f_\phi(\mathbf{y}_\theta^i) \right]$$

$\mathcal{O}(\mathbb{Q})$ is the observable that describes how well the event $\mathbb{Q}$ is described by the class of geometric objects $\mathbb{P}$.

Maximize $\phi \rightarrow \phi + \nabla_\phi \mathrm{EMD}_\phi$

Lipschitz NN

Each particle is passed individually to a Lipschitz 1 neural network $f_\phi(\mathbf{x})$ with parameters ϕ. Linear layers are weight normed such that

$$\|W^{(1)}\|_{p,\infty} \prod_{l=2}^{L} \|W^{(l)}\|_\infty \leq 1$$

To approximate the EMD well, the NN architecture needs to be a universal approximator of Lip 1 functions. So we use GroupSort activation.

Backward pass

Forward pass