Quantum Wasserstein distance based on an optimization over separable states
Quantum 7, 914 (2023)

G. Tóth[1,2,3,4,5] and J. Pitrik[5,6,7]

[1]University of the Basque Country UPV/EHU, Bilbao, Spain
[2]EHU Quantum Center, University of the Basque Country UPV/EHU, Spain
[3]Donostia International Physics Center (DIPC), San Sebastián, Spain
[4]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain
[5]Wigner Research Centre for Physics, Budapest, Hungary
[6]Alfréd Rényi Institute of Mathematics, Budapest, Hungary
[7]Department of Analysis,Budapest University of Technology and Economics, Budapest, Hungary

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Outline

1. **Motivation**
   - Connecting Wasserstein distance to entanglement theory

2. **Background**
   - Quantum Wasserstein distance
   - Quantum Fisher information

3. **Wasserstein distance and separable states**
   - Quantum Wasserstein distance based on an optimization over separable states
   - Relation to entanglement conditions

Motivation

- Many distance measures are maximal for orthogonal states.
- Recently, the Wasserstein distance appeared, which is different and this makes it very useful.
- For the quantum case, surprisingly, the self-distance can be nonzero.
- Can we connect these to entanglement theory and/or quantum metrology?

Outline

Classical Wasserstein distance - a very long past

- Monge, 1781;
  Kantorovich, Nobel Memorial Prize in Economic Sciences, 1975.

- Distance between probability distributions defined as

$$W_p(\mu, \nu) = \left(\min_{\pi} \int d(x, y)^p \pi(x, y) dxdy \right)^{1/p},$$

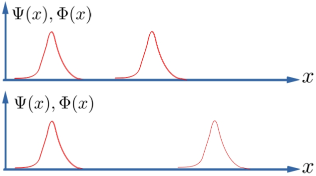
  where $d(x, y)$ is the distance of x and y, $\pi(x, y)$ is a distribution with marginals $\mu(x)$ and $\nu(y)$, p is a number, and $p = 2$ is a good choice.

- "cost of moving sand from a distribution to the other one."

- Used in very many applications in machine learning, engineering, various optimization problems.

Quantum Wasserstein distance - recent efforts

- Many distance measures are maximal for orthogonal states, e.g., for the following state-pairs.



- In the second example, the two states are further apart from each other, based on common sense.

- The quantum Wasserstein distance should recognize this since it is related to the "cost of moving sand from a distribution to the other one."

- Indeed, because of that the quantum Wasserstein distance can be used for machine learning.

G. De Palma, M. Marvian, D. Trevisan, and S. Lloyd,
IEEE Transactions on Information Theory 67, 6627 (2021).

Quantum Wasserstein distance

- **Definition.**—The square of the distance between two quantum states described by the density matrices ϱ and σ is

$$
\begin{aligned}
D_{\mathrm{DPT}}(\varrho,\sigma)^2 = \frac{1}{2}\min_{\varrho_{12}} \sum_{n=1}^{N} \quad & \mathrm{Tr}[(H_n^T \otimes \mathbb{1} - \mathbb{1} \otimes H_n)^2 \varrho_{12}], \\
\text{s. t.} \quad & \varrho_{12} \in \mathcal{D}, \\
& \mathrm{Tr}_2(\varrho_{12}) = \varrho^T, \\
& \mathrm{Tr}_1(\varrho_{12}) = \sigma,
\end{aligned}
$$

  where $\mathcal{D}$ is the set of density matrices, and H_n are Hermitian matrices.

- Note the relation to the representability problem.

  G. De Palma and D. Trevisan, Quantum optimal transport with quantum channels, Ann. Henri Poincaré 22, 3199 (2021).

  Examples of other approaches: Życzkowski, Slomczynski; Caglioti, Golse, Mouhot, Paul; Bistron, Cole, Eckstein, Friedland, Życzkowski.

Self-distance can be nonzero (unlike in the classical case)

- The self-distance of a state is

$$D_{\mathrm{DPT}}(\varrho,\varrho)^2 = \sum_{n=1}^{N} I_\varrho(H_n),$$

where the Wigner-Yanase skew information is defined as

$$I_\varrho(H) = \mathrm{Tr}(H^2\varrho) - \mathrm{Tr}(H\sqrt{\varrho}H\sqrt{\varrho}).$$

- This connects Wasserstein distance and quantum metrology.

- The classical case corresponds to $[\varrho, H_n] = 0$. For that, $D_{\mathrm{DPT}}(\varrho,\varrho)^2 = 0$.

G. De Palma and D. Trevisan,
Quantum optimal transport with quantum channels,
Ann. Henri Poincaré 22, 3199 (2021).

How to compute the Wasserstein distance?

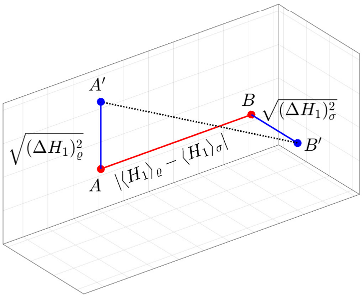
- The distance can be computed by semidefinite programming.
  → This might be the reason that it has appeared recently.

- For a pure ϱ and a mixed σ, the distance is given as

$$D_{\mathrm{DPT}}(\varrho,\sigma)^2$$
$$= \frac{1}{2}\sum_{n=1}^{N}\left[(\Delta H_n)^2{}_{\varrho} + (\Delta H_n)^2{}_{\sigma} + (\langle H_n\rangle_{\varrho} - \langle H_n\rangle_{\sigma})^2\right],$$

  see the following figure, where $(\Delta H_n)^2$ is the variance.

How to compute the Wasserstein distance? II



- $N = 1$, a single operator H_1 is given.
- ϱ is pure, σ is mixed.
- The quantum Wasserstein distance equals $1/\sqrt{2}$ times the usual Euclidean distance between A' and B'.

GT and J. Pitrik,
Quantum Wasserstein distance based on an optimization over separable states,
Quantum 7, 914 (2023).

Recent efforts to prove the triangle inequality

- For any ϱ, τ, and σ the modified triangle inequality holds

$$D_{\mathrm{DPT}}(\varrho, \sigma) \leq D_{\mathrm{DPT}}(\varrho, \tau) + D_{\mathrm{DPT}}(\tau, \tau) + D_{\mathrm{DPT}}(\tau, \sigma).$$

- Conjecture: a modified version of the quantum optimal transport defined by

$$d(\varrho, \omega) := \sqrt{D^2_{\mathrm{DPT}}(\varrho, \omega) - [D^2_{\mathrm{DPT}}(\varrho, \varrho) + D^2_{\mathrm{DPT}}(\omega, \omega)]/2}.$$

  is a metric.

  G. De Palma and D. Trevisan, Ann. Henri Poincaré 22, 3199 (2021).

- Triangle inequality for quantum Wasserstein divergences

$$d(\tau, \varrho) + d(\varrho, \omega) \leq d(\tau, \omega)$$

  holds for any mixed τ, ω, any pure ϱ and any quadratic cost + strong numerical evidence for general states.

  G. Bunth, J. Pitrik, T. Titkos, and D. Virosztek, arxiv:2402.13150.

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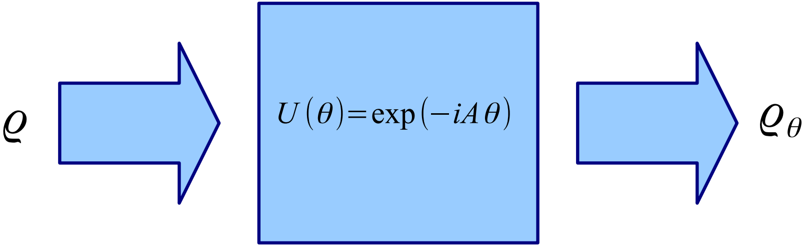
Quantum metrology

- Fundamental task in metrology



- We have to estimate θ in the dynamics

$$U = \exp(-iA\theta).$$

The quantum Fisher information

- Cramér-Rao bound on the precision of parameter estimation

$$(\Delta\theta)^2 \geq \frac{1}{mF_Q[\varrho, A]},$$

where $F_Q[\varrho, A]$ is the quantum Fisher information, and m is the number of independent repetitions.

- The quantum Fisher information is

$$F_Q[\varrho, A] = 2\sum_{k,l} \frac{(\lambda_k - \lambda_l)^2}{\lambda_k + \lambda_l} |\langle k|A|l\rangle|^2,$$

where $\varrho = \sum_k \lambda_k |k\rangle\langle k|$.

Formula based on convex roofs

The quantum Fisher information is the convex roof of the variance times four

$$F_Q[\varrho, A] = 4 \min_{\{p_k, |\psi_k\rangle\}} \sum_k p_k (\Delta A)^2_{\psi_k},$$

where

$$\varrho = \sum_k p_k |\psi_k\rangle\langle\psi_k|.$$

GT, D. Petz, Phys. Rev. A 87, 032324 (2013); S. Yu, arXiv1302.5311 (2013);
GT, I. Apellaniz, J. Phys. A: Math. Theor. 47, 424006 (2014).

Formula based on concave roofs

The variance is the concave roof of itself

$$(\Delta A)^2{}_{\varrho} = \max_{\{p_k,|\psi_k\rangle\}} \sum_k p_k (\Delta A)^2{}_{\psi_k},$$

where

$$\varrho = \sum_k p_k |\psi_k\rangle\langle\psi_k|.$$

GT, D. Petz, Phys. Rev. A 87, 032324 (2013);

GT, I. Apellaniz, J. Phys. A: Math. Theor. 47, 424006 (2014).

A single relation for the QFI and the variance

For any decomposition $\{p_k, |\psi_k\rangle\}$ of the density matrix ϱ we have

$$\frac{1}{4}F_Q[\varrho, A] \leq \sum_k p_k (\Delta A)^2_{\psi_k} \leq (\Delta A)^2_{\varrho},$$

where the upper and the lower bounds are both tight.

- Note that

$$\frac{1}{4}F_Q[\varrho, A] \leq (\Delta A)^2_{\varrho},$$

  where for pure states we have an equality.

- The QFI is strongly related to the variance.

Formula based on an optimization in the two-copy space

- Two-copy formulation for the variance

$$(\Delta H)^2{}_{\Psi} = \mathrm{Tr}(\Omega|\Psi\rangle\langle\Psi| \otimes |\Psi\rangle\langle\Psi|),$$

where we define the operator

$$\Omega = H^2 \otimes \mathbb{1} - H \otimes H.$$

We can reformulate the convex roof as

$$\begin{aligned} F_Q[\varrho, H] = \min_{\varrho_{12}} \quad & 4\mathrm{Tr}(\Omega\varrho_{12}), \\ \text{s. t.} \quad & \varrho_{12} \in \mathcal{S}', \\ & \mathrm{Tr}_2(\varrho_{12}) = \varrho. \end{aligned}$$

Here $\mathcal{S}'$ is the set of symmetric separable states.

GT, T. Moroder, and O. Gühne,
Evaluating convex roof entanglement measures,
Phys. Rev. Lett. 114, 160501 (2015).

Formula based on an optimization in the two-copy space II

We can further reformulate the convex roof as

$$\begin{aligned} F_Q[\varrho, H] = \min_{\varrho_{12}} \quad & 4\mathrm{Tr}[(H^2 \otimes \mathbb{1} - H \otimes H)\varrho_{12}], \\ \text{s. t.} \quad & \varrho_{12} \in \mathcal{S}, \\ & \mathrm{Tr}_2(\varrho_{12}) = \varrho, \\ & \mathrm{Tr}_1(\varrho_{12}) = \varrho. \end{aligned}$$

Here $\mathcal{S}$ is the set of separable states.

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Quantum Wasserstein distance based on an optimization over separable states

- **Definition**—We can also define

$$D_{\rm sep}(\varrho,\sigma)^2 = \frac{1}{2}\min_{\varrho_{12}} \sum_{n=1}^{N} \quad {\rm Tr}[(H_n^T \otimes \mathbb{1} - \mathbb{1} \otimes H_n)^2 \varrho_{12}],$$

$$\text{s. t.} \quad \varrho_{12} \in \mathcal{S},$$

$$\mathrm{Tr}_2(\varrho_{12}) = \varrho^T,$$

$$\mathrm{Tr}_1(\varrho_{12}) = \sigma,$$

where $\mathcal{S}$ is the set of separable states.

GT and J. Pitrik,
Quantum Wasserstein distance based on an optimization over separable states,
Quantum 7, 914 (2023).

Quantum Wasserstein distance based on an optimization over separable states II

- For two-qubits, it is computable numerically with semidefinite programming.
- For systems of larger dimensions, one can obtain a very good lower bound based on an optimization over states with a positive partial transpose (PPT).
- Even better lower bounds can be obtained.

P. Horodecki, Phys. Lett. A 232, 333 (1997);
A. Peres, Phys. Rev. Lett. 77, 1413 (1996);
A. C. Doherty, P. A. Parrilo, and F. M. Spedalieri, Phys. Rev. A 69, 022308 (2004).

Self-distance

- The self-distance for $N = 1$ is

$$D_{\rm sep}(\varrho,\varrho)^2 = \frac{1}{4} F_Q[\varrho, H_1].$$

- Note that

$$I_\varrho(A) \le \frac{1}{4} F_Q[\varrho, A] \le (\Delta A)^2{}_\varrho.$$

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Entanglement of ϱ_{12}

- In general,

$$D_{\rm sep}(\varrho,\sigma)\geq D_{\rm DPT}(\varrho,\sigma).$$

- If the relation

$$D_{\rm sep}(\varrho,\sigma)>D_{\rm DPT}(\varrho,\sigma)$$

  holds, then all the optimal ϱ_{12} couplings for $D_{\rm DPT}(\varrho,\sigma)$ are entangled.

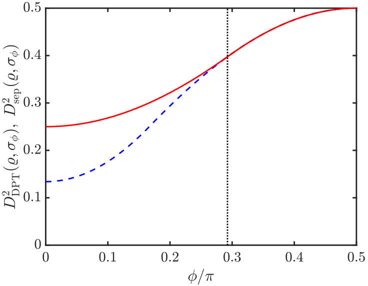
- Thus, an entangled ϱ_{12} can be cheaper than a separable one.

Comparison of the two types of Wasserstein distance

- Let us consider the distance between two single-qubit mixed states
$$\varrho = \frac{1}{2}|1\rangle\langle 1|_x + \frac{1}{2}\cdot\frac{\mathbb{1}}{2},$$
and
$$\sigma_\phi = e^{-i\frac{\sigma_y}{2}\phi}\varrho e^{+i\frac{\sigma_y}{2}\phi},$$
and
$$H_1 = \sigma_z.$$

$F_Q[\varrho,\sigma_z]/4 = 0.25 \rightarrow$

$I_\varrho(\sigma_z) \approx 0.13 \rightarrow$



Bounds on the distance

- Entanglement condition: Let us choose a set of H_n such that

$$\frac{1}{2}\sum_n \left\langle (H_n^T \otimes \mathbb{1} - \mathbb{1} \otimes H_n)^2 \right\rangle \geq \text{const.}$$

  holds for separable states.

- E. g., $\{H_n\} = \{j_x, j_y, j_z\}$ and "const."$= j$.

- If the inequality

$$D_{\text{DPT}}(\varrho, \sigma)^2 < \text{const.}$$

  holds, then all optimal ϱ_{12} states for $D_{\text{DPT}}(\varrho, \sigma)$ are entangled.

- Then, we will have a minimal distance

$$D_{\text{sep}}(\varrho, \sigma)^2 \geq \text{const.}$$

Summary

- For the quantum Wasserstein distance, we restrict the optimization to separable states.
- Then, the self-distance equals the quantum Fisher information over four.
- We found a fundamental connection from quantum optimal transport to quantum entanglement theory and quantum metrology.

G. Tóth and J. Pitrik, Quantum 7, 914 (2023).

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