Numerical method for feasible and approximately optimal solutions of multi-marginal optimal transport beyond discrete measures

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Multi-marginal optimal transport (MMOT)

- **Given:**
  - N probability measures $\mu_1, \ldots, \mu_N$ on Polish spaces $(\mathcal{X}_1, d_{\mathcal{X}_1}), \ldots, (\mathcal{X}_N, d_{\mathcal{X}_N})$;
  - $\boldsymbol{\mathcal{X}} := \mathcal{X}_1 \times \cdots \times \mathcal{X}_N$, $d_{\boldsymbol{\mathcal{X}}} := \bigoplus_{i=1}^N d_{\mathcal{X}_i}$;
  - cost function $f : \mathcal{X}_1 \times \cdots \times \mathcal{X}_N \to \mathbb{R}$.
- **Goal:** minimization over the set of couplings of $\mu_1, \ldots, \mu_N$:

$$\inf_{\mu \in \Gamma(\mu_1, \ldots, \mu_N)} \int_{\boldsymbol{\mathcal{X}}} f(x_1, \ldots, x_N)\, \mu(\mathrm{d}x_1, \ldots, \mathrm{d}x_N), \tag{MMOT}$$

where

$$\Gamma(\mu_1, \ldots, \mu_N) := \big\{\mu \in \mathcal{P}(\boldsymbol{\mathcal{X}}) : \text{the marginal of } \mu \text{ on } \mathcal{X}_i \text{ is } \mu_i \quad \forall 1 \leq i \leq N\big\}.$$

- **Dual problem** (MMOT*):

$$\sup \left\{ \sum_{i=1}^N \int_{\mathcal{X}_i} g_i \, \mathrm{d}\mu_i : \sum_{i=1}^N g_i(x_i) \leq f(x_1, \ldots, x_N) \quad \forall (x_1, \ldots, x_N) \in \boldsymbol{\mathcal{X}} \right\}.$$

Applications of MMOT

- **Multi-population matching** (a.k.a. matching for teams) in theoretical economics
- Wasserstein barycenter (special case of multi-population matching)
- Density functional theory in quantum mechanics
- Mathematical finance
- **Distributionally robust optimization** (DRO) in operations research

Existing approaches: discretization & regularization

- **Assuming discrete marginals**: Benamou, Carlier, Cuturi, Nenna, and Peyré [2015], Puccetti, Rüschendorf, and Vanduffel [2020], Tupitsa, Dvurechensky, Gasnikov, and Uribe [2020], . . .
- **Replacing non-discrete marginals by discrete approximations**: Carlier, Oberman, and Oudet [2015], Eckstein, Guo, Lim, and Obłój [2021], . . .
- **Entropic regularization and the Sinkhorn algorithm**: Cuturi [2013], Benamou, Carlier, and Nenna [2019], Peyré and Cuturi [2019], . . .
- **Regularization + neural networks**: Eckstein and Kupper [2019], Henry-Labordère [2019], Eckstein, Kupper, and Pohl [2020], Cohen, Arbel, and Deisenroth [2020], De Gennaro Aquino and Eckstein [2020], . . .
- Do not produce feasible solutions of the primal nor the dual of MMOT.

Contributions

- We develop a numerical algorithm for approximately solving the MMOT problem.
- The algorithm produces a feasible solution of the dual MMOT through relaxation.

  $\Rightarrow$ **lower bound**
- The algorithm produces a feasible solution of the primal MMOT.

  $\Rightarrow$ **upper bound**
- For any $\tilde{\epsilon} > 0$, we are able to control upper bound $-$ lower bound $\leq \tilde{\epsilon}$.

  $\Rightarrow$ **$\tilde{\epsilon}$-optimal primal and dual solutions**

Relaxation

- Relax the marginal constraints into finitely many linear constraints.
  - Fixing a marginal can be seen as having infinitely many linear constraints.
- Couplings are replaced by a *moment set*:

Definition (Moment set)

For $i = 1, \ldots, N$, $[\mu_i]_{\mathcal{G}_i}$ is called a moment set centered at μ_i characterized by functions $\mathcal{G}_i \subset \mathcal{L}^1(\mathcal{X}_i, \mu_i)$: $\quad \nu_i \in [\mu_i]_{\mathcal{G}_i} \quad \Leftrightarrow \quad \int_{\mathcal{X}_i} g_i \,\mathrm{d}\mu_i = \int_{\mathcal{X}_i} g_i \,\mathrm{d}\nu_i \; \forall g_i \in \mathcal{G}_i$.
Moreover,

$$\Gamma([\mu_1]_{\mathcal{G}_1}, \ldots, [\mu_N]_{\mathcal{G}_N}) := \Big\{\mu \in \Gamma(\nu_1, \ldots, \nu_N) : \nu_i \in [\mu_i]_{\mathcal{G}_i} \; \forall 1 \leq i \leq N\Big\}.$$

- **Relaxed MMOT problem**:

$$\inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \ldots, [\mu_N]_{\mathcal{G}_N})} \int_{\boldsymbol{\mathcal{X}}} f(x_1, \ldots, x_N) \, \mu(\mathrm{d}x_1, \ldots, \mathrm{d}x_N). \qquad (\mathrm{MMOT}_{\mathrm{relax}})$$

Constructing a feasible solution of the primal MMOT

Definition (Reassembly)

Let $\bar{\mathcal{X}}_i := \mathcal{X}_i$ for $i = 1, \ldots, N$. $\tilde{\mu}$ is called a reassembly of $\hat{\mu} \in \mathcal{P}(\mathcal{X}_1 \times \cdots \times \mathcal{X}_N)$ with the marginals $\mu_1, \ldots, \mu_N$ if there exists a probability measure $\gamma \in \mathcal{P}(\mathcal{X}_1 \times \cdots \times \mathcal{X}_N \times \bar{\mathcal{X}}_1 \times \cdots \times \bar{\mathcal{X}}_N)$ such that:

1. the marginal of γ on $\mathcal{X}_1 \times \cdots \times \mathcal{X}_N$ is $\hat{\mu}$;
2. for $i = 1, \ldots, N$, the marginal $\gamma_i \in \Gamma(\hat{\mu}_i, \mu_i)$ of γ on $\mathcal{X}_i \times \bar{\mathcal{X}}_i$ satisfies $\int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} d_{\mathcal{X}_i}(x, y)\, \gamma_i(\mathrm{d}x, \mathrm{d}y) = W_1(\hat{\mu}_i, \mu_i)$;
3. the marginal of γ on $\bar{\mathcal{X}}_1 \times \cdots \times \bar{\mathcal{X}}_N$ is $\tilde{\mu}$.

The set of *reassemblies* is denoted by $R(\hat{\mu}; \mu_1, \ldots, \mu_N) \subset \Gamma(\mu_1, \ldots, \mu_N)$.

- Idea: morphing $\hat{\mu}$ in an "optimal" way to turn its marginals into $\mu_1, \ldots, \mu_N$.
- Allows us to construct a feasible solution of (MMOT) via an infeasible one.

Controlling the approximation error

Theorem (Approximation of MMOT)

Suppose that:

1. $f : \mathcal{X} \to \mathbb{R}$ *is* L_f*-Lipschitz continuous for* $L_f > 0$*;*
2. *for* $i = 1, \ldots, N$*,* $\mathcal{G}_i \subset \mathcal{L}^1(\mathcal{X}_i, \mu_i)$*;*
3. $\hat{\mu}$ *is an* ϵ*-optimizer of* $(\mathrm{MMOT}_{\mathrm{relax}})$ *for* $\epsilon > 0$*, i.e.,*

$$\int_{\mathcal{X}} f \, \mathrm{d}\hat{\mu} \leq \inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \ldots, [\mu_N]_{\mathcal{G}_N})} \left\{ \int_{\mathcal{X}} f \, \mathrm{d}\mu \right\} + \epsilon;$$

4. $\tilde{\epsilon} := \epsilon + L_f \left(\sum_{i=1}^{N} \sup_{\nu_i \in [\mu_i]_{\mathcal{G}_i}} \left\{ W_1(\mu_i, \nu_i) \right\} \right)$.

Then, every $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \ldots, \mu_N)$ *is an* $\tilde{\epsilon}$*-optimizer of* (MMOT)*, i.e.,*

$$\int_{\mathcal{X}} f \, \mathrm{d}\tilde{\mu} \leq \inf_{\mu \in \Gamma(\mu_1, \ldots, \mu_N)} \left\{ \int_{\mathcal{X}} f \, \mathrm{d}\mu \right\} + \tilde{\epsilon}.$$

Important questions

- **Question 1**: for any $\epsilon > 0$, can we obtain an ϵ-optimizer $\hat{\mu}$ of $(\text{MMOT}_{\text{relax}})$?
  - **Answer 1**: yes, through proving the strong duality between $(\text{MMOT}_{\text{relax}})$ and its dual problem, which is a linear semi-infinite programming (LSIP) problem. Subsequently, a suitable cutting-plane algorithm (e.g., Conceptual Algorithm 11.4.1 of Goberna and López [1998]) can be used to obtain an ϵ-optimizer $\hat{\mu}$ of $(\text{MMOT}_{\text{relax}})$.
- **Question 2**: can we explicitly construct a $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \ldots, \mu_N)$?
  - **Answer 2**: yes, we can explicitly construct a reassembly using the copula theory and Laguerre diagrams.
- **Question 3**: can we control $\sup_{\nu_i \in [\mu_i]_{\mathcal{G}_i}} \left\{ W_1(\mu_i, \nu_i) \right\}$ to be arbitrarily close to 0 for $i = 1, \ldots, N$?
  - **Answer 3**: yes, for any $\epsilon_i > 0$ we can explicitly construct a finite collection $\mathcal{G}_i \subset \mathcal{L}^1(\mathcal{X}_i, \mu_i)$ such that $\sup_{\nu_i \in [\mu_i]_{\mathcal{G}_i}} \left\{ W_1(\mu_i, \nu_i) \right\} \le \epsilon_i$.

Numerical algorithm

- Putting these pieces together, we develop a numerical algorithm, whose properties are summarized as follows.

Theorem (Properties of the proposed algorithm)

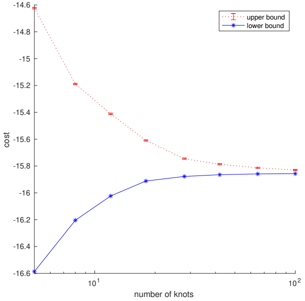
Under suitable conditions, for any $\tilde{\epsilon} > 0$, the proposed algorithm produces the outputs: $\tilde{\mu} \in \mathcal{P}(\boldsymbol{\mathcal{X}})$, $\hat{y}_0 \in \mathbb{R}$, $\hat{\boldsymbol{y}} \in \mathbb{R}^m$, $\mathrm{MMOT}^{\mathrm{LB}}$, $\mathrm{MMOT}^{\mathrm{UB}}$, and the following statements hold.

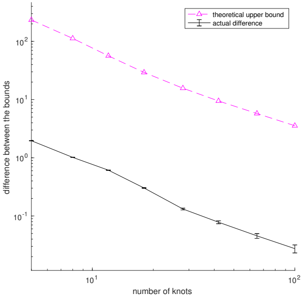
1. $\mathrm{MMOT}^{\mathrm{LB}} \leq (\mathrm{MMOT}) \leq \mathrm{MMOT}^{\mathrm{UB}}$;
2. $\hat{y}_0 + \langle \hat{\boldsymbol{y}}, \boldsymbol{g}(\cdot) \rangle$ *corresponds to an* $\hat{\epsilon}$*-optimizer of* (MMOT^*), *where* $\hat{\epsilon} := \mathrm{MMOT}^{\mathrm{UB}} - \mathrm{MMOT}^{\mathrm{LB}} \leq \tilde{\epsilon}$;
3. $\tilde{\mu}$ *is an* $\hat{\epsilon}$*-optimizer of* (MMOT), *where* $\hat{\epsilon} := \mathrm{MMOT}^{\mathrm{UB}} - \mathrm{MMOT}^{\mathrm{LB}} \leq \tilde{\epsilon}$.

A numerical example

- **Settings:**
  - $N = 50$;
  - $f(\boldsymbol{x}) := \left(\sum_{k=1}^{2} \left|\langle \boldsymbol{s}_k^+, \boldsymbol{x}\rangle - t_k^+\right|\right) - \left(\sum_{k=1}^{2} \left|\langle \boldsymbol{s}_k^-, \boldsymbol{x}\rangle - t_k^-\right|\right)$, where $\boldsymbol{s}_1^+$, $\boldsymbol{s}_2^+$, $\boldsymbol{s}_1^-$, $\boldsymbol{s}_2^-$ are uniformly randomly generated from the unit sphere in $\mathbb{R}^N$, and t_1^+, t_2^+, t_1^-, t_2^- are randomly generated real constants;
  - for $i = 1, \dots, N$, μ_i is a mixture of normal distributions with randomly generated parameters truncated to $[-10, 10]$.

- **Result:**





Further applications of the approximation scheme

- Multi-population matching (a.k.a. matching for teams)
  - Introduced by Carlier and Ekeland [2010] and includes the Wasserstein barycenter problem as a special case.
  - Carlier and Ekeland [2010] showed that the multi-population matching problem can be reformulated into an MMOT problem.
  - Therefore, we can apply the machinery we developed for solving MMOT problems to obtain an approximately optimal matching equilibrium.
  - Moreover, we adopt an alternative relaxation scheme to parametrize the transfer functions in the problem, which also results in an approximately optimal matching equilibrium.

Further application: two-stage DRO

- Two-stage distributionally robust optimization (DRO) with marginal constraints:

$$\inf_{\boldsymbol{a}\in S_1}\left\{\langle \boldsymbol{c}_1, \boldsymbol{a}\rangle + \sup_{\mu\in\Gamma(\mu_1,\ldots,\mu_N)}\int_{\mathcal{X}} Q(\boldsymbol{a},\boldsymbol{x})\,\mu(\mathrm{d}\boldsymbol{x})\right\},$$

where $Q(\boldsymbol{a},\boldsymbol{x})$ is the cost incurred by the second-stage problem:

$$\begin{aligned} Q(\boldsymbol{a},\boldsymbol{x}) := \quad & \underset{\boldsymbol{z}}{\text{minimize}} && \langle \boldsymbol{c}_2, \boldsymbol{z}\rangle \\ & \text{subject to} && \mathbf{A}_{\mathrm{in}}\boldsymbol{z} \le \mathbf{V}_{\mathrm{in}}\boldsymbol{a} + \mathbf{W}_{\mathrm{in}}\boldsymbol{x} + \boldsymbol{b}_{\mathrm{in}}, \\ & && \mathbf{A}_{\mathrm{eq}}\boldsymbol{z} = \mathbf{V}_{\mathrm{eq}}\boldsymbol{a} + \mathbf{W}_{\mathrm{eq}}\boldsymbol{x} + \boldsymbol{b}_{\mathrm{eq}}, \\ & && \boldsymbol{z} \in \mathbb{R}^{K_2}. \end{aligned}$$

- We can similarly replace $\Gamma(\mu_1,\ldots,\mu_N)$ by $\Gamma([\mu_1]_{\mathcal{G}_1},\ldots,[\mu_N]_{\mathcal{G}_N})$ for suitable $\mathcal{G}_i \subset \mathcal{L}^1(\mathcal{X}_i,\mu_i)$ for $i=1,\ldots,N$ to relax the two-stage DRO problem.

- Subsequently, we are able to compute an approximately optimal solution of the two-stage DRO problem such that the approximation error can be controlled to be arbitrarily close to 0.

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