Computational Optimal Transport

Regularized Optimal Transport methods for solving variational Mean-Field Games

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1 Quadratic 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 – leading to a so-called differential game – with the response to his choices depends on other agents' states and actions through a mean-field effect.

The general setup of a MFG has every agent penalize a running cost on the control and mean-field interaction, as well as a terminal cost on the its final position and the overall final distribution of agents (see [9]). The framework of [3, 4] focuses on games with agent dynamics $dX_t = \alpha_t dt + dW_t$ and quadratic running cost on the control α

$$\int_0^T L(\alpha_t) = \int_0^T \frac{\alpha_t^2}{2}$$

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

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

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

$$\rho_0$$
 given (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 a subset of the Euclidean space \mathbb{R}^d . The applications $f[\mu]$ and $g[\mu]$ are supposed to be derivatives of some real-valued functionals F and G on the space of measures. For instance, if $G(\mu)=\int_{\Omega}\Psi\,d\mu(x)$ then its derivative is $g[\mu](x)=\Psi(x)$.

Equations (1.1a) and (1.1b) form a coupled system of control (Hamilton-Jacobi-Bellman) and diffusion (Fokker-Planck) partial differential equations. They can be solved in some cases using finite-difference methods (see Achdou, Camilli, and Capuzzo-Dolcetta [1]).

2 Variational formulations for the quadratic MFG

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

$$W_2(\mu,\nu)^2 = \inf_{\gamma \in \Pi(\mu,\nu)} \int |x-y|^2 d\gamma \tag{2.1}$$

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 can be reformulated to the following variational problem:

$$\inf_{\rho,v} J(\rho,v) = \frac{1}{2} \int_0^T \int_{\Omega} |v_t|^2 d\rho_t(x) dt + \int_0^T F(\rho_t) dt + G(\rho_T)$$
s.t. $\partial_t \rho_t - \frac{1}{2} \Delta \rho_t + \operatorname{div}(\rho_t v) = 0$

$$\rho_0 \in \mathbb{W}_2(\Omega)$$
(2.2)

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 lying in a Sobolev space – see [3] for further discussion on regularity.

This point of view [3] is called *Eulerian*: we minimize over both the velocity v and the time-trajectory of the agents' density ρ . This can be solved by introducing Lagrange multipliers, exploiting duality, and using a finite element method, as shown in [3].

Benamou, Carlier, and Santambrogio [3] and Benamou et al. [4] also introduce a *Lagrangian* point of view, which allows to use tools from optimal transport theory: the variational problem is changed to optimize over the space of probability distributions on the space of agent trajectories.

2.1 Lagrangian formulation

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 measure¹.

Measures $Q \in \mathcal{P}(\mathcal{X})$ can also be seen as trajectories $(Q_t)_{t \in [0,T]}$ in $\mathcal{P}(\Omega)$ 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 $0 \le t_1 < \dots < t_N \le T$.

Marginals of the Wiener measure. In particular, R_t is the Lebesgue measure \mathcal{L}^d on \mathbb{R}^d , and we have that the final marginals have densities:

$$R_{s,t}(x,y) = P_{t-s}(y-x). (2.3)$$

where P_t is the standard d-dimensional heat kernel:

$$P_t(u) = \frac{1}{(2\pi t)^{d/2}} \exp\left(-\frac{|u|^2}{2t}\right)$$
 (2.4)

The N-marginals are given by

$$R_{t_1,\dots,t_N}(x_1,\dots,x_n) = \prod_{i=1}^{N-1} P_h(x_{i+1} - x_i)$$
(2.5)

Benamou, Carlier, and Santambrogio [3] and Benamou and Carlier [2] then re-cast the Eulerian variational game (2.2) into a Lagrangian optimization problem over the set of Borel probability measures. This new problem is also solved in [3] using a finite element method.

Integration Partial integration with respect to the 2-marginal measure $R_{0,h}$ is actually convolution with respect to the heat kernel P_h :

$$\int_{\Omega} u(x) R_{0,h}(x,y) \, dx = \int_{\Omega} u(x) P_h(y-x) \, dx = (u * P_h)(y)$$

The effect of integration against the N-marginal can then be deduced by induction.

2.2 Entropic Lagrangian

Instead of using finite element methods, Benamou et al. [4] propose using an entropy minimization approach to allow for a more computationally efficient method adapted from the Sinkhorn algorithm introduced by Cuturi [6]. This method introduces entropic regularization in the problem, but this time on the measure over the trajectory space

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

 \mathcal{X} . The resulting numerical algorithm becomes a regularization of the Lagrangian from [3, 2].

The entropic Lagrangian variational problem is

$$\inf_{Q \in \mathcal{P}(\mathcal{X})} H(Q|R) + \int_0^T F(Q_t) \, dt + G(Q_T) \quad \text{s.t. } Q_0 = \rho_0$$
 (2.6)

Intuitively, this is the same as fixing the marginals ρ_t , finding the optimal bridge Q between them that has minimal entropy relative to the Wiener measure, and then optimizing over the ρ_t .

2.3 Viscosity and the deterministic limit

We change the MFG problem to one following the agent dynamics $dX_t = \alpha_t dt + \sigma dW_t$ with a diffusion coefficient σ . The MFG equilibrium equations become

$$-\partial_t u - \frac{\sigma^2}{2} \Delta u + \frac{1}{2} |\nabla u|^2 = f[\rho_t]$$

$$\partial_t \rho - \frac{\sigma^2}{2} \Delta \rho - \operatorname{div}(\rho \nabla u) = 0$$
(2.7)

This can be used to approximate first-order MFGs by setting a low viscosity parameter σ . Denoting $\varepsilon = \sigma^2$, the entropic variational problem (2.6) becomes

$$\inf_{Q \in \mathcal{P}(\mathcal{X})} \varepsilon H(Q|\mathbf{R}_{\varepsilon}) + \int_{0}^{T} F(Q_{t}) dt + G(Q_{T}) \quad \text{s.t. } Q_{0} = \rho_{0}$$
 (2.8)

where R_{ε} is the Wiener measure associated with Wiener processes scaled by ε .

3 Numerical algorithm

3.1 Time discretization

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

Benamou et al. [4] propose a discretization of (2.6) obtained by connecting the marginals through a multimarginal OT problem:

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

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

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

Thus, the discretized entropy minimization problem can be written as

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

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

$$\inf_{\gamma \in \mathcal{P}(\Omega^{N+1})} \text{KL}(\gamma | R^N) + \iota_{\rho_0}(\mu_0) + \sum_{k=1}^{N-1} F(\mu_k) + G(\mu_N)$$
s.t. $\mu_k = P_{\#}^k \gamma$ (3.3)

where $i_{\rho_0}(\mu) = +\infty$ 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]:

$$\sup_{u} \int_{\Omega^{N+1}} \left(1 - \exp\left(\bigoplus_{k=0}^{N} u_k\right) \right) dR^N - i_{\rho_0}^*(-u_0) - \sum_{k=1}^{N-1} F^*(-u_k) - G^*(-u_N)$$
 (3.4)

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

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, ..., N and $(a_j)_{j \neq k}$

$$\mathcal{I}_{k}((a_{j})_{j \neq k})(\tilde{x}_{k}) = \int_{\Omega^{N}} \prod_{j \neq k} a_{j}(x_{j}) R^{N}(dx_{0:k-1}, \tilde{x}_{k}, dx_{k+1:N})$$

the partial integral of the $a_j, j \neq k$ with respect to R^N without variable x_k . For convenience we use the shorthand

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

for the nth iterate where we denote $a_j = \exp(-u_j)$.

Then we compute the dual potentials iteratively:

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

until convergence.

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

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

where

$$\operatorname{prox}_F^{\operatorname{KL}}(z) = \operatorname*{argmin}_s F(s) + \operatorname{KL}(s|z)$$

is the KL-proximal operator.

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 i_{ν} of any measure ν is given by $i_{\nu}^{*}(u) = \langle u, \nu \rangle$.
- The hard congestion constraint

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

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

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

• 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

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

3.2 Spatial discretization

For full numerical implementation, all measures are replaced by multi-dimensional arrays representing discrete histograms over a fixed grid of points x_i in \mathbb{R}^d of size $M = N_1 \times \cdots \times N_d$, and we naturally exchange convolution with the heat kernel for discrete convolution. This will be the main computational issue.

Projections. 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.

Proposition 1. The KL-projection on 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.

The KL-projection on the obstacle constraint is

$$\operatorname{prox}^{\operatorname{KL}}(\beta) = \beta \mathbb{1}_{\Omega \setminus \mathscr{O}} \tag{3.8}$$

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

$$\operatorname{prox}_{F}^{\mathrm{KL}}(\beta) = \min(\beta, \bar{m}) \mathbb{1}_{\Omega \setminus \mathcal{O}}. \tag{3.9}$$

Efficient convolution. Denote $\mathbf{R} \in \mathbb{R}^{M^N}$ the discretized measure R^N . Summation of multiple vectors u_0, \ldots, u_N with respect to \mathbf{R} is the following tensor contraction

$$\mathbf{R}[u_0, \dots, u_N] = \sum_{i_0, \dots, i_N} \mathbf{R}_{i_0, \dots, i_N} \prod_{k=0}^N u_{i_k}$$

The multi-marginal kernel **R** can be factorized as $\mathbf{R}_{i_0,\dots,i_N} = \prod_{k=0}^{N-1} \mathbf{P}_{i_k,i_{k+1}}$ where **P** is the discrete heat kernel on \mathbb{R}^M . This allows us to write the partial convolution \mathcal{I}_k (leaving the kth component out) as

$$\mathcal{I}_k = \mathbf{R}[(u_j)_{j \neq k}] = \mathbf{A}_{k-1} \odot \mathbf{B}_{k+1}$$
(3.10)

where $\mathbf{A}_k = \mathbf{P}^T(a_k \odot \mathbf{P}^T(a_{k-1} \odot \cdots))$ and $\mathbf{B}_k = \mathbf{P}(a_k \odot \mathbf{P}(a_{k+1} \odot \cdots))$.

4 Examples

4.1 Transport with a soft 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):

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

²https://github.com/cvxgrp/cvxpy

³Steven 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.

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:

$$\inf_{\gamma} \langle \Psi, \gamma^T \mathbb{1} \rangle + \varepsilon \operatorname{KL}(\gamma | \mathbf{R})$$
s.t. $\gamma \mathbb{1} = \rho_0, \quad \gamma^T \mathbb{1} \odot \mathbb{1}_{\mathscr{Q}} = 0$ (4.1)

In this two-marginal case, the matrix $\mathbf{R} = \mathbf{P}$ is the discretization of the heat kernel P_h as discussed in section 3.2:

$$\mathbf{R}_{i,j} = P_{h\varepsilon}(x_j - x_i)$$

for all grid indices i, j.

In this problem we want to observe the optimal target distribution $\rho_1^* = (\gamma^*)^T \mathbb{1}$ the agents reach at the final time t = 1.

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

$$a_0^* = e^{-u_0^*/\varepsilon} = \frac{\rho_0}{\mathbf{R}a_1^*}$$

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

$$\gamma^* = \mathbf{R} \odot (a_0^* \otimes a_1^*)$$

It satisfies, as expected, that $\gamma_{i,j}^* = 0$ for all $j \in \mathcal{O}$. The final distribution of agents is

$$\rho_1 = \gamma^T \mathbb{1} = a_1^* \odot \mathbf{R} a_0^*$$

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 \mathcal{O}), and when lowering the viscosity parameter $\sigma = \sqrt{\varepsilon}$ (see figs. 2b and 2c).

Since the kernel ${\bf R}$ on the domain is separable, the convolution can be sped up [10, ch. 4].

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 [11], as well as the discrete MFG fig. 3b.

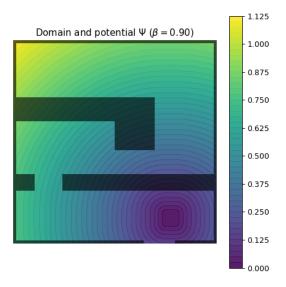


Figure 1: Computational domain of the game Ω with set of obstacles \mathscr{O} (transparent grey), and contour of the potential function $\Psi(x) = d(x, \mathscr{A})^{\beta}$.

4.1.2 Three time steps

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

$$\inf_{\gamma,\rho_{1},\rho_{2}} \langle \Psi, \rho_{2} \rangle + \varepsilon \operatorname{KL}(\gamma | \mathbf{R})$$
s.t. $P_{\#}^{k} \gamma = \rho_{k}, \ k = 0, 1, 2$

$$\rho_{1} \leq \bar{m}$$

$$\rho_{1} \odot \mathbb{1}_{\mathscr{O}} = 0$$

$$\rho_{2} \odot \mathbb{1}_{\mathscr{O}} = 0$$
(4.2)

Contraction/convolution with the kernel R in this case satisfies

$$\mathbf{R}[\cdot, v, w] = \mathbf{P}(v \odot \mathbf{P}w)$$

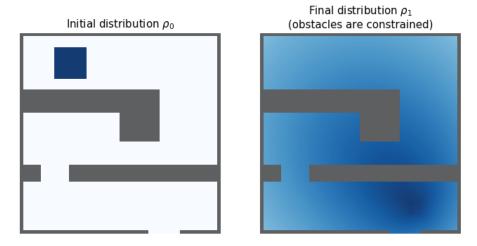
$$\mathbf{R}[u, \cdot, w] = (\mathbf{P}^T u) \odot (\mathbf{P}w)$$

$$\mathbf{R}[u, v, \cdot] = \mathbf{P}^T (v \odot \mathbf{P}^T u)$$

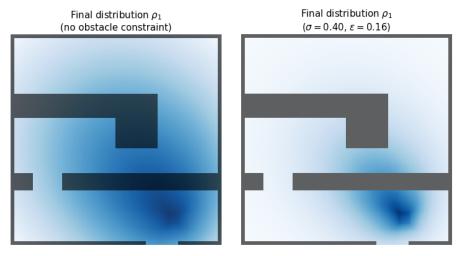
Proposition 3. The Lagrange multipliers u_i^* at the optimum satisfy the fixed-point conditions:

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

$$a_1^* = \min\left(\frac{\bar{m}}{\mathbf{R}[a_0^*, \cdot, a_2^*]}, 1\right)$$

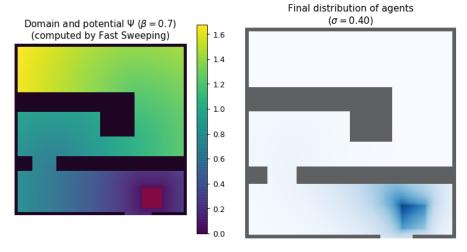


(a) Result of the "fuzzy" transport problem with enforcement of the obstacle constraints and viscosity parameter $\sigma=1.$



(b) Final distribution ρ_1^* without en- (c) Obstacles are constrained as in forcing the obstacles. The mass of the fig. 2a, but with viscosity parameter distribution "bleeds" through the ob- $\sigma=0.4$. stacles.

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



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

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

The marginals are obtained as

$$\rho_1^* = a_1^* \odot \mathbf{R}[a_0^*, \cdot, a_2^*] = a_1^* \odot (\mathbf{P}^T a_0^*) \odot (\mathbf{P} a_2^*)$$

and

$$\rho_2^* = a_2^* \odot \mathbf{R}[a_0^*, a_1^*, \, \cdot \,] = a_2^* \odot \mathbf{P}^T(a_1^* \odot \mathbf{P}^T a_0^*)$$

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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