Breaking the Curse of Dimension in Multi-marginal Kantorovich Optimal Transport on Finite State Spaces

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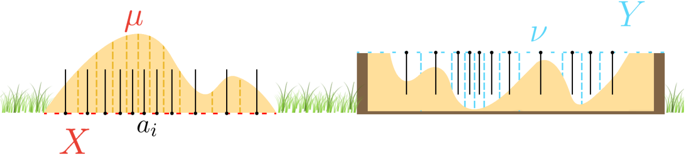
31.01.2019

Kantorovich optimal transport

Consider $X = \{a_1, \ldots, a_\ell\}$ with $a_i \neq a_j$ for $i, j \in \{1, \ldots, \ell\}, i \neq j$.

Prototypical marginal: Uniform measure $\overline{\lambda} := \sum_{i=1}^{\ell} \frac{1}{\ell} \delta_{a_i}$.

This marginal measure arises via equi-mass discretization from continuous problems.



Kantorovich OT problem

Minimize

$$\int_{X^N} c_N(x_1, x_2, \ldots, x_N) \; d\gamma(x_1, \ldots, x_N)$$

over all $\gamma \in \mathcal{P}_{sym}(X^N)$ with given marginals $\overline{\lambda}, \ldots, \overline{\lambda}$.

Kantorovich optimal transport

Definition (Kantorovich coupling)

In the given setting a probability measure γ on X^N is called a Kantorovich coupling if it fulfills

- $\gamma \in \mathcal{P}_{sym}(X^N)$
- γ has marginals $\overline{\lambda}, ..., \overline{\lambda}$, shorthand notation: $\gamma \mapsto \overline{\lambda}$

Number of unknowns: $\binom{N+\ell-1}{\ell-1}$

Monge optimal transport

Definition ((Symmetrized) Monge state)

A probability measure on X^N is a (symmetrized) Monge state if it is of the form

$$\sum_{\nu=1}^{\ell} \frac{1}{\ell} S\left(\delta_{T_1(a_\nu)} \otimes \ldots \otimes \delta_{T_N(a_\nu)}\right)$$

for N permutations $T_1, \ldots, T_N : X \to X$.

Number of unknowns: $\ell \cdot (N-1)$

Here the linear symmetrization operator $S : \mathcal{P}(X^N) \to \mathcal{P}(X^N)$ is given by

$$(S\gamma)(A_1 \times \ldots \times A_N) = \sum_{\sigma \in S_N} \frac{1}{|S_N|} \gamma(A_{\sigma(1)} \times \ldots \times A_{\sigma(N)}) \text{ for all } A_1, \ldots, A_N \subseteq X.$$

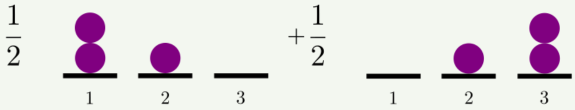
Is there always a Monge state minimizing the considered Kantorovich OT problem?

Example (Particles connected by springs [Friesecke;2018])

Consider for $N = 3$ and $X = \{1, 2, 3\} \subset \mathbb{R}$ the cost function given by $c_3(x_1, x_2, x_3) = \sum_{1 \leq i < j \leq 3} c(|x_i - x_j|)$ with $c(r) := (r - \frac{3}{4})^2$.

Then the unique optimizer of the considered Kantorovich OT problem is given by

$$\gamma_* = S\gamma \text{ where } \gamma = \frac{1}{2}(\delta_1 \otimes \delta_1 \otimes \delta_2 + \delta_2 \otimes \delta_3 \otimes \delta_3).$$



This γ_* is not a Monge state!

Monge states and a low-dimensional enlargement

Quasi-Monge states

Recall:

Definition (Monge state)

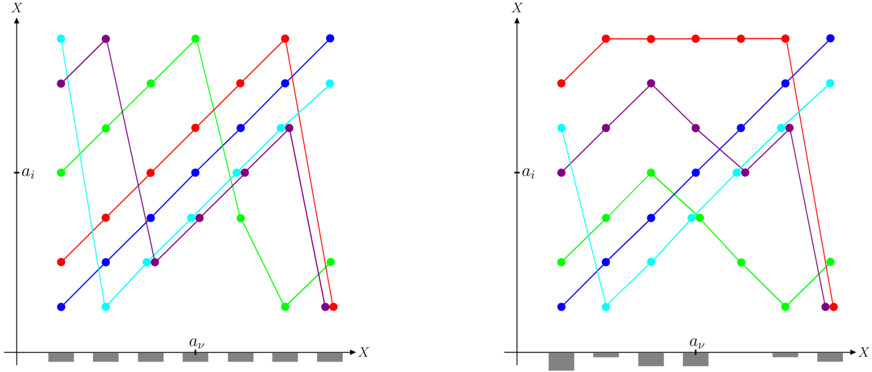
A probability measure on X^N is a Monge state if it is of the form

$$\sum_{\nu=1}^{\ell} \frac{1}{\ell} S\left(\delta_{T_1(a_\nu)} \otimes \dots \otimes \delta_{T_N(a_\nu)}\right)$$

for N permutations $T_1, \dots, T_N : X \to X$.

Monge states and a low-dimensional enlargement

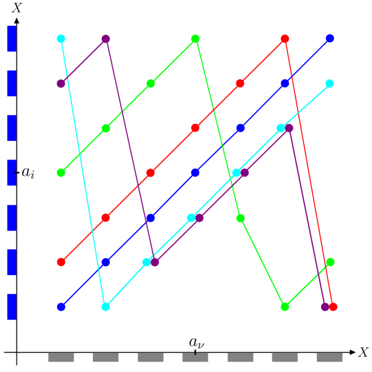
Quasi-Monge states

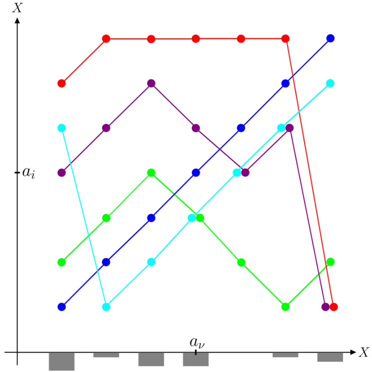


Idea: Drop the constraint that each map preserves the uniform measure (i.e. is a permutation) and demand this only "on average".

Monge states and a low-dimensional enlargement

Quasi-Monge states





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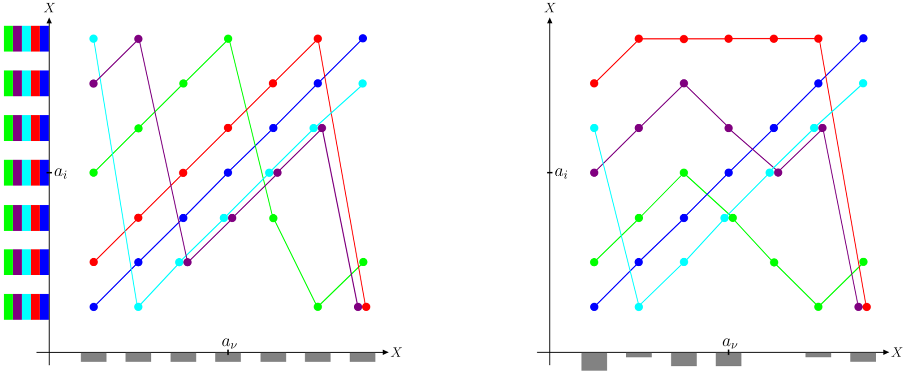

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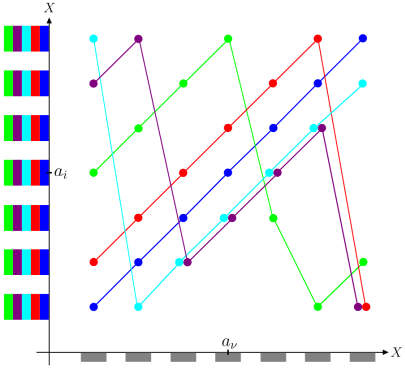

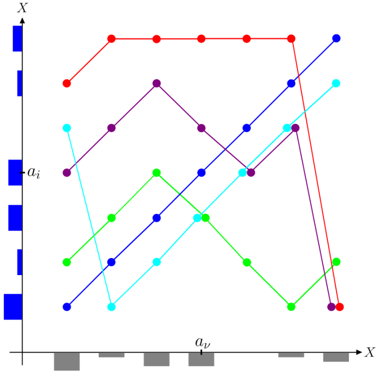

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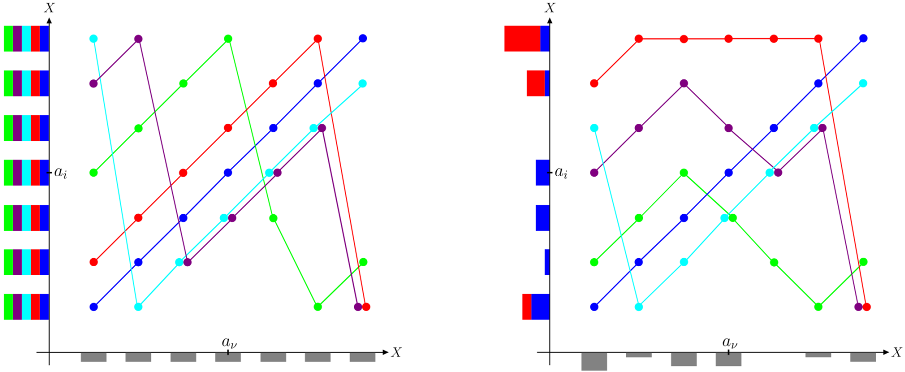

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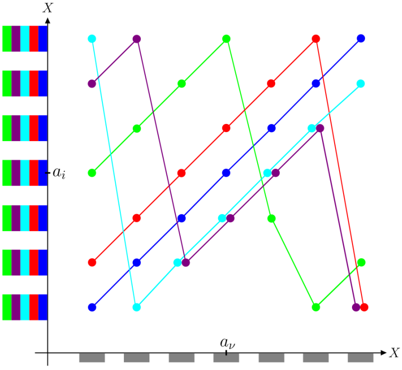

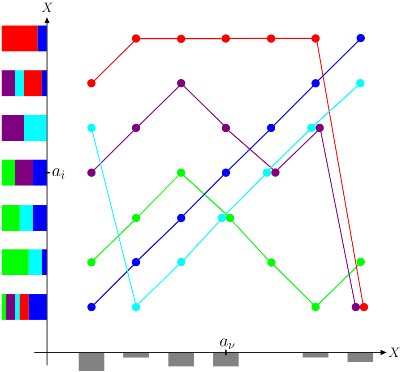

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Monge states and a low-dimensional enlargement

Quasi-Monge states

Definition

A probability measure on X^N is a Monge state if it is of the form

$$\sum_{\nu=1}^{\ell} \frac{1}{\ell} S\left(\delta_{T_1(a_\nu)} \otimes \ldots \otimes \delta_{T_N(a_\nu)}\right)$$

for N permutations $T_1, \ldots, T_N : X \to X$.

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Monge states and a low-dimensional enlargement

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Definition

A probability measure on X^N is a Quasi-Monge state if it is of the form

$$\sum_{\nu=1}^{\ell} \alpha^{(\nu)} S\left(\delta_{T_1(a_\nu)} \otimes \ldots \otimes \delta_{T_N(a_\nu)}\right)$$

for some $\alpha^{(\nu)} \geq 0$ with $\sum \alpha^{(\nu)} = 1$ and for N permutations $T_1, \ldots, T_N : X \to X$.

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for some $\alpha^{(\nu)} \geq 0$ with $\sum \alpha^{(\nu)} = 1$ and for N maps $T_1, \ldots, T_N : X \to X$ such that

$$\frac{1}{N} \sum_{k=1}^{N} T_k \# \alpha = \overline{\lambda}.$$

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$$\frac{1}{N} \sum_{k=1}^{N} T_k \# \alpha = \bar{\lambda}.$$

Number of unknowns: $\ell \cdot (N+1)$

A new characterization of Monge states

It is obvious that every Monge state is a Quasi-Monge state with the site weights being equal to $\frac{1}{\ell}$, i.e. $\alpha^{(1)} = ... = \alpha^{(\ell)} = \frac{1}{\ell}$. The converse is not obvious but true:

Theorem (Friesecke and V.:Characterization of Monge states)

A probability measure on X^N is a Monge state if and only if it is a Quasi-Monge state with all the site weights being equal to $\frac{1}{\ell}$, i.e. $\alpha^{(1)} = ... = \alpha^{(\ell)} = \frac{1}{\ell}$.

Breaking the curse of dimension

Theorem (Friesecke and V.:Breaking the curse of dimension)

For

- *any number $N \geq 2$ of marginals*
- *any finite state space X*
- *any cost function $c_N : X^N \to \mathbb{R} \cup \{+\infty\}$*
- *any prescribed marginal $\lambda_* \in \mathcal{P}(X)$*

Breaking the curse of dimension

Theorem (Friesecke and V.:Breaking the curse of dimension Part 1)

For

- *any number $N \geq 2$ of marginals*
- *any finite state space X*
- *any cost function $c_N : X^N \to \mathbb{R} \cup \{+\infty\}$*
- *any prescribed marginal $\lambda_* \in \mathcal{P}(X)$*

the considered Kantorovich OT problem admits a solution which is a Quasi-Monge state.

Breaking the curse of dimension

Theorem (Friesecke and V.:Breaking the curse of dimension Part 2)

If the cost c_N has pairwise-symmetric structure, i.e. $c_N(x_1, ..., x_N) = \sum_{1 \le i < j \le N} c(x_i, x_j)$ for some symmetric $c : X^2 \to \mathbb{R} \cup \{+\infty\}$, then the Kantorovich OT problem reduces to the problem:

Minimize

$$\sum_{1 \le i < j \le N} \int_X c(T_i(x), T_j(x)) \, d\alpha(x)$$

subject to

$$\frac{1}{N} \sum_{k=1}^{N} T_k \# \alpha = \lambda_*$$

$$\alpha \in \mathcal{P}(X)$$

$$T_1, .., T_N : X \to X$$

Breaking the curse of dimension

Proof.

Careful analysis of extreme points of the set of N-marginal Kantorovich couplings on $\{1, \dots, \ell\}$, for general N and ℓ. $\square$

Summary: Breaking the curse of dimension

	Number of unknowns	Sufficient to obtain optimal cost
Kantorovich coupling	$\binom{N+\ell-1}{\ell-1}$	*Yes*
Monge state	$\ell \cdot (N-1)$	*No*
Quasi-Monge state (our work)	$\ell \cdot (N+1)$	*Yes*

Literatur

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