Optimal Transport

An Application to Color Transfer

Said Gounane
MIMSC Laboratory
EST Essaoira
https://github.com/sgounane/workshop_mimsc_25

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Overview

1. Reminders on Optimal Transport
2. Example: Bakeries and Cafés
3. Sinkhorn Algorithm for Entropy Regularized Optimal Transport
4. Application to color transfer

Optimal Transport

- Optimal Transport is a theory that allows us to compare two (weighted) points clouds (X, a) and (Y, b), where $X \in \mathbb{R}^{n \times d}$ and $Y \in \mathbb{R}^{m \times d}$ are the locations of the n (resp. m) points in dimension d, and $a \in \mathbb{R}^n$, $b \in \mathbb{R}^m$ are the weights.
- The total weights should sum to one, i.e.

$$\sum_{i=1}^{n} a_i = \sum_{j=1}^{m} b_j = 1$$

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- The basic idea of Optimal Transport is to "transport" the mass located at points X to the mass located at points Y.

Optimal Transport

- Let us denote by

$$\mathcal{U}(a,b) = \left\{ P \in \mathbb{R}^{n\times m} \mid P \geq 0, \sum_{j=1}^{m} P_{ij} = a_i, \sum_{i=1}^{n} P_{ij} = b_j \right\}$$

  the set of admissible transport plans.

- If $P \in \mathcal{U}(a,b)$, the quantity $P_{ij} \geq 0$ should be regarded as the mass transported from point X_i to point Y_j.
- For this reason, it is called a **transport plan**.

Optimal Transport

- We will also consider a **cost matrix** $C \in \mathbb{R}^{n \times m}$. C_{ij} is cost for transporting one unit of mass from X_i to Y_j.
- This cost is usually computed using the positions X_i and Y_j, for example

$$C_{ij} = \|X_i - Y_j\| or C_{ij} = \|X_i - Y_j\|^2.$$

- Then transporting mass according to $P \in \mathcal{U}(a, b)$ has a total cost of $\sum_{ij} P_{ij} C_{ij}$.
- The goal In Optimal Transport is to find a transport plan $P \in \mathcal{U}(a, b)$ that will minimize its total cost.

Optimal Transport

- In other words, we want to solve

$$\min_{P \in \mathcal{U}(a,b)} \sum_{ij} C_{ij} P_{ij}.$$

- This problem is a Linear Program. We can thus solve this problem using classical Linear Programming algorithms.
- The solution P^* is an optimal transport plan between (X, a) and (Y, b)
- $\sum_{ij} P^*_{ij} C_{ij}$ is the optimal transport distance between (X, a) and (Y, b): it is the **minimal** amount of "**energy**" that is necessary to transport the initial mass located at points X to the target mass lcoated at points Y.

Example

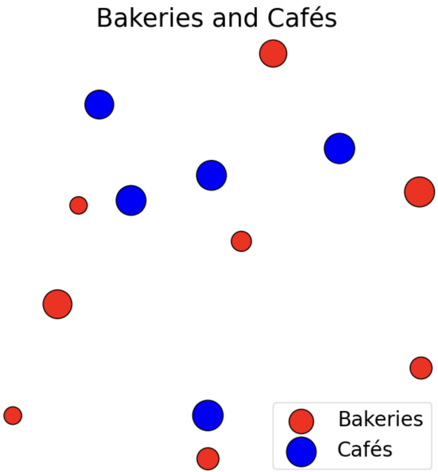


Figure: Bakeries and Cafés example

Example

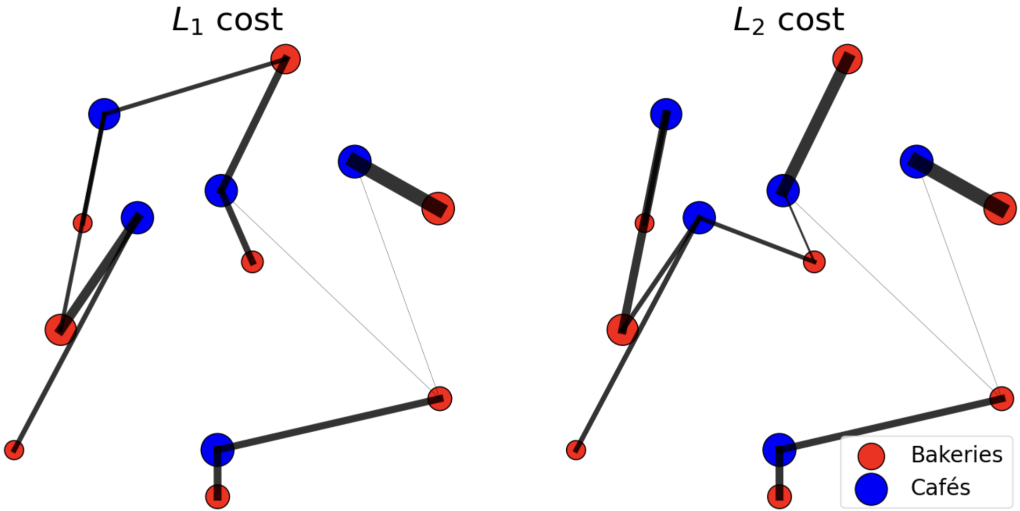


Figure: Bakeries and Cafés example

Sinkhorn Algorithm

- In real applications, and especially in Machine Learning, we often have to deal with huge numbers of points.
- In this case, the linear programming algorithms which have cubic complexity will take too much time to run.
- That's why in practice we can minimize another criterion given by

$$\min_{P \in \mathcal{U}(a,b)} \langle C, P \rangle + \epsilon \sum_{ij} P_{ij}[\log(P_{ij}) - 1].$$

- When ϵ is sufficiently small, we can consider that a solution is a good approximation of a real optimal transport plan.

Sinkhorn Algorithm

- To solve this problem, one can remark that the optimality conditions imply that a solution P_ϵ^* necessarily is of the form $P_\epsilon^* = \mathrm{diag}(u)\, K\, \mathrm{diag}(v)$, where $K = \exp(-C/\epsilon)$ and u, v are two non-negative vectors.
- P_ϵ^* should verify the constraints, i.e. $P_\epsilon^* \in \mathcal{U}(a, b)$, so that

$$P_\epsilon^* 1_m = a \text{ and } (P_\epsilon^*)^T 1_n = b$$

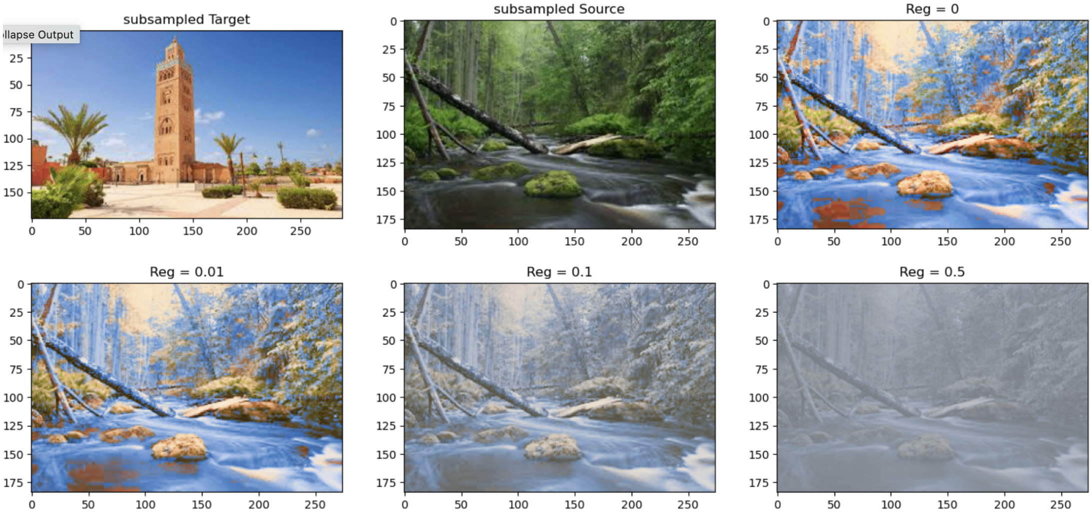
which can be rewritten as

$$u \odot (Kv) = a \text{ and } v \odot (K^T u) = b$$

Then Sinkhorn's algorithm alternate between the resolution of these two equations, and reads

$$u \leftarrow \frac{a}{Kv} \text{ and } v \leftarrow \frac{b}{K^T u}$$

Applications



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References

Presentation and code samples extracted from:
Machine Learning Summer School 2019
Moscow
Russia
https://smiles.skoltech.ru/mlss2019
Tutorial - Computational Optimal Transport:
https://youtu.be/lHrLAkYeHkk?si=cp-3iUaMfC-gaOW9

The End