Study of *Optimal transport mapping via input convex neural networks*

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Context

μ, ν probability distributions on $\mathbb{R}^d$.

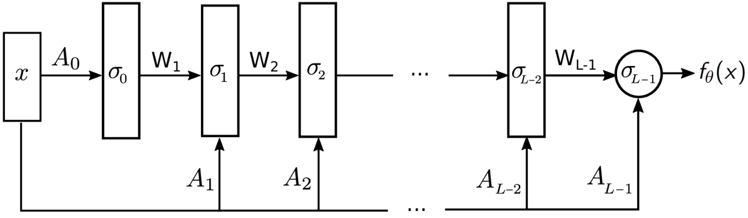
- Monge: $\min_{T \mid T_{\#}\mu = \nu} \int_{\mathbb{R}^d} c(x, T(x)) d\mu(x)$.
- Kantorovitch: $W_2^2(\mu, \nu) = \min_{\gamma \in \Pi(\mu,\nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\gamma(x, y)$.
- Dual:

$$W_2^2(\mu, \nu) = \sup_{\substack{f \text{ convex} \\ f^* \in L^1(\nu)}} \inf_{g \text{ convex}} \mathcal{V}_{\mu,\nu}(f, g) + C_{\mu,\nu},$$

with $\mathcal{V}_{\mu,\nu}(f, g) = -\mathbb{E}_\mu [f(X)] - \mathbb{E}_\nu [\langle Y, \nabla g(Y) \rangle - f(\nabla g(Y))]$.

Theorem: if (f, g) is optimal, and μ has a density w.r.t. Lebesgue measure, then ∇f solve Monge problem.

Input Convex Neural Networks (ICNN)



- All coefficients of the weight matrices W_l are non-negative.
- The activation functions σ_l are convex for $l = 0, \ldots, L-1$.
- The activation functions σ_l are non-decreasing for $l = 1, \ldots, L-1$.

Then $x \mapsto f_\theta(x)$ is convex.

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The problem

$$W_2^2(\mu,\nu) = \sup_{\substack{f \text{ convex} \\ f^* \in L^1(\nu)}} \inf_{g \text{ convex}} \left(-\mathbb{E}_\mu\left[f(X)\right] - \mathbb{E}_\nu\left[\langle Y, \nabla g(Y)\rangle - f\left(\nabla g(Y)\right)\right]\right) + C_{\mu,\nu}$$

is thus approximated by

$$\sup_{f \in \mathrm{ICNN}(\mathbb{R}^d)} \inf_{g \in \mathrm{ICNN}(\mathbb{R}^d)} \left(-\mathbb{E}_\mu\left[f(X)\right] - \mathbb{E}_\nu\left[\langle Y, \nabla g(Y)\rangle - f\left(\nabla g(Y)\right)\right]\right) + C_{\mu,\nu},$$

with $C_{\mu,\nu} = \dfrac{1}{2}\mathbb{E}_{X\sim\mu, Y\sim\nu}\left[\|X\|_2^2 + \|Y\|_2^2\right]$.

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Algorithm

Algorithm

Require: Samples from μ and ν, batch size M, generator iterations K, total iterations T

for $t = 1$ to T **do**
  for $k = 1$ to K **do**
    Sample $\{X_i\}_{i=1}^M \sim \mu$, $\{Y_i\}_{i=1}^M \sim \nu$
    Update g to minimize J using Adam
  end for
  Sample $\{X_i\}_{i=1}^M \sim \mu$, $\{Y_i\}_{i=1}^M \sim \nu$
  Update f to maximize J using Adam
  $w \leftarrow \max(w, 0)$ for all coefficients w of W_l in θ_f, $l = 1, \ldots, L-1$
end for

$$J(\theta_f, \theta_g) = \frac{1}{M} \sum_{i=1}^{M} \left(f\left(\nabla g(Y_i)\right) - \langle Y_i, \nabla g(Y_i)\rangle - f(X_i)\right) + \lambda \sum_{W_l \in \theta_g} \| \max(-W_l, 0)\|_F^2. \quad (1)$$

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Theoretical guarantees

$$\varepsilon_1(f,g) = \mathcal{V}_{\mu,\nu}(f,g) - \inf_{\tilde{g} \text{ convex}} \mathcal{V}_{\mu,\nu}(f,\tilde{g})$$

$$\varepsilon_2(f) = \sup_{\tilde{f} \text{ convex}} \inf_{\tilde{g} \text{ convex}} \mathcal{V}_{\mu,\nu}(\tilde{f},\tilde{g}) - \inf_{\tilde{g} \text{ convex}} \mathcal{V}_{\mu,\nu}(f,\tilde{g}).$$

Theorem: Assume ν has a density with respect to Lebesgue measure, and let ∇g^* be the optimal transport from ν to μ.
Then for any (f,g) such that f is α-strongly convex, the following holds:

$$\|\nabla g - \nabla g^*\|^2_{L^2(\nu)} \leq \frac{2}{\alpha}\left(\varepsilon_1(f,g) + \varepsilon_2(f)\right).$$

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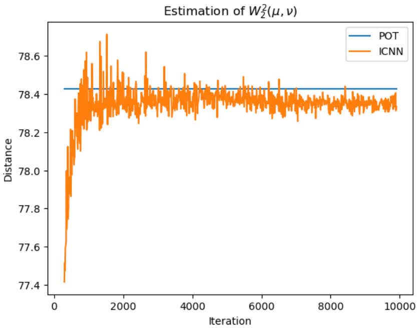
Experiments



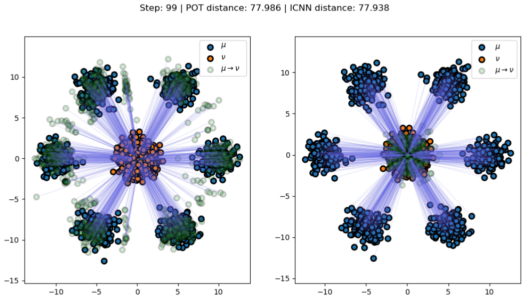


Figure: Gaussian mixture with 6 components, and Gaussian distribution. Estimated distance and optimal transport.

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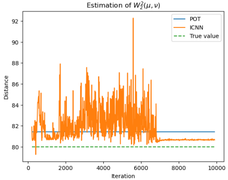
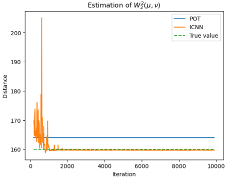
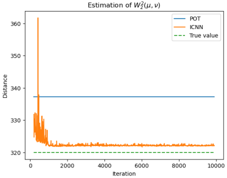
Experiments



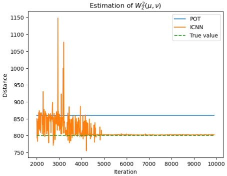
(a) Gaussian in $\mathbb{R}^5$



(b) Gaussian in $\mathbb{R}^{10}$



(c) Gaussian in $\mathbb{R}^{20}$



(d) Gaussian in $\mathbb{R}^{50}$

Figure: Translated Gaussian distributions in higher dimensions.

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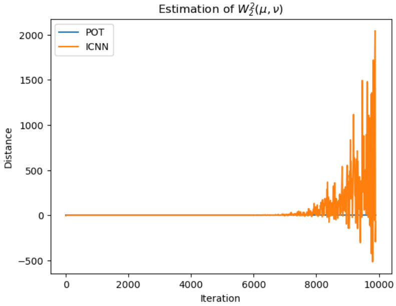
Experiments



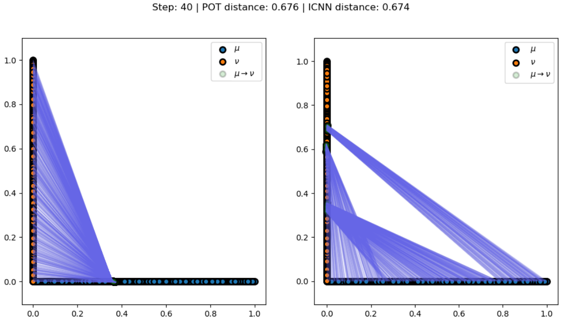
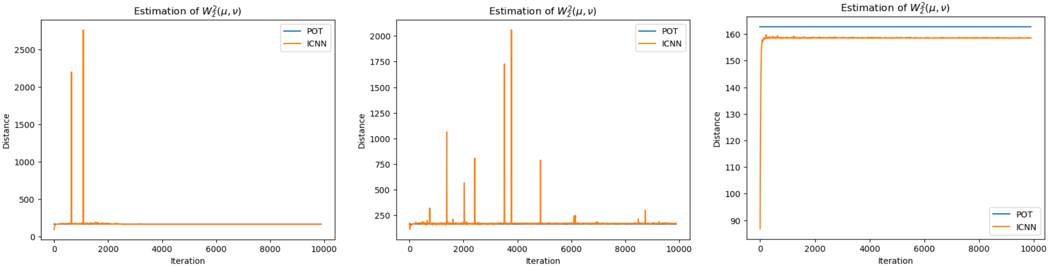


Figure: μ and ν without density (true value: $\frac{2}{3}$)

Experiments



(a) Penalty for g's coefficients (b) Positive coefficients for g (c) No constraints on g

Figure: Impact of enforcing positivity of g's coefficients

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Conclusion

- Can be slow
- Not always stable: need to carefully tune hyperparameters
- The choice of hyperparameters is not discussed in the paper

- Scalable to high dimensions and large datasets
- Easy to implement
- Some theoretical guarantees

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References

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