Quantum OT: quantum channels and qubits Tutorial 1

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Plan



Quantum Systems

- From Classical to Quantum
- Systems of many qubits
- Quantum channels
- Classical Optimal Transport
 Monge and Kantorovich
 Wasserataia distance
 - Wasserstein distance
- An overview of Quantum OT
 The GMPC approach

Bibliography

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2 Classical Optimal Transport

3 An overview of Quantum OT

Bibliography

E (discrete)

e ∈ *E*

 $A \subseteq E$

 $f: E \to \mathbb{C}$ bounded real-valued non-negative (psd) $|f|^2$

 $\sum_{x \in E} f(x)$ $\ell^{p}(E) = \left\{ f : \sum_{x \in E} |f(x)|^{p} < \infty \right\}$ H Hilbert space $|\psi
angle\in H$ V < H (closed subspace

A : $D(A) \subseteq H \rightarrow H$ linear operator bounded operator self-adjoint non-negative $|A|^2 = A^{\dagger}A$

 $\operatorname{Tr}[A]$ $\ell^{p}(H) = \left\{ A : \operatorname{Tr}[(A^{\dagger}A)^{p/2}] < \infty \right\}$

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probability densities p

 δ_X

Markov operator (transition kernel)

Product $E \times F$ Partial sum $\sum_{x} f(x, y)$ $\sum_{(x,y)} f(x, y) = \sum_{x} \sum_{y} f(x, y)$ Marginal $p_E(x) = \sum_{y} p(x, y)$

 $\begin{aligned} \mathcal{S}(p) &= -\sum_{x} p(x) \ln p(x) \\ \mathcal{D}(p||q) &= \sum_{x} p(x) \ln(p(x)/q(x)) \end{aligned}$

quantum states $ho \in \mathcal{S}(H)$ $|\psi
angle\langle\psi|$ (pure state) CPTP operator

Product space $H \otimes K$ Partial trace $Tr_H[A]$ $Tr[A] = Tr_K[Tr_H[A]]$ Marginal $\rho_H = Tr_K[\rho]$

$$\begin{split} S(\rho) &= -\operatorname{Tr}[\rho \ln \rho] \\ D(\rho || \sigma) &= \operatorname{Tr}[\rho (\ln \rho - \ln \sigma)] \end{split}$$

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States and density matrices

Given a state π on a (finite dimensional) space *H*, pick basis $(|\psi_i\rangle)_i$ and write its density matrix $(\pi_{i,j})_{ij}$:

$$\pi = \sum_{i,j} \pi_{i,j} |\psi_i\rangle \langle \psi_j|.$$

Then:

- $(\pi_{i,j})_{ij}$ is Hermitian positive semidefinite
- The diagonal $(\pi_{i,i})_i$ is a classical probability density
- By the spectral theorem one can always diagonalize

$$\pi = \sum_{i} \boldsymbol{p}_{i} |\varphi_{i}\rangle \langle \varphi_{i}|$$

but the basis $(|\varphi_i\rangle)_i$ depends on π .

From Classical to Quantum

Partial trace and density matrices

Given a state π on the product space $H \otimes K$, pick basis $(|\psi_i\rangle)_i$, $(|\varphi_j\rangle)_j$, and write its density matrix $(\pi_{ij,k\ell})_{ijk\ell}$:

$$\pi = \sum_{i,j,k,\ell} \pi_{ij,k\ell} |\psi_i\rangle \otimes |\phi_j\rangle \langle \psi_k| \otimes \langle \phi_\ell|.$$

Then

$$\operatorname{Tr}_{H}[\pi] = \sum_{j,\ell} \left(\sum_{i} \pi_{ij,i\ell} \right) |\phi_{j}\rangle \langle \phi_{\ell}|,$$

$$\operatorname{Tr}_{K}[\pi] = \sum_{i,k} \left(\sum_{j} \pi_{ij,kj} \right) |\psi_{i}\rangle \langle \psi_{\ell}|,$$

Well-defied (do not depend on the basis).

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Well-defied (do not depend on the basis).

Exercises

On Hilbert spaces $H, K, p, q \in [0, 1]$, orthonormal $(|\psi_i\rangle)_i \in H, (|\varphi_i)_i \in K$,

- Define $\rho_p = (1 p)|\psi_0\rangle\langle\psi_0| + p|\psi_1\rangle\langle\psi_1|$. Show that $\rho_p \in \mathcal{S}(H)$ and compute $\mathcal{S}(\rho_p)$.
- 3 Define $|\psi_p\rangle = \sqrt{(1-p)}|\psi_0\rangle + \sqrt{p}|\psi_1\rangle$ and compute $S(|\psi_p\rangle\langle\psi_p|)$.

Onsider the (Bell) state

$$|\Phi^+\rangle:=\frac{1}{\sqrt{2}}|\psi_0\rangle\otimes|\varphi_0\rangle+\frac{1}{\sqrt{2}}|\psi_1\rangle\otimes|\varphi_1\rangle$$

Compute

$$\mathsf{Tr}_{\mathcal{H}}[|\Phi^{+}\rangle\langle\Phi^{+}|],\quad\mathsf{Tr}_{\mathcal{K}}[|\Phi^{+}\rangle\langle\Phi^{+}|].$$

Qubits systems

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

$$H = (\mathbb{C}^2)^{\otimes n}$$

The standard (computational) basis

 $\{|s
angle\}$ with $s\in\{0,1\}^n,$ e.g. for n=1 $\{|0
angle,|1
angle\},$ for n=2,

```
\{|00\rangle,|01\rangle,|10\rangle,|11\rangle\}.
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Quantum states on systems of qubits

On *n*-qubits σ , $\rho \in \mathcal{S}(\mathbb{C}^2)^{\otimes n}$,

- States are 2ⁿ × 2ⁿ complex matrices (Hermitian, positive semi-definite, with unit trace).
- Pure states are rank-one matrices, corresponding to unit norm vectors

$$\sigma = |\psi\rangle \langle \psi|$$

but not necessarily $\psi \in \{0, 1\}^n$.

• Classical probabilities $(p(s))_{s \in \{0,1\}^n}$ correspond to diagonal states:

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

Systems of many qubits

Quantum computing

(Most) quantum computing architectures are based on systems of *n* qubits (ideally $n \gg 1$) with sequence of unitary operations (gates) acting on a small subset of them (e.g., up to 3 at the time). Examples:

• Singe qubit gates:

$$X = \left(\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array}\right), \quad H = \frac{1}{\sqrt{2}} \left(\begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array}\right),$$

Two-qubits gates:

$$CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad SWAP = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

• Three-qubits gates: Toffoli gate (CCX)

Exercise: Show that the above are unitary operators.

11/34

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Postulates of Quantum Mechanics

• A wave function $|\psi_0\rangle \in H$ in a closed (isolated) quantum system evolves according to Schrödinger's equation

$$\partial_t |\psi_t\rangle = iA |\psi_t\rangle$$

for a self-adjoint A. Integration gives

$$|\psi_t\rangle = U_t |\psi_0\rangle$$
, with $U_t = e^{itA}$ unitary.

Probability (Born's rule) A measurement of a system is described by an orthonormal basis $(|\phi_v\rangle)_v \subseteq H$. If the state is $|\psi\rangle \in H$, the outcome has value v with probability (Born's rule)

$$p(v) = |\langle \phi_v | \psi \rangle|^2.$$

After the measurement, the system is in state $|\phi_v\rangle$ with probability p(v), i.e., the state is mixed:

$$\sum_{\mathbf{v}} \mathbf{p}(\mathbf{v}) |\phi_{\mathbf{v}}\rangle \langle \phi_{\mathbf{v}} |.$$

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For the unitary evolution of closed systems:

 $\rho \mapsto U_t \rho U_t^{\dagger},$

3 For the measurement $(|\phi_v\rangle)_v \subseteq H$:

$$\rho \mapsto \sum_{\mathbf{v}} |\phi_{\mathbf{v}}\rangle \left(\langle \phi_{\mathbf{v}} | \rho | \phi_{\mathbf{v}} \rangle \right) \langle \phi_{\mathbf{v}} |.$$

Can one interpolate between these two, describing open quantum systems which interact with an external environment?

Notice that both transformations are linear and map states into states.

13/34

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Can one interpolate between these two, describing open quantum systems which interact with an external environment?

Notice that both transformations are linear and map states into states.

We need a further property for a linear transformation of a quantum system H, $\Phi : \rho \mapsto \Phi(\rho)$ which maps states into states to be a quantum channel.

Complete positivity: enlarging *H* to any system $H \otimes K$ and acting with $\Phi \otimes \mathbb{I}_K$ still maps joint states into states.

Quantum channels Φ therefore are defined as maps that are

• linear:
$$\Phi(\lambda \rho + \sigma) = \lambda \Phi(\rho) + \Phi(\sigma)$$
,

- completely positive: $\Phi \otimes \mathbb{I}_{\mathcal{K}}(\rho)$ is positive (semidefinite) whenever ρ is so,
- trace preserving: $Tr[\Phi(\rho)] = Tr[\rho]$ (so that states are mapped into states).

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Representations of quantum channels

These are useful ways to write (and think of) a channel Φ :

• (Kraus) There exists linear operators $(B_k)_k$ such that

$$\sum_{k} B_{k}^{\dagger} B_{k} = \mathbb{I}$$

and representing Φ as

$$\Phi(\rho) = \sum_{k} B_k \rho B_k^{\dagger}.$$

• (Stinespring) There exists an auxiliary quantum system K, a state $|0_K\rangle \in K$ and unitary U acting on $H \otimes K$ such that, for every ρ .

$$\Phi(\rho) = \operatorname{Tr}_{K}[U(\rho \otimes |\mathsf{0}_{K}\rangle\langle\mathsf{0}_{K}|) U^{\dagger}].$$

One can choose K as (a copy of) H.

Exercise: describe the two representations for unitary evolutions of closed systems and measurements.

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15/34

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4 Bibliography

Monge's Optimal Transport problem

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

How to transport soil during a construction with minimal expenses?

A discrete formulation: given a

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

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

• 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

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

Monge and Kantorovich

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A random instance of OT in the plane



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Kantovorich and linear programming

Relax a map T with a coupling

$$\pi(\mathbf{x}_i,\mathbf{y}_j) \geq \mathbf{0}$$

such that

$$\sum_{j} \pi(\mathbf{x}_i, \mathbf{y}_j) = \sigma(\mathbf{x}_i), \quad \sum_{i} \pi(\mathbf{x}_i, \mathbf{y}_j) = \rho(\mathbf{y}_j).$$

The problem becomes linear optimization with linear constraints:

$$\min_{\pi} \sum_{i} \sum_{j} c(x_i, y_j) \pi(x_i, y_j)$$

that can be solved via simplex algorithm.

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

$$W_1(\sigma, \rho) = \min_{\pi} \sum_i \sum_j d(x_i, y_j) \pi(x_i, y_j)$$

defines a distance between (discrete) probability densities.

Called Wasserstein distance of order 1 (aka Kantorovich-Rubinstein distance, or Earth Mover's distance).

Exercise: $(x, y) \mapsto d(x, y)^p$, with $p \in (0, 1)$, is a distance. What is $\lim_{p \to 0^+} W_{d^p}(\sigma, \rho)?$

For p > 1, one defines a distance via

$$W_{p}(\sigma,\rho) = \left(\min_{T} \sum_{i} \sum_{j} d(x_{i}, y_{j})^{p} T(x_{i}, y_{j})\right)^{1/p}$$

21/34

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Duality

Kantorovich provided also the dual formulation for W₁:

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

Inequality \geq is trivial, the other follows from minmax theorems.

- It gives a definition of *W*₁ without transport plans, using only *d*-Lipschitz functions *f*.
- The formula also yields that $W_1(\sigma, \rho) = \|\sigma \rho\|_{W_1}$ is induced by a norm.
- For general c(x, y) duality uses conjugate functions (f, g):

$$f(x)-g(y)\leq c(x,y).$$

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Inequality \geq is trivial, the other follows from min max theorems.

- It gives a definition of W₁ without transport plans, using only d-Lipschitz functions f.
- The formula also yields that $W_1(\sigma, \rho) = \|\sigma \rho\|_{W_1}$ is induced by a norm.
- For general c(x, y) duality uses conjugate functions (f, g):

$$f(x)-g(y)\leq c(x,y).$$

22/34

Benamou-Brenier formula

• From a probabilist perspective

$$\min_{\pi} \sum_{i} \sum_{j} c(x_i, y_j) \pi(x_i, y_j) = \min_{X \sim \sigma, Y \sim \rho} \mathbb{E} \left[c(X, Y) \right]$$

• On \mathbb{R}^d and $c(x, y) = |x - y|^p$, we have

$$|x-y|^p \leq \int_0^1 |\dot{x}_t|^p dt$$

along any (smooth) path $(x_t)_t$ with $x_0 = x$, $x_1 = y$.

For any stochastic process (X_t)_t with X₀ ∼ X, X₁ ∼ Y:

$$\mathbb{E}\left[|X-Y|^{p}\right] \leq \mathbb{E}\left[\int_{0}^{1}|\dot{X}_{t}|^{p}dt\right]$$

• Benamou and Brenier (1999) proved that

$$W^{p}_{\rho}(\sigma,\rho) = \min_{(X_{t})_{t}:X_{0}\sim\sigma,X_{1}\sim\rho} \mathbb{E}\left[\int_{0}^{1} |\dot{X}_{t}|^{\rho} dt\right]$$

23/34

Other "distances" between probabilities

Total Variation distance

$$\|\rho - \sigma\|_{TV} = \frac{1}{2} \sum_{x} |\sigma(x) - \rho(x)|$$



$$H^{2}(\sigma,\rho) = \frac{1}{2} \sum_{x} |\sqrt{\sigma(x)} - \sqrt{\rho(x)}|^{2} = 1 - \sum_{x} \sqrt{\sigma(x)} \sqrt{\rho(x)}$$

3 Kullback-Leibler divergence

$$D_{KL}(\sigma||
ho) = \sum_{x} \sigma(x) \ln (\sigma(x)/
ho(x)).$$

No use of geometry of the space, i.e. the distance d(x, y) between positions.

Exercise: Show that TV is Wasserstein distance w.r.t. $d(x, y) = 1_{\{x \neq y\}}$

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Plan

Quantum Systems

- 2) Classical Optimal Transport
- An overview of Quantum OT
 The GMPC approach
 - Bibliography

An overview of Quantum OT

Classical distances between probabilities have quantum analogues:

- Total variation \rightarrow Trace distance $\frac{1}{2} \| \rho \sigma \|_1 = \frac{1}{2} \operatorname{Tr}[|\rho \sigma|]$
- Hellinger distance \rightarrow Fidelity $F(\rho, \sigma) = \|\sqrt{\rho}\sqrt{\sigma}\|_{1}^{2}$.
- Kullback-Leibler divergence \rightarrow Relative entropy $S(\rho \| \sigma)$.

As their classical counterparts:

- + Quite general, easy to compute or approximate
- Not adapted to specific geometry, i.e., unitarily invariant:

 $\boldsymbol{d}(\rho,\sigma) = \boldsymbol{d}(\boldsymbol{U}\rho\boldsymbol{U}^{\dagger},\boldsymbol{U}\sigma\boldsymbol{U}^{\dagger}).$

What about Quantum Optimal Transport distances?

26/34

An overview of Quantum OT

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26/34

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What about Quantum Optimal Transport distances?

Quantum OT theories: a timeline

- 1992 Connes/Lott: 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: quantum Kantorovich problem (plans)
- 2019 De Palma/T.: quantum optimal transport with channels (couplings)
- 2020 De Palma/Marvian/T./Lloyd: Wasserstein distance on qubits (Hamming)

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The GMPC approach

The GMPC approach

Consider a quantum system H and states $\sigma, \rho \in \mathcal{S}(H)$. Following Kantorovich, we need

• Couplings: any $\Pi \in \mathcal{S}(H \otimes H)$ with

$$\operatorname{Tr}_{\mathbf{1}} \Pi = \rho, \quad \operatorname{Tr}_{\mathbf{2}} \Pi = \sigma$$

• Transportation cost: any observable C on $H \otimes H$. **Example:** fix R_1, \ldots, R_d "quadratures" on H, set

$$C = \sum_{i=1}^{d} (R_i \otimes \mathbb{I} - \mathbb{I} \otimes R_1)^2.$$

The GMPC transportation problem is

$$\inf_{\Pi} \operatorname{Tr}[C\Pi].$$

Problems

The GMPC transportation problem is

inf Tr[C∏]. ⊓

- Show that the inf is attained (assuming H finite dimensional, or C bounded). Are minimizers unique?
- 2 Describe the set of couplings if σ (or ρ) is a pure state.
- (*) On the *n*-qubit system, assume that ρ, σ and C are diagonal in the computational basis (hence identified with classical functions and probabilities).
 Is the GMPC transportation cost the same as the classical transportation?

Plan

Quantum Systems

- 2) Classical Optimal Transport
- 3 An overview of Quantum OT





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