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 $(\mathcal{X}, \mu)$ and $(\mathcal{Y}, \nu)$ 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 $(\mathcal{X}, \mu)$ and $(\mathcal{Y}, \nu)$, or an optimal coupling, is a coupling minimize

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

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

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

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

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.

In order to decrease the number of variables, we can derive the dual problem of discrete optimal transport.

$$\begin{aligned} &\max_{\lambda,\eta} \sum_{i=1}^{m} \mu_i\lambda_i + \sum_{j=1}^{n} \nu_j\eta_j \\ &s.t. c_{ij} - \lambda_i - \eta_j \geq 0, \forall i, j \end{aligned} \tag{3}$$

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Although this formulation only has m + n variables, there are still challenges including the recovery of π from λ and η and the great number of constraints.

3 Algorithms

3.1 ADMM for Primal Problem

We first implement a first order algorithm called **alternative direction method of multipliers** (ADMM). According to a reformulation of primal problem,

$$\begin{aligned} \min_{\pi} & \sum_{i=1}^{m}\sum_{j=1}^{n} c_{ij}\pi_{ij} + \mathbb{I}_{+}(\hat{\pi}) \\ s.t. & \sum_{j=1}^{n} \pi_{ij} = \mu_i, \forall i \\ & \sum_{i=1}^{m} \pi_{ij} = \nu_j, \forall j \\ & \pi = \hat{\pi} \end{aligned} \tag{4}$$

where $\mathbb{I}_{+}$ is indicator of $\mathbb{R}_{+}^{m\times n}$. The augmented Lagrangian can be written as

$$\begin{aligned} \mathcal{L}_{\rho}(\pi, \hat{\pi}, \lambda, \eta, e) = & \sum_{i=1}^{m}\sum_{j=1}^{n} c_{ij}\pi_{ij} + \mathbb{I}_{+}(\hat{\pi}) \\ & + \sum_{i=1}^{m} \lambda_i \left(\mu_i - \sum_{j=1}^{n} \pi_{ij}\right) + \sum_{j=1}^{n} \eta_j \left(\nu_j - \sum_{i=1}^{m} \pi_{ij}\right) + \sum_{i=1}^{m}\sum_{j=1}^{n} e_{ij}\left(\pi_{ij} - \hat{\pi}_{ij}\right) \\ & + \frac{\rho}{2}\sum_{i=1}^{m}\left(\mu_i - \sum_{j=1}^{n} \pi_{ij}\right)^2 + \frac{\rho}{2}\sum_{j=1}^{n}\left(\nu_j - \sum_{i=1}^{m} \pi_{ij}\right)^2 + \frac{\rho}{2}\sum_{i=1}^{m}\sum_{j=1}^{n}\left(\pi_{ij} - \hat{\pi}_{ij}\right)^2 \end{aligned} \tag{5}$$

The minimizer of $\hat{\pi}$ can be written easily as

$$argmin_{\hat{\pi}}\mathcal{L}_{\rho}(\pi, \hat{\pi}, \lambda, \eta, e) = max\left(\pi + \frac{e}{\rho}, 0\right) \tag{6}$$

For the minimizer of π, we can derive the following equation:

$$\sum_{k=1}^{n} \pi_{ik} + \sum_{k=1}^{m} \pi_{kj} + \pi_{ij} = \frac{1}{\rho}\left(-e_{ij} + \lambda_i + \eta_j - c_{ij}\right) + \mu_i + \upsilon_j + \hat{\pi}_{ij} \equiv r_{ij} \tag{7}$$

It's a linear equation of π_{ij} for the given r_{ij}, which can be solved directly.

$$\pi_{ij} = r_{ij} - \frac{1}{n+1}\sum_{k=1}^{n}\left(r_{ik} - \frac{1}{m+n+1}\sum_{l=1}^{m} r_{lk}\right) - \frac{1}{m+1}\sum_{k=1}^{m}\left(r_{kj} - \frac{1}{m+n+1}\sum_{l=1}^{n} r_{kl}\right) \tag{8}$$

Then, we can write the explicit form of ADMM algorithm. This algorithm is implemented in **ADMM_primal.py**.

Algorithm 1: Alternating direction method of multipliers for the primal problem

Input: input data c, μ, ν, step sizeα, penalty scalar ρ and maximum iteration N
Output: solution π

initializing $k = 0$
$\pi^{(k)}, \hat{\pi}^{(k)}, e^{(k)}, \lambda^{(k)}, \eta^{(k)} := 0$
while $k < N$ **do**
  $\pi^{(k+1)} := argmin_{\pi} \mathcal{L}_{\rho}(\pi, \hat{\pi}^{(k)}, \lambda^{(k)}, \eta^{(k)}, e^{(k)})$
  $\hat{\pi}^{(k+1)} := argmin_{\hat{\pi}} \mathcal{L}_{\rho}(\pi^{(k+1)}, \hat{\pi}, \lambda^{(k)}, \eta^{(k)}, e^{(k)})$
  $\lambda^{(k+1)} := \lambda^{(k)} + \alpha\rho(\mu - \sum_{j=1}^{n} \pi_{ij})$
  $\eta^{(k+1)} := \eta^{(k)} + \alpha\rho(\nu - \sum_{i=1}^{m} \pi_{ij})$
  $e^{(k+1)} := e^{(k)} + \alpha\rho(\pi - \hat{\pi})$
  $k := k + 1$
end
return $\hat{\pi}$

3.2 ADMM for Dual Problem

According the reformulation of dual problem,

$$\begin{aligned} &\min_{\lambda,\eta} -\sum_{i=1}^{m} \mu_i \lambda_i - \sum_{j=1}^{n} \nu_j \eta_j + \mathbb{I}_{+}(e) \\ &s.t. c_{ij} - \lambda_i - \eta_j - e_{ij} = 0, \forall i, j \end{aligned} \tag{9}$$

we can write down the augmented Lagrangian as

$$\begin{aligned} \mathcal{L}_{\rho}(\lambda, \eta, e, d) = &-\sum_{i=1}^{m} \mu_i \lambda_i - \sum_{j=1}^{n} \nu_j \eta_j + \mathbb{I}_{+}(e) \\ &+ \sum_{i=1}^{m} \sum_{j=1}^{n} d_{ij}(c_{ij} - \lambda_i - \eta_j - e_{ij}) + \frac{\rho}{2} \sum_{i=1}^{m} \sum_{j=1}^{n} (c_{ij} - \lambda_i - \eta_j - e_{ij})^2 \end{aligned} \tag{10}$$

The minimizer of e can be done directly by solving for zero gradient and projection, while the minimizer of λ and η can be done by solving for zero gradient.

$$\begin{aligned} argmin_{e_{ij}} \mathcal{L}_{\rho}(\lambda, \eta, e, d) =& max\left(c_{ij} + \frac{d_{ij}}{\rho} - \lambda_i - \eta_j, 0\right) \\ argmin_{\lambda_i} \mathcal{L}_{\rho}(\lambda, \eta, e, d) =& \frac{1}{n}\left((\mu_i + \sum_{j=1}^{n} d_{ij})/\rho + \sum_{j=1}^{n}(c_{ij} - \eta_j - e_{ij})\right) \\ argmin_{\eta_j} \mathcal{L}_{\rho}(\lambda, \eta, e, d) =& \frac{1}{m}\left((\nu_j + \sum_{i=1}^{m} d_{ij})/\rho + \sum_{i=1}^{m}(c_{ij} - \lambda_i - e_{ij})\right) \end{aligned} \tag{11}$$

The algorithm is implemented in **ADMM_dual.py**. Solution π can be recovered by $\pi = -d$ from KKT conditions.

Algorithm 2: Alternating direction method of multipliers for the primal problem

Input: input data c, μ, ν, step sizeα, penalty scalar ρ and maximum iteration N
Output: solution π

initializing $k = 0$
$\lambda^{(k)}, \eta^{(k)}, e^{(k)}, d^{(k)} := 0$
while $k < N$ **do**
    $\lambda_i^{(k+1)} := argmin_{\lambda_i} \mathcal{L}_\rho(\lambda, \eta^{(k)}, e^{(k)}, d^{(k)})$
    $\eta_j^{(k+1)} := argmin_{\eta_j} \mathcal{L}_\rho(\lambda^{(k+1)}, \eta, e^{(k)}, d^{(k)})$
    $e_{ij}^{(k+1)} := argmin_{e_{ij}} \mathcal{L}_\rho(\lambda^{(k+1)}, \eta^{(k+1)}, e, d^{(k)})$
    $d_{ij}^{(k+1)} := d_{ij}^{(k)} + \alpha\rho(c_{ij} - \lambda_i - \eta_j - e_{ij})$
    $k := k + 1$
end
return $\pi = -d$

3.3 Sinkhorn Method with Entropy Regularization

The discrete entropy of a coupling matrix is defined as

$$\mathbf{H}(\mathbf{P}) \stackrel{\text{def}}{=} -\sum_{i,j} \mathbf{P}_{i,j} \left(\log\left(\mathbf{P}_{i,j}\right) - 1\right) \tag{12}$$

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:

$$\mathrm{L}_{\mathrm{C}}^{\varepsilon}(\mathbf{a}, \mathbf{b}) \stackrel{\text{def}}{=} \min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \langle \mathbf{P}, \mathbf{C} \rangle - \varepsilon \mathbf{H}(\mathbf{P}) \tag{13}$$

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

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

$$\mathbf{P}_{i,j} = \mathbf{u}_i \mathbf{K}_{i,j} \mathbf{v}_j \tag{14}$$

where $\mathbf{K}_{i,j} = e^{-\mathbf{C}_{i,j}/\epsilon}$ 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:

$$\mathcal{L}(\mathbf{P}, \mathbf{f}, \mathbf{g}) = \langle \mathbf{P}, \mathbf{C} \rangle - \varepsilon \mathbf{H}(\mathbf{P}) - \langle \mathbf{f}, \mathbf{P}\mathbf{1}_n - \mathbf{a} \rangle - \left\langle \mathbf{g}, \mathbf{P}^{\mathrm{T}}\mathbf{1}_n - \mathbf{b} \right\rangle \tag{15}$$

take first order gradient and we get

$$\frac{\partial \mathcal{L}(\mathbf{P}, \mathbf{f}, \mathbf{g})}{\partial \mathbf{P}_{i,j}} = \mathbf{C}_{i,j} + \varepsilon \log\left(\mathbf{P}_{i,j}\right) - \mathbf{f}_i - \mathbf{g}_j = 0 \tag{16}$$

$$\Rightarrow \mathbf{P}_{i,j} = e^{\mathbf{f}_i/\varepsilon} e^{-\mathbf{C}_{i,j}/\varepsilon} e^{\mathbf{g}_j/\varepsilon} \tag{17}$$

Based on the constrain that:

$$\operatorname{diag}(\mathbf{u}) \mathbf{K} \operatorname{diag}(\mathbf{v}) \mathbf{1}_m = \mathbf{a} \tag{18}$$

$$\operatorname{diag}(\mathbf{v}) \mathbf{K}^{\top} \operatorname{diag}(\mathbf{u}) \mathbf{1}_n = \mathbf{b} \tag{19}$$

or :

$$\mathbf{u} \odot (\mathbf{K}\mathbf{v}) = \mathbf{a} \quad \text{and} \quad \mathbf{v} \odot \left(\mathbf{K}^{\mathrm{T}}\mathbf{u}\right) = \mathbf{b} \tag{20}$$

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

$$\mathbf{u}^{(\ell+1)} = \frac{\mathbf{a}}{\mathbf{K}\mathbf{v}^{(\ell)}} \text{ and } \mathbf{v}^{(\ell+1)} = \frac{\mathbf{b}}{\mathbf{K}^{\mathrm{T}}\mathbf{u}^{(\ell+1)}} \tag{21}$$

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

4 Numerical Result and Interpretation

4.1 Description of datasets

In order to compare the performance of differnet algorithms, we have to use some classic and challenging datasets.

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Use unnumbered third level headings for the acknowledgments. All acknowledgments go at the end of the paper. Do not include acknowledgments in the anonymized submission, only in the final paper.

References

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