Quantum Optimal Transport

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Abstract

In this work, we study the Quantum Optimal Transport problem with the goal of finding new more efficient algorithms than the current existing ones in the literature. Our key idea is to find Quantum equivalents of existing linear programming algorithms solving the classical optimal transport problem such as Sinkhorn Algorithm, Hungarian Algorithm, etc.

1 Introduction and context

1.1 Classical Optimal Transport Problem

Let us first formulate the Classical OT Problem. Suppose you have $m > 0$ factories producing and amount G for goods which has to be distributed to n consumers. Assume that $x_{i,j}^{AB}$ is the proportions of goods shipped from factory i to consumer j and x_i^A and x_j^B respectively the amount of good produced by factory i and the amount of good received by consumer j. We then have:

$$\forall (i,j) \in [n] \times [m],\ x_i^A = \sum_{j=1}^{n} x_{i,j}^{AB} \text{ and } x_j^B = \sum_{i=1}^{m} x_{i,j}^{AB} \ (1)$$

Where $[n] = \{1, \dots, n\}$ and $[m] = \{1, \dots, m\}$.
Let $\Gamma(x^A, x^B)$ be the set of elements $X^{AB} = (x_{i,j}^{AB})_{i,j} \in \mathcal{M}_{n,m}(\mathbb{R}^+)$ satisfying (1), where $x^A = (x_1^A, \dots, x_m^A)^T$ and $x^B = (x_1^B, \dots, x_n^B)^T$.
Assuming $n = m$, let $C = (c_{i,j}) \in \mathcal{M}_n(\mathbb{R}^+)$ such that for all i, j, $c_{i,j}$ represents the cost of transporting goods from factory i to factory j and for all $i, j, k \in [n]$, $c_{i,j} \leq c_{i,k} + c_{k,j}$.
The Classical optimal transport is then formulated as:

$$T_C(x^A, x^B) = \min_{X \in \Gamma(x^A, x^B)} Tr(CX^T)$$

There are many Algorithms solving this problem, which are in polynomial time.

1.2 A different perspective on $\mathcal{M}_{n^2}(\mathbb{C})$

In order to make things clearer and coherent with the literature, and before presenting the quantum optimal transport, we will give another perspective on $\mathcal{M}_{n^2}(\mathbb{C})$. Let M be a an element of $\mathcal{M}_{n^2}(\mathbb{C})$. M can be written as follows:

$$M = \begin{pmatrix} A_{1,1} & \dots & A_{1,n} \\ \vdots & \ddots & \vdots \\ A_{n,1} & \dots & A_{n,n} \end{pmatrix}$$

where for all $i, j \in [n]$, $A_{i,j}$ is a matrix in $\mathcal{M}_n(\mathbb{C})$.
Considering this, we can represent the matrix M with a sequence of 4 indices instead of 2, $M = (m_{i_1,i_2,j_1,j_2})_{i_1,i_2,j_1,j_2 \in [n]}$ such that for all $i_1, i_2, j_1, j_2 \in [n]$, $m_{i_1,i_2,j_1,j_2} = [A_{i_1,j_1}]_{i2,j2}$.

1.3 Quantum Optimal Transport Problem

Let $\mathcal{S}_m^+(\mathbb{C})$ be the set of density matrices, i.e. positive semi-definite elements of $\mathcal{M}_n(\mathbb{C})$ of trace equal to 1. Let $\rho^A \in \mathcal{S}_m^+(\mathbb{C})$ and $\rho^B \in \mathcal{S}_n^+(\mathbb{C})$. ρ^A and ρ^B describe two n dimensional quantum states. A coupling of ρ^A and ρ^B is a matrix $\rho^{AB} = (\rho^{AB}_{i,j,k,l})_{i,k \in [m],\, j,l \in [n]} \in \mathcal{S}_{nm}^+(\mathbb{C})$ such that

$$Tr_A(\rho^{AB}) = \left(\sum_{i=1}^{m} \rho^{AB}_{i,p,i,q}\right)_{p,q \in [n]} = \rho^B \text{ and } Tr_B(\rho^{AB}) = \left(\sum_{p=1}^{n} \rho^{AB}_{i,p,j,p}\right)_{i,j \in [m]} = \rho^A$$

Using the classical representation of $\mathcal{M}_{n^2}(\mathbb{C})$, the two equalities above can also be written as

$$Tr_A(\rho^{AB}) = \sum_{i=1}^{n} \rho_{i,i} \text{ and } Tr_B(\rho^{AB}) = (Tr(\rho_{p,q}))_{p,q \in [n]}$$

where

$$\rho^{AB} = \begin{pmatrix} \rho_{1,1} & \dots & \rho_{1,n} \\ \vdots & \ddots & \vdots \\ \rho_{n,1} & \dots & \rho_{n,n} \end{pmatrix}$$

We denote $\Gamma^Q(\rho^A, \rho^B)$ the set of all couplings of ρ^A and ρ^B that we will call the set of bipartite density matrices and consider C a hermitian matrix of order mn. The quantum optimal problem, abbreviated as QOT, is then formulated as:

$$T_C^Q(\rho^A, \rho^B) = \min_{\rho^{AB} \in \Gamma^Q(\rho^A, \rho^B)} Tr(C\rho^{AB})$$

The key difference between this problem and the previous problem is that it is a SDP problem, which is known to be more difficult. Notice here that since the objective function could be a complex number, we are minimizing its real part.

2 Extremal points of $\Gamma^Q(\rho^A, \rho^B)$

2.1 Extremal points of rank one

In this part, we assume $m = n$, $x^A = x^B = (1, \dots, 1)^T$, and $\rho^A = \rho^B = I$. In this case, $T_C(x^A, x^B)$ is the set of bistochastic matrices.
Our first idea was to study the extremal points of the set $\Gamma^Q(\rho^A, \rho^B)$. Our intuition was that since extremal points in the classical case were matrices with many coefficients equal to 0, the equivalent of this property would be some upper bound on the rank of the matrix. It is hence natural to ask ourselves the following question: what are the matrices of rank 1 that are extremal in $\Gamma^Q(\rho^A, \rho^B)$? This led us to the following result:

Proposition 2.1.

All matrices of rank one in $\Gamma^Q(\rho^A, \rho^B)$

1. Can be written as $M = uu^T$ where $u = (x_1^T, \ldots, x^{nT})^T$ such that for all $i \in [n]$, $x_i \in \mathbb{R}^n$ and $(x_1, \ldots, x_n)$ is an orthonormal basis of $\mathbb{R}^n$.
2. Are extremal points of $\Gamma^Q(\rho^A, \rho^B)$.

Proof. In order to prove this, we will use the following result

Lemma 2.2.

The extremal directions of the cone $\mathcal{C} = \{\rho \in \mathcal{M}_{n^2}(\mathbb{C}),\ \rho \text{ positive semi definite}\}$ are exactly the matrices that can be written as uu^T such that $u \in \mathbb{R}^{n^2}$.

Let $M = uu^T$ be a rank one matrix in $\Gamma^Q(\rho^A, \rho^B)$ where $u = (x_1^T, \ldots, x^{nT})^T$.
The matrix M can be written as block matrix $M = (x_i x_j^T)_{i,j}$. The condition $M \in \Gamma^Q(\rho^A, \rho^B)$ is equivalent to

$$Tr_A(M) = \sum_{i=1}^{n} x_i x_i^T = I \text{ and } Tr_B(M) = \big(Tr(x_i x_j^T)\big)_{i,j\in[n]} = (x_j^T x_i)_{i,j\in[n]} = I$$

The second equality gives for all $i, j \in [n]$ the following property $x_j^T x_i = \delta_{i,j}$, i.e. $(x_1, \ldots, x_n)$ is an orthonormal basis of $\mathbb{R}^n$. Note that when this property is verified, $Tr_A(M) = \sum_{i=1}^n x_i x_i^T = I$ is also true. Hence, the first property has been proven.
Using Lemma 2.2, it is easy to see that if $M_1, M_2 \in \Gamma^Q(\rho^A, \rho^B)$ and $\lambda \in [0, 1]$, then

$$M = \lambda M_1 + (1 - \lambda) M_2 \Longrightarrow \lambda \in \{0, 1\}$$

i.e. M is an extremal point of $\Gamma^Q(\rho^A, \rho^B)$.

2.2 General case

After proving this result, our first attempt to find the extremal points of $\Gamma^Q(\rho^A, \rho^B)$ was to try to find an equivalent to the extremal points of $\Gamma(x^A, x^B)$ in the quantum case. It turns out that the equivalent of $\Gamma(x^A, x^B)$ in $\Gamma^Q(\rho^A, \rho^B)$ is the set of diagonal matrices in $\Gamma^Q(\rho^A, \rho^B)$. We see this using the following bijective map:

$$\psi : \begin{cases} \Gamma(x^A, x^B) & \longrightarrow \Gamma^Q(\rho^A, \rho^B) \cap \mathcal{D} \\ M & \longmapsto diag(L_1(M), \ldots, L_n(M)) \end{cases}$$

Where $\mathcal{D}$ is the set of diagonal matrices of $\mathcal{M}_{n^2}(\mathbb{C})$, and $diag(L_1(M), \ldots, L_n(M))$ the diagonal matrix induced by the rows of $M = (m_{i,j})_{i,j\in[n]}$, i.e.

$$diag(L_1(M), \ldots, L_n(M)) = \begin{pmatrix} m_{1,1} & & & & & & & \\ & \ddots & & & & & 0 & \\ & & m_{1,n} & & & & & \\ & & & \ddots & & & & \\ & & & & \ddots & & & \\ & 0 & & & & m_{n,1} & & \\ & & & & & & \ddots & \\ & & & & & & & m_{n,n} \end{pmatrix}$$

Notice that the constraints in $\Gamma^Q(\rho^A, \rho^B)$ are indeed giving the wanted constraints in $\Gamma(x^A, x^B)$:

$$Tr_A(\psi(M)) = I \iff \forall i \in [n] \sum_{k=1}^{n} m_{k,i} = 1$$

In the set of bistochastic matrices, the extremal points are exactly permutation matrices, i.e. matrices that take the following form: $M = (\delta_{i,\sigma(j)})_{i,j \in [n]}$ where $\sigma \in \mathcal{S}_n$. The equivalent of these matrices in $\Gamma^Q(\rho^A, \rho^B)$ can be written as $\rho = (\delta_{i,k}\delta_{j,l}\delta_{\sigma(i),k})_{i,j,k,l \in [n]}$. Those matrices are basically diagonal matrices with n coefficients equal to 1 and the other coefficients are equal to 0. Our intuition was that these matrices are extremal points in $\Gamma^Q(\rho^A, \rho^B)$ which unfortunately turned out to be wrong. Here is a counter example. Assume $n = 2$. We consider the following matrices:

$$A = \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} = u_1 u_1^T,\ B = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} = u_2 u_2^T \text{ and } C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

where $u_1 = \begin{pmatrix} 1 & 0 & 0 & -1 \end{pmatrix}^T$ and $u_2 = \begin{pmatrix} 1 & 0 & 0 & 1 \end{pmatrix}^T$. A and B are elements of $\Gamma^Q(\rho^A, \rho^B)$, and $C = \psi(I)$ is the equivalent of the identity matrix in $\Gamma^Q(\rho^A, \rho^B)$. If our intuition was correct, C should be an extremal point of $\Gamma^Q(\rho^A, \rho^B)$. However, we can see that

$$C = \frac{1}{2}A + \frac{1}{2}B$$

which means that C is not extremal. According to [4], the extremal points of $\Gamma^Q(\rho^A, \rho^B)$ for $n = 2$ are maximally entangled pure states, i.e. exactly the rank one matrices we found when we started studying the problem. Furthermore, [4] cites a correspondence between completely positive linear $CP_{n,m}$ maps from $\mathcal{M}_n(\mathbb{C})$ to $\mathcal{M}_m(\mathbb{C})$ and bipartite density matrices proven in [2] using the isomorphism $\sigma : \phi \longmapsto \sum_{i,j \in [n]} E_{i,j} \otimes \phi(E_{i,j})$ where the equivalent of the condition on partial traces in the space of completely positive linear maps becomes $\phi(I) = \rho^A$ and $\phi^*(I) = \rho^B$ (see definition of ϕ^* in [4] or in section 3.2.2) and hence establishes that using this result, finding the extremal points of $\Gamma^Q(\rho^A, \rho^B)$ is equivalent to finding extremal points of

$$CP_{m,n}(\rho^A, \rho^B) = \{\phi \in CP_{n,m},\ \phi(I) = \rho^A \text{ and } \phi^*(I) = \rho^B\}$$

Theorem 4 in [4] give a very elegant characterisation of extremal points of $CP_{m,n}(\rho^A, \rho^B)$

Theorem 2.3.

Let $\phi : \mathcal{M}_n(\mathbb{C}) \longrightarrow \mathcal{M}_m(\mathbb{C})$ be a linear map. ϕ is extremal in the convex set $CP_{n,m}(\rho^A, \rho^B)$ if and only if for all $A \in \mathcal{M}_n(\mathbb{C})$,

$$\phi(A) = \sum_{i=1}^{r} V_i^* A V_i$$

where for all i, $V_i \in \mathbb{C}^{n \times m}$ such that

$$\sum_{i=1}^{r} V_i^* V_i = \rho^A \text{ and } \sum_{i=1}^{r} V_i V_i^* = \rho^B$$

and $\{V_i^* V_j \oplus V_j V_i^*,\ i, j \in [r]\}$ is a linearly independent set.

However, this theorem cannot be more explicitly written in $\Gamma^Q(\rho^A, \rho^B)$.

3 Sinkhorn Algorithm

After studying the extremal points of $\Gamma^Q(\rho^A, \rho^B)$, out second idea was to find an equivalent to the Sinkhorn Algorithm in the quantum case.

3.1 Classical Sinkhorn Algorithm

Let us formulate the regularized version of the classical optimal transport problem

$$T_C^\lambda(x^A, x^B) = \min_{x \in \Gamma(x^A, x^B)} Tr(CX^T) - \frac{1}{\lambda} h(X)$$

Where

$$h(X) = \sum_{i,j \in [n]} x_{ij} \log x_{ij}$$

The Lagrangian of this minimization problem can be written as

$$L^\lambda(X, (\alpha_i^A)_j, (\alpha_j^B)_j) = \sum_{i,j \in [n]} c_{ij} x_{ij} - \frac{1}{\lambda} \sum_{i,j \in [n]} x_{ij} \log x_{ij} - \sum_{i=1}^n \alpha_i^A \left(\sum_{j=1}^n x_{ij} - x_i^A \right)$$
$$- \sum_{j=1}^n \alpha_j^B \left(\sum_{i=1}^n x_{ij} - x_i^B \right)$$

At optimality, we have for all $i, j \in [n]$,

$$\frac{\partial L^\lambda}{\partial x_{ij}} = c_{ij} - \frac{1}{\lambda}(1 + \log x_{i,j}) - \alpha_i^A - \alpha_j^B = 0$$

i.e.

$$x_{i,j} = e^{\lambda \alpha_i^A} e^{1 - \lambda c_{ij}} e^{\alpha_j^B}$$

This problem is equivalent to the following: given a matrix $M \in \mathcal{M}_n(\mathbb{R})$, find diagonal matrices D^1 and D^2 such that the matrix $X^* = D^1 M D^2$ verifies condition (1) stated in section 1.1.

A very well known way to solve this problem is the Sinkhorn Algorithm, which is an iterative method consisting of scaling rows and columns at each iteration. This gives us a sequence defined by the following:

$$M_0 = M, \; M_{k+1} = D_{k+1}^1 M_k \text{ if } k \text{ odd}, \; M_{k+1} = M_k D_{k+1}^2 \text{ else}$$

Where for all k,

$$D_{k+1}^1 = diag\left(\frac{x_1^A}{\sum_{j=1}^n [M_k]_{1j}}, \dots, \frac{x_n^A}{\sum_{j=1}^n [M_k]_{nj}} \right)$$
$$D_{k+1}^2 = diag\left(\frac{x_1^B}{\sum_{i=1}^n [M_k]_{i1}}, \dots, \frac{x_n^B}{\sum_{i=1}^n [M_k]_{in}} \right)$$

When the matrix M has positive coefficients, the Sinkhorn algorithm converges to a solution of the problem, i.e. the two sequences $(D_{2k+1}^1 \dots D_1^1)_k$ and $(D_0^2 \dots D_{2k}^2)_k$ converge respectively to matrices D^1 and D^2 verifying the wanted property.

3.2 Quantum Sinkhorn Algorithm

Before talking about our work on the quantum Sinkhorn Algorithm, let us mention that in [5] Peyré and al. gave some quantum version of the Sinkhorn Algorithm. However, the algorithm does not solve the actual quantum optimal transport problem but rather another version of it with relaxed constraints.

3.2.1 Sinkhorn resulting from the dual problem

In this section, we will explain our first try to find a quantum equivalent to Sinkhorn Algorithm.
The regularized problem related to the quantum optimal transport problem can be written as

$$T_C^{Q,\lambda}(\rho^A, \rho^B) = \min_{X \in \Gamma^Q(\rho^A, \rho^B)} Tr(CX^T) + \frac{1}{\lambda} h(X) \quad \textbf{(P)}$$

Where

$$h(X) = X \log X := \sum_{i \in [n]} x_i \log x_i$$

such that $(x_i)_i$ are the eigenvalues of X. The lagrangian of this problem can be written as

$$\begin{aligned} L^{Q,\lambda}(X, \alpha^A, \alpha^B) &= \langle C,\, X\rangle - \langle \alpha^A,\, Tr_B(X) - \rho^A\rangle - \langle \alpha^B,\, Tr_A(X) - \rho^B\rangle + \frac{1}{\lambda}h(X) \\ &= \langle C,\, X\rangle - \langle \alpha^A,\, Tr_B(X)\rangle - \langle \alpha^B,\, Tr_A(X)\rangle + \langle \alpha^A,\, \rho^A\rangle + \langle \alpha^B,\, \rho^B\rangle + \frac{1}{\lambda}h(X) \\ &= \langle C,\, X\rangle - \langle \alpha^A \otimes I,\, X\rangle - \langle I \otimes \alpha^B,\, X\rangle + \langle \alpha^A,\, \rho^A\rangle + \langle \alpha^B,\, \rho^B\rangle + \frac{1}{\lambda}h(X) \\ &= \langle C - \alpha^A \otimes I - I \otimes \alpha^B,\, X\rangle + \frac{1}{\lambda}h(X) + \langle \alpha^A,\, \rho^A\rangle + \langle \alpha^B,\, \rho^B\rangle \end{aligned}$$

The dual problem can be then written as

$$\sup_{\alpha^A, \alpha^B \in \mathcal{M}_n(\mathbb{C})} \inf_{X \succeq 0} L^{Q,\lambda}(X, \alpha^A, \alpha^B)$$

The function $\hat{L} : X \longmapsto L^{Q,\lambda}(X, \alpha^A, \alpha^B)$ has an infinite derivative at the boundary of the cone of semi definite positive matrices, hence $\hat{L}$ necessarily reaches its minimum in the interior of the cone of semi definite positive matrices.

To prove this result, we consider matrix X in the boundary of $S_{n^2}^{+}(\mathbb{C})$, i.e. $X = \sum_{k=1}^{r} u_i u_i^T$ where $k < n^2$ and $(u_1, ..., u_k)$ is an orthonormal family. Let us assume the the minimum of h is reached at X. Let $\bar{X}$ be a matrix in $S_{n^2}^{++}(\mathbb{C})$, we have

$$\frac{h(X + t\bar{X}) - h(X)}{t} \xrightarrow[t \to 0^+]{} -\infty$$

By taking $t > 0$ small enough such that $\frac{h(X+t\bar{X})-h(X)}{t} = \alpha < 0$, we can see that $h(X + t\bar{X}) < h(X)$, a contradiction.
Once this result proven, we can say the $\hat{L}$ reaches its minimum in a matrix $\hat{X}$ in $S_{n^2}^{++}(\mathbb{C})$, and that

$$\frac{\partial \hat{L}}{\partial X}(\hat{X}) = 0$$

i.e.

$$C - \alpha^A \otimes I - I \otimes \alpha^B + \frac{1}{\lambda}(\log \hat{X} + I) = 0$$

i.e.

$$\hat{X} = exp(-I - \lambda(C - \alpha^A \otimes I - I \otimes \alpha^B))$$

The dual problem can then be rewritten as

$$\sup_{\alpha^A, \alpha^B \in \mathcal{M}_n(\mathbb{C})} L^{Q,\lambda}(\hat{X}, \alpha^A, \alpha^B)$$

Where

$$\begin{aligned}
L^{Q,\lambda}(\hat{X},\alpha^A,\alpha^B) &= \left\langle C-\alpha^A\otimes I - I\otimes\alpha^B,\ \hat{X}\right\rangle + \frac{1}{\lambda}h(\hat{X}) + \langle\alpha^A,\ \rho^A\rangle + \langle\alpha^B,\ \rho^B\rangle \\
&= \left\langle -\frac{1}{\lambda}(I+\log\hat{X}),\ \hat{X}\right\rangle + \frac{1}{\lambda}\left\langle\hat{X},\ \log\hat{X}\right\rangle + \langle\alpha^A,\ \rho^A\rangle + \langle\alpha^B,\ \rho^B\rangle \\
&= -\frac{1}{\lambda}\left\langle I,\ \hat{X}\right\rangle + \langle\alpha^A,\ \rho^A\rangle + \langle\alpha^B,\ \rho^B\rangle \\
&= \langle\alpha^A,\ \rho^A\rangle + \langle\alpha^B,\ \rho^B\rangle - Tr(exp(-I-\lambda(C-\alpha^A\otimes I - I\otimes\alpha^B)))
\end{aligned}$$

We hence obtain the following form for the dual problem

$$\sup_{\alpha^A,\alpha^B\in\mathcal{M}_n(\mathbb{C})} \quad \langle\alpha^A,\ \rho^A\rangle + \langle\alpha^B,\ \rho^B\rangle - Tr(exp(-I-\lambda(C-\alpha^A\otimes I - I\otimes\alpha^B))) \qquad \textbf{(D)}$$

The only thing left to prove now is that the primal and dual problem are equivalent. In a similar way as the proof of corollary 2.3 in [1], using strong duality theorem in the case of strictly qualified constraints, we have the following proposition:

Proposition 3.1.

If the set of constraints of problem (P) is strictly feasible, i.e. there exists $\rho\succ 0$ such that $Tr_A(\rho)=\rho^B$ and $Tr_B(\rho)=\rho^A$, then $val(P)=val(D)$ and the two following propositions are equivalent

1. ρ is an optimal solution of (P)
2. $\rho\in\Gamma^Q(\rho^A,\rho^B)$ and there exists $\alpha^A,\alpha^B\in\mathcal{M}_n(\mathbb{C})$ such that

$$\rho = exp(-I-\lambda(C-\alpha^A\otimes I - I\otimes\alpha^B))$$

We consider $f_A:\mathcal{M}_n(\mathbb{C})\times\mathcal{M}_n(\mathbb{C})\longrightarrow\mathcal{M}_n(\mathbb{C})$ and $f_B:\mathcal{M}_n(\mathbb{C})\times\mathcal{M}_n(\mathbb{C})\longrightarrow\mathcal{M}_n(\mathbb{C})$ such that for all $\alpha^A,\alpha^B\in\mathcal{M}_n(\mathbb{C})$

$$\begin{aligned}
f_A(\alpha^A,\alpha^B) &= Tr_A(exp(-I+\lambda(C+\alpha^A\otimes I + I\otimes\alpha^B))) \\
f_B(\alpha^A,\alpha^B) &= Tr_B(exp(-I+\lambda(C+\alpha^A\otimes I + I\otimes\alpha^B)))
\end{aligned}$$

Taking this proposition 3.1 into account, we would like to solve the following system of equations

$$\begin{cases} f_A(\alpha^A,\alpha^B) &= \rho_B \\ f_B(\alpha^A,\alpha^B) &= \rho_A \end{cases}$$

In order to do that, we are getting inspired from the Sinkhorn Algorithm. We define the two sequence of matrices $(\alpha^{Ak})_k$ and $(\alpha^{Bk})_k$, such that

$$\begin{cases} \alpha_0^A,\alpha_0^B\in\mathcal{M}_n(\mathbb{C}) \\ \alpha_{k+1}^A = \alpha \text{ s.t. } f_B(\alpha,\alpha_k^B)=\rho^A \\ \alpha_{k+1}^B = \alpha \text{ s.t. } f_A(\alpha_{k+1}^A,\alpha)=\rho^B \end{cases}$$

Before trying to prove that this sequence indeed converges to a solution of our system of equations, we tried to see first if it is the case in practice.
In the figure above, d_k is used to see how well the algorithm converges and is defined as

$$d_k = \|f_A(\alpha_k^A,\alpha_k^B)-\rho^B\| + \|f_B(\alpha_k^A,\alpha_k^B)-\rho^A\|$$

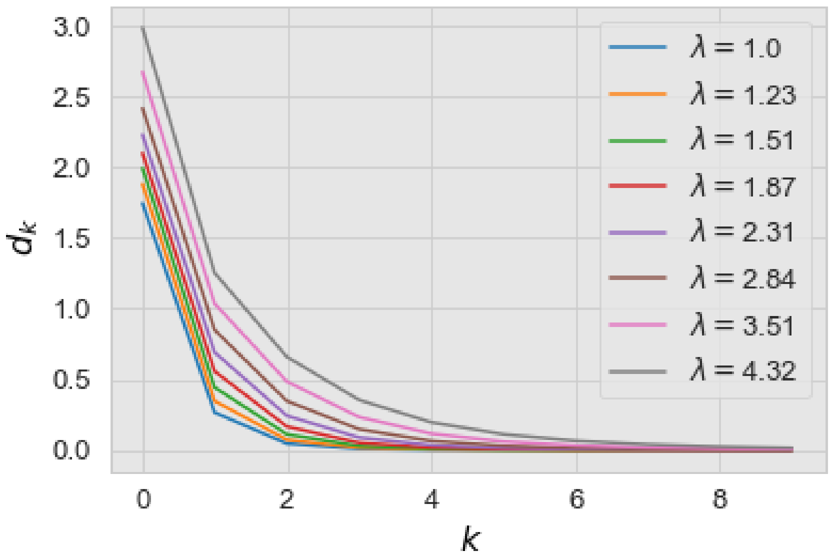

Figure 1: Testing algorithm convergence for different values of λ.

The simulations were made in the case $n = 4$. The cost matrix C and marginals ρ^A, ρ^B were initialized randomly and α_0^A, α_0^B were taken equal to 0.
This algorithm was simulated bu using Python's `scipy.optimize.root` to solve the two equations at each iteration. Simulations show that the algorithm indeed converges. However, we are seeking for solutions for big values of λ, and it seems convergence gets more difficult as λ gets bigger.
Noting for all $k \in \mathbb{N}$, $\alpha_{k+1}^A = \varphi(\alpha_k^B)$ and $e^{\alpha_{k+1}^A} = \psi(e^{\alpha_k^B})$, our houpe was to find that either φ or ψ were decreasing for Loewener order, or stricly contracting for the following metric on the cone of positive definite matrices

$$d_H(A, B) := \sup \log Spec(A^{-1}B) - \inf \log Spec(A^{-1}B)$$

i.e. we can find a real number $k \in [0, 1]$ such that for all $A, B \in \mathcal{S}_n^+(\mathbb{C})$

$$d_H(\varphi(A), \varphi(B)) \leq k d_H(A, B)$$

unfortunately, none of the two properties above are true. Simulations show that neither φ or ψ are decreasing and φ is not a contracting application for the metric d_H.
In figure 2, A and B for each value of λ, we use 50 random samples of A and B.

3.2.2 Independent Sinkhorn Algorithm

Knowing the correspondence between completely completely positive linear maps and bipartite density matrices, we started exploring the scaling problem in the space of completely positive linear matrices independently of the quantum optimal transport problem. We denote the set of completely positive linear maps from $\mathcal{M}_n(\mathbb{C})$ to $\mathcal{M}_m(\mathbb{C})$ as $CP_{n,m}$. Operators in $CP_{n,m}$ can be written as follows: for all $X \in \mathcal{M}_n(\mathbb{C})$,

$$T(X) = \sum_{i=1}^{r} V_i X V_i^*$$

Where for all i, $V_i \in \mathcal{M}_n(\mathbb{C})$. We also define T^* as

$$T^*(X) = \sum_{i=1}^{r} V_i^* X V_i$$

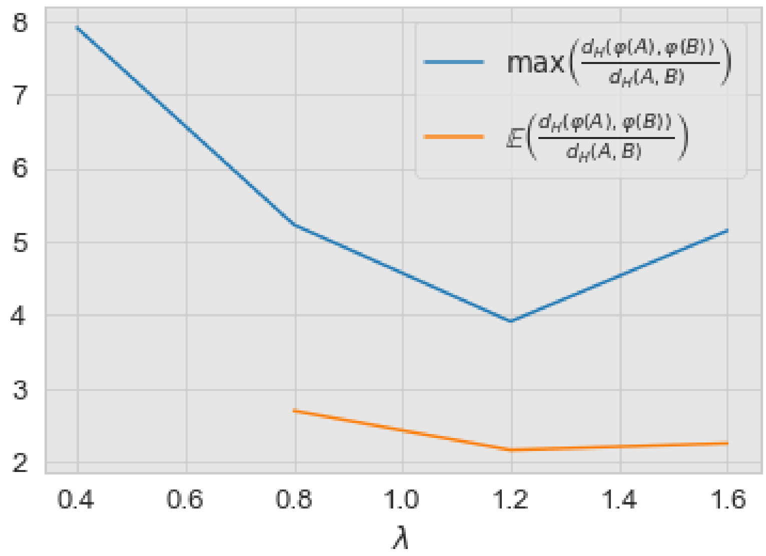

Figure 2: Computing $\frac{d_H(\varphi(A),\varphi(B))}{d_H(A,B)}$ for different values of λ

We would like to study the following scaling problem stated in [3].
We define the scaling operator S, given C_1 and C_2 by the following: for all $T \in CP_{n,m}$

$$S_{C_1,C_2}(T) = C_1 T(C_2^* X C_2) C_1^*$$

Given $T \in CP_{n,m}$, find $C_1, C_2 \in \mathcal{M}_n(\mathbb{C})$ such that

$$S_{C_1,C_2}(T)(I) = I \text{ and } S_{C_1,C_2}(T^*)(I) = I$$

The two equalities above can be rewritten as

$$C_1 = (T(C_2 C_2^*))^{-1/2} \text{ and } C_2 = (T^*(C_1 C_1^*))^{-1/2}$$

i.e.

$$C_1 C_1^* = (T(C_2 C_2^*))^{-1} \text{ and } C_2 C_2^* = (T^*(C_1 C_1^*))^{-1}$$

Those two equalities gave us the idea of an iterative algorithm. In order to do that, we define the operator F by the following:

$$\forall X \in S_n^+(\mathbb{C}),\; F(X_1, X_2) = (T(X_2)^{-1}, (T^*(X_1))^{-1})$$

The iterative consists of computing a sequence $(X_n)_n = (X_1^n, X_2^n)_{n\in\mathbb{N}}$ defined by:

$$\begin{cases} X_0 \in \mathcal{S}_n^+(\mathbb{C}) \times \mathcal{S}_n^+(\mathbb{C}) \\ X_{n+1} = F(X_n) \end{cases}$$

Simulations in Python show that this sequence indeed converges and that if we take $C_1 = X_1^{n1/2}$ and $C_2 = X_2^{n1/2}$ for n large enough, obtain that

$$S_{C_1,C_2}(T)(I) \simeq I \text{ and } S_{C_1,C_2}(T^*)(I) \simeq I$$

4 Conclusion and next steps

In this first step of this project, three main conclusions can be made:

1. The extremal points of $\Gamma^Q(\rho^A, \rho^B)$ can be easily expressed in an explicit way when $n = 2$, however, for higher values of n, even though there is a characterisation of extremal points using Choi's representation, it does not seem easy to write $EXTR(\Gamma^Q(\rho^A, \rho^B))$ in a more explicit way.

2. We attempted to find a quantum version of the Sinkhorn algorithm by using the dual version of the Quantum Optimal transport problem, but eventually found out that both functions φ and ψ are not monotonous nor contracting, which makes it complicated to have a theoretical proof of the convergence of our first quantum Sinkhorn algorithm.

3. We are currently studying another version of Sinkhorn's algorithm suggested by [3]. Simulations show that we can indeed empirically solve the scaling problem for marginals equal to the identity matrix. We are planning to see if it is possible to do the same for marginals other than I and prove the convergence theoretically.

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