Control of ensembles via structured optimal transport

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This is based on joint work with Yongxin Chen[1], Isabel Haasler[2], and Johan Karlsson[2].

[1] Isabel Haasler, Johan Karlsson, and Axel Ringh. Control and estimation of ensembles via structured optimal transport: A computational approach based on entropy-regularized multi-marginal optimal transport. *IEEE Control Systems Magazine*, In press, 2021

[2] Isabel Haasler, Axel Ringh, Yongxin Chen, and Johan Karlsson. Multi-marginal optimal transport with tree-structured cost and the Schrödinger bridge problem. Accepted to *SIAM Journal on Control and Optimization*, 2021.

[3] Axel Ringh, Isabel Haasler, Yongxin Chen, and Johan Karlsson. Efficient computations of multi-species mean field games via graph-structured optimal transport. *Submitted*, 2021.

[4] Isabel Haasler, Axel Ringh, Yongxin Chen, and Johan Karlsson. Scalable computation of dynamic flow problems via multi-marginal graph-structured optimal transport. *In preparation*, 2021.

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Outline

- Introduction: a matching problem
- Optimal transport: discrete and continuous formulation
- Matching, minimum energy control, and optimal steering of a swarm
- Numerical solution method: Sinkhorn iterations

Introduction: A matching problem

- Consider two sets of N agents $x^{(0)} := \{x_i^{(0)}\}_{i=1}^N$ and $x^{(1)} := \{x_j^{(1)}\}_{j=1}^N$ in the state space $\mathbb{R}^d$.
- Can define a distance between the two sets as the solution to a matching (assignment) problem

$$d(x^{(0)}, x^{(1)}) := \underset{\phi \in \text{perm}(\{1,2\ldots,N\})}{\text{minimize}} \sum_{i=1}^{N} \|x_i^{(0)} - x_{\phi(i)}^{(1)}\|_2^2.$$

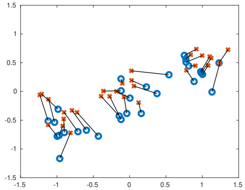


Figure: Example of an optimal association between two distributions of agents.

- Drawback: combinatorial problem! Intractable even for modest N.

Reformulate the problem:

- Parametrize the permutation in terms of the permutation matrix: $M = [M_{ij}]_{i,j=1}^{N}$ with

$$M_{ij} = \begin{cases} 1, & \text{if agent } x_i^{(0)} \text{ and agent } x_j^{(1)} \text{ are associated,} \\ 0, & \text{otherwise.} \end{cases}$$

- Introduce the cost matrix $C_{x^{(0)},x^{(1)}} = [C_{ij}]$, where $C_{ij} = \|x_i^{(0)} - x_j^{(1)}\|_2^2$.
- The optimization problem for $d(x^{(0)}, x^{(1)})$ can be rewritten as

$$\begin{aligned} \underset{M\in\{0,1\}^{N\times N}}{\text{minimize}} \quad & \sum_{i=1}^{N}\sum_{j=1}^{N} C_{ij}M_{ij} \\ \text{subject to} \quad & \sum_{j=1}^{N} M_{ij} = 1,\ i = 1,\dots,N \\ & \sum_{i=1}^{N} M_{ij} = 1\ j = 1,\dots,N \end{aligned} \quad \Longleftrightarrow \quad \begin{aligned} \underset{M\in\{0,1\}^{N\times N}}{\text{minimize}} \quad & \langle C_{x^{(0)},x^{(1)}}, M\rangle \\ \text{subject to} \quad & M\mathbf{1} = \mathbf{1} \\ & M^T\mathbf{1} = \mathbf{1}. \end{aligned}$$

- **Note:** M is a doubly stochastic matrix.

Introduction: A matching problem

- Relax the variables $M_{ij} \in \{0, 1\}$ to $0 \leq M_{ij} \leq 1$.
- Birkhoff's theorem: permutation matrices are the extreme points of the polytope of doubly stochastic matrices [1].
- All linear programs with an optimal solution has an optimal solution which is an extreme point of the constraint polytope [2].

Theorem

The optimization problems

$$\underset{\phi \in \mathrm{perm}(\{1,2\ldots,N\})}{\text{minimize}} \sum_{i=1}^{N} \|x_i^{(0)} - x_{\phi(i)}^{(1)}\|_2^2 \qquad \textit{and} \qquad \begin{aligned} \underset{M \in [0,1]^{N \times N}}{\text{minimize}} \quad & \langle C_{x^{(0)}, x^{(1)}}, M \rangle \\ \text{subject to} \quad & M\mathbf{1} = \mathbf{1} \\ & M^T\mathbf{1} = \mathbf{1} \end{aligned}$$

attain the same optimal value, and any optimal matrix $\hat{M}$ which is an extreme point of the constraints corresponds to an optimal permutation $\hat{\phi}$.

Note: solving the linear program with the simplex method guarantees that any obtained optimal solution is an optimal permutation matrix.

Note: the linear program is a special instance of a discrete optimal transport problem.

[1] G. Birkhoff, Tres observaciones sobre el algebra lineal, Univ. Nac. Tucuman, Ser. A, vol. 5, pp. 147154, 1946.
[2] D. Luenberger and Y. Ye, Linear and nonlinear programming. Cham: Springer, 2016.

The discrete optimal transport problem is given by

$$\begin{aligned} \underset{M \in \mathbb{R}_+^{N \times N}}{\text{minimize}} \quad & \langle C, M \rangle \\ \text{subject to} \quad & M\mathbf{1} = \mu_0 \\ & M^T\mathbf{1} = \mu_1. \end{aligned}$$

where

- $\mu_0, \mu_1 \in \mathbb{R}_+^N$ are given marginals; must have same total mass: $\mathbf{1}^T \mu_0 = \mathbf{1}^T \mu_1$.
- $C = [C_{ij}]_{i,j=1}^N$ is a cost matrix; C_{ij} = the cost of moving mass from point i to point j.
- $M = [M_{ij}]_{i,j=1}^N$ is the transport plan; M_{ij} = the mass moved from point i to point j.

Interpretation: a classical minimum-cost flow problem on a complete bipartite graph

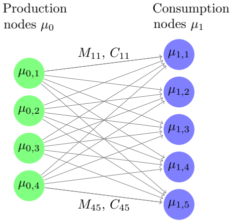


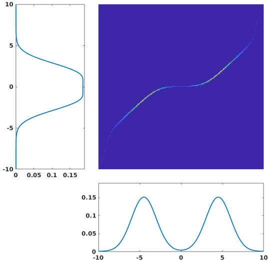
Figure: Small minimum-cost flow problem.

The discrete formulation can be generalized to a continuous setting:

$$\begin{aligned} \underset{m\in\mathcal{M}_+(X\times X)}{\text{minimize}} \quad & \int_{X\times X} c(x_0,x_1)m(x_0,x_1)dx_0dx_1 \\ \text{subject to} \quad & \int_X m(x_0,x_1)dx_1 = \mu_0(x_0), \\ & \int_X m(x_0,x_1)dx_0 = \mu_1(x_1). \end{aligned}$$

where

- $X \subset \mathbb{R}^d$ is the state space.
- $\mathcal{M}_+(\cdot) =$ the set of nonnegative distributions.
- $\mu_0,\ \mu_1 \in \mathcal{M}_+(X)$ are given marginals; must have same total mass: $\int_X \mu_0(x)dx = \int_X \mu_1(x)dx$.
- $c(\cdot,\cdot)$ is a continuous cost function; $c(x_0,x_1) =$ cost of moving mass from x_0 to x_1.
- $m(\cdot,\cdot) \in \mathcal{M}_+(X\times X)$ is the transport plan; $m(x_0,x_1) =$ the mass moved from x_0 to x_1.



This is the so-called Kantorovich formulation of the optimal transport problem.

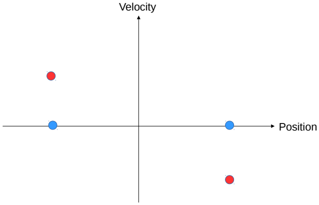
The discrete problem can be seen as a specific instance where, for $k=1,2$,

$$\mu_k(x_k) = \sum_{i=1}^{N} \mu_{k,i}\delta(x-x_i)$$

Matching and minimum energy control

Returning to the matching problem

$$\underset{\phi \in \text{perm}(\{1,2\ldots,N\})}{\text{minimize}} \sum_{i=1}^{N} \|x_i^{(0)} - x_{\phi(i)}^{(1)}\|_2^2.$$



- If X is a state space, distance $\|x_i^{(0)} - x_j^{(1)}\|_2^2$ might not be "relevant".
- Can the dynamics be included in the formulation?

Note: $\|x_i^{(0)} - x_j^{(1)}\|_2^2$ is the geodesic distance in Euclidean space.

Can be formulated as

$$\|x_i^{(0)} - x_j^{(1)}\|_2^2 = \begin{array}{rl} \underset{\gamma \in C([0,1])}{\text{minimize}} & \int_0^1 \|\dot{\gamma}(t)\|_2^2 dt \\ \text{subject to} & \gamma(0) = x_i^{(0)}, \quad \gamma(1) = x_j^{(1)} \end{array} = \begin{array}{rl} \underset{u \in L_2([0,1])}{\text{minimize}} & \int_0^1 \|u(t)\|_2^2 dt \\ \text{subject to} & \dot{x}(t) = u(t), \\ & x(0) = x_i^{(0)}, \quad x(1) = x_j^{(1)}. \end{array}$$

This is a minimum energy control problem for d independent integrators!

Introducing underlying dynamics in the matching problem

This means that the matching problem can be rewritten as

$$\underset{\phi\in\text{perm}(\{1,2\dots,N\})}{\text{minimize}} \sum_{i=1}^{N} \|x_i^{(0)} - x_{\phi(i)}^{(1)}\|_2^2 \quad = \quad \begin{aligned} \underset{\substack{\phi\in\text{perm}(\{1,2\dots,N\})\\ u_i\in L_2([0,1])}}{\text{minimize}} \quad & \sum_{i=1}^{N}\int_0^1 \|u_i(t)\|_2^2 dt \\ \text{subject to} \quad & \dot{x}_i(t) = u_i(t), \\ & x_i(0) = x_i^{(0)}, \quad x_i(1) = x_{\phi(i)}^{(1)}. \end{aligned}$$

Now we can introduce dynamics:

$$\begin{aligned} \underset{\substack{\phi\in\text{perm}(\{1,2\dots,N\})\\ u_i\in L_2([0,1])}}{\text{minimize}} \quad & \sum_{i=1}^{N}\int_0^1 \|u_i(t)\|_2^2 dt \\ \text{subject to} \quad & \dot{x}_i(t) = Ax_i(t) + Bu_i(t), \\ & x_i(0) = x_i^{(0)}, \quad x_i(1) = x_{\phi(i)}^{(1)}. \end{aligned} \quad = \quad \underset{\phi\in\text{perm}(\{1,2\dots,N\})}{\text{minimize}} \sum_{i=1}^{N} c^{A,B}(x_i^{(0)}, x_{\phi(i)}^{(1)})$$

where $c^{A,B}$ is the "control energy distance"

$$\begin{aligned} c^{A,B}(x_0, x_1) \; = \; \underset{u\in L_2([0,1])}{\text{minimize}} \quad & \int_0^1 \|u(t)\|_2^2 dt \\ \text{subject to} \quad & \dot{x}(t) = Ax(t) + Bu(t), \\ & x(0) = x_0, \quad x(1) = x_1. \end{aligned}$$

Dynamics can be included by changing the cost function!

Introducing underlying dynamics in the matching problem

The "control energy distance" has a closed form expression:

$$c^{A,B}(x_0, x_1) = (x_1 - \text{expm}(A)x_0)^T \Sigma_{A,B}^{-1}(x_1 - \text{expm}(A)x_0)$$

where $\Sigma_{A,B}$ is the controllability Gramian $\Sigma_{A,B} = \int_0^1 \text{expm}(A(1-s))BB^T\text{expm}(A^T(1-s))ds$.

The arguments for rewriting the combinatorial problem as a linear program still hold!

- Parametrize ϕ with permutation matrix $M \in \{0,1\}^{N\times N}$.
- Introduce cost $C^{A,B}_{x^{(0)},x^{(1)}} = [C^{A,B}_{ij}]_{i,j=1}^N$, where $C^{A,B}_{ij} = c^{A,B}(x_i^{(0)}, x_j^{(1)})$.
- Write as $\underset{M\in\{0,1\}^{N\times N}}{\text{minimize}} \langle C^{A,B}_{x^{(0)},x^{(1)}}, M\rangle$ subject to $M\mathbf{1} = \mathbf{1}$ and $M^T\mathbf{1} = \mathbf{1}$.
- Relax $M \in \{0,1\}^{N\times N}$ to $M \in [0,1]^{N\times N}$ and use Birkhoff's theorem.

.

$\rightsquigarrow$ Can solve the problem by solving $\underset{M\in[0,1]^{N\times N}}{\text{minimize}} \langle C^{A,B}_{x^{(0)},x^{(1)}}, M\rangle$ subject to $M\mathbf{1} = \mathbf{1}$ and $M^T\mathbf{1} = \mathbf{1}$.

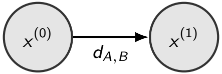
Note: it holds for general nonlinear dynamics, as long as $c(x_0, x_1)$ can be computed effectively.

$$\begin{aligned} c(x_0,x_1) \; = \; & \underset{u\in L_2([0,1])}{\text{minimize}} && \int_0^1 \|u(t)\|_2^2 dt \\ & \text{subject to} && \dot{x}(t) = f(x,u), \\ &&& x(0) = x_0, \quad x(1) = x_1. \end{aligned}$$

Optimal steering of a swarm based on the matching problem

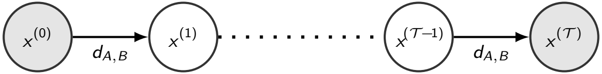
$$\begin{aligned} d_{A,B}(x^{(0)}, x^{(1)}) \; := \; \underset{\substack{\phi \in \mathrm{perm}(\{1,2\dots,N\}) \\ u_i \in L_2([0,1])}}{\text{minimize}} \quad & \sum_{i=1}^{N} \int_0^1 \|u_i(t)\|_2^2 dt & = \underset{M \in [0,1]^{N \times N}}{\text{minimize}} \quad & \langle C^{A,B}_{x^{(0)},x^{(1)}}, M \rangle \\ \text{subject to} \quad & \dot{x}_i(t) = A x_i(t) + B u_i(t), & \text{subject to} \quad & M\mathbf{1} = \mathbf{1} \\ & x_i(0) = x_i^{(0)}, \quad x_i(1) = x^{(1)}_{\phi(i)} & & M^T \mathbf{1} = \mathbf{1}. \end{aligned}$$

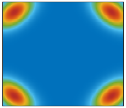
We illustrate such problems graphically as below, where grey circles means known agent distributions.



Next step: can we solve control problems of type $\underset{x^{(i)}}{\text{minimize}} \sum_{i=0}^{\mathcal{T}-1} d_{A,B}(x^{(i)}, x^{(i+1)})$ with given $x^{(0)}$, $x^{(\mathcal{T})}$?

Illustrated with the below graph, where white circles means unknown distributions to be optimized over.



	?	?	?	?	?	?	?
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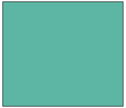
?	?	?	?	?	?	?	

Optimal steering of a swarm based on the matching problem
Relaxation to convex problem

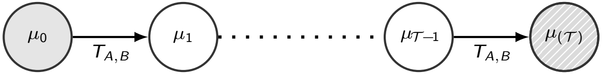
Issue: $d_{A,B}(x^{(0)}, x^{(1)})$ is not convex in the agent positions! (To see this: $C^{A,B}_{ij} = c^{A,B}(x^{(0)}_i, x^{(1)}_j)$).
Remedy: the optimal transport interpretation!

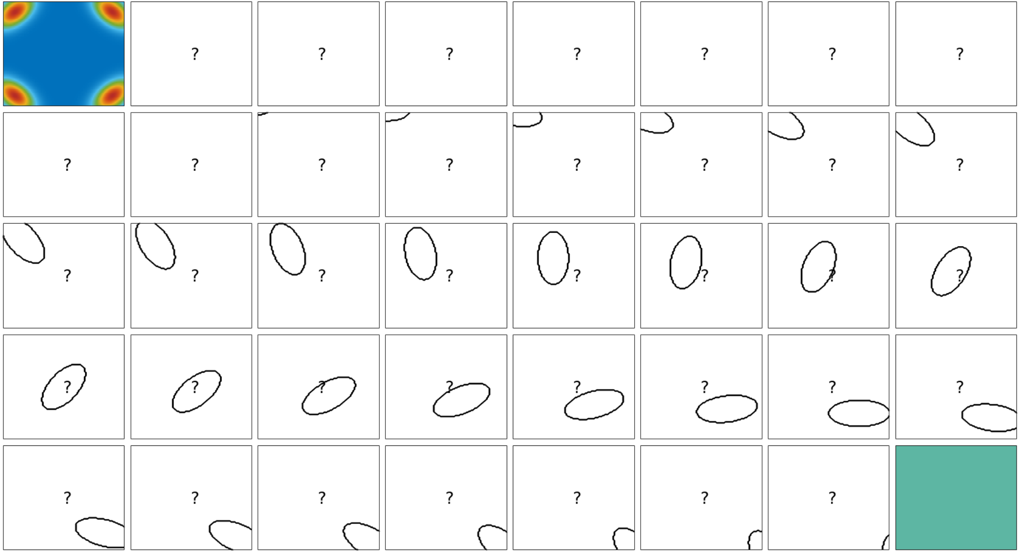
$$d_{A,B}(x^{(0)}, x^{(1)}) = \begin{array}{ll} \underset{M\in[0,1]^{N\times N}}{\text{minimize}} & \langle C^{A,B}_{x^{(0)},x^{(1)}}, M\rangle \\ \text{subject to} & M\mathbf{1} = \mathbf{1} \\ & M^T\mathbf{1} = \mathbf{1} \end{array} \rightsquigarrow \begin{array}{ll} \underset{m\in\mathcal{M}_+(X\times X)}{\text{minimize}} & \displaystyle\int_{X\times X} c^{A,B}(x_0, x_1)m(x_0, x_1)dx_0 dx_1 =: T_{A,B}(\mu_0, \mu_1) \\ \text{subject to} & \displaystyle\int_X m(x_0, x_1)dx_1 = \mu_0(x_0), \\ & \displaystyle\int_X m(x_0, x_1)dx_0 = \mu_1(x_1). \end{array}$$

Relax it to a general density control problem.

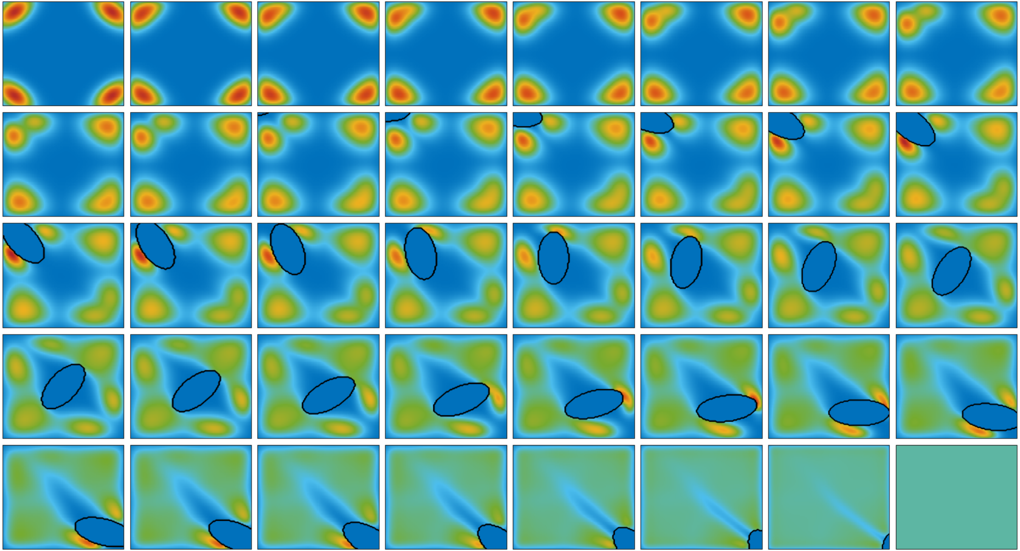
- Corresponds to having two densities of infinitesimal agents, each with dynamics $\dot{x} = Ax + Bu$.
- The optimal transport problem $T_{A,B}(\mu_0, \mu_1)$ is convex in the marginals!

Change $\underset{x^{(i)}}{\text{minimize}} \sum_{i=0}^{\mathcal{T}-1} d_{A,B}(x^{(i)}, x^{(i+1)})$ for the density control problem $\underset{\mu_i}{\text{minimize}} \sum_{i=0}^{\mathcal{T}-1} T_{A,B}(\mu_i, \mu_{i+1})$.
Illustrated with the below graph, where white circles means unknown distributions to be optimized over.
We can also introduce constraints on the unknown marginals.





Optimal steering of a swarm based on the matching problem
Example with constraints



To solve $\underset{\mu_i}{\text{minimize}} \sum_{i=0}^{\mathcal{T}-1} T_{A,B}(\mu_i, \mu_{i+1})$ numerically, we must first understand how to solve $T_{A,B}(\mu_0, \mu_1)$.

Answer: Discretize the state space and solve discrete problem!

State space $\mathbb{R}^d$ with each dimension discretized into $\mathcal{N}$ grid points $\rightsquigarrow$ $\mathcal{N}^d$ grid points $(y_i)_{i=1}^{\mathcal{N}^d}$

- $\rightsquigarrow$ marginals μ_0 and μ_1 are vectors in $\mathcal{N}^d$.
- $\rightsquigarrow$ cost matrix $C^{A,B} \in \mathbb{R}_+^{\mathcal{N}^d \times \mathcal{N}^d} = \mathbb{R}_+^{\mathcal{N}^{2d}}$, with elements $C_{ij}^{A,B} = c^{A,B}(y_i, y_j)$.
- $\rightsquigarrow$ transport plan M with $\mathcal{N}^{2d}$ variables!
  An explosion in the number of variables!
  Even for small numbers like $d = 2$ and $\mathcal{N} = 100$, this gives $100^4 = 10^8 =$ 100 million variables

$$\begin{aligned} \underset{M \in [0,1]^{N \times N}}{\text{minimize}} \quad & \langle C^{A,B}_{x(0),x(1)}, M \rangle \\ \text{subject to} \quad & M\mathbf{1} = \mathbf{1} \\ & M^T\mathbf{1} = \mathbf{1} \end{aligned}$$

- $+$ N^2 varaibles, where N is number of agents; independent of dimension of state space.
- $-$ Not convex in agent position.

$$\begin{aligned} \underset{M \in \mathbb{R}_+^{\mathcal{N}^d \times \mathcal{N}^d}}{\text{minimize}} \quad & \langle C^{A,B}, M \rangle \\ \text{subject to} \quad & M\mathbf{1} = \mu_0 \\ & M^T\mathbf{1} = \mu_1 \end{aligned}$$

- $-$ $\mathcal{N}^{2d} \gg N^2$ variables; huge, and exponential in the dimension of state space.
- $+$ Convex in agent position.

Recently proposed to solve via entropy regularization [1]: $KL(M \mid \mathbf{1}\mathbf{1}^T) = \sum_{i,j=1}^{\mathcal{N}^d} (M_{ij}\log(M_{ij}) - M_{ij} + 1)$,

$$\begin{aligned} \min_{M \in \mathbb{R}_+^{\mathcal{N}^d \times \mathcal{N}^d}} \quad & \langle C, M \rangle + \epsilon KL(M \mid \mathbf{1}\mathbf{1}^T) \\ \text{subject to} \quad & M\mathbf{1} = \mu_0 \\ & M^T\mathbf{1} = \mu_1. \end{aligned}$$

- Let $\exp(\,\cdot\,)$, $\log(\,\cdot\,)$, $./$, $\odot$ denotes the element-wise function.
- For $K = \exp(-C/\epsilon)$, the solution is of the form

$$M = \mathrm{diag}(u)K\mathrm{diag}(v).$$

Theorem (Sinkhorn iterations [2])

For any matrix K with positive elements there are diagonal matrices $\mathrm{diag}(u), \mathrm{diag}(v)$ such that $M = \mathrm{diag}(u)K\mathrm{diag}(v)$ has prescribed row- and column-sums μ_0 and μ_1. The vectors u and v can be obtained by alternating perform:

$$u = \mu_0./(Kv)$$

$$v = \mu_1./(K^T u).$$

[1] M. Cuturi. Sinkhorn distances: Lightspeed computation of optimal transport. In *Advances in Neural Information Processing Systems*, pages 2292–2300, 2013.
[2] R. Sinkhorn. Diagonal equivalence to matrices with prescribed row and column sums. *The American Mathematical Monthly*, 74(4), 402–405, 1967.

Recently proposed to solve via entropy regularization [1]: $KL(M \mid \mathbf{1}\mathbf{1}^T) = \sum_{i,j=1}^{\mathcal{N}^d} (M_{ij}\log(M_{ij}) - M_{ij} + 1)$,

$$\min_{M \in \mathbb{R}_+^{\mathcal{N}^d \times \mathcal{N}^d}} \quad \langle C, M \rangle + \epsilon KL(M \mid \mathbf{1}\mathbf{1}^T)$$

subject to $M\mathbf{1}$

Reduces the number of variables from $\mathcal{N}^{2d}$ to $2\mathcal{N}^d$!

- Let $\exp(\cdot)$
- For $K = \exp(-C/\epsilon)$, the solution is of the form:

$$M = \mathrm{diag}(u) K \mathrm{diag}(v).$$

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[2] R. Sinkhorn. Diagonal equivalence to matrices with prescribed row and column sums. *The American Mathematical Monthly*, 74(4), 402–405, 1967.

More in-depth on how to derive the Sinkhorn iterations: consider

$$\begin{aligned} \min_{M \in \mathbb{R}_+^{\mathcal{N}^d \times \mathcal{N}^d}} \quad & \langle C, M \rangle + \epsilon KL(M \mid \mathbf{1}\mathbf{1}^T) \\ \text{subject to} \quad & M\mathbf{1} = \mu_0 \\ & M^T\mathbf{1} = \mu_1. \end{aligned}$$

- Using Lagrangian relaxation gives

$$L(M, \lambda, \zeta) = \langle C, M \rangle + \epsilon KL(M \mid \mathbf{1}\mathbf{1}^T) + \lambda^T(\mu_0 - M\mathbf{1}) + \zeta^T(\mu_1 - M^T\mathbf{1}).$$

- Given dual variables λ, ζ, the minimum M_{ij} is

$$0 = \frac{\partial L(M, \lambda, \zeta)}{\partial M_{ij}} = C_{ij} + \epsilon \log(M_{ij}) - \lambda_i - \zeta_j$$

- Solve for M_{ij} to get

$$M_{ij}^* = e^{\lambda_i/\epsilon} e^{-C_{ij}/\epsilon} e^{\zeta_j/\epsilon}.$$

- Change of variables: $u = \exp(\lambda/\epsilon)$, $v = \exp(\zeta/\epsilon)$. The optimal solution is of the form

$$M^* = \text{diag}(u) K \text{diag}(v)$$

  where $K = \exp(-C/\epsilon)$.

One way to interpreted the Sinkhorn iterations: coordinate ascent in the Lagrangian dual.

- Lagrangian relaxation gave optimal form of the primal variable

$$M^* = \mathrm{diag}(u)K\mathrm{diag}(v)$$

- The Lagrangian dual function:

$$\varphi(u,v) := \min_{M \in \mathbb{R}_+^{\mathcal{N}^d \times \mathcal{N}^d}} L(M,u,v) = L(M^*,u,v) = \ldots = \epsilon \log(u)^T \mu_0 + \epsilon \log(v)^T \mu_1 - \epsilon u^T K v + \epsilon \mathcal{N}^{2d}.$$

- The dual problem is thus

$$\max_{u,v \in \mathbb{R}_+^{\mathcal{N}^d}} \varphi(u,v)$$

- Taking the gradient w.r.t u and putting it equal to zero gives

$$\epsilon \mu_0./u - \epsilon K v = 0 \quad \rightsquigarrow \quad u = \mu_0./(Kv),$$

and w.r.t v gives

$$\epsilon \mu_1./v - \epsilon \left(u^T K\right)^T = 0 \quad \rightsquigarrow \quad v = \mu_1./(K^T u).$$

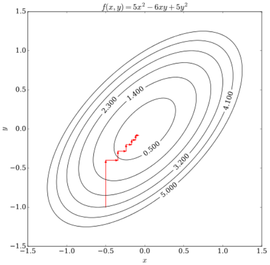

Figure from Wikipedia

These are the Sinkhorn iterations! (cf. [1])

[1] P. Tseng. Dual ascent methods for problems with strictly convex costs and linear constraints: A unified approach. *SIAM Journal on Control and Optimization*, 28(1), 214–242, 1990.

Summary and take-home message:

- Optimal transport can be used to solve matching problems for sets of dynamic agents;
- With this as basis, it can be used to solve optimal control problems for swarm of agents;
- The problems can be solve numerically by developing numerical methods along the lines of the Sinkhorn iterations.

Optimal transport - a viable framework for many problems and applications!

Thank you for your attention!

Questions?