Computational Optimal Transport - Numerical tours

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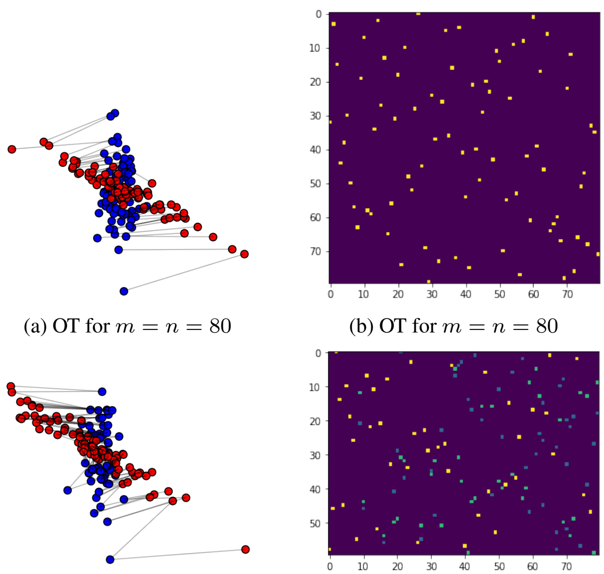
1. Optimal Transport with Linear programming

1.1. Optimal transport between rotated Gaussians

First, we consider two point clouds $(X_i)_{i=1}^n$ and $(Y_j)_{j=1}^m$ with $X_i \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \Sigma)$ and $Y_j \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, R\Sigma R^T)$ where $\Sigma = \text{Diag}(0.1, 5)$, and R is the rotation matrix of angle $\pi/5$.
We consider the quadratic cost $c(x, y) = \|x - y\|_2^2$.
The result can be seen in Fig. 1. We see that for $m = n$, we get a permutation matrix.



(a) OT for $m = n = 80$ (b) OT for $m = n = 80$

(c) OT for $m = 80, n = 60$ (d) OT for $m = 80, n = 60$

Figure 1. Optimal transport between rotated Gaussians

We also see, as has been said during the lecture, that the optimal transport is *not* a rotation.

In fact, we know by Brenier's theorem that the optimal transport from $\mathcal{N}(0, \Sigma)$ to $\mathcal{N}(0, R\Sigma R^T)$ is given by $T : x \mapsto Ax$, with $A = \Sigma^{-1/2}(\Sigma^{1/2} R \Sigma R^T \Sigma^{1/2})^{1/2} \Sigma^{-1/2}$.
We display this optimal transport in Fig. 2. Note that of course, the optimal transport between Gaussians and the optimal transport between point clouds do not perfectly coincide.

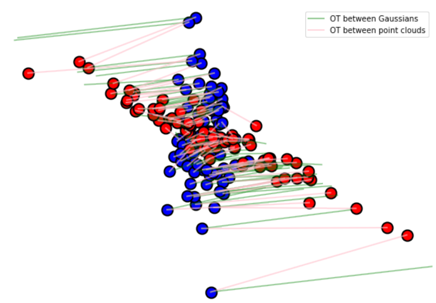


Figure 2. Optimal transport between rotated Gaussians, and between corresponding point clouds

1.2. Optimal transport for $p \neq 2$

We can look at the result when $p \neq 2$.
This is shown in Fig. 3.

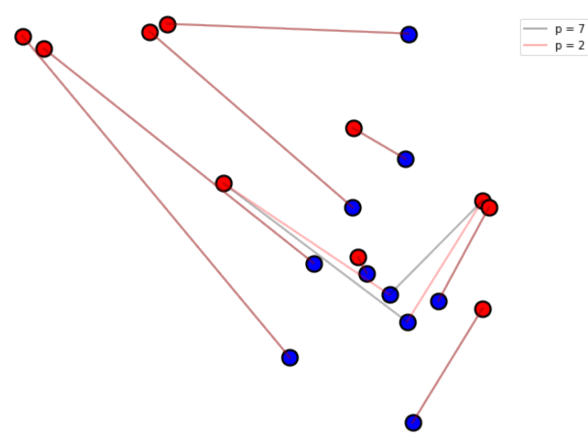


Figure 3. Optimal transport for $p = 2$ and $p = 7$

We see that there has been a switch between the two norms, which do not have the same sensibility to high distances.

1.3. Displacement interpolation between a circle and a horse

Of course, what was done previously can also work on more complex point clouds.
For instance, we can consider the two point clouds in Fig. 4.

Figure 4. A horse and a circle

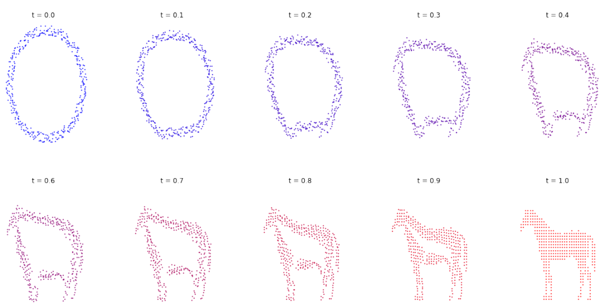


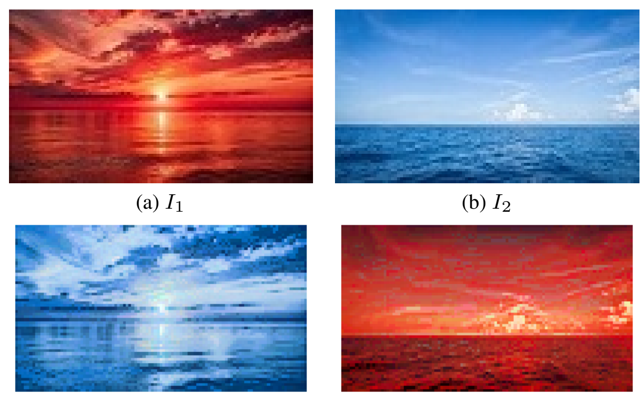
Figure 5. Displacement interpolation between a circle and a horse

The Optimal Transport is visible in Fig. 5.

1.4. Color transfer for images

This application is inspired by page 3 of [1].
Consider two colored images I_1 and I_2 of same size.
Each pixel $I(i,j)$ can be seen as a point in the Red-Green-Blue 3D coordinate system.
Thus, we can find an optimal transport between $(I_1(i,j))_{i,j}$ and $(I_2(i,j))_{i,j}$, and replace the pixels' color accordingly.

Using only `cvxpy`, this can be quite complicated: this problem is large-scale, and the default solver is not really adapted. But, with small enough images, and with some adaptation of the solver's parameters, we get the result shown in Fig. 6.
The result is not entirely satisfying, and adding some regularization to smoothen the colors would most likely help.



(a) I_1 (b) I_2

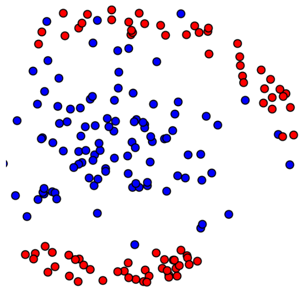
(c) I_1 using colors of I_2 (d) I_2 using colors of I_1

Figure 6. Optimal transport between two images

2. Entropic Regularization of Optimal Transport

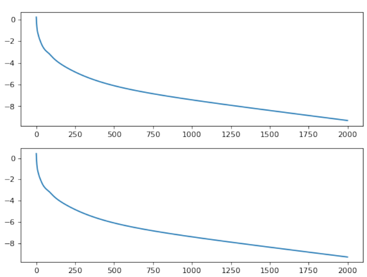
2.1. Transport between point clouds

We consider the following dataset.

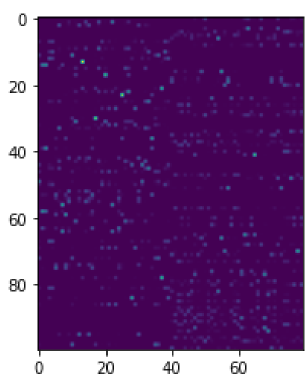


Exercise 1

Using Sinkhorn with $\varepsilon = 0.01$ yields Fig. 7.



(a) Convergence of the marginals



(b) Transport plan

Figure 7. Sinkhorn algorithm with $\varepsilon = 0.01$

To compute the marginals, we use for instance

$$\begin{aligned} P^{(k+1)}\mathbb{1} &= \mathrm{diag}(u^{(k+1)})K\mathrm{diag}(v^{(k+1)})\mathbb{1} \\ &= \mathrm{diag}(u^{(k+1)})Kv^{(k+1)} \\ &= \frac{a}{Kv^{(k+1)}} \odot Kv^{(k+1)}. \end{aligned}$$

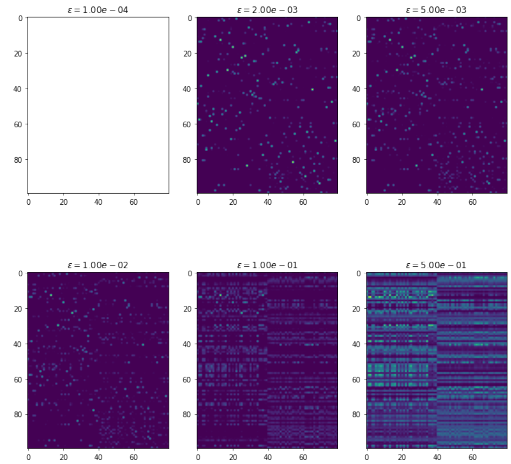


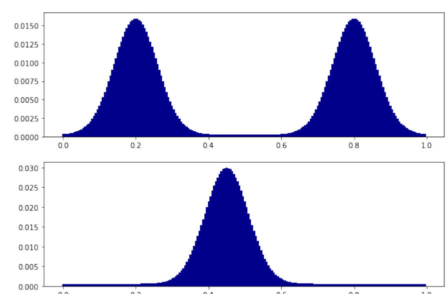
Figure 8. Sinkhorn for several ε

Exercise 2 - Impact of ε

Fig. 8 shows the results obtained for several values of ε. Theoretically, when $\varepsilon = 0$ the optimal coupling is the solution to Kantorovitch problem, and when $\varepsilon = +\infty$ the coupling is $\alpha \otimes \beta$.
In practice, whenever ε is too small, underflow happens, hence the result for $\varepsilon = 10^{-4}$.

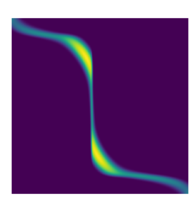
2.2. Transport between histograms

We consider the following histograms.

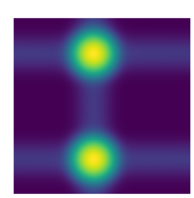


Exercise 3

The result of Sinkhorn algorithm is shown in Fig. 9.



(a) $\epsilon = 10^{-3}$



(b) $\varepsilon = 10$

Figure 9. Sinkhorn algorithm with $\varepsilon = 0.01$

The transport plan for $\varepsilon = 10^{-3}$ is shown in Fig. 10.

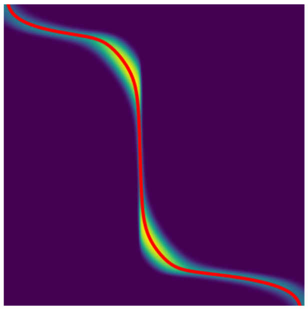


Figure 10. Transport plan with Sinkhorn algorithm for $\varepsilon = 0.01$

For large values of ε (here, $\varepsilon = 10$) we recover as expected the coupling $\alpha \otimes \beta$.

2.3. Wasserstein barycenters

Exercises 4 & 5

Below, we display the Wasserstein barycenters of four images for several values of the coefficients.
The images are very different from one another, so some of the barycenters are not very nice looking. However, the ones in the last row and the ones in the last column are interesting.

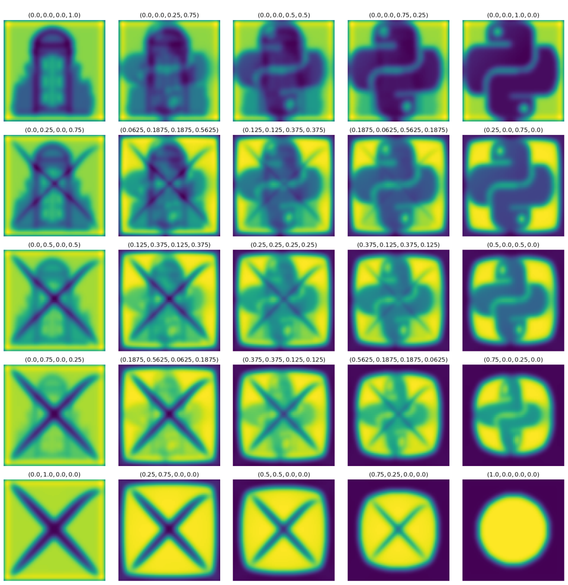


Figure 11. Wasserstein barycenters

References

[1] Numerical Optimal Transport - Applications. https://optimaltransport.github.io/slides-peyre/Applications.pdf. Accessed: 2024-12-17.