Un invito al Trasporto Ottimo Quantistico[1]

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[1] Based on joint works with G. De Palma, M. Marvian, S. Lloyd, T. Titkos and D. Virosztek

Outline

Plan

Monge's transport problem

Monge (1781): *sur la théorie des déblais et des remblais*.

How to transport soil during a construction with minimal expenses?

The assignment problem

A discrete formulation: given a

- cost $c(x, y)$ of moving unit of soil from position x to position y, e.g.

$$c(x, y) = |x - y|,$$

- Source distribution of soil $\sigma = (\sigma(x_i))_i$
- Target distribution (dump) $\rho = (\rho(y_j))_j$

Find $T : \{x_i\} \to \{y_j\}$ that moves σ into ρ with minimal transport cost

$$\sum_i c(x_i, T(x_i))\sigma(x_i).$$

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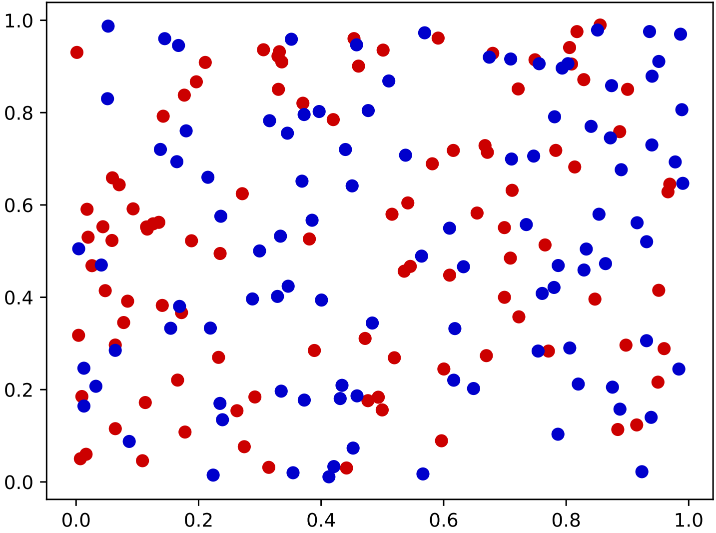
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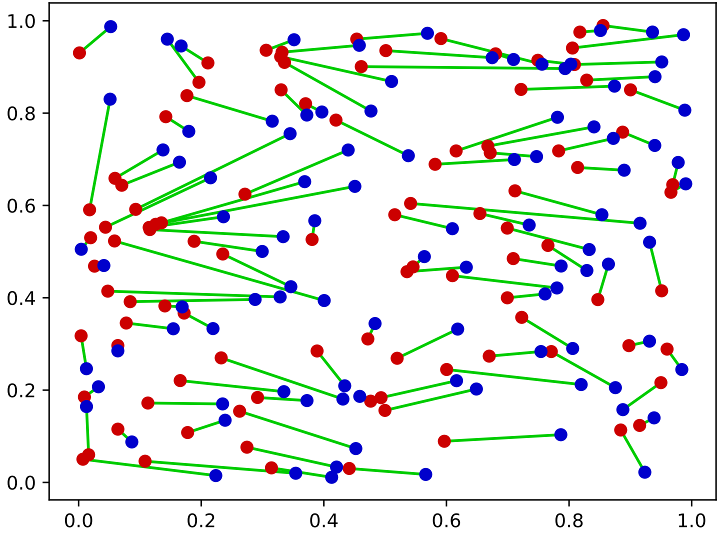

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Kantorovich and linear programming

Relax the map T to a transport plan

$$T(x_i, y_j) \geq 0$$

such that

$$\sum_j T(x_i, y_j) = \sigma(x_i), \quad \sum_i T(x_i, y_j) = \rho(y_j).$$

Probabilistic intepretation:

$$K(y_j|x_i) := \frac{T(x_i, y_j)}{\sigma(x_i)} \in [0, 1].$$

The variational problem becomes

$$\min_T \sum_i \sum_j c(x_i, y_j) T(x_i, y_j)$$

$\Rightarrow$ linear programming!

From soil to probabilities

- For a transport plan T it must be

$$\sum_i \sigma(x_i) = \sum_i \sum_j T(x_i, y_j) = \sum_j \sum_i T(x_i, y_j) = \sum_j \rho(y_j).$$

- We assume that ρ, σ are probability mass functions (discrete densities):

$$\sum_i \sigma(x_i) = \sum_j \rho(y_j) = 1.$$

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Earth Mover's distance and duality

- If $c(x, y) = d(x, y)$ is a distance, then

$$W_1(\sigma, \rho) = \min_T \sum_i \sum_j d(x_i, y_j) T(x_i, y_j)$$

induces a distance (Wasserstein-Kantorovich, Earth Mover's).

- Kantorovich duality:

$$W_1(\sigma, \rho) = \max \left\{ \sum_i f(x_i)\sigma(x_i) - \sum_j f(y_j)\rho(y_j) \ : \ |f(x) - f(y)| \le d(x, y) \right\}.$$

- Buy at price $f(y_j)$ and sell at price $f(x_i)$ $\Rightarrow$ maximize the profit!

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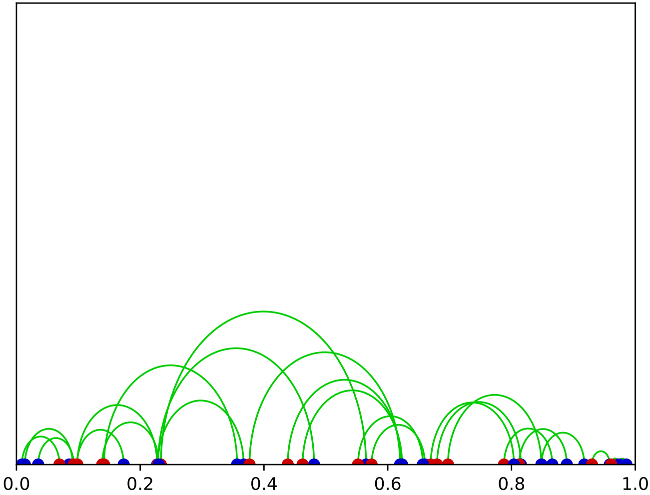
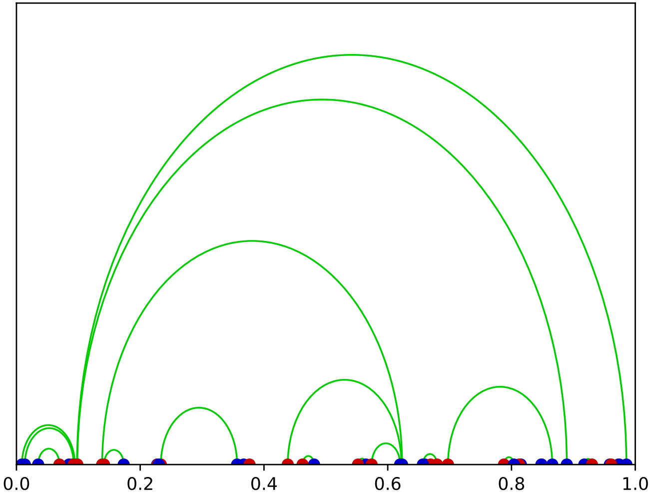
$c(x, y) = |x - y|^p, p = 1$



$c(x, y) = |x - y|^p, p = 0.6$



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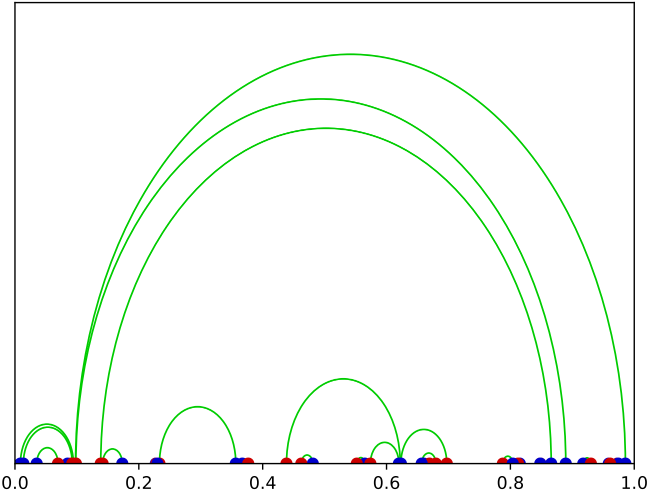

Some applications of optimal transport:

1. comparison between point clouds
2. geometric interpolation between distributions
3. discriminator in generative AI models (WGANs)
4. functional inequalities (isoperimetric, concentration of measure)
5. PDE's as gradient flows
6. geometry (synthetic Ricci curvature bounds)

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Classical vs Quantum: a dictionary

Classical	Quantum
	

Classical vs Quantum: a dictionary

E (finite set)	H Hilbert space ($\mathbb{C}^d$)
$e \in E$	$\lvert\psi\rangle \in H$
$A \subseteq E$	$V < H$
$f : E \to \mathbb{C}$ real-valued non-negative $\lvert f\rvert^2$	$A : H \to H$ linear self-adjoint (observable) non-negative $\lvert A\rvert^2 = A^\dagger A$
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probabilities $p \in \mathcal{P}(E)$ Dirac $p = \delta_x$	quantum states $\rho \in S(H)$ pure states $\rho = \|\psi\rangle\langle\psi\|$
Markov (transition) operator $K : \mathcal{P}(E) \to \mathcal{P}(E)$ $(Kp)(y) = \sum_{x \in E} K(y\|x)p(x)$	CPTP operator (quantum channel) $\Phi : S(H) \to S(H)$ $\Phi(\rho) = \sum_j B_j \rho B_j^\dagger$
Shannon's entropy $S(p) = -\sum_x p(x) \log p(x)$	Von Neumann entropy $S(\rho) = -\operatorname{Tr}[\rho \log \rho]$
Relative entropy (KL divergence) $D(p\|\|q) = \sum_x p(x) \log(p(x)/q(x))$	(Umegaki) relative entropy $D(\rho\|\|\sigma) = \operatorname{Tr}[\rho(\log \rho - \log \sigma)]$

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Single qubit system

A quantum analogue of $\{0, 1\}$. Set

$$H = \mathbb{C}^2.$$

Standard (computational) basis

$$\{|0\rangle, |1\rangle\} = \{(1, 0), (0, 1)\},$$

Pauli operators

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Parametrization of states:

$$\rho = \frac{1}{2} \left(\mathbb{I}_{\mathbb{C}^2} + b_x \sigma_x + b_y \sigma_y + b_z \sigma_z \right),$$

with

$$(b_x, b_y, b_z) \in \mathbb{R}^3, \quad b_x^2 + b_y^2 + b_z^2 \leq 1.$$

$$\rho = |\psi\rangle\langle\psi| \quad \text{is pure} \quad \Leftrightarrow \quad b_x^2 + b_y^2 + b_z^2 = 1.$$

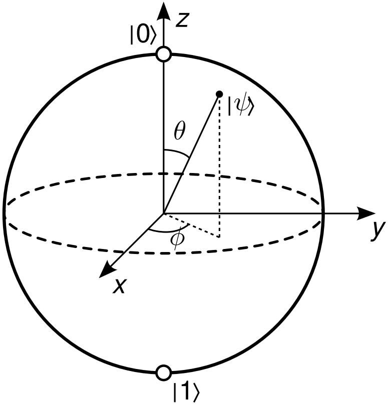

Figure: The Bloch representation of a pure state $\rho = |\psi\rangle\langle\psi| \in \mathbb{C}^2$.

Many-qubits systems

A quantum analogue of $\{0,1\}^n$:

$$H_n = (\mathbb{C}^2)^{\otimes n} \sim \mathbb{C}^{2^n}.$$

Standard (computational) basis

$$\{|s\rangle \ : s \in \{0,1\}^n\}.$$

Pure states are $\rho = |\psi\rangle\langle\psi|$ but not necessarily $\psi \in \{0,1\}^n$:

$$|\psi\rangle = \frac{1}{2^{n/2}} \sum_{s\in\{0,1\}^n} |s\rangle \qquad \text{(uniform superposition)}$$

$$|\Phi^+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \qquad \text{(Bell state, } n = 2)$$

"Classical" probabilities on $\{0,1\}^n$ are diagonal in the computational basis:

$$\rho = \sum_{s\in\{0,1\}^n} p(s)|s\rangle\langle s|.$$

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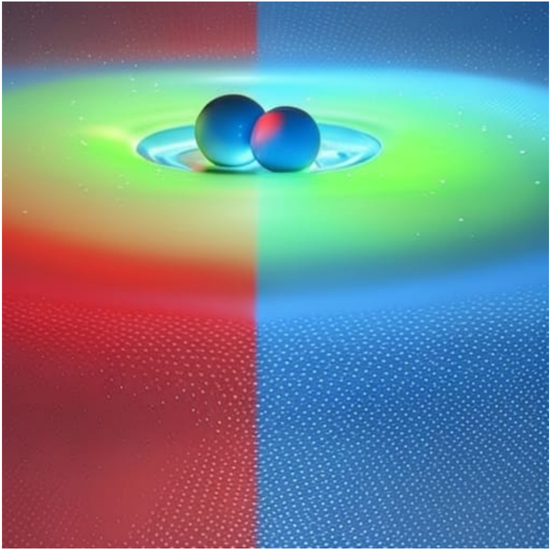
Why Quantum Optimal Transport?



Why Quantum Optimal Transport?

Classical distances between probabilities have quantum analogues:

- Total variation $\to$ Trace distance
- Hellinger distance $\to$ Fidelity
- KL divergence $\to$ Relative entropy

Like their classical counterparts:

+ Quite general, easy to compute or approximate
- Not adapted to specific geometry

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spectral distance in non-commutative geometry

1997 - Zyczkowski/Slomczynski:
Wasserstein distance of Husimi distributions

2012 - Maas/Carlen:
quantum analogue of Benamou-Brenier formula

2013 - Agredo:
1-Wasserstein extending any distance on basis vectors

2016 - Golse/Mouhot/Paul:
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2019 - De Palma/T.:
Quantum optimal transport using channels

2020 - De Palma/Marvian/T./Lloyd:
Earth mover's distance on qubits

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Transport via quantum channels

- Any Kantorovich transport plan $T(x_i, y_j)$ yields a transition kernel

$$K(y_j|x_i) = \frac{T(x_i, y_j)}{\sigma(x_i)},$$

such that

$$K\sigma = \rho$$

- Fix real-valued functions $(g_\ell)_{\ell=1}^d$ and choose a "quadratic" cost

$$c(x, y) = \sum_{\ell=1}^{d} (g_\ell(x) - g_\ell(y))^2.$$

$$\sum_i \sum_j c(x_i, y_j) T(x_i, y_j)$$
$$= \sum_\ell \sum_i g_\ell^2(x_i)\sigma(x_i) + \sum_j g_\ell^2(y_j)\rho(y_j) - 2\sum_i g_\ell(x_i)(K^\dagger g_\ell)(x_i)\sigma(x_i),$$

where

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- Given $\rho, \sigma \in \mathcal{S}(H)$, define transport plans as quantum channels

$$\Phi : \mathcal{S}(H) \to \mathcal{S}(H), \quad \Phi(\tau) = \sum_j B_j \tau B_j^\dagger$$

such that

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- Fix observables $\mathcal{R} = (R_\ell)_{\ell=1}^d$ and define

$$C_{\mathcal{R}}(\Phi) = \sum_\ell \mathrm{Tr}[R_\ell^2 \sigma] + \mathrm{Tr}[R_\ell^2 \rho] - 2\,\mathrm{Tr}[R_\ell \sqrt{\sigma} (\Phi^\dagger R_\ell) \sqrt{\sigma}],$$

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Is $D_{\mathcal{R}}(\rho, \sigma) = \sqrt{D^2_{\mathcal{R}}(\rho, \sigma)}$ a distance?

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Problem: Describe the isometries $J : \mathcal{S}(H) \to \mathcal{S}(H)$

$$D_{\mathcal{R}}(J(\rho), J(\sigma)) = D_{\mathcal{R}}(\rho, \sigma) \quad \forall \rho, \sigma.$$

Theorem (Titkos-Virosztek 2022)

Consider the single qubit space $H = \mathbb{C}^2$.

But failure of bijectivity can happen only on pure states (on the sphere)!

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- Aim: define a quantum analogue of earth mover's distance with respect to the Hamming distance on binary strings:

$$|x-y|_{\mathrm{H}} = \sum_{i=1}^{n} |x_i - y_i| \quad \text{for } x, y \in \{0,1\}^n.$$

- Recall the Kantorovich duality:

$$W_1(\sigma,\rho) = \max \left\{ \sum_{x \in \{0,1\}^n} f(x)(\sigma(x) - \rho(x)) \ : \ |f(x) - f(y)| \leq |x-y|_{\mathrm{H}} \right\}.$$

- Setting: n-qubits system $H_n = (\mathbb{C}^2)^{\otimes n}$. Strategy:
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Quantum Lipschitz constant

- Classical L-Lipschitz functions with respect to the Hamming distance have bounded differences:

$$|f(x) - f(y)| \leq L \quad \forall x, y \in \{0,1\}^n \text{ differing in only one site.}$$

- Equivalently:

$$\|f\|_{Lip} = 2 \max_{i=1,\dots,n} \min \left\{ \|f - g_i\|_\infty \ : \ g_i : \{0,1\}^n \to \mathbb{R} \text{ independent of site } i \right\}$$

- Given an observable A on $H_n = (\mathbb{C}^2)^{\otimes n}$, define

$$\|A\|_{Lip} = 2 \max_{i=1,\dots,n} \min \left\{ \|A - A_i \otimes \mathbb{I}_{\mathbb{C}^2}\|_\infty \ : \ A_i \text{ observable on } H_{n-1} \right\}.$$

- We define the quantum earth mover's distance by duality:

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Gaussian concentration

- Let $\sigma = 2^{-n}\mathbb{I}_{(\mathbb{C}^2)^{\otimes n}}$ (corresponding to a classical uniform distribution)
- Quantom Marton's inequality: for any state ρ,

$$W_1(\sigma, \rho) \leq \sqrt{\frac{n}{2} S(\rho \| \sigma)}.$$

- Duality $\Rightarrow$ if A satisfies $\mathrm{Tr}[A] = 0$ and $\|A\|_{Lip} \leq 1$, then

$$\dim\left(A \geq k\sqrt{n}\mathbb{I}_{(\mathbb{C}^2)^{\otimes n}}\right) \leq 2^n e^{-2k^2}.$$

- Informally:

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$$W_1(\sigma, \rho) \leq \sqrt{\frac{n}{2} S(\rho \| \sigma)}.$$

- Duality $\Rightarrow$ if A satisfies $\mathrm{Tr}[A] = 0$ and $\|A\|_{Lip} \leq 1$, then

$$\dim \left(A \geq k\sqrt{n}\mathbb{I}_{(\mathbb{C}^2)^{\otimes n}} \right) \leq 2^n \mathrm{e}^{-2k^2}.$$

- Informally:

$$A \approx 2^{-n}\,\mathrm{Tr}[A] \pm \|A\|_{Lip}\sqrt{n}.$$

Gaussian concentration

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Plan

Perspectives

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Quantum OT has already found applications:

- Non-commutative Ricci curvature bounds
- Quantum machine learning (generative models, quantum neural nets)
- Equilibrium measures on quantum spin systems

…many others just around the corner?

Further mathematical developments:

- Algorithms (classical/quantum)
- Geometry induced by OT (isometries, inequalities)
- Structural properties of optimizers
- Connections among different approaches…

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