Practical session 1: optimal transport on the real line

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The aim of this practical session is to familiarize ourselves with the various objects in optimal transport theory in the most simple setting: the real line $\mathbb{R}$ with the cost $c(x, y) = |y - x|^2$. This will be the occasion to observe in a concrete setting the behaviors that we have exhibited so far (stability, existence of transport maps, geodesics). You may use the language of your choice (Python, Julia, Matlab,...) and return a short report as a jupyter notebook or pdf file (with concise and justified answers, full proofs are not required).

Optimal transport via sorting. In this first part, we consider empirical distributions of the form $\mu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$ and $\nu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{y_i}$ for $n \in \mathbb{N}^*$ and points $x_i, y_i \in \mathbb{R}$.

1. Write a function that takes as input the $n$-vectors $(x_i)_{i=1}^{n}$ and $(y_i)_{i=1}^{n}$ and returns the permutation of indices that characterize the optimal transport plan.

2. Let $\mu = \frac{3}{4} \mathcal{L}_{[0,2/3]} + \frac{3}{4} \mathcal{L}_{[2/3,1]}$ and $\nu = \frac{3}{4} \mathcal{L}_{[1/3,1]} + \frac{3}{4} \mathcal{L}_{[0,1/3]}$ where $\mathcal{L}$ is the Lebesgue measure. What is the optimal transport map between $\mu$ and $\nu$?

3. Draw $n$ independent samples from $\mu$ and from $\nu$ and represent the optimal transport plan between the empirical distributions $\hat{\mu}_n$ and $\hat{\nu}_n$ on $[0,1]^2$ (plot is via a point cloud). Plot for $n = 20$ and $n = 50$.

4. Compute the $2$-Wasserstein distance between $\mu_n$ and $\nu_n$ and plot it as a function of $n$, for $n = 1$ to $n = 500$. What is the (almost sure) limit of $W_2(\mu_n, \nu_n)$?

5. (optional) Take a random sample with large $n$ (say, $n = 1000$) and represent the $W_2$ geodesic between $\mu_n$ and $\nu_n$ at times $t \in \{0, 1/4, 1/2, 3/4, 1\}$ (you may plot it using a histogram). What is the exact expression for the geodesic between $\mu$ and $\nu$ at $t = 1/2$?

Optimal transport via quantile functions. We now consider probability distributions that are given by their discretized density on a uniform grid. More specifically, we consider a fixed uniform grid $(x_i)_{i=1}^{n}$ on $[0, 1]$ with $x_i = i/n - 1/(2n)$ (say, with $n = 200$) and measures of the form $\mu_a = \sum_{i=1}^{n} a_i \delta_{x_i}$ where $a \in \mathbb{R}_+^n$ satisfies $\sum a_i = 1$.

6. Write a function that takes as input two $n$-vectors $a$ and $b$ in $\mathbb{R}_+^n$ such that $\sum a_i = \sum b_j = 1$ and returns the discrete optimal transport plan represented by a matrix $P \in \mathbb{R}_+^{n \times n}$ (i.e. such that the optimal transport plan between $\mu_a$ and $\mu_b$ is $\sum_{i,j} P_{i,j} \delta(x_i, x_j)$).

7. Let $\mu_a$ and $\mu_b$ be the discretization of truncated Gaussian distributions of $(\text{mean}, \text{variance})$ $(0.2, 0.1^2)$ and $(0.6, 0.2^2)$ respectively (do not forget to normalize the weight vectors after discretization). Represent the optimal transport plan in greyscale on $[0, 1]^2$.

8. (optional) Because of the discretization, we see that the optimal transport plan is not deterministic (while it should be in the continuous world). A workaround is to define the barycentric projection map

$$T(x_i) = \frac{\sum_{j=1}^{n} x_j P_{i,j}}{\sum_{j=1}^{n} P_{i,j}}$$

which is well-defined whenever $a_i = \sum_{j=1}^{n} P_{i,j} > 0$. Using this map, plot the (approximate) geodesic between $\mu_a$ and $\mu_b$ at times $t \in \{0, 1/4, 1/2, 3/4, 1\}$.

9. (optional) What is the $2$-Wasserstein distance between two Gaussians $\mathcal{N}(m_1, \sigma_1)$ and $\mathcal{N}(m_2, \sigma_2)$? You can make a conjecture using numerical experiments and prove it by constructing a monotone transport map.