Stochastic Algorithm for Optimal Transport

Zehui Xuan

September 14th, 2022

Supervisor: Olivier Wintenberger, Antoine Godichon-Baggioni

Content

- Introduction
- 2 Theoretical Analysis
 - Analysis on the upper bound of regret for the Sinkhorn Divergence
 - \bullet Analysis on the upper bound of regret for Regularized Wasserstein distance with fixed ε
- 3 Experiments
 - Calculation of the true value of the squared Wasserstein distance
 - Approximation in discrete case
 - Approximation in semi-discrete case
- Conclusion



Introduction

- - Analysis on the upper bound of regret for the Sinkhorn Divergence
 - Analysis on the upper bound of regret for Regularized Wasserstein distance with
- - Calculation of the true value of the squared Wasserstein distance
 - Approximation in discrete case
 - Approximation in semi-discrete case

What is Optimal Transport?

Optimal Transport:

- Moving one distribution of mass to another
- Minimizing the cost of transport

Example:

Introduction

000000

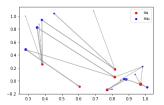


Figure 1: Example of OT in discrete case

Kantorovich formulation [4]:

$$W(\mu, \nu) = \min_{P \in U(\mu, \nu)} \sum_{i,j} c_{i,j} P_{i,j}$$
 (1)

where

$$U(\mu, \nu) = \{ P \in \mathbb{R}_+^{I \times J} : P \mathbf{1}_J = \mu \text{ and } P^\top \mathbf{1}_I = \nu \}$$
 and c is a cost matrix.

Preliminaries (1/4)

Introduction

000000

Kantorovich formulation in continuous setting [4]:

$$\forall (\mu, \nu) \in \mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{Y}), W(\mu, \nu) \stackrel{\text{def.}}{=} \min_{\pi \in \Pi(\mu, \nu)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\pi(x, y) \tag{2}$$

Preliminaries (1/4)

Introduction

0000000

Kantorovich formulation in continuous setting [4]:

$$\forall (\mu, \nu) \in \mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{Y}), W(\mu, \nu) \stackrel{\text{def.}}{=} \min_{\pi \in \Pi(\mu, \nu)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\pi(x, y) \tag{2}$$

Squared Wasserstein Distance [1]:

$$W_2^2(\mu,\nu) \stackrel{\text{def.}}{=} \min_{\pi \in \Pi(\mu,\nu)} \int_{\mathcal{X} \times \mathcal{Y}} \|x_i - y_j\|^2 \mathrm{d}\pi(x,y)$$
 (3)

Preliminaries (1/4)

Introduction

0000000

Kantorovich formulation in continuous setting [4]:

$$\forall (\mu, \nu) \in \mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{Y}), W(\mu, \nu) \stackrel{\text{def.}}{=} \min_{\pi \in \Pi(\mu, \nu)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\pi(x, y)$$
 (2)

Squared Wasserstein Distance [1]:

$$W_2^2(\mu,\nu) \stackrel{\text{def.}}{=} \min_{\pi \in \Pi(\mu,\nu)} \int_{\mathcal{X} \times \mathcal{Y}} \|x_i - y_j\|^2 \mathrm{d}\pi(x,y)$$
 (3)

Regularized OT Cost [2]:

$$W_{\varepsilon}(\mu,\nu) \stackrel{\text{def.}}{=} \min_{\pi \in \Pi(\mu,\nu)} \int_{\mathcal{X} \times \mathcal{Y}} c(x,y) d\pi(x,y) + \varepsilon KL(\pi \mid \mu \otimes \nu)$$
 (4)

Introduction

0000000

The semi-dual formulation in the discrete case [3]:

$$W_{\varepsilon}(\mu,\nu) = \max_{\mathbf{v} \in \mathbb{R}^J} \bar{H}_{\varepsilon}(\mathbf{v}) = \sum_{i=1}^J \bar{h}_{\varepsilon}(x_i,\mathbf{v}) \mu_i, \tag{5}$$

where

$$\bar{h}_{\varepsilon}(x, \mathbf{v}) = \sum_{j=1}^{J} \mathbf{v}_{j} \nu_{j} + \begin{cases} -\varepsilon \ln \left(\sum_{j=1}^{J} \exp \left(\frac{\mathbf{v}_{j} - c(x, y_{j})}{\varepsilon} \right) \nu_{j} \right) - \varepsilon & \text{if } \varepsilon > 0, \\ \min_{j} \left(c(x, y_{j}) - \mathbf{v}_{j} \right) & \text{if } \varepsilon = 0. \end{cases}$$
(6)

Preliminaries (2/4)

The semi-dual formulation in the discrete case [3]:

$$W_{\varepsilon}(\mu,\nu) = \max_{\mathbf{v} \in \mathbb{R}^J} \bar{H}_{\varepsilon}(\mathbf{v}) = \sum_{i=1}^J \bar{h}_{\varepsilon}(x_i,\mathbf{v})\mu_i, \tag{5}$$

where

$$\bar{h}_{\varepsilon}(x, \mathbf{v}) = \sum_{j=1}^{J} \mathbf{v}_{j} \nu_{j} + \begin{cases} -\varepsilon \ln \left(\sum_{j=1}^{J} \exp \left(\frac{\mathbf{v}_{j} - c(x, y_{j})}{\varepsilon} \right) \nu_{j} \right) - \varepsilon & \text{if } \varepsilon > 0, \\ \min_{j} \left(c(x, y_{j}) - \mathbf{v}_{j} \right) & \text{if } \varepsilon = 0. \end{cases}$$
(6)

In the case of semi-discrete, the semi-dual problem is in a form of maximization of expectation as follows [3].

$$W_{\varepsilon}(\mu,\nu) = \max_{\mathbf{v} \in \mathbb{R}^J} \mathbb{E}_X \left[\bar{h}_{\varepsilon}(X, \mathbf{v}) \right] \tag{7}$$

where $X \sim \mu$.

Preliminaries (3/4)

Introduction

0000000

The gradient of function \bar{h}_{ε} :

$$\nabla_{\mathbf{v}}\bar{h}_{\varepsilon}(\mathbf{x},\mathbf{v}) = \mathbf{v} - \chi_{(c(\mathbf{x},\mathbf{y}_{\ell})-\mathbf{v}_{\ell})_{\ell}}^{\varepsilon}, \quad \text{where} \quad \forall \varepsilon > 0, (\chi_{r}^{\varepsilon})_{j} \stackrel{\text{def.}}{=} e^{-\frac{r_{j}}{\varepsilon}} \mathbf{v}_{j} \left(\sum_{\ell} e^{-\frac{r_{\ell}}{\varepsilon}} \mathbf{v}_{\ell} \right)^{-1}.$$
(8)

We mainly use two algorithms which utilize the gradient information. Consider the discrete OT setting where $\mu = \sum_{i=1}^{J} \mu_i \delta_{x_i}$ and $\nu = \sum_{i=1}^{J} \nu_i \delta_{v_i}$:

Algorithm 1 Stochastic Average Gradient (SAG) for Discrete OT between μ and ν

```
Input: \alpha
Output: v
     \mathbf{v} \leftarrow \mathbb{O}_{I}, \mathbf{d} \leftarrow \mathbb{O}_{I}, \forall i, \mathbf{g}_{i} \leftarrow \mathbb{O}_{I}
      for k = 1, 2, ... do
                Sample i \in \{1, 2, ..., I\} uniform.
               \mathbf{d} \leftarrow \mathbf{d} - \mathbf{g}_i
               \mathbf{g}_i \leftarrow \mu_i \nabla_{\mathbf{v}} h_{\varepsilon}(\mathbf{x}_i, \mathbf{v})
               \mathbf{d} \leftarrow \mathbf{d} + \mathbf{g}_i
                \mathbf{v} \leftarrow \mathbf{v} + \alpha \mathbf{d}
      end for
```

Preliminaries (4/4)

Introduction

0000000

Consider the discrete OT setting where μ is a continuous measure and $\nu = \sum_{i=1}^{J} \nu_i \delta_{\nu_i}$:

Algorithm 2 Averaged SGD for Semi-Discrete OT

```
Input: \alpha
Output: v
      \tilde{\mathbf{v}} \leftarrow \mathbb{O}_{I}, \, \mathbf{v} \leftarrow \tilde{\mathbf{v}}
       for k = 1, 2, ... do
                  Sample x_k from \mu
                 \tilde{\mathbf{v}} \leftarrow \tilde{\mathbf{v}} + \frac{\alpha}{\sqrt{k}} \nabla_{\mathbf{v}} \bar{h}_{\varepsilon}(\mathbf{x}_k, \tilde{\mathbf{v}})
                  \mathbf{v} \leftarrow \frac{1}{k} \mathbf{\tilde{v}} + \frac{k-1}{k} \mathbf{v}
       end for
```

Motivation

Introduction

000000

Why is it difficult to resolve an OT problem?

- Computational burden
- Large bias of the estimators

Motivation

Introduction

Why is it difficult to resolve an OT problem?

- Computational burden
- Large bias of the estimators

Our goal: Estimating the squared Wasserstein distance in semi-discrete setting.

Motivation

Introduction 000000

Why is it difficult to resolve an OT problem?

- Computational burden
- Large bias of the estimators

Our goal: Estimating the squared Wasserstein distance in semi-discrete setting.

Our ideas:

We use the empirical Sinkhorn Divergence as our estimator. Sinkhorn Divergence:

$$S_{arepsilon}(\mu,
u) \stackrel{\mathsf{def.}}{=} W_{arepsilon}(\mu,
u) - rac{1}{2} \left(W_{arepsilon}(\mu,\mu) + W_{arepsilon}(
u,
u)
ight)$$

② We use a ε_t which decreases with iteration t, for example $\varepsilon_t = \frac{\varepsilon_0}{\sqrt{t}}$.

- Introduction
- 2 Theoretical Analysis
 - Analysis on the upper bound of regret for the Sinkhorn Divergence
 - \bullet Analysis on the upper bound of regret for Regularized Wasserstein distance with fixed ε
- 3 Experiments
 - Calculation of the true value of the squared Wasserstein distance
 - Approximation in discrete case
 - Approximation in semi-discrete case
- 4 Conclusion

Analysis of the bounds for

- $\sum_{t=1}^{T} \left| \mathbb{E}\left[\hat{S}_{\varepsilon,n}^{(t)}\right] W_2^2 \right|$, where $\hat{S}_{\varepsilon,n}^{(t)}$ is an approximation of the empirical Sinkhorn Divergence using SAG algorithm at iteration t;
- $\sum_{t=1}^{T} \left| \mathbb{E} \left[\hat{W}_{\varepsilon}^{(t)} \right] W_{2}^{2} \right|$, where $\hat{W}_{\varepsilon}^{(t)}$ is an approximation of regularized Wasserstein distance using ASGD algorithm at iteration t.

- Theoretical Analysis
 - Analysis on the upper bound of regret for the Sinkhorn Divergence
 - Analysis on the upper bound of regret for Regularized Wasserstein distance with
- - Calculation of the true value of the squared Wasserstein distance
 - Approximation in discrete case
 - Approximation in semi-discrete case

Decomposition

Consider the decomposition:

$$\begin{split} \left| \mathbb{E} \left[\hat{S}_{\varepsilon,n}^{(t)} \right] - W_2^2 \right| &\leq \left| \mathbb{E} \left[\hat{S}_{\varepsilon,n}^{(t)} \right] - \hat{S}_{\varepsilon,n} \right| + \left| \hat{S}_{\varepsilon,n} - \mathbb{E} \left[\hat{S}_{\varepsilon,n} \right] \right| \\ &+ \mathbb{E} \left[\left| \hat{S}_{\varepsilon,n} - S_{\varepsilon} \right| \right] + \left| S_{\varepsilon} - W_2^2 \right| \end{split}$$

with the bound for each component:

$$\left| S_{\varepsilon}(\mu, \nu) - W_2^2(\mu, \nu) \right| \le O(\varepsilon^2),$$

$$\mathbb{E}\left[\left| S_{\varepsilon}(\hat{\mu}_n, \nu) - S_{\varepsilon}(\mu, \nu) \right| \right] \lesssim \left(1 + \varepsilon^{-d'/2} \right) n^{-1/2},$$

$$\left| \hat{S}_{\varepsilon, n} - \mathbb{E}\left[\hat{S}_{\varepsilon, n} \right] \right| \lesssim \sqrt{\ln(2/\delta)} \cdot \sqrt{1/n + J}$$

with probability $1 - \delta$, and finally

$$\left|\mathbb{E}\left[\hat{S}_{\varepsilon,n}^{(t)}\right] - \hat{S}_{\varepsilon,n}\right| \leq \frac{1}{t}\left(C_{11}n^{-1}\varepsilon^{-1} + C_{12}\varepsilon^{-1} + C_{21}n^{2}\varepsilon + C_{22}\varepsilon + C_{31}n + C_{32}\right)$$

where C_{11} , C_{12} , C_{21} , C_{22} , C_{31} , C_{32} and C_{4} are constants. (Details in Appendix 2)

Fixed ε - Result

We have

$$\sum_{t=1}^{T} \left| \mathbb{E} \left[\hat{S}_{\varepsilon,n}^{(t)} \right] - W_2^2 \right| \lesssim \left(\ln(T) + 1 \right) \left(C_{11} n^{-1} \varepsilon^{-1} + C_{12} \varepsilon^{-1} + C_{21} n^2 \varepsilon + C_{22} \varepsilon + C_{31} n + C_{32} \right) + T \left(\varepsilon^2 + n^{-1/2} + n^{-1/2} \varepsilon^{-d'/2} + C_4 \sqrt{n^{-1} + J} \right)$$

where C_{11} , C_{12} , C_{21} , C_{22} , C_{31} , C_{32} and C_{4} are constants. (Details in Appendix 2)

Fixed ε - Analysis (1/3)

Let $\varepsilon = A_{\varepsilon} T^a$ and $n = A_n T^b$, where $A_{\varepsilon}, A_n > 0$ and $a, b \in \mathbb{R}$. We rewrite the bound B_{T} as follows.

$$B_{T} = (\ln T + 1) \left(\frac{C_{11}}{A_{\varepsilon} A_{n}} T^{-(a+b)} + \frac{C_{12}}{A_{\varepsilon}} T^{-a} + C_{21} A_{\varepsilon} A_{n}^{2} T^{a+2b} + C_{22} A_{\varepsilon} T^{a} + C_{31} A_{n} T^{b} + C_{32} \right)$$

$$+ T \left(A_{\varepsilon}^{2} T^{2a} + A_{n}^{-\frac{1}{2}} A_{\varepsilon}^{-\frac{d'}{2}} T^{-\frac{d'}{2}a - \frac{1}{2}b} + A_{n}^{-\frac{1}{2}} T^{-\frac{1}{2}b} + C_{4} \sqrt{A_{n}^{-1} T^{-b} + J} \right)$$

Based on the expression of B_T , we set the following objective.

$$\mathop{\rm minimize}_{a,b \in \mathbb{R}} \ \max\{-a-b, -a, a+2b, a, b, 2a+1, -\frac{d'}{2}a - \frac{1}{2}b+1, -\frac{1}{2}b+1\}$$

Fixed ε - Analysis (2/3)

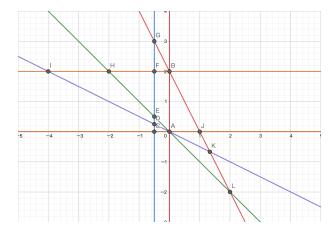


Figure 2: Illustration of the objective on \mathbb{R}^2

Fixed ε - Analysis (3/3)

а	Ь	-a - b	— <i>а</i>	a + 2b	2a + 1	$-\frac{1}{2}b - \frac{d'}{2}a + 1$	$-\frac{1}{2}b+1$	max
0	0	0	0	0	1	1	1	1
0	2	-2	0	4	1	0	0	4
$-\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{d'}{4}+1$	1	$\geq \frac{3}{2}$
$-\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{2}$	0	0	$\frac{d'}{4} + \frac{7}{8}$	78	$\geq \frac{3}{2}$ $\geq \frac{11}{8}$
$-\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{d'}{4} + \frac{3}{4}$	8 3 4	$\geq \frac{5}{4}$
$-\frac{1}{2}$	2	$-\frac{3}{2}$	$\frac{1}{2}$	$\frac{7}{2}$	0	$\frac{d'}{4}$	0	$\geq \frac{7}{2}$
$-\frac{1}{2}$ $-\frac{1}{2}$ -2	$\frac{d'}{2} + 2$	$-\frac{d'}{2}-\frac{3}{2}$	$\frac{1}{2}$	$d' + \frac{7}{2}$	0	0	$-\frac{d'}{4}$	$\geq \frac{7}{2}$ $\geq \frac{11}{2}$
-2	2	0	2	2	-3	d'	0	≥ 2
-4	2	2	4	0	-7	2d'	0	≥ 4
$\frac{2}{d'}$	0	$-\frac{2}{d'_2}$	$-\frac{2}{d'_4}$	$\frac{2}{d'}$	$\frac{4}{d'} + 1$	0	1	3
$\frac{\frac{4}{2d'-1}}{\frac{2}{d'-1}}$	$\frac{-2}{2d'-1}$	$\frac{-2}{2d'-1}$	$\frac{-4}{2d'-1}$	0	$\frac{8}{2d'-1}+1$	0	$\frac{1}{2d'-1}+1$	3 11 3 5
$\frac{2}{d'-1}$	$\frac{2d'-1}{\frac{-2}{d'-1}}$	0	$\frac{-2}{d'-1}$	$\frac{-2}{d'-1}$	$rac{8}{2d'-1} + 1 \ rac{4}{d'-1} + 1$	0	$\frac{\frac{1}{2d'-1}+1}{\frac{1}{d'-1}+1}$	5

Table 1: Analysis of order of T

References

Decreasing ε - Result

We have

$$\begin{split} \sum_{t=1}^{T} \left| \hat{S}_{\varepsilon_{t},n}^{(t)} - W_{2}^{2} \right| \lesssim & (\ln T + 1) (C_{31}n + C_{32} + \varepsilon_{0}^{2}) \\ &+ \left((T+1)^{\frac{d'}{4}+1} - 1 \right) n^{-\frac{1}{2}} \varepsilon_{0}^{-\frac{d'}{2}} \cdot \frac{4}{d'+4} \\ &+ T \left(n^{-\frac{1}{2}} + C_{4} \sqrt{n^{-1} + J} \right) \\ &+ \left(2T^{\frac{1}{2}} - 1 \right) (C_{11}n^{-1} + C_{12}) \varepsilon_{0}^{-1} \\ &+ \left(3 - 2T^{-\frac{1}{2}} \right) (C_{21}n^{2} + C_{22}) \varepsilon_{0} \end{split}$$

where C_{11} , C_{12} , C_{21} , C_{22} , C_{31} , C_{32} and C_{4} are constants. (Details in Appendix 2)

Decreasing ε - Analysis (1/2)

Let $n = AT^a$. We rewrite the bound B_T as follows.

$$\begin{split} B_T = & (\ln T + 1)(C_{31}AT^a + C_{32} + \varepsilon_0^2) \\ & + \left((T+1)^{\frac{d'}{4}+1} - 1 \right)A^{-\frac{1}{2}}T^{-\frac{a}{2}}\varepsilon_0^{-\frac{d'}{2}} \cdot \frac{4}{d'+4} \\ & + T\left(A^{-\frac{1}{2}}T^{-\frac{a}{2}} + C_4\sqrt{A^{-1}T^{-a} + J}\right) \\ & + \left(2T^{\frac{1}{2}} - 1\right)(C_{11}A^{-1}T^{-a} + C_{12})\varepsilon_0^{-1} \\ & + \left(3 - 2T^{-\frac{1}{2}}\right)(C_{21}A^2T^{2a} + C_{22})\varepsilon_0 \end{split}$$

Based on the expression of B_T , we set the following objective.

$$\underset{a \in \mathbb{R}}{\text{minimize}} \ \max \left\{ a, \frac{d'}{4} + 1 - \frac{a}{2}, \frac{1}{2} - a, 2a \right\}$$

Introduction

Decreasing ε - Analysis (2/2)

а	$\frac{d'}{4} + 1 - \frac{a}{2}$	$\frac{1}{2} - a$	2 <i>a</i>	max
0	$\frac{d'}{4} + 1$	$\frac{1}{2}$	0	$\geq \frac{3}{2}$
$\frac{1}{4}$	$\frac{\dot{d'}}{4} + \frac{7}{8}$	$\frac{\overline{1}}{4}$	$\frac{1}{2}$ $\underline{d'} \perp \underline{4}$	$\geq \frac{\overline{11}}{8}$
$\frac{\frac{1}{4}}{\frac{d'}{6} + \frac{2}{3}}$	$\frac{d'}{6} + \frac{2}{3}$	$-\frac{d'}{6}-\frac{1}{6}$	$\frac{d'}{3} + \frac{4}{3}$	≥ 2
$-\frac{d'}{2} - 1$	$\frac{d'}{2} + \frac{3}{2}$	$\frac{d'}{2} + \frac{3}{2}$	-d' - 2	$\geq \frac{5}{2}$
$-\frac{d'}{2} - 1$ $\frac{d'}{10} + \frac{2}{5}$	$\frac{d'}{2} + \frac{3}{2}$ $\frac{d'}{5} + \frac{4}{5}$	$-\frac{d'}{10} + \frac{1}{10}$	$\frac{d'}{5} + \frac{4}{5}$	$\begin{array}{c} 3 \\ > 11 \\ > 2 \\ > 5 \\ > 5 \\ > 5 \\ > 5 \end{array}$
$\frac{1}{6}$	$\frac{d}{4} + \frac{11}{12}$	$\frac{1}{3}$	$\frac{1}{3}$	$\geq \frac{17}{12}$

Table 2: Analysis of order of T

Analysis on the upper bound of regret for Regularized Wasserstein distance with fixed arepsilon

- 1 Introduction
- 2 Theoretical Analysis
 - Analysis on the upper bound of regret for the Sinkhorn Divergence
 - \bullet Analysis on the upper bound of regret for Regularized Wasserstein distance with fixed ε
- 3 Experiments
 - Calculation of the true value of the squared Wasserstein distance
 - Approximation in discrete case
 - Approximation in semi-discrete case
- 4 Conclusion

Analysis on the upper bound of regret for Regularized Wasserstein distance with fixed arepsilon

Decomposition

Consider the decomposition:

$$\left| \mathbb{E} \left[\hat{W}_{\varepsilon}^{(t)} \right] - W_2^2 \right| \leq \left| \mathbb{E} \left[\hat{W}_{\varepsilon}^{(t)} \right] - W_{\varepsilon} \right| + \left| W_{\varepsilon} - W_2^2 \right|$$

where

$$\left|W_{\varepsilon}(\mu,\nu)-W_{2}^{2}(\mu,\nu)\right|\leq O\left(\varepsilon\ln\left(\frac{1}{\varepsilon}\right)\right),$$

$$\left| \mathbb{E} \left[W_{\varepsilon}^{(t)} - W_{\varepsilon} \right] \right| \leq 2 \left(\frac{D^2}{\alpha} + 4\alpha \right) \frac{2 + \ln t}{\sqrt{t}}.$$

Analysis on the upper bound of regret for Regularized Wasserstein distance with fixed arepsilon

Result and analysis

We have

$$\sum_{t=1}^{T} \left| \mathbb{E} \left[\hat{W}_{\varepsilon}^{(t)} \right] - W_2^2 \right| \lesssim T \varepsilon \ln \left(\frac{1}{\varepsilon} \right) + C_5 (2 + \ln T) \cdot T^{\frac{1}{2}}$$

where

$$C_5 = 4\left(\frac{D^2}{\alpha} + 4\alpha\right).$$

As long as we set the hyperparameter $\varepsilon = O(T^a)$ where $a < -\frac{1}{2}$ in advance, we can get a bound of order $O(T^{\frac{1}{2}} \ln T)$.

- - Analysis on the upper bound of regret for the Sinkhorn Divergence
 - Analysis on the upper bound of regret for Regularized Wasserstein distance with
- **Experiments**
 - Calculation of the true value of the squared Wasserstein distance
 - Approximation in discrete case
 - Approximation in semi-discrete case

Contents

- Calculation of the true values of $W_2^2(\mu,\nu)$ which are used for comparison with experimental results.
- Approximation of $W_2^2(\mu, \nu)$ in discrete setting,
 - with fixed ε :
 - with decreasing ε_t .
- Approximation of $W_2^2(\mu, \nu)$ in semi-discrete setting,
 - with fixed ε :
 - with decreasing ε_t .

Calculation of the true value of the squared Wasserstein distance

- - Analysis on the upper bound of regret for the Sinkhorn Divergence
 - Analysis on the upper bound of regret for Regularized Wasserstein distance with
- **Experiments**
 - Calculation of the true value of the squared Wasserstein distance
 - Approximation in discrete case
 - Approximation in semi-discrete case

Calculation of the true value of the squared Wasserstein distance

Methods

In decrease setting:

- Solve the problem directly by using linear programming solver.
- ② Calculate the total transport cost.

In semi-discrete setting:

- **1** Solve the regularized problem by using ASGD algorithm with $\varepsilon = 0$.
- 2 Discretize μ with sample size N.
- Ocalculate the total transport cost.

Calculation of the true value of the squared Wasserstein distance

Verification of the method in semi-discrete setting

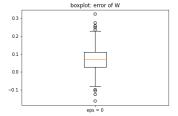


Figure 3: Boxplot of error of W

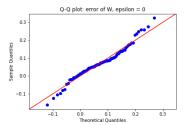


Figure 4: Q-Q plot of error of W

Approximation in discrete case

- - Analysis on the upper bound of regret for the Sinkhorn Divergence
 - Analysis on the upper bound of regret for Regularized Wasserstein distance with
- **Experiments**
 - Calculation of the true value of the squared Wasserstein distance
 - Approximation in discrete case
 - Approximation in semi-discrete case

Approximation in discrete case

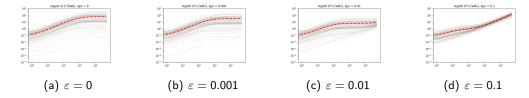


Figure 5: Regret of \hat{S}_{ε} (SAG), discrete case

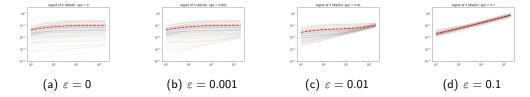


Figure 6: "Regret" of \hat{S}_{ε} (ASGD), discrete case

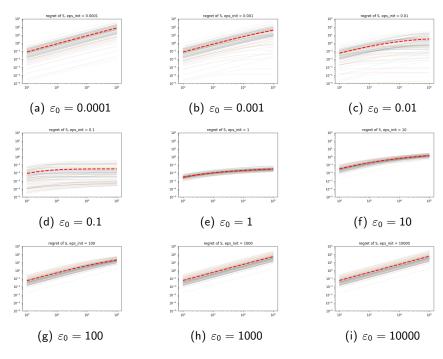


Figure 7: "Regret" of \hat{S}_{ε_t} , discrete case

- - Analysis on the upper bound of regret for the Sinkhorn Divergence
 - Analysis on the upper bound of regret for Regularized Wasserstein distance with
- **Experiments**
 - Calculation of the true value of the squared Wasserstein distance
 - Approximation in discrete case
 - Approximation in semi-discrete case

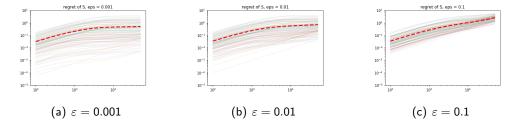


Figure 8: "Regret" of \hat{S}_{ε} , semi-discrete case

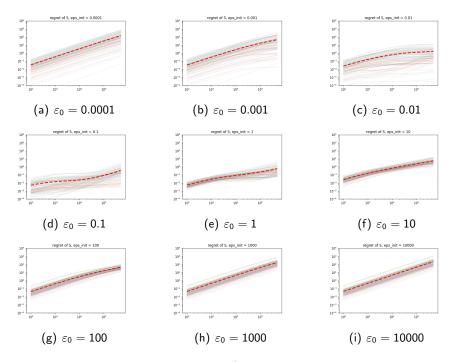


Figure 9: "Regret" of \hat{S}_{ε_t} , semi-discrete case

- - Analysis on the upper bound of regret for the Sinkhorn Divergence
 - Analysis on the upper bound of regret for Regularized Wasserstein distance with
- - Calculation of the true value of the squared Wasserstein distance
 - Approximation in discrete case
 - Approximation in semi-discrete case
- Conclusion

Conclusion

- Theoretical analysis on the upper bound of regret:
 - The upper bound of regret of the empirical Sinkhorn divergence by using SAG could not avoid a large order with respect to *T*.
 - The upper bound of regret of the regularized Wasserstein distance by using ASGD has a smaller order of T.
- Numerical experiments:
 - Error in estimating W_2^2 directly using ASGD is not negligible.
 - Results for SAG is heavily influenced by the choice of ε or ε_0 .

Thank you

Introduction

Thank you for listening!

Bibliography

- [1] Lenaic Chizat, Pierre Roussillon, Flavien Léger, François-Xavier Vialard, and Gabriel Peyré. Faster Wasserstein Distance Estimation with the Sinkhorn Divergence. arXiv:2006.08172 [math, stat], October 2020.
- [2] Marco Cuturi. Sinkhorn Distances: Lightspeed Computation of Optimal Transport. In Advances in Neural Information Processing Systems, volume 26. Curran Associates, Inc., 2013.
- [3] Aude Genevay, Marco Cuturi, Gabriel Peyré, and Francis Bach. Stochastic Optimization for Large-scale Optimal Transport. arXiv:1605.08527 [cs, math], May 2016.
- [4] Leonid Kantorovich. On the transfer of masses. *Doklady Akademii Nauk USSR*, 1942.



- Sample of the second of the
 - Semi-dual formulation of regularized OT in continuous setting
 - List of constants in the regret analysis for the Sinkhorn Divergence



- 6 Appendix
 - Semi-dual formulation of regularized OT in continuous setting
 - List of constants in the regret analysis for the Sinkhorn Divergence

Semi-dual formulation of regularized OT in continuous setting

The semi-dual formulation of regularized OT problem [3]:

$$W_{\varepsilon}(\mu,\nu) = \max_{\mathbf{v} \in \mathcal{C}(\mathcal{Y})} H_{\varepsilon}(\mathbf{v}) \stackrel{\text{def.}}{=} \int_{\mathcal{X}} \mathbf{v}^{\mathbf{c},\varepsilon}(\mathbf{x}) \mathrm{d}\mu(\mathbf{x}) + \int_{\mathcal{Y}} \mathbf{v}(\mathbf{y}) \mathrm{d}\nu(\mathbf{y}) - \varepsilon$$

where $v^{c,\varepsilon}(x)$ is the c-transform and the approximation for any $v \in \mathcal{C}(\mathcal{Y})$:

$$\forall x \in \mathcal{X}, \quad v^{c,\varepsilon}(x) \stackrel{\text{def.}}{=} \begin{cases} \min_{y \in \mathcal{Y}} c(x,y) - v(y) & \text{if } \varepsilon = 0 \\ -\varepsilon \ln \left(\int_{\mathcal{Y}} \exp \left(\frac{v(y) - c(x,y)}{\varepsilon} \right) d\nu(y) \right) & \text{if } \varepsilon > 0 \end{cases}$$



Appendix

- Semi-dual formulation of regularized OT in continuous setting
- List of constants in the regret analysis for the Sinkhorn Divergence

List of constants in the regret analysis for the Sinkhorn Divergence

$$\begin{split} &C_{11} = 128 \|\mathbf{v}_{1}^{0} - \mathbf{v}_{1}^{*}\|^{2} + 64 \|\mathbf{v}_{2}^{0} - \mathbf{v}_{2}^{*}\|^{2}, \\ &C_{12} = 64 \|\mathbf{v}_{3}^{0} - \mathbf{v}_{3}^{*}\|^{2}, \\ &C_{21} = 2\sigma_{1}^{2} + \sigma_{2}^{2}, \\ &C_{22} = J\sigma_{3}^{2}, \\ &C_{31} = 32 \left(\bar{H}_{\varepsilon}^{1}(\mathbf{v}_{1}^{*}) - \bar{H}_{\varepsilon}^{1}(\mathbf{v}_{1}^{0}) \right) + 16 \left(\bar{H}_{\varepsilon}^{2}(\mathbf{v}_{2}^{*}) - \bar{H}_{\varepsilon}^{2}(\mathbf{v}_{2}^{0}) \right), \\ &C_{32} = 16J \left(\bar{H}_{\varepsilon}^{3}(\mathbf{v}_{3}^{*}) - \bar{H}_{\varepsilon}^{3}(\mathbf{v}_{3}^{*}) \right), \\ &C_{4} = \sqrt{\ln(2/\delta)}. \end{split}$$

$$\begin{split} W_{\varepsilon}(\hat{\mu}_{n},\nu_{J}) &= \max_{\mathbf{v}_{1} \in \mathbb{R}^{J}} \bar{H}_{\varepsilon}^{1}(\mathbf{v}_{1}) = \frac{1}{n} \sum_{i=1}^{n} \bar{h}_{\varepsilon}^{1}(x_{i},\mathbf{v}_{1}), \\ \bar{h}_{\varepsilon}^{1}(x,\mathbf{v}) &= \sum_{j=1}^{J} \mathbf{v}_{j} \nu_{j} - \varepsilon \ln \left(\sum_{j=1}^{J} \exp \left(\frac{\mathbf{v}_{j} - c\left(x,y_{j}\right)}{\varepsilon} \right) \nu_{j} \right) - \varepsilon, \\ W_{\varepsilon}(\hat{\mu}_{n},\hat{\mu}_{n}) &= \max_{\mathbf{v}_{2} \in \mathbb{R}^{n}} \bar{H}_{\varepsilon}^{2}(\mathbf{v}_{2}) = \frac{1}{n} \sum_{i=1}^{n} \bar{h}_{\varepsilon}^{2}(x_{i},\mathbf{v}_{2}), \\ \bar{h}_{\varepsilon}^{2}(x,\mathbf{v}) &= \frac{1}{n} \sum_{i=1}^{n} \mathbf{v}_{i} - \varepsilon \ln \left(\frac{1}{n} \sum_{i=1}^{n} \exp \left(\frac{\mathbf{v}_{i} - c\left(x,x_{i}\right)}{\varepsilon} \right) \right) - \varepsilon, \\ W_{\varepsilon}(\nu_{J},\nu_{J}) &= \max_{\mathbf{v}_{3} \in \mathbb{R}^{J}} \bar{H}_{\varepsilon}^{3}(\mathbf{v}_{3}) = \sum_{j=1}^{J} \bar{h}_{\varepsilon}^{3}(y_{j},\mathbf{v}_{3}) \nu_{j}, \\ \bar{h}_{\varepsilon}^{3}(y,\mathbf{v}) &= \sum_{j=1}^{J} \mathbf{v}_{j} \nu_{j} - \varepsilon \ln \left(\sum_{j=1}^{J} \exp \left(\frac{\mathbf{v}_{j} - c\left(y,y_{j}\right)}{\varepsilon} \right) \nu_{j} \right) - \varepsilon. \end{split}$$

$$\begin{split} & \left| \mathbb{E} \left[\hat{S}_{\varepsilon,n}^{(t)} \right] - \hat{S}_{\varepsilon,n} \right| \\ & \leq \left| \mathbb{E} \left[\bar{H}_{\varepsilon}^{1}(\mathbf{v}_{1}^{(t)}) \right] - \bar{H}_{\varepsilon}^{1}(\mathbf{v}_{1}^{*}) \right| + \frac{1}{2} \left| \mathbb{E} \left[\bar{H}_{\varepsilon}^{2}(\mathbf{v}_{2}^{(t)}) \right] - \bar{H}_{\varepsilon}^{2}(\mathbf{v}_{2}^{*}) \right| + \frac{1}{2} \left| \mathbb{E} \left[\bar{H}_{\varepsilon}^{3}(\mathbf{v}_{3}^{(t)}) \right] - \bar{H}_{\varepsilon}^{3}(\mathbf{v}_{3}^{*}) \right| \end{split}$$

where

$$\begin{split} \left| \mathbf{E} \left[\bar{H}_{\varepsilon}^{1}(\mathbf{v}_{1}^{(t)}) \right] - \bar{H}_{\varepsilon}^{1}(\mathbf{v}_{1}^{*}) \right| &\leq \frac{32n}{t} \left(\bar{H}_{\varepsilon}^{1}(\mathbf{v}_{1}^{*}) - \bar{H}_{\varepsilon}^{1}(\mathbf{v}_{1}^{0}) + \frac{4}{n^{2}\varepsilon} \|\mathbf{v}_{1}^{0} - \mathbf{v}_{1}^{*}\|^{2} + \frac{\sigma_{1}^{2}n\varepsilon}{16} \right) \\ &\frac{1}{2} \left| \mathbf{E} \left[\bar{H}_{\varepsilon}^{2}(\mathbf{v}_{2}^{(t)}) \right] - \bar{H}_{\varepsilon}^{2}(\mathbf{v}_{2}^{*}) \right| &\leq \frac{16n}{t} \left(\bar{H}_{\varepsilon}^{2}(\mathbf{v}_{2}^{*}) - \bar{H}_{\varepsilon}^{2}(\mathbf{v}_{2}^{0}) + \frac{4}{n^{2}\varepsilon} \|\mathbf{v}_{2}^{0} - \mathbf{v}_{2}^{*}\|^{2} + \frac{\sigma_{2}^{2}n\varepsilon}{16} \right) \\ &\frac{1}{2} \left| \mathbf{E} \left[\bar{H}_{\varepsilon}^{3}(\mathbf{v}_{3}^{(t)}) \right] - \bar{H}_{\varepsilon}^{3}(\mathbf{v}_{3}^{*}) \right| &\leq \frac{16J}{t} \left(\bar{H}_{\varepsilon}^{3}(\mathbf{v}_{3}^{*}) - \bar{H}_{\varepsilon}^{3}(\mathbf{v}_{3}^{0}) + \frac{4}{J\varepsilon} \|\mathbf{v}_{3}^{0} - \mathbf{v}_{3}^{*}\|^{2} + \frac{\sigma_{3}^{2}\varepsilon}{16} \right) \end{split}$$