Computational Optimal Transport – Project report:

Optimal Transport and Entropic methods for solving variational Mean-Field Games

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1 General setting: variational mean-field games

A mean-field game [8, 9] is a strategic decision-making problem with a very large, continuously-distributed number of interacting agents inside a state space: the overall theory developed by Lasry and Lions can be used as a means to model large, computationally intractable games. In the continuous-time setting explored in [9], each agent evolves according to some dynamics and makes choices, but the response to his choices are affected by the states and choices of the numerous other agents – leading to a so-called *differential game* – through a *mean-field* effect.

Several ways of modeling agent cross-interaction exist. More recently, [3] have focused on games where agent interactions take a variational form, allowing to penalize phenomenons such as congestion inside areas of the agent state space.

The (Nash) equilibrium agent-control dynamics can be summarized by the system of coupled nonlinear partial differential equations:

$$-\partial_t u - \frac{1}{2}\Delta u + \frac{1}{2}|\nabla u|^2 = f[\rho_t] \quad (t,x) \in (0,T)\times\Omega \tag{1.1a}$$

$$\partial_t \rho_t - \frac{1}{2}\Delta \rho_t - \mathrm{div}(\rho_t \nabla u) = 0 \tag{1.1b}$$

$$\rho_0 \text{ given} \tag{1.1c}$$

$$u(T,\cdot) = g[\rho_T] \tag{1.1d}$$

where and $t \mapsto \rho_t$ is a trajectory in the space of measures, and Ω is the standard Euclidean space $\mathbb{R}^d$. The applications f and g are supposed to be derivatives of some real-valued functionals F and G. For instance, if $G(\mu) = \int_\Omega \Psi\, d\mu(x)$ then its derivative is $g[\mu](x) = \Psi(x)$.

The equations (1.1a)–(1.1b) form a coupled system of control (Hamilton-Jacobi-Bellman) and diffusion (forward Kolmogorov) equations. They can be solved in some cases using finite-difference methods (see [1]).

1.1 The variational problem

The first idea of [3] is to cast the MFG partial differential equations to a variational problem over an appropriate function space. Denote $\mathbb{W}_2(\Omega) = (\mathcal{P}_2(\Omega), \mathcal{W}_2)$ the set of probability measures with finite second moment, equipped with the Wasserstein metric

$$\mathcal{W}_2(\mu,\nu)^2 = \inf_{\gamma\in\Pi(\mu,\nu)} \int |x-y|^2 d\gamma \tag{1.2}$$

where $\Pi(\mu, \nu) = \{\gamma \in \mathcal{P}_2(\Omega \times \Omega) : P^1_\# \gamma = \mu,\ P^2_\# \gamma = \nu\}$ is the set of transport plants from μ to ν. Then, $\mathcal{C}([0, T], \mathbb{W}_2(\Omega))$ is the Wiener space of continuous $\mathbb{W}_2$-valued trajectories. Benamou, Carlier, and Santambrogio [3] show that the MFG be reformulated to the following variational problem:

$$\inf_{\rho,v} J(\rho, v) = \frac{1}{2}\int_0^T \int_\Omega |v_t|^2 \, d\rho_t(x) \, dt + \int_0^T F(\rho_t) \, dt + G(\rho_T) \tag{1.3a}$$

$$\text{s.t. } \partial_t \rho_t - \frac{1}{2}\Delta\rho_t + \operatorname{div}(\rho_t v) = 0 \tag{1.3b}$$

$$\rho_0 \in \mathbb{W}_2(\Omega) \tag{1.3c}$$

where $\rho = (\rho_t)_{t\in[0,T]} \in \mathcal{C}([0, T], \mathbb{W}_2(\Omega))$ is a trajectory in $\mathbb{W}_2$ and v is a sufficiently regular function on $[0, T] \times \Omega$ (most likely a Sobolev space).

Benamou et al. [4] also introduce the following partial problem:

$$\mathrm{FP}_h(\mu, \nu) = \inf_{\rho,v} \int_0^h \int_\Omega |v_t|^2 d\rho_t(x) \, dt \quad \text{s.t. } \partial_t\rho_t - \frac{1}{2}\Delta\rho_t + \operatorname{div}(\rho_t v),\ \rho_0 = \mu,\ \rho_h = \nu \tag{1.4}$$

It can be used to connect approximations of the solution measure to our MFG problem at discrete times $t_k = kh$, $k = 0, \dots, N$.

This point of view [3] is called *Eulerian*: we minimize over both the velocity v and the time-trajectory of the agents' density ρ. It is not very practical because of the structure of the constraint (a Fokker-Planck equation). Instead, we could minimize over measures in the space of individual agents' trajectories, which is the base of the *Lagrangian* formulation [2, 3] proposed by Benamou, Carlier, and Santambrogio and that we explore in the sequel.

2 Lagrangian dual formulation

2.1 Wiener space and measure

This new point of view involves a change in function spaces. We denote $\mathcal{X} = \mathcal{C}([0, T], \Omega)$ the Wiener space of (agents') trajectories $[0, T] \to \Omega$. Following [3, 2], we equip it with the Wiener measure (the law of a Wiener process with any starting point x)

$$R = \int_\Omega \delta_{x+W} \, dx$$

where W is a standard Wiener process in $\mathbb{R}^d$. It is an analogue in the space $\mathcal{X}$ to the usual finite-dimensional Lebesgue measure[1].

Measures $Q \in \mathcal{P}(\mathcal{X})$ can also be seen as trajectories $(Q_t)_{t\in[0,T]} \in \mathcal{C}([0, T], \mathcal{P}(\Omega))$, with

$$Q_t = e_{t\#} Q \in \mathcal{P}(\Omega)$$

the push-forward of Q by the evaluation map $e_t : \xi \in \mathcal{X} \longmapsto \xi(t)$. This naturally defines an injection $\underline{i} : \mathcal{P}(\mathcal{X}) \to \mathcal{C}([0, T], \mathcal{P}(\Omega))$. We also introduce the more general marginals $Q_{t_1,\dots,t_n} = (e_{t_1}, \dots, e_{t_n})_\# Q$ for $0 \le t_1 < \cdots < t_N \le T$.

[1] https://en.wikipedia.org/wiki/Infinite-dimensional_Lebesgue_measure

Marginals of the Wiener measure $\boldsymbol{R}$. We introduce the heat kernel $G_t(u) = \frac{1}{(2\pi t)^{d/2}} \exp\left(-\frac{|u|^2}{2t}\right)$. In particular, R_t is the Lebesgue measure $\mathcal{L}^d$ on $\mathbb{R}^d$, and

$$R_{s,t}(dx, dy) = G_{t-s}(x-y)\, dx\, dy. \tag{2.1}$$

Benamou, Carlier, and Santambrogio [3] and Benamou and Carlier [2] then re-cast the Eulerian variational game (1.3) into a so-called Lagrangian optimization problem over the set of Borel probability measures (more specifically that associated with the Sobolev subspace H^1 of $\mathcal{X}$). This new problem is solved in [3] using a finite element method, which is computationally expensive.

2.2 The entropic Lagrangian approach

Instead, Benamou et al. [4] propose using an entropy minimization approach to allow for a more computationally efficient method adapted from the Sinkhorn algorithm [6] developed by Cuturi.

This method, just like the Sinkhorn for OT between histograms (discrete measures), introduces some sort of entropic regularization [4], but this time on the measure over the trajectory space $\mathcal{X}$. The resulting numerical algorithm becomes a regularization of the Lagrangian from [3, 2].

The entropic Lagrangian variational problem is

$$\inf_{Q\in\mathcal{P}(\mathcal{X})} \mathrm{KL}(Q|R) + \int_0^T F(Q_t)\, dt + G(Q_T),\ \text{s.t. } Q_0 = \rho_0 \tag{2.2}$$

Partial transport problem Benamou et al. provide another partial transport problem:

$$S_h(\mu, \nu) = \inf\left\{\mathrm{KL}(Q|R) : Q \in \mathcal{P}(\mathcal{C}([0,h],\Omega)),\ Q_0 = \mu,\ Q_h = \nu\right\} \tag{2.3}$$

This problem can be seen as a continuous OT problem between the two measures μ and ν. Benamou et al. [4] show that it is linked to the partial Eulerian problem (1.4) as

$$S_h(\mu,\nu) = \mathrm{FP}_h(\mu,\nu) + \mathrm{Ent}\,\mu.$$

The dimensionality of problem (2.3) can be greatly simplified: [4] shows that we can rewrite it as a static OT problem

$$S_h(\mu,\nu) = \inf\left\{\mathrm{KL}(\gamma|R_{0,h}) : \gamma \in \Pi(\mu,\nu)\right\}. \tag{2.4}$$

2.3 Viscosity and the deterministic limit

We change the MFG problem to one following the agent-level dynamics $dX_t = v_t dt + \sigma dW_t$. The MFG equilibrium equations become

$$\begin{aligned} -\partial_t u - \frac{\sigma^2}{2}\Delta u + \frac{1}{2}|\nabla u|^2 &= f[\rho_t] \\ \partial_t \rho - \frac{\sigma^2}{2}\Delta\rho - \operatorname{div}(\rho\nabla u) &= 0 \end{aligned} \tag{2.5}$$

3 Numerical algorithm

Let N be the number of discrete steps for the time discretization of the problem, and $h = T/N$ the time step.

We consider the following multi-marginal OT problem

$$\mathcal{S}(\mu_0, \ldots, \mu_N) = \inf_{\gamma \in \Pi(\mu_0, \ldots, \mu_N)} H(\gamma | R^N) \tag{3.1}$$

where $t_k = kh$, $R^N = R_{t_0,\ldots,t_N}$ and the marginals $\mu_k \in \mathcal{P}_2(\Omega)$. Then, define

$$\mathcal{U}(\mu_0, \ldots, \mu_N) = h \sum_{k=1}^{N-1} F(\mu_k) + G(\mu_N). \tag{3.2}$$

Thus, the discretized entropy minimization problem can be written as

$$\inf \left\{ \mathcal{S}(\mu_0, \ldots, \mu_N) + \mathcal{U}(\mu_0, \ldots, \mu_N) : \mu_k \in \mathcal{P}_2(\Omega),\ \mu_0 = \rho_0 \right\}.$$

Expanding the inf-within-inf leads to the following convex optimization problem:

$$\begin{aligned} &\inf_{\gamma \in \mathcal{P}(\Omega^{N+1})} H(\gamma | R^N) + \imath_{\rho_0}(\mu_0) + \sum_{k=1}^{N-1} F(\mu_k) + G(\mu_N) \\ &\text{s.t. } \mu_k = P^k_{\#}\gamma \end{aligned} \tag{3.3}$$

where $\imath_{\rho_0}(\mu) = +\infty$ if $\mu \neq \rho_0$ and 0 otherwise is the convex indicatrix of the measure ρ_0. This is a generalized multimarginal optimal transport problem.

Benamou et al. [4] provide the corresponding dual problem involving the convex conjugates and potential functions, by using a multimarginal generalization of a result from Chizat et al. [5]:

$$\sup_u -\imath^*_{\rho_0}(-u_0) - \sum_{k=1}^{N-1} F^*(-u_k) - G^*(-u_N) - \int_{\Omega^{N+1}} \left(\exp\left(\oplus_{k=0}^N u_k \right) - 1 \right) dR^N \tag{3.4}$$

where the supremum is taken over $u = (u_0, \ldots, u_N) \in L^\infty(\Omega)^{N+1}$.

Benamou et al. [4] introduce a Sinkhorn-like iterative algorithm to solve the above dual problem. We rewrite it more explicitly with slightly different notations inspired by [5]

Algorithm 1. *Denote for $k = 0, \ldots, N$ and $(a_j)_{j \neq k}$*

$$\mathcal{I}_k((a_j)_{j\neq k})(z_k) = \int_{\Omega^N} \prod_{j \neq k} a_j(x_j)\, dR^N(x_{0:k-1}, z_k, x_{k+1:N})$$

the integral of functions $a_j, j \neq k$ with respect to R^N and variables x_j, $j \neq k$. For convenience we use the shorthand

$$\mathcal{I}_k^{(n)} = \mathcal{I}_k \left(\left(e^{u_j^{(n+1)}} \right)_{j<k}, \left(e^{u_j^{(n)}} \right)_{j>k} \right)$$

for the nth iterate.

Then we compute the dual potentials iteratively:

$$\begin{cases} u_0^{(n+1)} = \underset{v \in L^\infty}{\operatorname{argmax}} \displaystyle\int_\Omega (1 - e^{-v(x_0)}) \mathcal{I}_0^{(n)} \, dx_0 - \imath^*_{\rho_0}(v) \\ u_k^{(n+1)} = \underset{v \in L^\infty}{\operatorname{argmax}} \displaystyle\int_\Omega (1 - e^{-v(x_k)}) \mathcal{I}_k^{(n)} \, dx_k - hF^*(v), \quad 1 \leq k < N \\ u_N^{(n+1)} = \underset{v \in L^\infty}{\operatorname{argmax}} \displaystyle\int_\Omega (1 - e^{-v(x_N)}) \mathcal{I}_N^{(n)} \, dx_N - G^*(v) \end{cases} \tag{3.5}$$

until convergence.

Using duality, we find that the iterates $u_k^{(n)}$ satisfy

$$a_k^{(n)} = \exp(-u_k^{(n)}) = \frac{\operatorname{prox}_{F_k}^{\mathrm{KL}}(\mathcal{I}_k^{(n)})}{\mathcal{I}_k^{(n)}} \tag{3.6}$$

where

$$\operatorname{prox}_F^{\mathrm{KL}}(z) = \underset{s}{\operatorname{argmin}} \, F(s) + \mathrm{KL}(s|z).$$

Remark 1 (Some convex conjugates)**.** In practice, the convex conjugates of the cost functions are difficult to compute. For some of the examples in the paper, we have closed-form conjugates.

- The conjugate of the convex indicatrix $\imath_\nu$ of any measure ν is given by $\imath_\nu^*(u) = \langle u, \nu \rangle$.
- The hard congestion constraint

  $$C(\rho) = \begin{cases} 0 & \text{if } \rho \leq \bar{m} \\ +\infty & \text{otherwise} \end{cases}$$

  has convex conjugate (on the domain $\rho \geq 0$)

  $$C^*(u) = \sup_{\rho \leq \bar{m}} \langle u, \rho \rangle = \langle u^+, \bar{m}\mathbb{1} \rangle$$

- Obstacle constraints, given by

  $$F(\rho) = \int_\Omega V(x) \, d\rho(x) = \begin{cases} 0 & \text{if } \rho = 0 \text{ on } \mathscr{O} \\ +\infty & \text{otherwise} \end{cases} = \imath_0(\mathbb{1}_{\mathscr{O}}\rho)$$

  where V is the convex indicatrix of the complement $\Omega \backslash \mathscr{O}$ of the obstacles. Its conjugate is given by

  $$F^*(u) = \begin{cases} 0 & \text{if } u \leq 0 \text{ on } \Omega \backslash \mathscr{O} \\ +\infty & \text{otherwise} \end{cases}$$

3.1 Full discretization

For full numerical implementation, all measures are replaced by multi-dimensional arrays representing discrete histograms over a fixed grid of points in $\mathbb{R}^d$ of dimensionality $M = N_1 \times \cdots \times N_d$. Integration is exchanged with summation.

In the general case, the KL-projections in the Sinkhorn iterations can be solved using the Python library CVXPY[2,3]. Some can be computed explicitly.

[2] https://github.com/cvxgrp/cvxpy

[3] Steven Diamond and Stephen Boyd. "CVXPY: A Python-Embedded Modeling Language for Convex Optimization". In: *Journal of Machine Learning Research* 17.83 (2016), pp. 1–5.

Proposition 1. *The KL-projection under the hard congestion constraint of a measure $\beta \in \mathbb{R}^M$ is given by*

$$\operatorname{prox}_C^{\mathrm{KL}}(\beta) = \min(\beta, \overline{m}) \tag{3.7}$$

where the minimum is taken element-wise.

If we also add the obstacle constraint on a set $\mathscr{O}$ of points in the grid, then the proximal operator reads

$$\operatorname{prox}_F^{\mathrm{KL}}(\beta) = \min(\beta, \bar{m}\mathbb{1}_{\Omega\setminus\mathscr{O}}). \tag{3.8}$$

4 Examples

4.1 Transport with a "fuzzy" target

4.1.1 Two-marginal case

We start with a very simplified approximation of the crowd displacement problem on $\Omega = [0,1]^2$, with only the first step (with initial agent distribution) and final step decided by the terminal penalty function G.

We set G to be the obstacle constraint related to a subset $\mathscr{O}$ of Ω as well as a potential $\Psi(x) = d(x, \mathscr{A})^\beta$ for some $\beta > 0$, related to the distance to a target subset $\mathscr{A}$ (see fig. 1):

$$G(\mu) = \int_\Omega \Psi \, d\mu + \imath_0(\mu \mathbb{1}_{\mathscr{O}})$$

Thus, the agents engage in a one-round mean-field game where they are only concerned with moving to regions with lower potential Ψ – as close as possible to $\mathscr{A}$ – whilst obeying physical constraints related to the obstacles.

The discretized MFG problem with viscosity parameter $\varepsilon = \sigma^2$ can be written as the following transport problem:

$$\begin{aligned} &\inf_\gamma \langle \Psi, \gamma^T \mathbb{1}\rangle + \varepsilon H(\gamma | R_\varepsilon) \\ &\text{s.t. } \gamma\mathbb{1} = \rho_0, \quad \gamma^T\mathbb{1} \odot \mathbb{1}_{\mathscr{O}} = 0 \end{aligned} \tag{4.1}$$

The interesting aspect of this problem is observing what kind of optimal distribution $\rho_1^* = (\gamma^*)^T\mathbb{1}$ the agents reach.

Proposition 2. *Problem (4.1) can be solved in closed form: the Lagrange multiplier u_0^* for the marginal law constraint satisfies*

$$e^{-u_0^*} = \frac{\rho_0}{R_\varepsilon a_1^*}$$

where $a_1^* = e^{-\Psi/\varepsilon} \odot \mathbb{1}_{\Omega\setminus\mathscr{O}}$, and the optimal coupling is

$$\gamma^* = R_\varepsilon \odot (e^{-u^*} \otimes \hat{\varphi})$$

It satisfies, as expected, that $\gamma_{i,j}^* = 0$ for all $j \in \mathscr{O}$.

Numerical experiment We ran a numerical experiment by implementing the solutions given by proposition 2 to the discrete MFG (4.1). fig. 2a provides a representation of both . We also checked the results when removing the constraints on the obstacles (essentially setting $\mathscr{O}$), and when lowering the viscosity parameter $\sigma = \sqrt{\varepsilon}$ (see figs. 2b and 2c).

Of course, replacing G by a hard marginal constraint turns the problem into a classical regularized OT problem, and the above proposition leads to usual Sinkhorn iterations on the

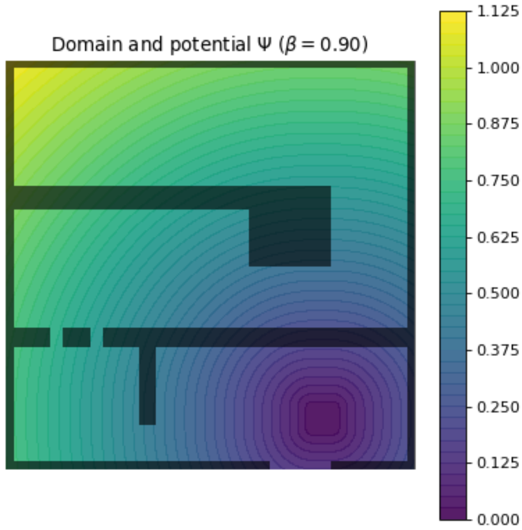


Figure 1: Computational domain of the game Ω with set of obstacles $\mathscr{O}$ (transparent grey), and contour of the potential function $\Psi(x) = d(x, \mathscr{A})^\beta$.

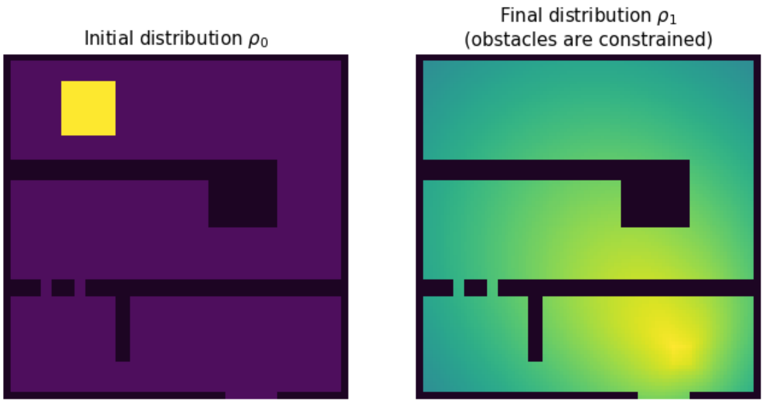
grid. The matrix-vector product in the Lagrange multiplier potentially becomes a computational bottleneck, but the separability of the heat kernel R_ε allows for fast computation using simple 1D convolutions.

Remark 2 (A "smarter" (more realistic) potential for crowd dynamics)**.** The results shown fig. 2 are satisfactory for the given potential Ψ – as expected the agents try to stay near the low-potential regions. However, for modeling of crowd dynamics they would be deeply nonphysical because the potential is inadequate. In a room evacuation scenario, for instance, agents would seek to minimize the time-to-exit: the literature shows this leads to the Eikonal equation, a kind of Hamilton-Jacobi PDE. We computed the adequate potential shown fig. 3a using the Fast Sweeping method [10] which we implemented in Cython.

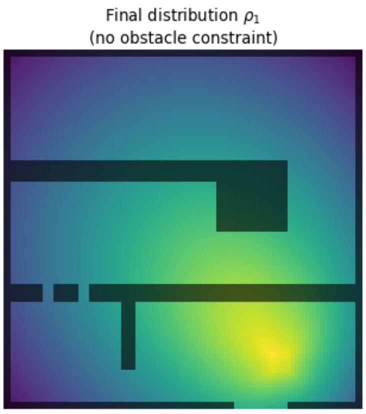
4.1.2 One intermediate time step

We now go up to three marginals (ρ_0, ρ_1, ρ_2). We assign to the single intermediate marginal ρ_1 the congestion constraint $\rho_1 \leq \bar{m}$ and the obstacle constraint. The primal problem then reads

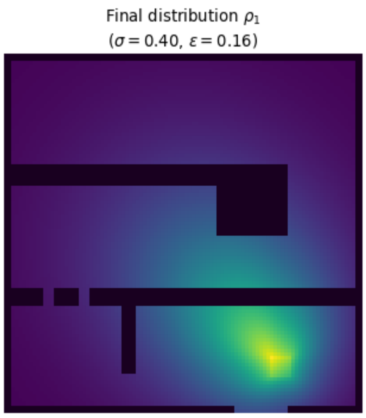
$$\begin{aligned} &\inf_{\gamma,\rho_1,\rho_2} \langle \Psi, \rho_2 \rangle + \varepsilon H(\gamma | R_\varepsilon) \\ \text{s.t. } &P^k_\# \gamma = \rho_k,\ k = 1, 2 \\ &\rho_1 \leq \bar{m} \\ &\rho_1 \odot \mathbb{1}_{\mathscr{O}} = 0 \\ &\rho_2 \odot \mathbb{1}_{\mathscr{O}} = 0 \end{aligned} \tag{4.2}$$



(a) Result of the "fuzzy" transport problem with enforcement of the obstacle constraints and viscosity parameter $\sigma = 1$.

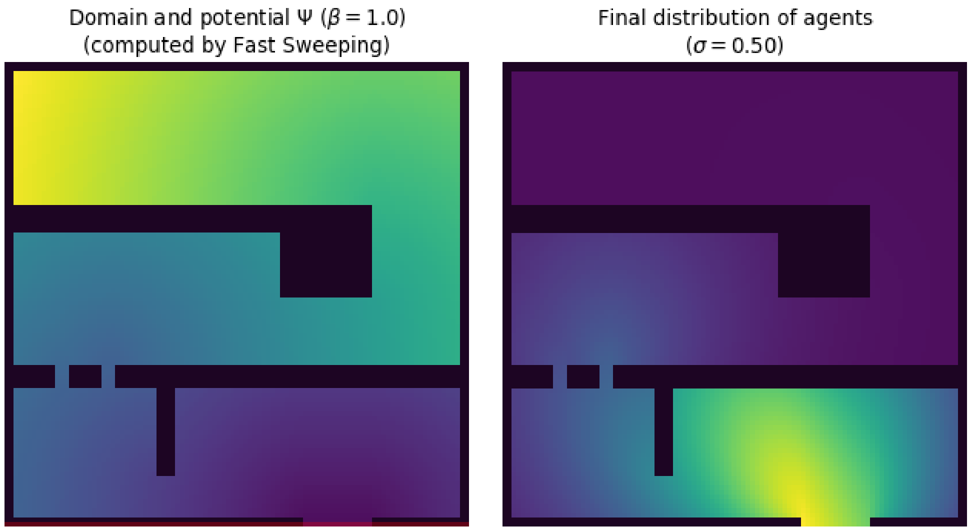


(b) Final distribution ρ_1^* without enforcing the obstacles. Notice that the mass of the distribution "bleeds" through the obstacles.



(c) Obstacles are constrained as in fig. 2a, but with a lower viscosity parameter $\sigma = 0.4$.

Figure 2: Marginal distributions of the solution of two-step MFG or "fuzzy transport" problem (4.1), with a few variations.



(a) Domain and potential associated with the fastest path distance.

(b) Optimal terminal distribution ρ_1^* of the discrete MFG with the potential from fig. 3a.

Figure 3: Setup and solution for the discrete MFG using the time-to-exit potential discussed in remark 2.

Proposition 3. *The Lagrange multipliers u_i^* at the optimum satisfy the fixed-point conditions:*

$$a_0^* = \frac{\rho_0}{R_\varepsilon[\cdot, a_1^*, a_2^*]}$$

$$a_1^* = \min\left(\frac{\bar{m}}{R_\varepsilon[a_0^*, \cdot, a_1^*]}\right)$$

where $a_i^* = \exp(-u_i^*)$, a_1^* is supported on $\Omega \backslash \mathscr{O}$ and $a_2^* = e^{-\Psi/\varepsilon} \odot \mathbb{1}_{\Omega\backslash\mathscr{O}}$, and we denote $R_\varepsilon[\cdot,\cdot,\cdot]$ the tensor product by R_ε.

The fixed point can then computed using an iterative algorithm à la generalized Sinkhorn, just as in the Algorithm 1 suggested by [4].

The issue of computational efficiency is more pronounced here than before due to the tensor product and need for multiple iterations until convergence.

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