QUANTUM WASSERSTEIN ISOMETRIES OF N-QUBIT STATE SPACES WITH RESPECT TO THE SYMMETRIC TRANSPORT COST

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ABSTRACT. I was introduced to the topic of quantum optimal transport by my supervisor last semester for my BSc thesis. The aim of this report is to provide a brief introduction to the theory of classical and quantum optimal transport and quantum Wasserstein isometries. After describing the main setup and the preliminaries, we focus on the new results of this semester. We give the spectral decomposition of the symmetric cost operator generated by the Pauli matrices in the n-qubit space. We also give a Wigner-type characterization of quantum Wasserstein isometries with respect to the symmetric cost.

1. INTRODUCTION

1.1. **Motivation and history.** The classical optimal transport problem was first introduced by the French mathematician Gaspard Monge in 1781, then reformulated and improved by Soviet mathematician and economist Leonid Kantorovich in the 1940s. He used linear programming to solve the problem and found a dual formulation. Since then, optimal transport theory has become a wide resarch topic in functional analysis with various application areas not only within mathematics, but also in fluid mechanics, machine learning, image processing and economics.

Translating the optimal transport problem into the formalism of quantum mechanics raises numerous new questions and enables various applications e.g. in quantum information theory.

Among the several possible approaches, we use the one with quantum channels introduced by De Palma and Trevisan in [1].

1.2. **The classical optimal transport problem.** Let us consider a country with factories that produce a product and shops that sell it. We are given the production quantities of each factory, the demand of each store and the cost of transporting one unit of the product from each factory to each store. Our aim is to find a suitable transport plan with minimal transport cost.

The measures spaces $(X, \mathcal{A}_X, \mu)$ and $(Y, \mathcal{A}_Y, \nu)$ describe the initial distribution of products on set X and the required final distribution of products on set Y, respectively [3].

The cost function $c(x, y) : X \times Y \to \overline{\mathbb{R}}_+$ describes the cost of transporting unit mass of the product from location x to location y.

Definition 1 (Transport plan). *A transport plan between the probability measures $\mu \in Prob(X)$ and $\nu \in Prob(Y)$ is a probability measure $\pi \in Prob(X \times Y)$ such that*

$$\int_Y d\pi(x,y) = d\mu(x) \text{ and } \int_X d\pi(x,y) = d\nu(y).$$

The transport cost corresponding to a probability measure π is

$$I[\pi] := \int_{X\times Y} c(x,y) d\pi(x,y).$$

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With $\Pi(\mu,\nu)$ denoting the set of transport plans from μ to ν, the goal is finding

$$\inf_{\pi\in\Pi(\mu,\nu)}\left(\int_{X\times Y} c(x,y)d\pi(x,y)\right).$$

If $X=Y$ and the cost function $c(x,y):=d(x,y)^p$ is a power of a metric, then a metric function between probability measures on X can be defined as

$$W_p(\mu,\nu):=\inf_{\pi\in\Pi(\mu,\nu)}\left(\int_{X\times X} d(x,y)^p d\pi(x,y)\right)^{1/p}.$$

This metric is called the Wasserstein distance of order p for any $p\geq 1$.

2. Quantum optimal transport

For reformulating the transport problem in the framework of quantum mechanics, we need the Pauli matrices, which are four 2×2 complex matrices that form a basis of the 2×2 Hermitian matrices over the real numbers and also a basis of all 2×2 complex matrices over the complex numbers.

$$\sigma_0=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad \sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

The underlying set of the quantum optimal transport problem is a Hilbert space $\mathcal{H}$, we investigate the case $\mathcal{H}=\mathbb{C}^{2^n}$. The set of quantum states on the Hilbert space $\mathbb{C}^{2^n}$ is

$$\mathcal{S}\left(\mathbb{C}^{2^n}\right)=\left\{\varrho\in\mathcal{L}\left(\mathbb{C}^{2^n}\right):\varrho\geq 0,\mathrm{tr}[\varrho]=1\right\}.$$

A state $\varrho\in\mathcal{S}\left(\mathbb{C}^{2^n}\right)$ is called a pure state if it is a rank 1 projection, i.e. there exists a unit vector $\psi\in\mathbb{C}^{2^n}$ such that $\varrho=|\psi\rangle\langle\psi|$. The set of pure states is $\mathcal{P}_1\left(\mathbb{C}^{2^n}\right)$.

Definition 2 (Partial trace)**.** *With $\mathcal{H}=\mathbb{C}^{2^n}$ and $\Pi\in\mathcal{L}(\mathcal{H}\otimes\mathcal{H}^*)$ the partial traces $tr_{\mathcal{H}}[\Pi]\in\mathcal{L}(\mathcal{H}^*)$ and $tr_{\mathcal{H}^*}[\Pi]\in\mathcal{L}(\mathcal{H})$ are linear operator such that*

$$tr_{\mathcal{H}}[tr_{\mathcal{H}^*}[\Pi]A]=tr_{\mathcal{H}\otimes\mathcal{H}^*}[\Pi(A\otimes I_{\mathcal{H}^*})] \text{ and } tr_{\mathcal{H}^*}[tr_{\mathcal{H}}[\Pi]A^T]=tr_{\mathcal{H}\otimes\mathcal{H}^*}[\Pi(I_{\mathcal{H}}\otimes A^T)] \text{ for all } A\in\mathcal{L}(\mathcal{H}).$$

For a linear operator $A\in\mathcal{L}(\mathcal{H})$ the notation $||A\rangle\rangle$ stands for its corresponding vector in $\mathcal{H}\otimes\mathcal{H}^*$ with respect to the canonical isomorphism $|\psi\rangle\langle\varphi|\leftrightarrow|\psi\rangle\otimes\langle\varphi|$ between $\mathcal{L}(\mathcal{H})$ and $\mathcal{H}\otimes\mathcal{H}^*$.

The set of couplings of states $\varrho,\omega\in\mathcal{S}(\mathcal{H})$ is defined as

$$C(\varrho,\omega)=\left\{\Pi\in\mathcal{S}(\mathcal{H}\otimes\mathcal{H}^*):\mathrm{tr}_{\mathcal{H}^*}[\Pi]=\omega,\mathrm{tr}_{\mathcal{H}}[\Pi]=\varrho^T\right\}.$$

The quantum Wasserstein distance of states ϱ and ω with respect to a cost operator C is defined as

$$D_C(\varrho,\omega)=\left(\inf_{\Pi\in C(\varrho,\omega)}\mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}^*}[\Pi C]\right)^{1/2}.$$

Definition 3 (Quantum Wasserstein isometry)**.** *A map $\Phi:\mathcal{S}(\mathcal{H})\to\mathcal{S}(\mathcal{H})$ is an isometry of the quantum Wasserstein distance D_C if*

$$D_C(\Phi(\varrho),\Phi(\omega))=D_C(\varrho,\omega)$$

holds for all states $\varrho,\omega\in\mathcal{S}(\mathcal{H})$.

3. New results

3.1. **Spectral decomposition of the symmetric cost operator.**

In the 2-dimensional case the symmetric cost operator is defined as

$$C^{(1)}_{\text{sym}} = \sum_{j=1}^{3} \left(\sigma_j \otimes I^T - I \otimes \sigma_j^T\right)^2 .$$

By simple direct calculations we obtain

$$C^{(1)}_{\text{sym}} = 8 \cdot \left(\frac{1}{2} \cdot \sum_{j=1}^{3} ||\sigma_j\rangle\rangle \, \langle\langle\sigma_j|| \right).$$

We define the symmetric cost operator analogously for the 2^n-dimensional case, but for computational convenience, we do not omit the term with only σ_0 matrices,

Definition 4 (2^n-dimensional symmetric cost operator)**.**

$$C^{(n)}_{sym} = \sum_{j_1,\dots,j_n=0}^{3} \left((\sigma_{j_1} \otimes \dots \otimes \sigma_{j_n}) \otimes I^T_{2^n} - I_{2^n} \otimes (\sigma_{j_1} \otimes \dots \otimes \sigma_{j_n})^T\right)^2 .$$

We derive the spectral decomposition form of the symmetric cost operator to provide an upper limit for the quantum Wasserstein distance of two arbitrary states.

Theorem 1.

$$C^{(n)}_{sym} = 2 \cdot 4^n \cdot I_{2^n} \otimes I^T_{2^n} - 2 \cdot 4^n \cdot \frac{1}{2^n} \, ||I_{2^n}\rangle\rangle \, \langle\langle I_{2^n}|| \, .$$

Corollary 2.

$$C^{(n)}_{sym} \leq 2 \cdot 4^n \cdot I_{2^n} \otimes I^T_{2^n},$$

where $\leq$ stands for the Loewner order.

The quantum Wasserstein distance of two states $\varrho, \omega \in \mathcal{S}\left(\mathbb{C}^{2^n}\right)$ can be estimated from above by taking the transport cost with respect to the trivial coupling $\omega \otimes \varrho^T$, which yields the following inequality.

Corollary 3.

$$\left(D^{(n)}_{sym}(\varrho, \omega)\right)^2 \leq 2 \cdot 4^n \quad \forall \varrho, \omega \in \mathcal{S}\left(\mathbb{C}^{2^n}\right).$$

We are interested in the pairs of states that realise the maximal possible quantum Wasserstein distance.

Definition 5 (Diameter of a qubit state space)**.**

$$diam\left(\mathcal{S}\left(\mathbb{C}^{2^n}\right), D_{sym}\right) = \sup_{\varrho,\omega\in\mathcal{S}(\mathbb{C}^{2^n})} D_{sym}(\varrho, \omega).$$

We obtained the last corollary by explicitly calculating the transport cost for the trivial coupling $\omega \otimes \varrho^T$:

$$\operatorname{tr}\left[C^{(n)}_{\text{sym}}(\omega \otimes \varrho^T)\right] = 2 \cdot 4^n \left(1 - \frac{1}{2^n} \operatorname{tr}\left[\omega\varrho\right]\right),$$

which yields the following corollary.

Corollary 4.

$$\left(D^{(n)}_{sym}(\varrho, \omega)\right)^2 = 2 \cdot 4^n \implies tr\left[\omega\varrho\right] = 0.$$

If at least one of the states is pure, the only coupling is the trivial, so the converse implication is also true.

3.2. **A Wigner-type characterization.** Our following result states that a state ϱ is pure if and only if there exists a 2^n-simplex in the space of states with maximal quantum Wasserstein distance between all its vertices and one of its vertices being ϱ.

Theorem 5. *For any state $\varrho \in \mathcal{S}(\mathbb{C}^{2^n})$ the following are equivalent:*

(i) $\varrho \in \mathcal{P}_1(\mathbb{C}^{2^n})$, i.e. ϱ is pure

(ii) $\exists \varrho_1 \varrho_2, \ldots, \varrho_{2^n-1} \in \mathcal{S}(\mathbb{C}^{2^n})$ such that

$$D_{sym}(\varrho_j, \varrho_k) = diam\left(\mathcal{S}(\mathbb{C}^{2^n}), D_{sym}\right)$$

for any $j \neq k \in \{0, 1, \ldots, 2^n - 1\}$ with $\varrho_0 = \varrho$.

Corollary 6. *If $\Phi : \mathcal{S}(\mathbb{C}^{2^n}) \to \mathcal{S}(\mathbb{C}^{2^n})$ is a D_{sym}-isometry, then Φ maps pure states to pure states.*

Definition 6. *An operator $T : \mathcal{S}(\mathbb{C}^{2^n}) \to \mathcal{S}(\mathbb{C}^{2^n})$ is a symmetry transformation if it preserves transition probabilities, i.e.*

$$tr[T(\varrho)T(\omega)] = tr[\varrho\omega] \quad \text{for all } \varrho, \omega \in \mathcal{S}(\mathbb{C}^{2^n}).$$

Theorem 7 (Wigner theorem)**.** *If $T : \mathcal{S}(\mathbb{C}^{2^n}) \to \mathcal{S}(\mathbb{C}^{2^n})$ is a symmetry transformation, then there exists a unitary or anti-unitary operator U such that*

$$T(\varrho) = U\varrho U^\dagger \quad \text{for all } \varrho \in \mathcal{S}(\mathbb{C}^{2^n}).$$

The following theorem gives a characterisation of D_{sym}-isometries in $\mathcal{S}(\mathbb{C}^{2^n})$, which is the generalisation of the previous result for the case $n = 1$ in [2].

Theorem 8. *Let $\Phi : \mathcal{S}(\mathbb{C}^{2^n}) \to \mathcal{S}(\mathbb{C}^{2^n})$ be a map.*

The following are equivalent:

(i) Φ is a D_{sym}-isometry

(ii) there exists a unitary or anti-unitary operator U such that

$$\Phi(\varrho) = U\varrho U^\dagger \quad \text{for all } \varrho \in \mathcal{S}(\mathbb{C}^{2^n}).$$

4. Conclusion and future goals

During the semester, the focus of the research was the characterisation of the isometries with respect to the symmetric cost operator in n-qubit state spaces.

It is an interesting phenomenon on the single qubit state space that removing one Pauli matrix from the set of generators of the cost operator makes the structure of quantum Wasserstein isometries dramatically different [2]. Therefore, one of our most direct future goals is to consider cost operators on n-qubit systems that are generated by a subset of all tensor products of Pauli operators. Furthermore, we plan to study quantum Wasserstein isometries on systems where the dimension of the underlying Hilbert space is not a power of two, and we will make steps towards infinite-dimensional generalizations of our n-qubit results, as well.

References

[1] Giacomo De Palma and Dario Trevisan. Quantum optimal transport with quantum channels. In *Annales Henri Poincaré*, volume 22, pages 3199–3234. Springer, 2021.

[2] György Pál Gehér, József Pitrik, Tamás Titkos, and Dániel Virosztek. Quantum Wasserstein isometries on the qubit state space. *J. Math. Anal. Appl.*, 522:126955, 2023.

[3] Cédric Villani. *Topics in optimal transportation*, volume 58. American Mathematical Soc., 2021.