Multi-marginal optimal transport and applications

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  Different potential teams have different efficiencies.
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- Different potential teams have different efficiencies.

Want to construct teams to make overall process as efficient as possible.
Introduction

$\mu_1 \rightarrow \mu_2 \rightarrow \mu_3$

$M_1 = \text{"carpenters"}$

$M_2 = \text{"plumbers"}$

$M_3 = \text{"electricians"}$
Introduction

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Multi-marginal optimal transport and applications

\( \mu_1 \)

\( M_1 = \text{“carpenters”} \)

\( x_1 \)

\( \mu_2 \)

\( M_2 = \text{“plumbers”} \)

\( x_2 \)

\( \mu_3 \)

\( M_3 = \text{“electricians”} \)

\( x_3 \)

\( b(x_1, x_2, x_3) = \text{“surplus” of team } (x_1, x_2, x_3) \)
Multi-marginal problem: Monge formulation

- $M_i \subseteq \mathbb{R}^n$, open and bounded, $i = 1, 2, ..., m$.
- $\mu_i$ Borel probability measures on $M_i$.
- $b : M_1 \times M_2 \times ... \times M_m \rightarrow \mathbb{R}$ smooth surplus function.
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**Monge Problem:**

maximize:

\[
\int_{M_1} b(x_1, F_2(x_1), F_3(x_1), \ldots, F_m(x_1)) d\mu_1(x_1)
\]

among \((m - 1)\)-tuples of maps \((F_2, F_3, \ldots, F_m)\) such that \( F_i : M_1 \to M_i \) pushes \( \mu_1 \) to \( \mu_i \).
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$F$ pushes $\mu_1$ to $\mu_2$. 

$\mu_2(A) = \mu_1(F_2^{-1}(A))$
Multi-marginal problem: Kantorovich formulation

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Kantorovich Problem:

maximize

$$\int_{M_1 \times M_2 \times \ldots \times M_m} b(x_1, x_2, \ldots, x_m) d\gamma(x_1, x_2, \ldots, x_m)$$

among measures $\gamma$ on $M_1 \times M_2 \times \ldots \times M_m$ that project to the $\mu_i$. 
Multi-marginal problem: Kantorovich formulation

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among measures $\gamma$ on $M_1 \times M_2 \times \ldots \times M_m$ that project to the $\mu_i$.
A Kantorovich solution $\gamma$ (or $(X_1, X_2, \ldots, X_m)$) always exists.
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\( \gamma \) projects to \( \mu_i \).
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\[
\begin{align*}
\mu_2(A) &= \gamma(M_1 \times A) \\
\mu_1(B) &= \gamma(B \times M_2)
\end{align*}
\]
Optimal transportation with **two marginals** \((m = 2)\) is an active and well established area of research.

Many diverse applications, including: fluid mechanics, cosmology, interacting gases, meteorology, image processing, economics, etc.

Brenier '87, Gangbo '95, Caffarelli '96, Gangbo-McCann '96, Levin '96: Assume \(\mu_1 \ll dx_1\) and that \(b\) is twisted, ie:

\[
x_2 \mapsto D_{x_1} b(x_1, x_2)
\]

is injective.

Then \(\gamma\) is concentrated on the graph of a function over \(x_1\) and is unique.

Example: \(b(x_1, x_2) = -|x_1 - x_2|^2\).
Multi-marginal problems have many emerging applications, in economics, physics, $m$-monotonicity, image processing, financial math, statistics, etc., but are not well understood.

For certain special surplus functions, the optimal $\gamma$ is unique and is concentrated on a graph over $x_1$:

$$\{(x_1, F_2(x_1), \ldots, F_m(x_1))\}.$$

**Gangbo-Swiech '98:** $b(x_1, x_2, \ldots, x_m) = -\sum_{i \neq j} |x_i - x_j|^2$

**Heinich '02:** $b(x_1, x_2, \ldots, x_m) = h(x_1 + x_2 + \ldots + x_m)$ where $h : \mathbb{R}^n \rightarrow \mathbb{R}$ is strictly convex.

**P '11:** Strong second order conditions on $b$. For example, when $m = 3$, we require, for all $x_1, x_2 \in M_1$, $x_2 \in M_2$, $x_3, x_3 \in M_3$, we have:

$$D^2_{x_2x_3} b[D^2_{x_1x_3} b]^{-1} D^2_{x_1x_2} b(x_1, x_2, x_3) - D^2_{x_2x_2} b(x_1, x_2, x_3) + D^2_{x_2x_2} b(x_1, x_2, x_3) > 0.$$

**Kim-P '13:** $b(x_1, x_2, \ldots, x_m) = -\inf_{y \in M} \left[ \sum_{i=1}^m d^2(x_i, y) \right]$ on a Riemannian manifold $M$. 
For other surplus functions, solutions can be non-unique and have high dimensional support. Examples:

- \( b(x_1, x_2, \ldots, x_m) = -\sum_{i \neq j}^{m} \frac{1}{|x_i - x_j|} \), arises in density functional theory for Coulombic electronic interactions in quantum physics (Cotar-Friesecke-Kluppelberg '11 and Buttazzo-De Pascale-Gori-Giorgi '12).

- \( b(x_1, x_2, \ldots, x_m) = \sum_{i \neq j}^{m} |x_i - x_j|^2 \), arises when Coulombic interactions are replaced by repulsive, harmonic oscillator interactions.

- \( b(x_1, x_2, \ldots, x_m) = \det(x_1, x_2, \ldots, x_m) \) (when \( n = m \)) Carlier-Nazaret '06.

- \( b(x_1, x_2, \ldots, x_m) = h(x_1 + x_2 + \ldots + x_m) \), \( h \) strictly concave.
Example application 1: multi-agent matching

- Model due to Carlier-Ekeland ’10 and Chiappori-McCann-Nesheim ’10.
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- Measure $\mu_1$ represents a distribution of buyer types, looking to buy, say, custom built houses; $\mu_i$ ($i \geq 2$) represents a distribution of a type of worker needed to build houses (ie, carpenters, plumbers, electricians, etc.)
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- Buyer $x_1$ has a preference $f_1(x_1, z)$ for a house type $z \in Z \subseteq \mathbb{R}^n$; worker $x_i$ ($i \geq 2$) has a preference $f_i(x_i, z)$ to build house of type $z$. 

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- Finding an equilibrium in this market is equivalent to solving an optimal transport problem with surplus

$$b(x_1, x_2, \ldots, x_m) = \sup_{z \in Z} \sum_{i=1}^{m} f_i(x_i, z)$$
Example application 2: density functional theory

- Model due to Cotar-Friesecke-Kluppelberg '11 and Buttazzo-De Pascale-Gori-Giorgi '12.

\[ \mu_i \text{ represent particle densities of semi-classical electrons.} \]

Electrons are indistinguishable \( \Rightarrow \mu_i = \mu \).

Given \( \mu \), the single particle density, want to find the \( m \)-particle density (a measure on \( \mathbb{R}^{nm} \)) minimizing the total interaction energy.

Leads to an optimal transport problem with

\[ b(x_1, x_2, \ldots, x_m) = -\sum_{i \neq j} 1 |x_i - x_j|. \]
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Given $\mu$, the single particle density, want to find the $m$-particle density (a measure on $\mathbb{R}^{nm}$) minimizing the total interaction energy.

Leads to an optimal transport problem with $b(x_1, x_2, \ldots, x_m) = -\sum_{i \neq j} \frac{1}{|x_i - x_j|}$.
Take $n = 1$. 

For $m = 2$, if $\frac{\partial^2 b}{\partial x_1 \partial x_2} > 0$, the optimal map $x_2 = F_2(x_1)$ is increasing. If $\frac{\partial^2 b}{\partial x_1 \partial x_2} < 0$, the optimal map is decreasing.

For $m = 3$, if $\frac{\partial^2 b}{\partial x_i \partial x_j} > 0$ for all $i \neq j$, there exist odd optimal maps $x_2 = F_2(x_1)$, $x_3 = F_3(x_1)$, both increasing (Carlier '03).

Coordinate invariant condition:

$$\frac{\partial^2 b}{\partial x_1 \partial x_2} \left[ \frac{\partial^2 b}{\partial x_3 \partial x_2} \right] - \frac{\partial^2 b}{\partial x_3 \partial x_1} > 0.$$
Simple Example: 1 dimensional case for 2 and 3 marginals

- Take \( n = 1 \).
- For \( m = 2 \), if \( \frac{\partial^2 b}{\partial x_1 \partial x_2} > 0 \), optimal map \( x_2 = F_2(x_1) \) is increasing.
  - If \( \frac{\partial^2 b}{\partial x_1 \partial x_2} < 0 \) the optimal map is decreasing.

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  - If \( \frac{\partial^2 b}{\partial x_1 \partial x_2} < 0 \) the optimal map is decreasing.
- For \( m = 3 \), if \( \frac{\partial^2 b}{\partial x_i \partial x_j} > 0 \), for all \( i \neq j \) \( \exists! \) optimal maps \( x_2 = F_2(x_1), x_3 = F_3(x_1) \), both increasing (Carlier '03)
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- For $m = 3$, if $\frac{\partial^2 b}{\partial x_i \partial x_j} > 0$, for all $i \neq j$ there exist optimal maps $x_2 = F_2(x_1), x_3 = F_3(x_1)$, both increasing (Carlier '03)
- Coordinate invariant condition: $\frac{\partial^2 b}{\partial x_1 \partial x_2} \left[ \frac{\partial^2 b}{\partial x_3 \partial x_2} \right]^{-1} \frac{\partial^2 b}{\partial x_3 \partial x_1} > 0$. 
When $m = 2$, if $\det(D^2_{x_1 x_2} b) \neq 0$, solution is concentrated on $n$-dimensional Lipschitz submanifold of the product space (McCann-P-Warren ’12 ).
Higher dimensional problems for 2 and 3 marginals

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- $D_{x_i x_j}^2 b$ is a bilinear mapping on the product of tangent spaces $T_{x_i} M_i \times T_{x_j} M_j$. 
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- $(D^2_{x_1x_2} b)[(D^2_{x_3x_2} b)]^{-1}(D^2_{x_3x_1} b)$ is a bilinear mapping on $T_{x_1} M_1 \times T_{x_1} M_1$.
Higher dimensional problems for 2 and 3 marginals

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- $D_{x_i x_j}^2 b$ is a bilinear mapping on the product of tangent spaces $T_{x_i} M_i \times T_{x_j} M_j$.
- $(D_{x_1 x_2}^2 b) [ (D_{x_3 x_2}^2 b) ]^{-1} (D_{x_3 x_1}^2 b)$ is a bilinear mapping on $T_{x_1} M_1 \times T_{x_1} M_1$!
- $(D_{x_1 x_2}^2 b) [ (D_{x_3 x_2}^2 b) ]^{-1} (D_{x_3 x_1}^2 b) > 0$ makes sense!
Let the signature of $G$ be $(\lambda +, \lambda - , \lambda, \lambda -)$. 

$spt(\gamma)$ is spacelike: $V^T \cdot G \cdot V \geq 0$ for all $V \in T(spt(\gamma))$ (P1). 

Its dimension is no more than $\lambda$: 

$\lambda = n$ iff 

$D_{x_1x_2} b \left[ D_{x_2x_3} b \right]^{\lambda - 1} \left[ D_{x_3x_2} b \right] > 0$.
Let the signature of $G$ be $(\lambda_+, \lambda_-, mn - \lambda_+ - \lambda_-)$. 

$$G = \begin{bmatrix}
0 & D^2_{x_1 x_2} b & D^2_{x_1 x_3} b \\
D^2_{x_2 x_1} b & 0 & D^2_{x_2 x_3} b \\
D^2_{x_3 x_1} b & D^2_{x_3 x_2} b & 0 \\
\end{bmatrix}$$
Structure of solutions

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- Let the signature of \( G \) be \( (\lambda_+, \lambda_-, mn - \lambda_+ - \lambda_-) \).
- \( spt(\gamma) \) is spacelike: \( V^T \cdot G \cdot V \geq 0 \) for all \( V \in T(spt(\gamma)) \) (P'11).
- It's dimension is no more than \( mn - \lambda_- \).
- \( mn - \lambda_- = n \) iff \( (D^2_{x_1 x_2} b)[(D^2_{x_3 x_2} b)]^{-1}(D^2_{x_3 x_1} b) > 0 \).
Examples: \( \det(x_1 x_2 \ldots x_m), -\sum_{i \neq j} \frac{1}{|x_i - x_j|}, \sum_{i \neq j} |x_i - x_j|^2 \).
Rotationally invariant repulsive surplus

- Examples: $\det(x_1x_2...x_m), -\sum_{i\neq j} \frac{1}{|x_i-x_j|}, \sum_{i\neq j} |x_i - x_j|^2$.
- Optimal measure $\gamma$ is rotationally symmetric. (see, e.g. Carlier-Nazaret '06)
Examples: \( \det(x_1x_2\ldots x_m) \), \(-\sum_{i \neq j} \frac{1}{|x_i - x_j|} \), \( \sum_{i \neq j} |x_i - x_j|^2 \).

Optimal measure \( \gamma \) is rotationally symmetric. (see, e.g. Carlier-Nazaret '06)

If \( x, y, z \in \text{spt}(\gamma) \), then
Rotationally invariant repulsive surplus

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- Optimal measure \( \gamma \) is rotationally symmetric. (see, e.g. Carlier-Nazaret '06)

- If \( x, y, z \in \text{spt}(\gamma) \), then

  \[(x, y, z) \in \arg\max_{|\bar{x}|=r, |\bar{y}|=s, |\bar{z}|=t} b(\bar{x}, \bar{y}, \bar{z}) \]

  \((Ax, Ay, Az) \in \text{spt}(\gamma)\) for any rotation matrix \( A \).
Examples: \( \det(x_1x_2...x_m), -\sum_{i \neq j} \frac{1}{|x_i-x_j|}, \sum_{i \neq j} |x_i - x_j|^2 \).

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Some rotations fix \( x \) but not \( y \), assuming \( x \) and \( y \) are not co-linear (get non Monge solutions).
Examples: $\det(x_1 x_2 \ldots x_m)$, $-\sum_{i \neq j} \frac{1}{|x_i - x_j|}$, $\sum_{i \neq j} |x_i - x_j|^2$.

Optimal measure $\gamma$ is rotationally symmetric. (see, e.g. Carlier-Nazaret '06)

If $x, y, z \in \text{spt}(\gamma)$, then

$$(x, y, z) \in \text{argmax}_{|\bar{x}|=r, |\bar{y}|=s, |\bar{z}|=t} b(\bar{x}, \bar{y}, \bar{z})$$

$(Ax, Ay, Az) \in \text{spt}(\gamma)$ for any rotation matrix $A$.

Some rotations fix $x$ but not $y$, assuming $x$ and $y$ are not co-linear (get non Monge solutions).

These rotational directions are extra spacelike directions for $G$. 


Monge solution and uniqueness results

For which surplus functions is the optimizer concentrated on the graph of a function over $x_1$?

For $m = 2$, the twist, injectivity of $x_2 \mapsto D x_1 b(x_1, x_2)$, suffices. For $m = 3$, these type of results hold for $b(x_1, x_2, x_3) = \sup_{z \in Z^3} \sum_{i=1}^3 f_i(x_i, z)$. This class includes $-\sum_{i=1}^3 |x_i - x_j|^2$ (Gangbo-Swiech surplus), $h(x_1 + x_2 + x_3)$, for strictly convex $h$, (Heinich surplus). Optimal maps factor through a measure on $Z$ (the generalized barycenter) Agueh-Carlier '10. Can easily calculate $(D^2 x_1 x_2 b)[(D^2 x_3 x_2 b)]^{-1} (D^2 x_3 x_1 b) > 0$ (under mild conditions on the $f_i$).

One can also prove Monge solutions and uniqueness under strong differential conditions on $b$ (P '11), or under a twist like condition on special sets (Kim-P (in preparation)).

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This class includes $-\sum_{i=1}^3 |x_i - x_j|^2$ (Gangbo-Swiech surplus), $h(x_1 + x_2 + x_3)$ for strictly convex $h$ (Heinich surplus).

Optimal maps factor through a measure on $Z$ (the generalized barycenter) Agueh-Carlier '10.

Can easily calculate $[D^2_{x_2} b(x_3, x_2)] - 1 [D^2_{x_3} b(x_1, x_3)] > 0$ (under mild conditions on the $f_i$).

One can also prove Monge solutions and uniqueness under strong differential conditions on $b$ (P '11), or under a twist like condition on special sets (Kim-P (in preparation)).
Monge solution and uniqueness results

- For which surplus functions is the optimizer concentrated on the graph of a function over $x_1$?
- For $m = 2$, the twist, injectivity of $x_2 \mapsto D_{x_1} b(x_1, x_2)$, suffices.
- For $m = 3$, these type of results hold for

$$b(x_1, x_2, x_3) = \sup_{z \in Z} \sum_{i=1}^{3} f_i(x_i, z)$$
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One can also prove Monge solutions and uniqueness under strong differential conditions on $b$ (P '11), or under a twist like condition on special sets (Kim-P (in preparation)).
In the limit as $m \to \infty$, the differences become even more pronounced.

For the surplus $- \int_0^1 \int_0^1 |x_s - x_t|^2 dstdt$, we get unique Monge type solutions (P '13).

For $- \lim_{m \to \infty} \left( \frac{1}{m} \right) \sum_{i \neq j}^m \frac{1}{|x_i - x_j|}$; the (unique) optimal measure is product measure (Cotar-Friesecke-P (in preparation)).