SCIE2500 Final Report

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Abstract

Optimal Transport is a well-known problem of Optimization and applied math. The report mainly introduces the definition of Optimal Transport under discrete case and the most common modern computational algorithm applied on Optimal Transport, called the Sinkhorn algorithm. Entropic regularization is introduced to solve the original optimal problem, which represents the solution a simple format by the restriction condition and Lagrange Mutiplier. Sinkhorn's algorithm can be applied under this format. Finally the convergence of Sinkhorn's algorithm will be claim by some basis algebraic inequality related the Hilbert Metric, which is a metric project the matrix to a line. The convergence is linear but the convergence ratio is too slow in pratice. The connection how the original optimal can be solve by adding one more term "entropic" in the evaluating function. Most of the proof make use of very basic algebraic knowledge in the discrete case. All the discrete cases can be modified to continuous case with respect to some measures, as well as the discrete case is just the discrete measure case.

1 Background and Motivation

Optimal transportation was born in France in 1781, with a very famous paper by Gaspard Monge. It has become a classicla subject in probability theory, economics and optimization since then. Recently it gained extremely popularity because many researchers from different mathematical areas found it has a strong link with their topic. For exmaple in the Riemannian manifolds [Gro85], geometry, partial differential equations, probability theory, functional analysis and fluid mechanics [Bre87].

As the development of computer science and algorithm, researchers in imaging, computer or more general data science found that optimal transport provide a strong tool to describe distribution in abstract context. Optimal transport not only has a closed relation to many traditional mathematical area but also some modern data science application, which is my strongest motivation for me to make a insight.

2 Definition of Optimal Transport under Discrete Case

Optimal transport is actually an assignment problem. Suppose there are total mass 1 distrebuted in m location, writtern as $\mathbf{a} \in \mathbb{R}^m, \sum_{k=1}^m a_k = 1, a_k \geq 0$. We want to transport it to the new n location, written as $b \in \mathbb{R}^n, \sum_{k=1}^n b_k = 1, b_k \geq 0$, with given Cost Matrix $\mathbf{C} \in \mathbb{R}_+^{n\times m}$, where C_{ij} represents the cost of 1 mass transports from i^{th} location (of $\mathbf{a}$) to j^{th} location (of $\mathbf{b}$).

The set of coupling matrices of given $\mathbf{a}, \mathbf{b}$ is naturally defined as:

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

where the $\mathbb{1}_m, \mathbb{1}_n$ vector notaiton is the vectoc with all entries 1 in $\mathbb{R}^m, \mathbb{R}^n$.

Noticed $\mathbf{U}(\mathbf{a}, \mathbf{b})$ is always bounded and constrained by $n+m$ equalities, which means it's a convex polytope. [Bru06].

Then optimal transport problem is:

$$m_{\mathbf{C}}(\mathbf{a}, \mathbf{b}) \overset{\text{def.}}{=} \min_{\mathbf{P}\in\mathbf{U}(\mathbf{a},\mathbf{b})} \langle \mathbf{C}, \mathbf{P} \rangle \overset{\text{def.}}{=} \sum_{i,j} C_{i,j} P_{i,j}$$

3 Entropic Regularization

For a coupling matrix $\mathbf{P}$, the discrete entropy is definied as:

$$\mathbf{H}(\mathbf{P}) \stackrel{\text{def.}}{=} \sum_{i,j} \mathbf{P}_{i,j}(1 - \log(\mathbf{P}_{i,j}))$$

it's always greater or equal 0 since $\mathbf{P}_{i,j} \in [0,1]$. The function $-H$ is 1-strongly convex since by computing the Hessian, $\partial^2 - H(P) = \text{diag}(1/\mathbf{P}_{i,j})$ and $\mathbf{P}_{i,j} \leq 1$. The idea of the entropic regularization is to make $-H$ the regularizing function ($m^{\varepsilon}_{\mathbf{C}}(\mathbf{a}, \mathbf{b})$) to approch solutions or approximation of $m_{\mathbf{C}}(\mathbf{a}, \mathbf{b})$, the original problem:

$$m^{\varepsilon}_{\mathbf{C}}(\mathbf{a}, \mathbf{b}) \stackrel{\text{def.}}{=} \min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \langle \mathbf{P}, \mathbf{C} \rangle - \varepsilon \mathbf{H}(\mathbf{P})$$

Due to it is ε-strongly convex function, then $m^{\varepsilon}_{\mathbf{C}}(\mathbf{a}, \mathbf{b})$ has a unique optimal solution.

3.1 Convergence with ε

For every different $\varepsilon > 0$, the solution P_{ε} of $m^{\varepsilon}_{\mathbf{C}}(\mathbf{a}, \mathbf{b})$ is unique due to convexity. Then we will claim P_{ε} converges to the original optimal solution with maximal entropic, exactly:

$$\mathbf{P}_{\varepsilon} \longrightarrow \arg \min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \{-\mathbf{H}(\mathbf{P}) : \langle \mathbf{P}, \mathbf{C} \rangle = m_{\mathbf{C}}(\mathbf{a}, \mathbf{b})\}, \text{ as } \varepsilon \to 0$$

In particular,

$$m^{\varepsilon}_{\mathbf{C}}(\mathbf{a}, \mathbf{b}) \longrightarrow m_{\mathbf{C}}(\mathbf{a}, \mathbf{b}), \text{ as } \varepsilon \to 0$$

Proof. Consider a sequnce $(\varepsilon_l)_l$ s.t. $\varepsilon_l \downarrow 0$. Denote $\mathbf{P}_l$ the solution of $L^{\varepsilon_l}_{\mathbf{C}}(\mathbf{a}, \mathbf{b})$. Noticed $\mathbf{U}(\mathbf{a}, \mathbf{b})$ is bounded, by Bazano-Weierstrass Theorem, there is a subsequnce such that $\mathbf{P}_k \to \mathbf{P}^*$, and $\mathbf{P}^* \in \mathbf{U}(\mathbf{a}, \mathbf{b})$ because $\mathbf{U}(\mathbf{a}, \mathbf{b})$ is closed.

Consider any $\mathbf{P}$ as the solution of $m_{\mathbf{C}}(\mathbf{a}, \mathbf{b})$, due to optimality:

$$\langle \mathbf{C}, \mathbf{P} \rangle \leq \langle \mathbf{C}, \mathbf{P}_k \rangle, \quad \langle \mathbf{C}, \mathbf{P}_k \rangle + \varepsilon_k \mathbf{H}(\mathbf{P}) \leq \langle \mathbf{C}, \mathbf{P}_k \rangle + \varepsilon_k \mathbf{H}(\mathbf{P})$$

$$\Longrightarrow 0 \leq \langle \mathbf{C}, \mathbf{P}_k \rangle - \langle \mathbf{C}, \mathbf{P} \rangle \leq \varepsilon_k (\mathbf{H}(\mathbf{P}_k) - \mathbf{H}(\mathbf{P}))$$

Noticed $\mathbf{H}$ is continuous, $\langle \mathbf{C}, \mathbf{P}^* \rangle = \langle \mathbf{C}, \mathbf{P} \rangle$ as $k \to \infty$. and $\mathbf{H}(\mathbf{P}) \leq \mathbf{H}(\mathbf{P}^*)$, which means that $\mathbf{P}^*$ is a solution in the set of all optimal solutions of $m_{\mathbf{C}}(\mathbf{a}, \mathbf{b})$ with maximal entropy. By strictly convexity, the solution is unique and just P^*.

□

4 Sinkhorn's Algorithm

We use Lagrangian to show that the unique solution of $m^{\varepsilon}_{\mathbf{C}}(\mathbf{a}, \mathbf{b})$ has specific form.

4.1 Proposition

There exist scaling variable $\mathbf{u} \in \mathbb{R}^n_+, \mathbf{v} \in \mathbb{R}^m_+$ such that the solution $\mathbf{P}$ of $m^{\varepsilon}_{\mathbf{C}}(\mathbf{a}, \mathbf{b})$ satisfying:

$$\mathbf{P}_{i,j} = \mathbf{u}_i \mathbf{K}_{i,j} \mathbf{v}_j, \quad 1 \leq i \leq n, 1 \leq j \leq m, i, j \in \mathbb{N}$$

where $\mathbf{K} \in \mathbb{R}^{n \times m}$ with $\mathbf{K}_{i,j} = e^{-\frac{\mathbf{C}_{i,j}}{\varepsilon}}$.

Proof. Consider the Lagrangian of $m^{\varepsilon}_{\mathbf{C}}(\mathbf{a}, \mathbf{b})$ with variable $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$ for all marginal constraints:

$$\mathbf{L}(\mathbf{P}, \mathbf{x}, \mathbf{y}) = \langle \mathbf{C}, \mathbf{P} \rangle - \varepsilon \mathbf{H}(\mathbf{P}) - \langle \mathbf{x}, \mathbf{P} \mathbb{1}_m - \mathbf{a} \rangle - \langle \mathbf{y}, \mathbf{P}^T \mathbb{1}_n - \mathbf{b} \rangle$$

By the first order condition,

$$\frac{\partial \mathbf{L}(\mathbf{P},\mathbf{x},\mathbf{y})}{\partial \mathbf{P}_{i,j}} = \mathbf{C}_{i,j} + \varepsilon \log(\mathbf{P}_{i,j}) - \mathbf{x}_i - \mathbf{y}_j = 0$$

$$\Longrightarrow \mathbf{P}_{i,j} = e^{\frac{\mathbf{x}_i}{\varepsilon}} e^{\frac{-\mathbf{C}_{i,j}}{\varepsilon}} e^{\frac{\mathbf{y}_j}{\varepsilon}}, \quad (\mathbf{u})_i = e^{\frac{\mathbf{x}_i}{\varepsilon}}, (\mathbf{v})_j = e^{\frac{\mathbf{y}_j}{\varepsilon}}$$

□

4.2 Definition of Sinkhorn's Algorithm

Noticed for the corrosponding $(\mathbf{u},\mathbf{v})$, $\mathbf{P} = \mathrm{diag}(\mathbf{u})\mathbf{K}\mathrm{diag}(\mathbf{v})$. Therefore the variable $(\mathbf{u},\mathbf{v})$ must satisfy the restriction of $\mathbf{U}(\mathbf{a},\mathbf{b})$:

$$\mathbf{u} \odot (\mathbf{K}\mathbf{v}) = \mathbf{a}, \mathbf{v} \odot (\mathbf{K}^T\mathbf{u}) = \mathbf{b}$$

where $\odot$ is the vector product under entrywise ($(\mathbf{a} \odot \mathbf{b})_i = a_i b_i$).

The naturally way to find $(\mathbf{u},\mathbf{v})$ is solve them iteratively, and the Sinkhorn's algorithm is defined by the idea:

$$\mathbf{u}^{(k+1)} \overset{\text{def.}}{=} \frac{\mathbf{a}}{\mathbf{K}\mathbf{v}^{(k)}}, \quad \mathbf{v}^{(k+1)} \overset{\text{def.}}{=} \frac{\mathbf{b}}{\mathbf{K}\mathbf{u}^{(k+1)}}$$

where the division is also entrywise and initialized with an arbitrary positive vector $\mathbf{v}^{(0)} = \mathbb{1}_m$. Noticed that if Sinkhorn's algorithm converges for any initialization(will be proced latet), different initialization may obtain different limit up to a multiplicative constant since if $(\mathbf{u},\mathbf{v})$ satisfies the $\mathbf{U}(\mathbf{a},\mathbf{b})$ restriction, then $(\lambda\mathbf{u}, \lambda^{-1}\mathbf{v})$ also.

4.3 Hilbert Projective Metric

The Hilbert metric [Hil03] is defined on $\mathbb{R}^n_+$:

$$\forall(\mathbf{u},\mathbf{u}') \in (\mathbb{R}^n_+)^2, \quad d_H(\mathbf{u},\mathbf{u}') \overset{\text{def.}}{=} \log \max_{i,j} \frac{\mathbf{u}_i\mathbf{u}'_j}{\mathbf{u}_j\mathbf{u}'_i}$$

It's actually a distance on the projective cone $\mathbb{R}^n_+/\sim$ with $\mathbf{u} \sim \mathbf{v}$ iff $\exists r > 0, \mathbf{v} = r\mathbf{u}$. There are some important property about Hilbert Metric [Bir57], for $\mathbf{K} \in \mathbb{R}^{n\times m}_+$, $(\mathbf{u},\mathbf{u}') \in (\mathbb{R}^m_+)^2$:

$$d_H(\mathbf{K}\mathbf{u},\mathbf{K}\mathbf{u}') \le \lambda(\mathbf{K}) d_H(\mathbf{u},\mathbf{u}'), \text{where} \begin{cases} \lambda(\mathbf{K}) = \frac{\sqrt{\mu(\mathbf{K})}-1}{\sqrt{\mu(\mathbf{K})}+1} < 1 \\ \mu(\mathbf{K}) = \max_{i,j,k,l} \frac{\mathbf{K}_{i,j}\mathbf{K}_{k,l}}{\mathbf{K}_{i,l}\mathbf{K}_{j,k}} \end{cases}$$

The proof is basically first shown on $\mathbb{R}^2_+$ then generalize to common case.

4.4 Convergence of Sinkhorn's Algorithm

It's first introcuced and proved by [FL89], used above inequality to claim the liniear convergence of Sinkhorn's algorithm. We first has the unique solution $\mathbf{P}^*$ of $m^\varepsilon_{\mathbf{C}}(\mathbf{a},\mathbf{b})$, by [Sin75], there exist $(\mathbf{u}^*,\mathbf{v}^*) \in \mathbb{R}^m \times \mathbb{R}^n$ such that:

$$\mathbf{P}^* = \mathrm{diag}(\mathbf{u}^*)\mathbf{K}\mathrm{diag}(\mathbf{v}^*), \quad \mathbf{u}^* \odot (\mathbf{K}\mathbf{v}^*) = \mathbf{a}, \mathbf{v}^* \odot (\mathbf{K}^T\mathbf{u}^*) = \mathbf{b}$$

Theorem

We have $(\mathbf{u}^{(k)},\mathbf{v}^{(k)}) \to (\mathbf{u}^*,\mathbf{v}^*)$ under Sinkhorn's algorithm, and:

$$d_H(\mathbf{u}^{(k)},\mathbf{u}^*) = O(\lambda(\mathbf{K})^{2k}), \quad d_H(\mathbf{v}^{(k)},\mathbf{v}^*) = O(\lambda(\mathbf{K})^{2k}) \tag{1}$$

$$d_H(\mathbf{u}^{(k)},\mathbf{u}^*) \le \frac{d_H(\mathbf{P}^{(k)}\mathbb{1}_m, \mathbf{a})}{1-\lambda(\mathbf{K})^2}, \quad d_H(\mathbf{v}^{(k)},\mathbf{v}^*) \le \frac{d_H(\mathbf{P}^{(k),T}\mathbb{1}_n, \mathbf{b})}{1-\lambda(\mathbf{K})^2} \tag{2}$$

$$||\log(\mathbf{P}^{(k)}) - \log(\mathbf{P}^*)||_\infty \le d_H(\mathbf{u}^{(k)},\mathbf{u}^*) + d_H(\mathbf{v}^{(k)},\mathbf{v}^*) \tag{3}$$

where $\mathbf{P}^{(k)} \overset{\text{def.}}{=} \text{diag}(\mathbf{u}^k)\mathbf{K}\text{diag}(\mathbf{v}^k)$, and denote $\mathbf{P}^*$ the unique solution of $m^\varepsilon_{\mathbf{C}}(\mathbf{a}, \mathbf{b})$:

Proof. Noticed by definition of Hilbert Metric,

$$\forall (\mathbf{u}, \mathbf{u}') \in (\mathbb{R}^m_+)^2, \quad d_H(\mathbf{u}, \mathbf{u}') = d_H(\mathbf{u}/\mathbf{u}', \mathbb{1}_m) = d_H(\frac{\mathbb{1}_m}{\mathbf{u}}, \frac{\mathbb{1}_m}{\mathbf{u}'})$$

That means,

$$\begin{aligned} d_H(\mathbf{u}^{(k+1)}, \mathbf{u}^*) &= d_H\left(\frac{\mathbf{a}}{\mathbf{K}\mathbf{v}^{(k)}}, \frac{\mathbf{a}}{\mathbf{K}\mathbf{v}^*}\right) = d_H\left(\frac{\mathbb{1}_m}{\mathbf{K}\mathbf{v}^{(k)}}, \frac{\mathbb{1}_m}{\mathbf{K}\mathbf{v}^*}\right) \\ &= d_H(\mathbf{K}\mathbf{v}^{(k)}, \mathbf{K}\mathbf{v}^*) \leq \lambda(\mathbf{K}) d_H(\mathbf{v}^{(k)}, \mathbf{v}^*) \end{aligned}$$

the last step used inequality proved above, and mutatis mutandis,

$$d_H(\mathbf{v}^{(k)}, \mathbf{v}^*) \leq \lambda(\mathbf{K}) d_H(\mathbf{u}^{(k)}, \mathbf{u}^*) \Longrightarrow d_H(\mathbf{u}^{(k+1)}, \mathbf{u}^*) \leq \lambda^2(\mathbf{K}) d_H(\mathbf{u}^{(k)}, \mathbf{u}^*)$$

which proves (1). Then consider Triangular inequality,

$$\begin{aligned} d_H(\mathbf{u}^{(k)}, \mathbf{u}^*) &\leq d_H(\mathbf{u}^{(k+1)}, \mathbf{u}^{(k)}) + d_H(\mathbf{u}^{(k+1)}, \mathbf{u}^*) \\ &\leq d_H\left(\frac{\mathbf{a}}{\mathbf{K}\mathbf{v}^{(k)}}, \mathbf{u}^{(l)}\right) + \lambda^2(\mathbf{K}) d_H(\mathbf{u}^{(k)}, \mathbf{u}^*) \\ &= d_H\left(\mathbf{a}, \mathbf{u}^{(k)} \odot \mathbf{K}\mathbf{v}^{(k)}\right) + \lambda^2(\mathbf{K}) d_H(\mathbf{u}^{(k)}, \mathbf{u}^*) \\ &= d_H\left(\mathbf{a}, \mathbf{P}^{(k)}\mathbb{1}_m\right) + \lambda^2(\mathbf{K}) d_H(\mathbf{u}^{(k)}, \mathbf{u}^*) \end{aligned}$$

$$\Longrightarrow d_H(\mathbf{u}^{(k)}, \mathbf{u}^*) \leq \frac{d_H(\mathbf{P}^{(k)}\mathbb{1}_m, \mathbf{a})}{1 - \lambda(\mathbf{K})^2}$$

This proves the first part of (2), the latter part is similar. (3) is proved from [FL89], Lem 3. Denote $M_k = \exp\left(d_H(\mathbf{u}^{(k)}, \mathbf{u}^*) + d_H(\mathbf{v}^{(k)}, \mathbf{v}^*)\right) > 1$. Noticed $\mathbf{P}^{(k)} = \text{diag}(\mathbf{u}^k)\mathbf{K}\text{diag}(\mathbf{v}^k)$, $\mathbf{P}^{(k)} = \text{diag}(\mathbf{u}^*)\mathbf{K}\text{diag}(\mathbf{v}^*)$:

$$\mathbf{P}^* = \text{diag}(\mathbf{u}^*/\mathbf{u}^{(k)})\mathbf{P}^{(k)}\text{diag}(\mathbf{v}^*/\mathbf{v}^{(k)})$$

$$d_H(\mathbf{u}^*, \mathbf{u}^{(k)}) = d_H(\mathbf{u}^*/\mathbf{u}^{(k)}, \mathbb{1}_m), d_H(\mathbf{u}^*, \mathbf{u}^{(k)}) = d_H(\mathbf{v}^*/\mathbf{v}^{(k)}, \mathbb{1}_n)$$

Let $(\mathbf{u}^*/\mathbf{u}^{(k)})_i$ be normalized by dividing the smallest entry among $(\mathbf{u}^*/\mathbf{u}^{(k)})_i$ to obtain $\left(\mathbf{u}^*/\mathbf{u}^{(k)}\right)'$.

$$1 \leq \left(\mathbf{u}^*/\mathbf{u}^{(k)}\right)'_i \leq M_k, \forall i$$

And times the value divided to $\left(\mathbf{v}^*/\mathbf{v}^{(k)}\right)$ to obtain $\left(\mathbf{v}^*/\mathbf{v}^{(k)}\right)'$.
By definition of $\mathbf{P}^*, \mathbf{P}^{(k)}$,

$$\mathbf{P}^{(k),T}\mathbb{1}_n = \mathbf{P}^{*,T}\mathbb{1}_m = \mathbf{b}$$

By the diagnoalization:

$$\text{diag}\left(\mathbf{v}^*/\mathbf{v}^{(k)}\right)'\mathbf{P}^{(k),T} = \mathbf{P}^{*,T}\text{diag}\left(\mathbf{u}^*/\mathbf{u}^{(k)}\right)'^{-1}$$

By the first equality,

$$\text{diag}\left(\mathbf{v}^*/\mathbf{v}^{(k)}\right)'\mathbf{b} = \text{diag}\left(\mathbf{v}^*/\mathbf{v}^{(k)}\right)\mathbf{P}^{(k),T}\mathbb{1}_m$$

By the second equality,

$$\text{diag}\left(\mathbf{v}^*/\mathbf{v}^{(k)}\right)'\mathbf{P}^{(k),T}\mathbb{1}_m = \mathbf{P}^{*,T}\text{diag}\left(\mathbf{u}^*/\mathbf{u}^{(k)}\right)^{-1}\mathbb{1}_m$$

Recall the range of $\left(\mathbf{u}^*/\mathbf{u}^{(k)}\right)$:

$$M_k^{-1} \leq \left(\mathbf{u}^*/\mathbf{u}^{(k)}\right)_i^{-1} \leq 1, \forall i$$

Consider "times" $\mathbf{P}^{*,T}$:

$$M_k^{-1}\mathbf{b}_j = M_k^{-1}\left(\mathbf{P}^{*,T}\mathbb{1}_m\right)_j \leq \left(\mathbf{P}^{*,T}\mathrm{diag}\left(\mathbf{u}^*/\mathbf{u}^{(k)}\right)^{-1}\mathbb{1}_m\right)_j \leq \left(\mathbf{P}^{*,T}\mathbb{1}_m\right)_j = \mathbf{b}_j$$

By the result from second equality and $\mathbf{P}^{(k),T}\mathbb{1}_m = \mathbf{b}$:

$$M_k^{-1}\mathbf{b}_j \leq \left[\left(\mathbf{v}^*/\mathbf{v}^{(k)}\right)'\mathbf{b}\right]_j \leq \mathbf{b}_j, \forall j \Longrightarrow 1 \leq \left(\mathbf{v}^*/\mathbf{v}^{(k)}\right)'_j \leq M_k$$

$$\Longrightarrow M_k^{-1} \leq \left(\mathbf{u}^*/\mathbf{u}^{(k)}\right)'_i\left(\mathbf{v}^*/\mathbf{v}^{(k)}\right)'_j = \left(\mathbf{u}^*/\mathbf{u}^{(k)}\right)_i\left(\mathbf{v}^*/\mathbf{v}^{(k)}\right)_j = \mathbf{P}^*_{ij}/\mathbf{P}^{(k)}_{ij} \leq M_k$$

which can be represented to the form (3).

□

Complexity and Application to Solve Original Problem

By assuming $n = m$ for simplicity, [AJ17] claimed that after adding a rounding step to ensure to compute a valid coupling $\mathbf{P}_0 \in \mathbf{U}(\mathbf{a}, \mathbf{b})$, we can obtain a $\mathbf{P}_0$ satifying:

$$\langle \mathbf{P}_0, \mathbf{C}\rangle \leq m_{\mathbf{C}}(\mathbf{a}, \mathbf{b}) + \varepsilon$$

in time $O(n^2 \log(n)\varepsilon^{-3})$. And recently improved by [PDK18].

5 Result from [AJ17]

Main Theorem

Sinkhorn's algorithm with a rounding step returns a point $\hat{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})$ satifying

$$\langle \hat{P}, \mathbf{C}\rangle \leq \min_{\mathbf{P}\in\mathbf{U}(\mathbf{a},\mathbf{b})} \langle \mathbf{P}, \mathbf{C}\rangle + \varepsilon$$

in time $O(n^2 L^3 (\log n)\varepsilon^{-3})$, where L in the underbound of entry of C.

Definition

The potential function is denote as

$$f(\mathbf{x}, \mathbf{y}) = \sum_{i,j} \mathbf{A}_{i,j} e^{(x_i, y_j)} - \langle \mathbf{r}, \mathbf{x}\rangle - \langle \mathbf{c}, \mathbf{y}\rangle$$

The Kullback-Leibler divergence is denote as

$$\mathcal{K}(\mathbf{p}||\mathbf{q}) = \sum_{k=1}^{n} \mathbf{p}_k \log \frac{\mathbf{p}_k}{\mathbf{q}_k}$$

5.1 Theorem 2

Sinkhorn with $dist(\mathbf{A}, \mathbf{U}(\mathbf{a}, \mathbf{b})) = ||\mathbf{r}(\mathbf{A}) - \mathbf{r}||_1 + ||\mathbf{c}(\mathbf{A}) - \mathbf{c}||_1$ returns a matrix $\mathbf{B}$ satifying $||\mathbf{r}(\mathbf{B}) - \mathbf{r}||_1 + ||\mathbf{c}(\mathbf{B}) - \mathbf{c}||_1 \leq \varepsilon_1$ in time $O(\varepsilon_1^{-2}\log(\frac{s}{l}))$ interation, where $s = \sum_{i.j} \mathbf{A}_{i,j}, l = \min_{i,j} \mathbf{A}_{i,j}$.

The proof of Theorem 2 is mainly from below lemma.

Lemma 1

$$\forall k \geq 2, \mathcal{K}(\mathbf{r}||\mathbf{r}(\mathbf{A}^{(k-1)})) + \mathcal{K}(\mathbf{c}||\mathbf{c}(\mathbf{A}^{(k-1)})) = f(\mathbf{x}^{k-1}, \mathbf{y}^{k-1}) - f(\mathbf{x}^{k}, \mathbf{y}^{k})$$

where $\mathbf{x}^k, \mathbf{y}^k, \mathbf{A}^{(k-1)}$ is the result from Sinkhorn's interation. The proof is just directly from the definition of f, KL divergence and Sinkhorn's interation.

Lemma 2

Let $\mathbf{A}_{i,j} > 0$ and $||\mathbf{A}||_1 \leq s$, $\mathbf{A}_{i,j} \geq l > 0$, then

$$f(\mathbf{x}^1, \mathbf{y}^1) \leq f(\mathbf{0}, \mathbf{0})$$

$$f(\mathbf{0}, \mathbf{0}) \leq \log \frac{s}{l} + \min_{\mathbf{x},\mathbf{y} \in \mathbb{R}^n} f(\mathbf{x}, \mathbf{y})$$

The proof of lemma 2 is mainly from a algebraic inequality below

Lemma 3 (Pinsker's inequality)

Let $\mathbf{p}, \mathbf{q} \in \mathbb{R}^n, \mathbf{p}_k, \mathbf{q}_k > 0, \sum_{k=1}^n \mathbf{p}_k = \sum_{k=1}^n \mathbf{q}_k = 1$,

$$\sum_{k=1}^{n} |\mathbf{p}_k - \mathbf{q}_k| \leq \sqrt{2 \sum_{k=1}^{n} \mathbf{p}_k \log(\frac{\mathbf{p}_k}{\mathbf{q}_k})}$$

Proof. By above leamma, we can prove Theorem 2.

Let l^* be the first k s.t. $||\mathbf{r}(\mathbf{A}^{(l^*)}) - \mathbf{r}||_1 + ||\mathbf{c}(\mathbf{A}^{(l^*)}) - \mathbf{c}||_1 \leq \varepsilon_1$. By Pinsker's inequality, $\forall k < l^*$,

$$2\mathcal{K}\left(\mathbf{r}||\mathbf{r}(\mathbf{A}^{(l^*)})\right) \geq ||\mathbf{r}(\mathbf{A}^{(l^*)}) - \mathbf{r}||_1^2$$

$$2\mathcal{K}\left(\mathbf{c}||\mathbf{c}(\mathbf{A}^{(l^*)})\right) \geq ||\mathbf{c}(\mathbf{A}^{(l^*)}) - \mathbf{c}||_1^2$$

$$\Longrightarrow 4\left(\mathcal{K}\left(\mathbf{r}||\mathbf{r}(\mathbf{A}^{(l^*)})\right) + \mathcal{K}\left(\mathbf{c}||\mathbf{c}\mathbf{A}^{(l^*)}\right)\right) \geq \left(||\mathbf{r}(\mathbf{A}^{(l^*)}) - \mathbf{r}||_1 + ||\mathbf{c}(\mathbf{A}^{(l^*)}) - \mathbf{c}||_1\right)^2 > \varepsilon_1^2$$

Then applied Lemma1, 2, denote $(\mathbf{x}^*, \mathbf{y}^*)$ be the smallest point of f, whose existence is insure by convexity.

$$\begin{aligned}\log \frac{s}{l} &\overset{lem2}{\geq} f(\mathbf{0}, \mathbf{0}) - f(\mathbf{x}^*, \mathbf{y}^*) \geq f(\mathbf{0}, \mathbf{0}) - f(\mathbf{x}^{l^*}, \mathbf{y}^{l^*}) \\ &\overset{lem1}{=} \sum_{i=1}^{l^*-1} \mathcal{K}\left(\mathbf{r}||\mathbf{r}(\mathbf{A}^{(i)})\right) + \mathcal{K}\left(\mathbf{c}||\mathbf{c}(\mathbf{A}^{(i)})\right) > \sum_{i=1}^{l^*-1} \frac{\varepsilon_1^2}{4} = \frac{\varepsilon_1^2 l^*}{4}\end{aligned}$$

whiche proves Theorem 2.

□

Then we concludes we add one more roungding step algorithm 2 for constraints of $\mathbf{U}(\mathbf{a}, \mathbf{b})$, which will leads to the main theorem.

$X \leftarrow \mathbf{D}(x)$ with $x_i = \frac{r_i}{r_i(F)} \wedge 1$
$F' \leftarrow XF$
$Y \leftarrow \mathbf{D}(y)$ with $y_j = \frac{c_j}{c_j(F')} \wedge 1$
$F'' \leftarrow F'Y$
$\mathrm{err}_r \leftarrow r - r(F'')$, $\mathrm{err}_c \leftarrow c - c(F'')$
Output $G \leftarrow F'' + \mathrm{err}_r \mathrm{err}_c^\top / \|\mathrm{err}_r\|_1$

Figure 1:

Lemma 4

Given $\mathbf{A}$, denote $\mathbf{H} = \text{diag}(\mathbf{x})\mathbf{A}\text{diag}(\mathbf{y})$, for any $\mathbf{a}, \mathbf{b}$, above algorithm return $\mathbf{G} \in \mathbf{U}(\mathbf{a}, \mathbf{b})$ in $O(n^2)$ satifying,

$$||\mathbf{G} - \mathbf{H}||_1 \leq 2\left[||\mathbf{r}(\mathbf{H}) - \mathbf{r}||_1 + ||\mathbf{c}(\mathbf{H}) - \mathbf{c}||_1\right]$$

Proof. Just directly check that the complexity of each step in above algorithm. □

Then combine all the result above, we can prove the main theorem.

6 Conclusion

As the development of computer science, people can use more stronger method to compute some tradictional question. By using the entropic as the regularization, the orginal optimal problem can be evaluated more easily due the convexity.

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