Efficient, Stable, and Analytic Differentiation of the Sinkhorn Loss

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Outline

Motivation and Problem Setting

Statistical Divergence

- Given two distributions p and q, define a function $D(p, q)$ such that:
  - $D(p, q) \geq 0$ for all p and q
  - $D(p, q) = 0 \Leftrightarrow p = q$

Statistical Divergence

- Given two distributions p and q, define a function $D(p, q)$ such that:
  - $D(p, q) \geq 0$ for all p and q
  - $D(p, q) = 0 \Leftrightarrow p = q$
- Examples:
  - Kullback–Leibler divergence
$$D_{\mathrm{KL}}(p \| q) = \int p(x) \log \left(\frac{p(x)}{q(x)} \right) \mathrm{d}x$$
  - Squared Hellinger distance
$$H^2(p, q) = 2 \int \left(\sqrt{p(x)} - \sqrt{q(x)} \right)^2 \mathrm{d}x$$
  - Wasserstein distance
$$W_r(p, q) = \left(\inf_{\gamma \in \Pi(p,q)} \mathbb{E}_{(X,Y)\sim\gamma} \|X - Y\|^r \right)^{1/r}$$
  - ...

Problem Setting

- Given data $X_1, \dots, X_n \sim p^*$ and a model p_θ
- Task 1: Evaluate or estimate the divergence $D(p^*, p_\theta)$
  - A measure of goodness-of-fit
  - Testing distributional difference
- Task 2: Evaluate or estimate the gradient $\nabla_\theta D(p^*, p_\theta)$
  - This gradient makes p_θ learnable
  - Enables us to find a good model p_θ that minimizes $D(p^*, p_\theta)$

Wasserstein Distance

- Wasserstein distance is a popular metric to quantify the difference between distributions
- Inspired many breakthroughs in deep learning such as the Wasserstein generative adversarial networks (WGAN)
- However, its computation is notoriously difficult

Wasserstein Distance

- Given two discrete distributions $X \sim p$ and $Y \sim q$

$$\mathbb{P}(X = x_i) = a_i, \quad \mathbb{P}(Y = y_j) = b_i, \quad \sum_{i=1}^{n} a_i = \sum_{j=1}^{m} b_j = 1$$

- Define the cost matrix M with $M_{ij} = \|x_i - y_j\|^r$
- The r-Wasserstein distance between p and q is

$$W_r(p, q) = \left[\min_{P \in \Pi(a,b)} \langle P, M \rangle \right]^{1/r}$$

$$\Pi(a, b) = \{ T \in \mathbb{R}_+^{n \times m} : T\mathbf{1}_m = a, T^{\mathrm{T}}\mathbf{1}_n = b \}$$

- Solving P is also called the optimal transport (OT) problem

Sinkhorn Loss as Approximate OT

- Assuming $m = n$, standard linear programming solvers cost $\mathcal{O}(n^3 \log n)$
- Cuturi (2013) proposes the entropic-regularized OT

$$\min_{T \in \Pi(a,b)} \langle T, M \rangle - \lambda^{-1} h(T), \quad h(T) = \sum_{i=1}^{n} \sum_{j=1}^{m} T_{ij}(1 - \log T_{ij})$$

- Let T_λ^* be the unique global solution, and then the Sinkhorn loss is defined as

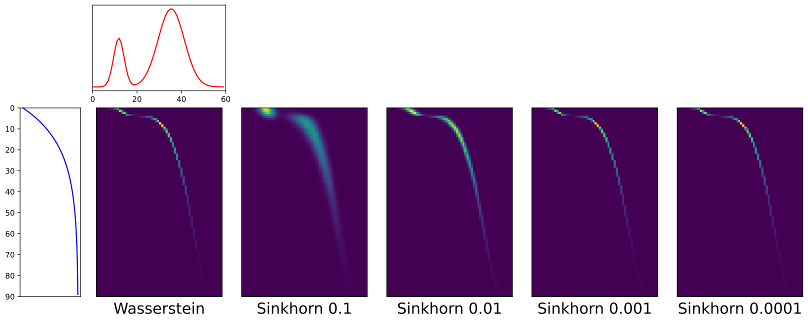
$$S_\lambda(M, a, b) = \langle T_\lambda^*, M \rangle$$

Sinkhorn Loss as Approximate OT

- Luise et al. (2018) shows that

$$|S_\lambda(M, a, b) - W_r^r(p, q)| \leq Ce^{-\lambda}$$

- For smaller and smaller λ^{-1}, $S_\lambda(M, a, b)$ is closer to the Wasserstein distance



Forward and Backward Pass

- Corresponding to the two tasks in the problem setting
- Forward pass of Sinkhorn loss
  - Compute $S_\lambda(M, a, b)$
  - Existing method: Sinkhorn's algorithm
- Backward pass of Sinkhorn loss
  - Compute $\nabla_M S_\lambda(M, a, b)$
  - Existing method: automatic differentiation

Sinkhorn's Algorithm

- Cuturi (2013) shows that T_λ^* can be expressed as

$$T_\lambda^* = \textbf{diag}(u^*) M_e \textbf{diag}(v^*)$$

for some vectors u^* and v^*, where $M_e = \left(e^{-\lambda M_{ij}}\right)$

- Interestingly, u^* and v^* can be solved using the iterations

$$u^{(k+1)} \leftarrow a \odot [M_e v^{(k)}]^{-1}, \quad v^{(k+1)} \leftarrow b \odot [M_e^{\mathrm{T}} u^{(k+1)}]^{-1}$$

- Notation: for vectors $u = (u_1, \ldots, u_k)^{\mathrm{T}}$, $v = (v_1, \ldots, v_k)^{\mathrm{T}}$,

$$u^{-1} = (u_1^{-1}, \ldots, u_k^{-1})^{\mathrm{T}}, \quad u \odot v = (u_1 v_1, \ldots, u_k v_k)^{\mathrm{T}}$$

Automatic Differentiation

- Note that the iterations in Sinkhorn's algorithm are all differentiable
- So one can use the automatic differentiation technique to compute $\nabla_M S_\lambda(M, a, b)$
- This requires "unrolling" the iterations
- Genevay et al. (2018) uses this method to learn generative models with the Sinkhorn loss

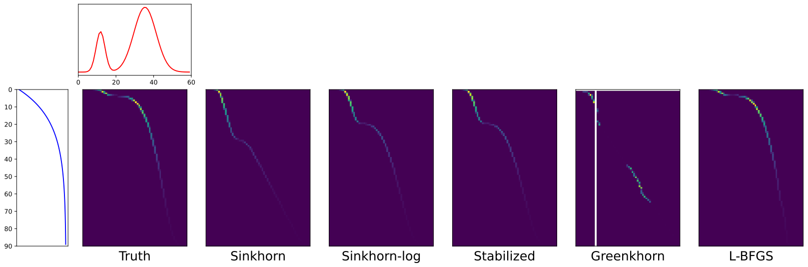
Our Contribution

Issues of Sinkhorn's Algorithm

- Numerical instability
  - M_e may underflow when λ is large
  - Making $M_e v^{(k)}$ and $M_e^{\mathrm{T}} u^{(k+1)}$ close to zero
  - $u^{(k+1)}$ and $v^{(k+1)}$ overflow
- Many works to improve
  - Log-domain iterations
  - Stabilized sparse scaling (Schmitzer, 2019)

Issues of Sinkhorn's Algorithm

- May be slow to converge
- Especially for large λ



Dual Problem

- The dual problem of the Sinkhorn optimization is $\max_{\alpha,\beta} \mathcal{L}(\alpha,\beta)$, where $\alpha \in \mathbb{R}^n$, $\beta \in \mathbb{R}^m$,

$$\mathcal{L}(\alpha,\beta) = \alpha^{\mathrm{T}} a + \beta^{\mathrm{T}} b - \lambda^{-1} \sum_{i=1}^{n} \sum_{j=1}^{m} e^{-\lambda(M_{ij}-\alpha_i-\beta_j)}$$

- This dual maximization problem is concave and unconstrained
- Once we get the optimal point (α^*, β^*), T^*_λ is recovered as

$$T^*_\lambda = \mathrm{e}_\lambda[\alpha^* \oplus \beta^* - M], \quad \mathrm{e}_\lambda[A] = (e^{\lambda A_{ij}})$$

- Notation: for vectors $u = (u_1, \dots, u_l)^{\mathrm{T}}$, $v = (v_1, \dots, v_k)^{\mathrm{T}}$,

$$u \oplus v = (u_i + v_j) \in \mathbb{R}^{l \times k}$$

Forward Pass

- (α, β) has one redundant degree of freedom, so globally set $\beta_m = 0$
- For a fixed β, the optimal α is

$$\alpha^*(\beta)_i = \lambda^{-1} \log a_i - \lambda^{-1} \log \left[\sum_{j=1}^{m} e^{\lambda(\beta_j - M_{ij})} \right]$$

- Then the optimization problem becomes

$$f(\beta) = -\alpha^*(\beta)^{\mathrm{T}} a - \beta^{\mathrm{T}} b + \lambda^{-1}$$

- We can also show that

$$\nabla_{\tilde{\beta}} f = \tilde{T}(\beta)^{\mathrm{T}} \mathbf{1}_n - \tilde{b}, \quad T(\beta) = \mathrm{e}_\lambda[\alpha^*(\beta) \oplus \beta - M]$$

- For a vector v or a matrix A, $\tilde{v}$ or $\tilde{A}$ means removing the last element or column

Stability of Solution

Theorem (informal)
Let f^* be the minimum value of $f(\beta)$, β^* an optimal solution, and $\alpha^* = \alpha^*(\beta^*)$. Then $f^* > -\infty$, β^* is unique, and α^*, β^* have computable bounds.

L-BFGS Algorithm

- The L-BFGS algorithm (Liu and Nocedal, 1989) is a well-known quasi-Newton method for smooth optimization problems
- It only requires evaluating $f(\beta)$ and $\nabla_{\tilde{\beta}} f$
- We provide theoretical guarantees for the L-BFGS algorithm on our problem

Convergence Analysis

Theorem (informal)
Let $\beta^{(k)}$ be the k-th iterate of β, and $f^{(k)} = f(\beta^{(k)})$, then

- *Objective function and iterates converge exponentially fast*

$$f^{(k)} - f^* \leq r^k (f^{(0)} - f^*) := \varepsilon^{(k)}, \quad \|\beta^{(k)} - \beta^*\|^2 \leq C_1 \varepsilon^{(k)}$$

- *Exponential decay of gradient*

$$\|\nabla_{\tilde{\beta}} f(\beta^{(k)})\|^2 = \|\tilde{T}^{(k)\mathrm{T}} \mathbf{1}_n - \tilde{b}\|^2 \leq C_2 \varepsilon^{(k)}$$

- *Stability of iterates*

$$0 < T_{ij}^{(k)} < \min\{a_i, b_j + \sqrt{C_2 \varepsilon^{(k)}}\}, \quad 1 \leq j \leq m-1$$

Backward Pass

- Instead of relying on automatic differentiation
- We develop an analytic expression for $\nabla_M S_\lambda(M, a, b)$
- Based on the implicit function theorem

Analytic Differentiation

Theorem
For a fixed $\lambda > 0$,

$$\nabla_M S_\lambda(M, a, b) = T^*_\lambda + \lambda(s_u \oplus s_v - M) \odot T^*_\lambda,$$

where

$$\begin{aligned} T^*_\lambda &= \mathrm{e}_\lambda[\alpha^* \oplus \beta^* - M] & D &= \mathbf{diag}(\tilde{b}) - \tilde{T}^{*\mathrm{T}}_\lambda \mathbf{diag}(a^{-1})\,\tilde{T}^*_\lambda \\ s_u &= a^{-1} \odot (\mu_r - \tilde{T}^* \tilde{s}_v) & \tilde{s}_v &= D^{-1}\left[\tilde{\mu}_c - \tilde{T}^{*\mathrm{T}}(a^{-1} \odot \mu_r)\right] \\ \mu_r &= (M \odot T^*)\mathbf{1}_m & \tilde{\mu}_c &= (\tilde{M} \odot \tilde{T}^*)^{\mathrm{T}}\mathbf{1}_n \end{aligned}$$

Error Bounds

Theorem
There exists a k_0 such that for every $k \geq k_0$,

$$\|\nabla_M S^{(k)} - \nabla_M S\|_F \leq C_S \sqrt{\varepsilon^{(k)}} = C_S \sqrt{f^{(0)} - f^*} \cdot r^{k/2}$$

Application and Experiments

Application: Deep Generative Models

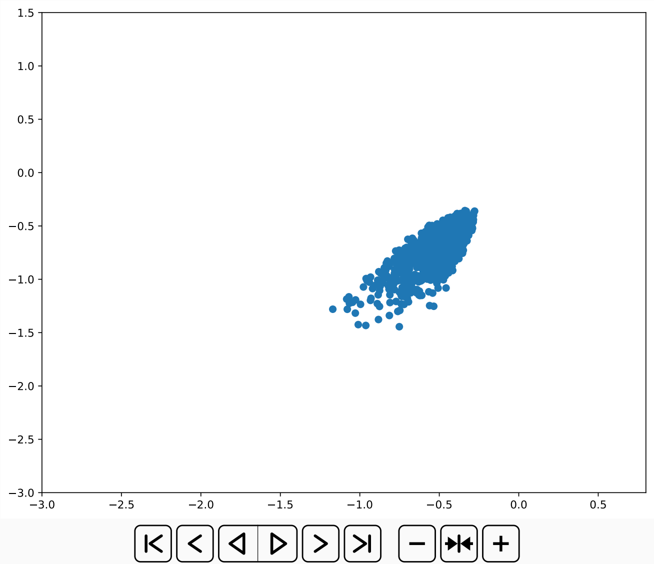
- Given a data set $X_1, \ldots, X_n \sim p^*$, find a deep neural network g_θ such that $g_\theta(Z) \sim p_\theta$ and $p_\theta \approx p^*$, where $Z \sim N(0, I_r)$
- This can be viewed as the implicit distribution estimation

Application: Deep Generative Models

- Given a data set $X_1, \ldots, X_n \sim p^*$, find a deep neural network g_θ such that $g_\theta(Z) \sim p_\theta$ and $p_\theta \approx p^*$, where $Z \sim N(0, I_r)$
- This can be viewed as the implicit distribution estimation

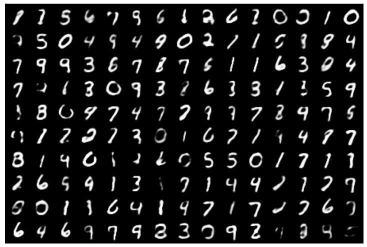
- Generate $Z_1, \ldots, Z_m \sim N(0, I_r)$, and let $Y_j = g_\theta(Z_j)$
- Cost matrix $(M_\theta)_{ij} = \|X_i - g_\theta(Z_j)\|^2$
- Find θ such that $\ell(\theta) = S_\lambda(M_\theta, n^{-1}\mathbf{1}_n, m^{-1}\mathbf{1}_m)$ is minimized

2D Example

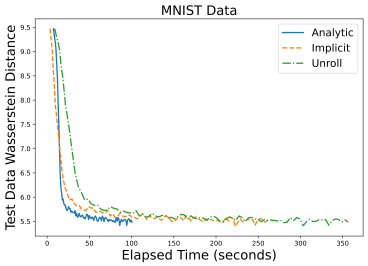


MNIST Dataset

- Compare the computing time of different methods
- Unroll: automatic differentiation; Implicit: existing software package; Analytic: proposed method

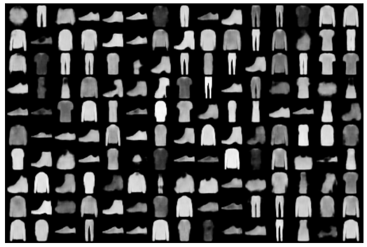


(a) Generated images

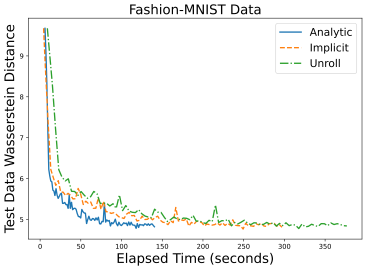


(b) Training process

Fasion-MNIST Dataset



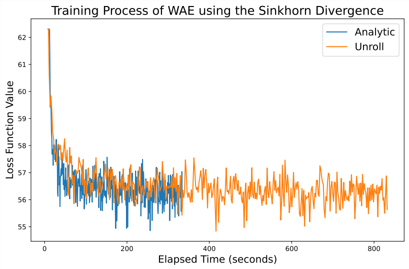
(c) Generated images



(d) Training process

CelebA Dataset

(e) Generated images



(f) Training process

Summary

- The Sinkhorn loss is an approximation to the popular Wasserstein distance
- We advocate the L-BFGS algorithm for forward pass, and analytic differentiation for the backward pass
- We rigorously prove that L-BFGS is stable and efficient for Sinkhorn loss
- Numerical results show the effiency of the advocated algorithms

THANK YOU!