

$$K_{HK_\lambda}(\mu, \nu) = \inf \int_{\Omega^2} c_\lambda(x, y) d\pi(x, y) + \underbrace{KL(P_{1\#}\pi|\mu)} + \underbrace{KL(P_{2\#}\pi|\nu)}$$

I think there should be a term  $4\lambda$  before the two KL divergence term.

Conjecture 1: Given Monge's formulation:

$$\pi = (I \times T)_{\#} \tilde{\mu}, \tilde{\mu} \ll \mu, T_{\#} \tilde{\mu} \ll \nu \int_T c_\lambda(x, y) d\pi(x, y) + 4\lambda KL(P_{1\#}\pi|\mu) + 4\lambda KL(P_{2\#}\pi|\nu) \quad (1)$$

where  $T: S \rightarrow \{y_j\}$  for some  $S \subset \{x_i\}$ , and  $\mu = Unif(\{x_1, \dots, x_n\})$ ,  $\nu = Unif(\{y_1, \dots, y_n\})$ ,

we claim: the optimal  $T$  is a 1-1 mapping.

It is equivalent to Corollary 3.3.

Proof: Given  $T$  which is not 1-1 mapping. We reindex  $x_i$  and  $y_j$  such that:

1.  $dom T = \{x_1, \dots, x_{n_T}\}$   
 $range T = \{y_1, \dots, y_{m_T}\}$ .
2.  $T(x_1) = \dots T(x_k) = y_1$  where  $k \geq 2$  and  $T(x_{k+1}) \neq y_1$ .
3.  $c_\lambda(x_1, y_1) \leq c_\lambda(x_l, y_1) \quad l = 2, \dots, k$ .

We define  $T'$  such that  $T'(x_1) = y_1$ ,  $T'(x_l) = T(x_l)$  for  $l = k + 1, \dots, n_T$ .

Let  $\pi$  and  $\pi'$  denote the optimal joint measure induced by  $T$  and  $T'$  respectively.

For convenience, let  $\pi(x_i, T(x_i)) = \tilde{\mu}(x_i) = \frac{p_i}{n}$  denote the mass of point  $(x_i, T(x_i))$  and similarly  $\pi'(x_i, T(x_i)) = \frac{p'_i}{n}$ . Now we analyze  $p_i$  for  $i = 1, 2, \dots, k$ .

The object function (1) becomes

$c_\lambda(x_i, y_1) \frac{p_i}{n} + 4\lambda \left( \frac{p_i}{n} \ln p_i - \frac{p_i}{n} \right) + 4\lambda \left( \frac{(p_1 + \dots + p_k)}{n} \ln(p_1 + \dots + p_k) - \frac{p_i}{n} \right) + C$  where  $C$  is a constant which is independent to  $p_i$ . Let  $L$  denote the function above.

Take derivative:  $\frac{d}{dp_i} L = \frac{1}{n} c_\lambda(x_i, y_1) + 4\lambda \frac{1}{n} \ln p_i + 4\lambda \frac{1}{n} \ln(p_1 + \dots + p_k)$

1. There exists  $p_i$  such that  $\frac{d}{dp_i} L = 0$  for each fixed  $p_j, j \neq i$ .

In fact, we have close form:

$$p_i = \frac{e^{-\frac{1}{4\lambda} c_\lambda(x_1, y_1)}}{\sqrt{e^{-\frac{1}{4\lambda} c_\lambda(x_1, y_1)} + \dots + e^{-\frac{1}{4\lambda} c_\lambda(x_k, y_1)}}}, (p_1 + \dots + p_k) = \sqrt{e^{-\frac{1}{4\lambda} c_\lambda(x_1, y_1)} + \dots + e^{-\frac{1}{4\lambda} c_\lambda(x_k, y_1)}}. \quad (1.1)$$

2.  $L$  is convex with respect to each  $p_i$ .

Why?  $\frac{d^2}{dp_i^2} L = \frac{4\lambda}{n} \frac{1}{p_i} + \frac{4\lambda}{n} \frac{1}{p_1 + \dots p_k} > 0$ .

Then the optimal  $p_i$  satisfies  $\frac{1}{n} c_\lambda(x_i, y_1) + 4\lambda \left( \frac{1}{n} \ln p_i + \frac{1}{n} \ln(p_1 + \dots p_k) \right) = 0$ .

Similarly, we have  $0 = \frac{d}{dp'_1} L = \frac{1}{n} c_\lambda(x_1, y_1) + \frac{2}{n} 4\lambda \ln p'_1$ .

That is  $p'_1 = e^{-\frac{1}{8\lambda} c_\lambda(x_1, y_1)}$ . (1.2)

By (1.1)(1.2), we have  $-2 \ln p'_1 + \ln p_1 + \ln(p_1 + \dots p_k) = 0$

Then  $p'_1 = \sqrt{p_1(p_1 + \dots p_k)} < (p_1 + \dots p_k)$ . (1.3)

For  $l > k$ , since  $T(x_l) = T'(x_l) \neq y_1$ , then  $p_i(x_l) = p'_i(x_l)$ .

Let  $F(\pi) = \int c_\lambda(x, y) d\pi(x, y) + 4\lambda KL(P_{\#1}\pi|\mu) + 4\lambda KL(P_{\#2}\pi|\nu)$ . We need to compare  $F(\pi), F(\pi')$ .

$F(\pi) - F(\pi')$

$= \left\{ \sum_{i=1}^k c_\lambda(x_i, y_1) \frac{p_i}{n} + 4\lambda \left( \sum_{i=1}^k \frac{p_i}{n} \ln p_i + \frac{(p_1 + \dots p_k)}{n} \ln(p_1 + \dots p_k) - 2 \sum_{i=1}^k \frac{p_i}{n} + 2 \right) \right\}$

$- \left\{ c_\lambda(x_1, y_1) \frac{p'_1}{n} + 4\lambda \left( \frac{p'_1}{n} \ln p'_1 + \frac{p'_1}{n} \ln(p'_1) - \frac{2p'_1}{n} + 2 \right) \right\}$

$= 8\lambda \left( \frac{p'_1}{n} - \sum_{i=1}^k \frac{p_i}{n} \right)$  by plugging in (1.1) (1.2)

$< 0$ . By (1.3)

Does it violate to the conjecture 1?

Particular example:

Consider the example:  $x_1 = 0, x_2 = 0.1, x_3 = 0.2, y_1 = 0, y_2 = 100, y_3 = 101. \lambda = \frac{1}{4}$ .

The optimal 1-1 mapping, denoted as  $T'$  is defined as  $x_1 \mapsto y_1$ .

We define  $T$  by  $x_1, x_2, x_3 \mapsto y_1$

Let  $\pi, \pi'$  denote the optimal joint distribution induced by  $T, T'$  respectively.

$F(\pi') = \frac{4}{3} = 2 - \frac{2}{3}$ . (0 transportation cost and  $4 \cdot \frac{1}{3}$  is the cost for destroying  $x_2, x_3$  and creating  $y_2, y_3$ .)

Now we define  $\pi(x_1, y_1) = \frac{1}{3} \frac{1}{\sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}}, \pi(x_2, y_1) = \frac{1}{3} \frac{\cos^2(0.1)}{\sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}},$

$$\pi(x_3, y_1) = \frac{1}{3} \frac{\cos^2(0.2)}{\sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}}$$

We have  $F(\pi) = \sum_{i=1}^3 c_\lambda(x_i, y_1) \frac{p_i}{3} + \sum_{i=1}^3 \frac{1}{3} \ln \frac{\pi(x_i, y_1)}{1/3} - \sum_{i=1}^3 \pi(x_i, y_i) + 1$

$$+ \frac{1}{3} \ln \frac{\sum_{i=1}^3 \pi(x_i, y_1)}{1/3} - \sum_{i=1}^3 \pi(x_i, y_i) + 1$$

$$= 0 - \ln \cos^2(0.1) \cdot \frac{1}{3} \frac{\cos^2(0.1)}{\sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}} - \ln \cos^2(0.2) \cdot \frac{1}{3} \frac{\cos^2(0.2)}{\sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}}$$

$$+ \frac{1}{3} \frac{1}{\sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}} \ln \frac{1}{\sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}} + \frac{1}{3} \frac{\cos^2(0.1)}{\sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}} \ln \frac{\cos^2(0.1)}{\sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}}$$

$$+ \frac{1}{3} \frac{\cos^2(0.2)}{\sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}} \ln \frac{\cos^2(0.2)}{\sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}}$$

$$+ \frac{1}{3} \sqrt{1 + \cos^2(0.1) + \cos^2(0.2)} \ln \sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}$$

$$- \frac{2}{3} \sqrt{1 + \cos^2(0.1) + \cos^2(0.2)} + 2$$

$$= 2 - \frac{2}{3} \sqrt{1 + \cos^2(0.1) + \cos^2(0.2)}$$

$$\approx 0.85 < \frac{4}{3}.$$

Note, given 1-1 mapping  $T$ , by (1.1), we can derive the closed form of

$$\pi = (I \times T)_{\#} \tilde{\mu}, \tilde{\mu} \ll \mu, T_{\#} \tilde{\mu} \ll \nu \int_{\mathbb{T}} c_{\lambda}(x, y) d\pi(x, y) + 4\lambda KL(P_{\#1}\pi|\mu) + 4\lambda KL(P_{\#2}\pi|\nu). \text{ Suppose } T: \{x_1, \dots, x_k\} \rightarrow \{y_1, \dots, y_k\}.$$

That is,  $\{x_1, \dots, x_k\} = I_{tran}$ ,  $\{x_{k+1}, \dots, x_n\} = I_{dest}$ .

$$\begin{aligned} \text{Then we have } F(\pi) &= \sum_{i=1}^k c_{\lambda}(x_i, y_i) \frac{p_i}{n} + 2 \sum_{i=1}^k \frac{p_i}{n} \ln p_i - 2 \sum_{i=1}^k \frac{p_i}{n} + 1 + 1 \\ &= 4\lambda \left( -2 \sum_{i=1}^k \frac{p_i}{n} + 2 \right) \\ &= 4\lambda \left( -\frac{2}{n} \sum_{i=1}^k e^{-\frac{1}{2}c_{\lambda}(x_i, y_i)} + 2 \right) \\ &= 4\lambda \left( -\frac{2}{n} \sum_{i=1}^k \overline{\cos} \left( \frac{\|x_i - y_i\|}{2\sqrt{\lambda}} \right) + 2 \right) \\ &= \sum_{i \in I_{tran}} 2 \frac{4\lambda}{n} \left( 1 - \overline{\cos} \left( \frac{\|x_i - y_i\|}{2\sqrt{\lambda}} \right) \right) + \sum_{i \in I_{dest}} 2 \cdot \frac{4\lambda}{n}. \end{aligned}$$

Compare to the result

**Proposition 3.2.** Let  $\mu = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$  and  $\nu = \frac{1}{n} \sum_{j=1}^n \delta_{y_j}$  where all  $x_i, y_j$  are distinct. Let  $T^*$  be the optimal transport map and define  $\mathcal{I}_{tran} = \{i : T^*(x_i) \neq x_i\}$  and  $\mathcal{I}_{dest} = \{i : T^*(x_i) = x_i\}$ . Then,

$$d_{HK_{\lambda}}(\mu, \nu)^2 = \sum_{i=1}^n (\mathbb{1}_{i \in \mathcal{I}_{tran}} D(x_i, T^*(x_i)) + 2\mathbb{1}_{i \in \mathcal{I}_{dest}} \bar{D})$$

where

$$\begin{aligned} D(x, y) &= \frac{4\lambda}{n} \left( 1 - \overline{\cos} \left( \frac{\|x - y\|}{2\sqrt{\lambda}} \right) \right) \\ \bar{D} &= \frac{4\lambda}{n}. \end{aligned}$$

I fee there is a typo at here. Consider  $n = 1$ . As  $\frac{\|x-y\|}{2\sqrt{\lambda}} \rightarrow \frac{\pi}{2}$ , the distance  $d_{HK_{\lambda}}(\mu, \nu)^2$  will not be a continuous function (with respect to  $\frac{\|x-y\|}{2\sqrt{\lambda}}$ ).

Conjecture 2: The solution of unbalanced OT problem/ Logarithmic Entropy-Transport/ Hellinger–Kantorovich OT problem:

$$\inf_{\pi} \int_{\mathcal{T}} c_{\lambda}(x, y) d\pi(x, y) + KL(P_{\#1}\pi|\mu) + KL(P_{\#2}\pi|\nu)$$

where  $\mu = \sum_{i=1}^n \frac{1}{n} \delta_{x_i}$ ,  $\nu = \sum_{i=1}^n \frac{1}{n} \delta_{y_i}$  is induced by a mapping  $T$ .

If  $\mu$  has a density then, as in the Wasserstein case, the minimiser  $\pi^*$  of the first Kantorovich form of HK is induced by a transport map [7, Theorem 6.6]. This means there exists  $T^* : \Omega \rightarrow \Omega$  and a measure  $\tilde{\mu} \in \mathcal{M}_+(\Omega)$  such that  $\pi^* = (\text{Id} \times T^*)_{\#} \tilde{\mu}$ . Unlike the Wasserstein case it is not true that  $\tilde{\mu}$  is equal to  $\mu$ , nor is  $T^*_{\#} \tilde{\mu}$  equal to  $\nu$ .

**Add here that this is also true if  $\mu = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$  and  $\nu = \frac{1}{n} \sum_{j=1}^n \delta_{y_j}$ ... and prove this!**

The related theorem is the following:

**Theorem 6.6** (Uniqueness) *Let  $\mu_i \in \mathcal{M}(X)$  and  $\gamma \in \text{Opt}_{\text{LE}}(\mu_1, \mu_2)$ .*

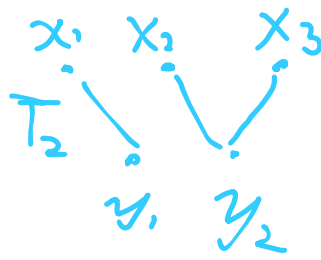
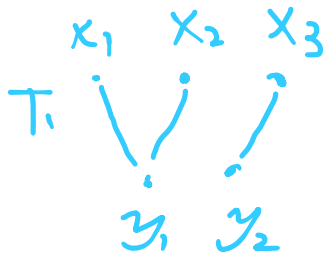
- (i) *The marginals  $\gamma_i = \pi_{\#}^i \gamma$  are uniquely determined.*
- (ii) *If  $X = \mathbb{R}$  with the usual distance then  $\gamma$  is the unique element of  $\text{Opt}_{\text{LE}}(\mu_1, \mu_2)$ .*
- (iii) *If  $X = \mathbb{R}^d$  with the usual distance,  $\mu_1 \ll \mathcal{L}^d$  is absolutely continuous, and  $A_i \subset \mathbb{R}^d$  and  $\sigma_i : A_i \rightarrow (0, \infty)$  are as in Theorem 6.3 b), then  $\sigma_1$  is approximately differentiable at  $\mu_1$ -a.e. point of  $A_1$  and  $\gamma$  is the unique element of  $\text{Opt}_{\text{LE}}(\mu_1, \mu_2)$ . The transport plan  $\gamma$  is concentrated on the graph of a function  $t : \mathbb{R}^d \rightarrow \mathbb{R}^d$  satisfying*

$$\begin{aligned} t(x_1) &= x_1 - \frac{\arctan(|\xi(x_1)|)}{|\xi(x_1)|} \xi(x_1), \\ \xi(x_1) &= -\frac{1}{2} \tilde{D} \log \sigma_1(x_1) \end{aligned} \tag{6.29}$$

Consider the following example:

$$x_1 = -2, x_2 = 0, x_3 = 2$$

$$y_1 = -1, y_2 = 1, y_3 = 100$$



We first consider the following two mappings:

$$T_1: \{x_1, x_2\} \mapsto y_1, x_3 \mapsto y_2$$

$$T_2: x_1 \mapsto y_1, \{x_2, x_3\} \mapsto y_2. \text{ We aim to show } T_1, T_2 \text{ are not optimal mappings.}$$

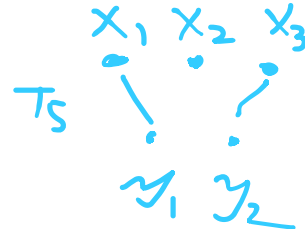
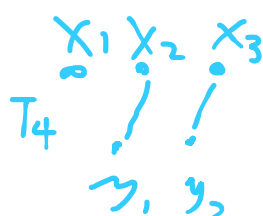
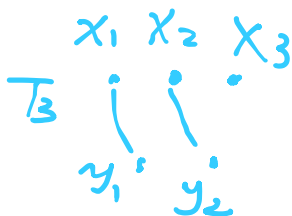
$$\text{We have: } F(T_1) = F(T_2).$$

Let  $\pi_1, \pi_2$  denoted the optimal joint distribution induced by  $T_1, T_2$  respectively. We have:

$$P_{2,\#}\pi_1 \neq P_{2,\#}\pi_2, \text{ indeed, } P_{2,\#}\pi_1(y_1) > P_{1,\#}\pi_1(x_1) \text{ while } P_{2,\#}\pi_2(y_1) = P_{1,\#}\pi_2(x_1).$$

Then by Theorem 6.6 (i), both  $T_1, T_2$  can not be optimal mappings.

Similarly, we consider the following mappings  $T_3, T_4, T_5$ .



$$T_3: x_1 \mapsto y_1, x_2 \mapsto y_2$$

$$T_4: x_2 \mapsto y_1, x_3 \mapsto y_2$$

$$T_5: x_1 \mapsto y_1, x_3 \mapsto y_2$$

We have  $F(T_3) = F(T_4) = F(T_5)$ . But  $P_{1,\#}\pi(T_3), P_{1,\#}\pi(T_4), P_{1,\#}\pi(T_5)$  are pair-wisely different.

Then  $T_3, T_4, T_5$  can not be the optimal mappings.

We do not have other choices of (monotonic increasing) mapping  $T$ .

So, does it violate the conjecture 2?

