
Large-scale Optimal Transport

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Abstract

1 Introduction to Optimal Transport

2 Problem Statement

The standard formulation of optimal transport are derived from couplings. [Villani2009] That is, let (\mathcal{X}, μ) and (\mathcal{Y}, ν) be two probability spaces, and a probability distribution π on $\mathcal{X} \times \mathcal{Y}$ is called *coupling* if $proj_{\mathcal{X}}(\pi) = \mu$ and $proj_{\mathcal{Y}}(\pi) = \nu$. An optimal transport between (\mathcal{X}, μ) and (\mathcal{Y}, ν) , or an optimal coupling, is a coupling minimize

$$\int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\pi(x, y) \quad (1)$$

Optimal transport problems can be categorized according to the discreteness of μ and ν . In this report, we only consider discrete optimal transport problems, where the two distributions are distributions of finite weighted points.

A discrete optimal transport problem can be formulated into a linear program as

$$\begin{aligned} \min_{\pi} \quad & \sum_{i=1}^m \sum_{j=1}^n c_{ij} \pi_{ij} \\ \text{s.t.} \quad & \sum_{j=1}^n \pi_{ij} = \mu_i, \forall i \\ & \sum_{i=1}^m \pi_{ij} = \nu_j, \forall j \\ & \pi_{ij} \geq 0, \end{aligned} \quad (2)$$

where c stands for the cost and s for the transportation plan, while μ and ν are restrictions. Note that we always suppose $c \geq 0$, $\mu \geq 0$, $\nu \geq 0$ and $\sum_{i=1}^m \mu_i = \sum_{j=1}^n \nu_j = 1$ implicitly. From realistic background, c is always valued the squared Euclidean distanced or some other norms. Note that there are mn variables in this formulation, and this leads to intensive computation.

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3 Algorithms

3.1 ADMM for Primal Problem

3.2 ADMM for Dual Problem

3.3 Sinkhorn Method with Entropy Regularization

The discrete entropy of a coupling matrix is defined as

$$\mathbf{H}(\mathbf{P}) \stackrel{\text{def}}{=} - \sum_{i,j} \mathbf{P}_{i,j} (\log (\mathbf{P}_{i,j}) - 1) \quad (3)$$

The function \mathbf{H} is strongly concave.

The idea of the entropic regularization of optimal transport is to use $-\mathbf{H}$ as a regularizing function to obtain approximate solutions to the original transport problem:

$$\mathbf{L}_C^\varepsilon(\mathbf{a}, \mathbf{b}) \stackrel{\text{def}}{=} \min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \langle \mathbf{P}, \mathbf{C} \rangle - \varepsilon \mathbf{H}(\mathbf{P}) \quad (4)$$

(Actually, this can be interpreted as $\text{KL}(\mathbf{P}||\mathbf{K})$)

One can show that the solution to 4 has the form of

$$\mathbf{P}_{i,j} = \mathbf{u}_i \mathbf{K}_{i,j} \mathbf{v}_j \quad (5)$$

where $\mathbf{K}_{i,j} = e^{-\mathbf{C}_{i,j}/\varepsilon}$ by calculating the KKT condition: Introducing two dual variables $\mathbf{f} \in \mathbb{R}^n, \mathbf{g} \in \mathbb{R}^n$ and calculate the lagrangian:

$$\mathcal{L}(\mathbf{P}, \mathbf{f}, \mathbf{g}) = \langle \mathbf{P}, \mathbf{C} \rangle - \varepsilon \mathbf{H}(\mathbf{P}) - \langle \mathbf{f}, \mathbf{P} \mathbf{1}_n - \mathbf{a} \rangle - \langle \mathbf{g}, \mathbf{P}^\top \mathbf{1}_n - \mathbf{b} \rangle \quad (6)$$

take first order gradient and we get

$$\frac{\partial \mathcal{L}(\mathbf{P}, \mathbf{f}, \mathbf{g})}{\partial \mathbf{P}_{i,j}} = \mathbf{C}_{i,j} + \varepsilon \log (\mathbf{P}_{i,j}) - \mathbf{f}_i - \mathbf{g}_j = 0 \quad (7)$$

$$\Rightarrow \mathbf{P}_{i,j} = e^{\mathbf{f}_i/\varepsilon} e^{-\mathbf{C}_{i,j}/\varepsilon} e^{\mathbf{g}_j/\varepsilon} \quad (8)$$

Based on the constrain that:

$$\text{diag}(\mathbf{u}) \mathbf{K} \text{diag}(\mathbf{v}) \mathbf{1}_m = \mathbf{a} \quad (9)$$

$$\text{diag}(\mathbf{v}) \mathbf{K}^\top \text{diag}(\mathbf{u}) \mathbf{1}_n = \mathbf{b} \quad (10)$$

or :

$$\mathbf{u} \odot (\mathbf{K} \mathbf{v}) = \mathbf{a} \quad \text{and} \quad \mathbf{v} \odot (\mathbf{K}^\top \mathbf{u}) = \mathbf{b} \quad (11)$$

(where \odot means entry-wise multiplication of vectors) we can develop our algorithm as iteratively updating \mathbf{u} and \mathbf{v} :

$$\mathbf{u}^{(\ell+1)} = \frac{\mathbf{a}}{\mathbf{K} \mathbf{v}^{(\ell)}} \quad \text{and} \quad \mathbf{v}^{(\ell+1)} = \frac{\mathbf{b}}{\mathbf{K}^\top \mathbf{u}^{(\ell+1)}} \quad (12)$$

with $\mathbf{v}^{(0)} = \mathbf{1}_m$ and $\mathbf{K}_{i,j} = e^{-\mathbf{C}_{i,j}/\varepsilon}$.

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References

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size to small (9 point) when listing the references. **Remember that you can go over 8 pages as long as the subsequent ones contain *only* cited references.**

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