Primal-Dual Randomized Coordinate Descent for Entropy regularized Optimal Transport using Sparse Structure

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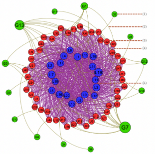
Abstract of my research topic

- Computational Difficulties
  - The optimal transport problem is computationally expensive.
  - Several algorithms have been proposed to solve the entropy regularized optimal transport.
    - Sinkhorn Algorithm
    - Adaptive Primal-Dual Accelerate Gradient Descent
    - etc.
- Issues
  - Among them, we focus on Accelerated Primal-Dual Randomized Coordinate Descent (APDRCD).
  - APDRCD and other primal-dual algorithms have large dimensionality of the primal (or dual) variables.
  - Updating all variables takes a lot of time per iteration.
- Proposal
  - By taking advantage of the sparsity of matrix A in the constraint condition, the update of the primal variables can be reduced to only nonzero elements of the sampled rows of A.
  - We tried to improve by block sampling using the sparse structure of A.

Optimal Transport

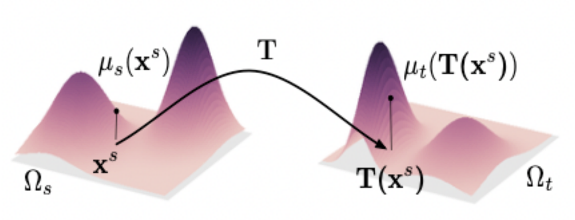
- Optimal transport (OT) is a tool for comparing distances between probability distributions
- It is becoming increasingly popular in machine learning.
  - Clustering
  - Supervised Learning
  - Domain Adaptation
  - Generative Adversarial Network



What is Optimal Transport?

- OT is the problem of finding the minimum energy to transport from a source to a target.
- The total energy for transportation

$$\sum_{i=1,j=1}^{n,m} C_{i,j} X_{i,j}$$



Formulation of the optimal transport problem

- OT formulation

$$\min_{X \in \mathbb{R}_{+}^{n \times m}} \quad \langle C, X \rangle \quad s.t.\ X\mathbf{1}_m = r,\ X^T\mathbf{1}_n = l$$

- $r \in \mathbb{R}^n$, $l \in \mathbb{R}^m$: input vector
- $C \in \mathbb{R}^{n \times m}$: cost matrix
- $X \in \mathbb{R}^{n \times m}$: transport matrix

- OT is a linear programming problem.
- It can be solved by the interior point method, with a best known practical complexity of $\tilde{O}(n^3)$.
- It cannot be used effectively in machine learning where the number of dimensions n becomes large.

Entropy regularized Optimal Transport [Cuturi, 2013]

$$\min_{X \in \mathcal{U}(r,l)} \quad \langle C, X \rangle - \eta H(X)$$

where

$$\mathcal{U}(r,l) \coloneqq \{X \in \mathbb{R}^{n \times m} : X\mathbf{1}_m = r, X^T\mathbf{1}_n = l\}$$

- [Cuturi, 2013] showed that the OT can be easily solved by adding an entropy regularization term.
- Sinkhorn Algorithm

$$u_{k+1} = \frac{r}{Kv_k}, \quad v_{k+1} = \frac{l}{K^T u_{k+1}}$$

- Computational Complexity $O(\frac{n^2}{\epsilon^2})$

Reformulate the entropy regularized optimal transport

$$\min_{x} \quad c^T x - \eta H(x) \quad s.t.\ Ax = b$$

where $(n = 3, m = 3)$

$$A = \begin{pmatrix} 1 & 1 & 1 & & & & & & \\ & & & 1 & 1 & 1 & & & \\ & & & & & & 1 & 1 & 1 \\ 1 & & & 1 & & & 1 & & \\ & 1 & & & 1 & & & 1 & \\ & & 1 & & & 1 & & & 1 \end{pmatrix}, \quad b = \begin{pmatrix} r \\ l \end{pmatrix} = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ l_1 \\ l_2 \\ l_3 \end{pmatrix}$$

- For simplicity, let n=m.
- $A \in \mathbb{R}^{2n \times n^2}$, $b \in \mathbb{R}^{2n}$, $c \in \mathbb{R}^{n^2}$, $x \in \mathbb{R}^{n^2}$
- $H(x) = -\sum_i x_i(\log x_i - 1)$
- $c = (C_{1,1}, C_{1,2}, \cdots, C_{n,n})^T$, $x = (X_{1,1}, X_{1,2}, \cdots, X_{n,n})^T$

General Problem and Primal-Dual Formulation

- We consider the optimization problem:

$$\min_{x \in \mathcal{X}} \quad f(x) \quad s.t. \ Ax = b$$

  - $f(x)$: smooth
  - A : linear operator.
- Lagrange dual problem:

$$\min_{y \in \mathcal{Y}} \left\{ \phi(y) := \langle y, b \rangle + \max_{x \in \mathcal{X}} \quad \left\{ -f(x) - \langle A^T y, x \rangle \right\} \right\}$$

- $\nabla \phi(y)$ is Lipschitz-continuous:

$$||\nabla \phi(y_1) - \nabla \phi(y_1)||_2 \leq L||y_1 - y_2||_2$$

Primal-Dual Method for Optimal Transport

- In the case of OT, Lagrange dual problem is as follows:

$$
\begin{aligned}
&\min_{x \in \mathcal{X}} \quad c^T x - \eta H(x) \quad s.t.\ Ax = b \\
\iff &\min_{y \in \mathcal{Y}} \phi(y) := \langle y, b \rangle + \max_{x \in \mathcal{X}} \quad \Big\{ -c^T x + \eta H(x) - \langle A^T y, x \rangle \Big\}
\end{aligned}
$$

- The updates for the primal and dual variables are as follows:

$$
\begin{aligned}
x^{k+1} &= \arg\max_x \Big\{ -c^T x + \eta H(x) - \langle A^T y^k, x \rangle \Big\} \\
&= \exp\left(-\frac{c + A^T y_k}{\eta} \right) \\
y^{k+1} &= y^k - \frac{1}{L} \nabla \phi(y^k) \\
&= y_k - \frac{1}{L} (A x^{k+1} - b)
\end{aligned}
$$

Primal-Dual Randomized Coordinate Descent Method

- Primal-Dual Randomized Coordinate Descent is a stochastic extension of the primal-dual method:

1. Update primal variables for all $i \in \{1, 2, \ldots, n^2\}$

$$x_i^{k+1} = \exp\left(-\frac{c_i + (A^T y^k)_i}{\eta}\right)$$

2. Randomly sample one coordinate $j_k \in \{1, 2, \ldots, 2n\}$
3. Update dual variables

$$y_{j_k}^{k+1} = y_{j_k}^k - \frac{1}{L}\nabla_{j_k}\phi(y^k)$$

- [Guo et al., 2020] proposed an accelerated algorithm based on this primal-dual randomized coordinate descent method.
  - Accelerated Primal-Dual Randomized Coordinate Descent (APDRCD)

Proposed Method 1

- Issues with APDRCD
  - Update all of the primal variables (all coordinates)
  - Updating all variables takes a lot of time per iteration.
- Our Methods
  - Update only variables x_i with related to y_{j_k} that was updated.
  - No need to update for x_i with related to y_{j_k} that was not updated.

$$x_i^{k+1} = \exp\left(\frac{-c_i - (A^T y^{k+1})_i}{\eta}\right)$$

Proposed Algorithm: Sparsity-Aware APDRCD

1. Randomly sample one coordinate $j_k \in \{1, 2, \ldots, 2n\}$
2. Update dual variables

$$y_{j_k}^{k+1} = y_{j_k}^{k} - \frac{1}{L} \nabla_{j_k} \phi(y^k)$$

3. Find x_i^{k+1} to update using $y_{j_k}^{k+1}$

$$I(j_k) = \left\{ i \in \{1, 2, \ldots, n\} : \ A_{j_k, i} \neq 0 \right\}$$

4. Update primal variables for all $i \in I(j_k)$

$$x_i^{k+1} = \exp\left(\frac{-c_i - (A^T y^{k+1})_i}{\eta} \right)$$

Proposed Method 2

- A has a special sparse structure.

$$A = \begin{pmatrix} 1 & 1 & 1 & & & & & & \\ & & & 1 & 1 & 1 & & & \\ & & & & & & 1 & 1 & 1 \\ 1 & & & 1 & & & 1 & & \\ & 1 & & & 1 & & & 1 & \\ & & 1 & & & 1 & & & 1 \end{pmatrix}$$

- Block sampling might can further simplify variable updates.
- Experiment with various sampling methods that are aware of the sparse structure of A.

greedy

$$A = \begin{pmatrix} 1 & 1 & 1 & & & & & & \\ & & & 1 & 1 & 1 & & & \\ & & & & & & 1 & 1 & 1 \\ 1 & & & 1 & & & 1 & & \\ & 1 & & & 1 & & & 1 & \\ & & 1 & & & 1 & & & 1 \end{pmatrix}$$

cyclic

$$A = \begin{pmatrix} 1 & 1 & 1 & & & & & & \\ & & & 1 & 1 & 1 & & & \\ & & & & & & 1 & 1 & 1 \\ 1 & & & 1 & & & 1 & & \\ & 1 & & & 1 & & & 1 & \\ & & 1 & & & 1 & & & 1 \end{pmatrix}$$

original

$$A = \begin{pmatrix} 1 & 1 & 1 & & & & & & \\ & & & 1 & 1 & 1 & & & \\ & & & & & & 1 & 1 & 1 \\ 1 & & & 1 & & & 1 & & \\ & 1 & & & 1 & & & 1 & \\ & & 1 & & & 1 & & & 1 \end{pmatrix}$$

vertical

$$A = \begin{pmatrix} 1 & 1 & 1 & & & & & & \\ & & & 1 & 1 & 1 & & & \\ & & & & & & 1 & 1 & 1 \\ 1 & & & 1 & & & 1 & & \\ & 1 & & & 1 & & & 1 & \\ & & 1 & & & 1 & & & 1 \end{pmatrix}$$

nblock

$$A = \begin{pmatrix} 1 & 1 & 1 & & & & & & \\ & & & 1 & 1 & 1 & & & \\ & & & & & & 1 & 1 & 1 \\ 1 & & & 1 & & & 1 & & \\ & 1 & & & 1 & & & 1 & \\ & & 1 & & & 1 & & & 1 \end{pmatrix}$$

20block

$$A = \begin{pmatrix} 1 & 1 & 1 & & & & & & \\ & & & 1 & 1 & 1 & & & \\ & & & & & & 1 & 1 & 1 \\ 1 & & & 1 & & & 1 & & \\ & 1 & & & 1 & & & 1 & \\ & & 1 & & & 1 & & & 1 \end{pmatrix}$$

20batch

$$A = \begin{pmatrix} 1 & 1 & 1 & & & & & & \\ & & & 1 & 1 & 1 & & & \\ & & & & & & 1 & 1 & 1 \\ 1 & & & 1 & & & 1 & & \\ & 1 & & & 1 & & & 1 & \\ & & 1 & & & 1 & & & 1 \end{pmatrix}$$

vblock

$$A = \begin{pmatrix} 1 & 1 & 1 & & & & & & \\ & & & 1 & 1 & 1 & & & \\ & & & & & & 1 & 1 & 1 \\ 1 & & & 1 & & & 1 & & \\ & 1 & & & 1 & & & 1 & \\ & & 1 & & & 1 & & & 1 \end{pmatrix}$$

Experiments

- Comparison
  - Execution time between the original APDRCD and the Sparsity-Aware APDRCD.
  - Compared original APDRCD with various block sampling methods.
- Dataset
  - Two probability distributions generated by uniform random numbers are used as input.

Experiments: APDRCD vs Sparsity-Aware APDRCD

- Original APDRCD converges a little faster than Sparsity-Aware.
- Sparsity-Aware APDRCD takes less time for each iteration than original one.

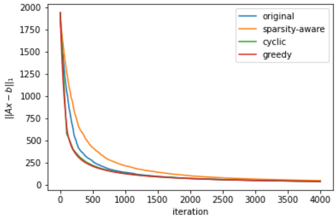


Figure 1: Distance to the transportation polytope per iteration

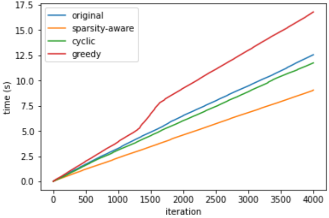


Figure 2: Execution time per iteration

Experiments: APDRCD vs APDRCD with block sampling

- In the error, "nblock" has the fastest descent along with "greedy".
- (Block sampling algorithms are not comparable in execution time to the other algorithms.)

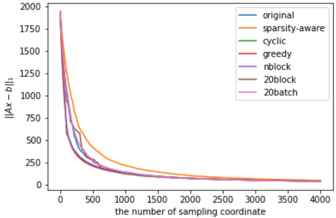


Figure 3: Distance to the transportation polytope/the number of sampled coordinates

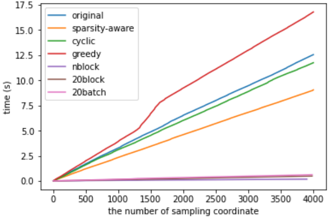


Figure 4: Execution time/the number of sampled coordinates

Comparison between block sampling algorithms

- In the error, "nblock" has a faster descent, but they are all about the same.
- "20batch" takes longer time than "20block".

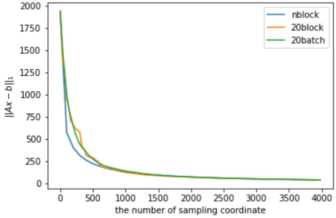


Figure 5: Distance to the transportation polytope/the number of sampled coordinates

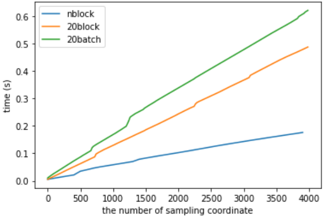


Figure 6: Execution time/the number of sampled coordinates because

Discussion

- Proposal 1
  - "sparsity-aware": shortest execution time
    - reduce the number of variables to be updated per iteration
  - "greedy": longest execution time
    - It took a long time to find the largest gradient of dual objective function.
- Proposal 2
  - "20batch" takes longer time than "20block".
    - It took a lot of time for sampling minibatches.

Future Work

- Experiment on real-world data and data with high dimensionality
- Convergence analysis of APDRCD algorithms with block sampling
- Compare proposed algorithm with other stochastic algorithms
- Find a suitable OT application for this algorithm

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