

A Particle System for Global Optimization

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Abstract—A particle algorithm for global optimization is presented, based on concepts from optimal transport. The particle flow is constructed by considering a time-stepping variational problem, and the resulting flow is interpreted as a gradient flow with respect to a certain (pseudo-) metric. The construction requires to solve an Euler-Lagrange boundary value problem at each time step, and a Galerkin procedure is described to approximate its solution. The algorithm is illustrated by a numerical example.

I. INTRODUCTION

We consider a global optimization problem

$$\min_{x \in \mathbb{R}^d} h(x), \quad (1)$$

where $h : \mathbb{R}^d \rightarrow \mathbb{R}$ is a real-valued continuously differentiable bounded function. The objective is to obtain, using a simulation-based method, the *global minimizer*

$$\bar{x} = \arg \min_{x \in \mathbb{R}^d} h(x).$$

We will assume that such a minimizer exists and is unique.

In this paper, we introduce an interacting particle algorithm based on a gradient-flow construction; cf., [6]. The particle system is comprised of N stochastic processes $\{X_t^i : 1 \leq i \leq N\}$: The value $X_t^i \in \mathbb{R}$ is the state of the i^{th} particle at time t .

In our approach, the dynamics of the i^{th} particle is defined by a controlled system:

$$dX_t^i = -\varepsilon \nabla h(X_t^i) dt + (1 - \varepsilon) dU_t^i \quad (2)$$

where the initial condition X_0^i is sampled from a given initial distribution $p^*(x, 0)$, $\varepsilon \in (0, 1)$ is a small parameter, and U_t^i is the control input that models the interaction with the population. The motivation comes from ‘consensus-type’ control used in the convex optimization literature; cf., [3].

We cast the synthesis of control input as an optimization problem. The optimal control input is obtained via solution of an associated Euler-Lagrange (E-L) boundary value problem (BVP). In particular, the optimal control input is given by,

$$dU_t^i = u(X_t^i, t) dt,$$

and the *control function* $u(x, t) = \nabla \phi(x, t)$ is obtained by solving an E-L BVP:

$$\begin{aligned} \nabla \cdot (p(x, t) \nabla \phi(x, t)) &= (h(x) - \hat{h}) p(x, t), \\ \int \phi(x, t) p(x, t) dx &= 0, \end{aligned} \quad (3)$$

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where p denotes the distribution of X_t^i , and $\hat{h} := \mathbb{E}[h(X_t^i)] = \int h(x) p(x, t) dx$. In numerical implementations, we approximate $\hat{h} \approx \frac{1}{N} \sum_{i=1}^N h(X_t^i) =: \hat{h}^{(N)}$. Note that the control function needs to be obtained for each value of time t .

The contributions of this paper are as follows:

- **Variational formulation.** The particle system (2) - (3) is obtained by considering a certain variational problem based on a time-stepping iterative procedure that is introduced in Sec. II. At each time-step, the procedure seeks to minimize the expected value of the function h , referred to as *energy*. The dynamics of the particle system (2) may thus be regarded as a gradient flow, or a steepest descent, for the energy.

It is noted that the particle dynamics is entirely deterministic, without any selection or reproduction.

- **Convergence.** We show that the particle system solves the optimization problem (1) in the following sense: Suppose $p(x, 0) > 0$ and the control function u is obtained as a solution of (3), then,

$$\int h(x) p(x, t) dx \rightarrow h(\bar{x}) \quad \text{as } t \rightarrow \infty. \quad (4)$$

This implies that the empirical distribution of the population will concentrate at the unique global minimizer \bar{x} .

- **Numerical algorithm.** We present a Galerkin algorithm to approximate the control function $u(x, t)$. The algorithm is completely adapted to data (That is, it does not require an explicit construction of $p(x, t)$ or computation of derivatives). Certain closed-form approximations for the control function are also presented. The conclusions are illustrated with a numerical example.

We next present a brief review of the relevant literature:

Literature review: Population-based methods, including interacting particle algorithms, are widely used for global optimization. Some examples include genetic algorithms, differential evolution and controlled random search (see recent survey articles [2], [1]). Whereas these algorithms can lack a model for how the particle distribution evolves, the interacting particle algorithm presented in [8] extends the simulated annealing algorithm via a Feynman-Kac construction with Markov exploration and selection kernels. The selection favors particles with higher Metropolis ratio (see also [7]).

More recently, model-based random search methods (see [13]) have been developed. These methods update the particles according to a prescribed reference distribution (model) whose evolution has the desired convergence properties. Various methods have been proposed based on the choice of the reference distribution and its evolution: i) the

cross entropy method ([9]) uses an optimal importance sampling distribution, ii) the model reference adaptive search in [4] updates the reference distribution via an application of the Bayes' recursion, iii) a particle filtering algorithm appears in [12], and iv) the reference model in [10] evolves according to the replicator dynamics, which is closely related to our work. Since the reference distributions may be implicit, particles are often sampled from a parameterized distribution, that at each iteration approximates (e.g., with respect to the Kullback-Leibler divergence) the reference distribution; cf., [5].

The outline of the remainder of this paper is as follows. The variational time-stepping procedure appears in Sec. II. The equations for the density and the particle system are described in Sec. III and Sec. IV, respectively. Finally, Sec. V provides a numerical example. The proofs appear in the Appendix.

Notation: C^k is used to denote the space of k -times continuously differentiable functions on \mathbb{R}^d ; C_c^k denotes the subspace of functions in C_k with compact support; L^∞ denotes the space of bounded functions on \mathbb{R}^d ; $L^2(\mathbb{R}^d; \rho)$ is used to denote the Hilbert space of functions on \mathbb{R}^d that are square-integrable with respect to density ρ ; and $H^k(\mathbb{R}^d; \rho)$ is used to denote the Hilbert space of functions whose first k -derivatives (defined in the weak sense) are in $L^2(\mathbb{R}^d; \rho)$.

For a function f , $\nabla f = \frac{\partial f}{\partial x_i}$ is used to denote the gradient and $D^2 f = \frac{\partial^2 f}{\partial x_i \partial x_j}$ is used to denote the Hessian. The derivatives are interpreted in the weak-sense.

II. TIME-STEPPING PROCEDURE

The considerations of this section – construction of a gradient flow – is motivated by the optimal transport literature, in particular, the work of Otto and co-workers on the variational interpretation of the Fokker-Planck-Kolmogorov equation [6].

The time-stepping scheme involves a sequence of minimization problems in the space of probability densities,

$$\mathcal{P} := \left\{ \rho : \mathbb{R}^d \rightarrow [0, \infty) \text{ meas. density} \mid \mathcal{M}(\rho) < \infty \right\}$$

where $\mathcal{M}(\rho) := \int |x|^2 \rho(x) dx$. We consider a finite-time interval $[0, T]$ with an associated discrete-time sequence $\{0, t_1, t_2, \dots, t_L\}$ with $t_L = T$, and denote $\Delta t_l := t_l - t_{l-1}$. Set $\rho_0 = \rho_0^* \in \mathcal{P}$ and inductively define $\{\rho_l\}_{l=1}^L \subset \mathcal{P}$ by taking $\rho_l \in \mathcal{P}$ to minimize the functional

$$I_l(\rho) := M(\rho \mid \rho_{l-1}) + \Delta t_l \int h(x) \rho(x) dx, \quad (5)$$

where $E(\rho) := \int h(x) \rho(x) dx$ is the energy associated with the objective function $h(x)$.

The following choices for the (pseudo-) metric $M(\rho \mid \rho_{l-1})$ are considered:

- 1) Kullback-Leibler (K-L) divergence:

$$D(\rho \mid \rho_{l-1}) = \int \rho(x) \ln \left(\frac{\rho(x)}{\rho_{l-1}(x)} \right) dx. \quad (6)$$

- 2) Wasserstein distance:

$$\frac{1}{2} W_2^2(\rho \mid \rho_{l-1}) = \frac{1}{2} \inf_{p \in \mathbb{P}(\rho_{l-1}, \rho)} \int_{\mathbb{R}^d \times \mathbb{R}^d} |x - y|^2 p(dx dy) \quad (7)$$

with $\mathbb{P}(\rho_{l-1}, \rho)$ as the set of all probability measures whose first marginal is ρ_{l-1} and second marginal is ρ .

- 3) Convex combination of the two:

$$\varepsilon \frac{1}{2} W_2^2(\rho \mid \rho_{l-1}) + (1 - \varepsilon) D(\rho \mid \rho_{l-1}), \quad (8)$$

where $\varepsilon \in (0, 1)$ is a small parameter.

The third case is ultimately of more interest – the related result follows from combining the results for the first and the second cases.

The sequence of minimizers $\{\rho_l\}_{l=0}^L$ is used to construct, via interpolation, a density function $\rho^{(L)}(x, t)$ for $t \in [0, T]$: Define $\rho^{(L)}(x, t)$ by setting

$$\rho^{(L)}(x, t) := \rho_l(x), \quad \text{for } t \in [t_l, t_{l+1}) \quad (9)$$

for $l = 0, 1, 2, \dots, L - 1$. Sec. III is concerned with convergence analysis in the limit $\Delta t_l \rightarrow 0$.

Remark 1: The minimizer of (5) with only the K-L divergence is given by the following recursion related to the stochastic annealing algorithm:

$$\begin{aligned} \rho_0(x) &= p_0^*(x) \in \mathcal{P}, \\ \rho_l(x) &= \frac{\rho_{l-1}(x) \exp(-\Delta t_l h(x))}{\int \rho_{l-1}(y) \exp(-\Delta t_l h(y)) dy}. \end{aligned} \quad (10)$$

Indeed, by Jensen's formula,

$$I_l(\rho) \geq -\ln \left(\int \rho_{l-1}(y) \exp(-\Delta t_l h(y)) dy \right),$$

with equality if and only if $\rho = \rho_l$.

Although the optimizer is known for the K-L divergence, a careful look at the first order optimality equations associated with ρ_l leads to i) the PDE (13) for evolution of the density (in Sec. III), and ii) a particle algorithm with mean-field control that approximates of the density (in Sec. IV).

The analysis with different choices of $M(\rho \mid \rho_{l-1})$ in (5) yields different algorithms.

Throughout the paper, the following assumptions are made for the prior distribution ρ_0^* and for function h :

Assumption A1 The probability density $\rho_0^* \in \mathcal{P}$ is of the form $\rho_0^*(x) = e^{-\mathcal{G}_0(x)}$, where $\mathcal{G}_0 \in C^2$, $\nabla \mathcal{G}_0 = O(|x|)$ as $|x| \rightarrow \infty$, and $D^2 \mathcal{G}_0 \in L^\infty$.

Assumption A2 The function $h \in C^2$ with $h, \nabla h, D^2 h \in L^\infty$.

III. VARIATIONAL ANALYSIS

A. First order optimality condition

The analysis proceeds by first obtaining the first variation as described in the following Lemma. The proof appears in Appendix A.

Lemma 1: Consider the minimization problem (5) under Assumptions (A1)-(A2). The minimizer ρ_l satisfies the following Euler-Lagrange equation:

- (i) If $M(\rho | \rho_{l-1}) = D(\rho | \rho_{l-1})$, the K-L divergence defined in (6), then ρ_l satisfies

$$\int [\nabla \cdot \zeta + \nabla \ln(\rho_{l-1}) \cdot \zeta - \Delta t_l \nabla h \cdot \zeta] \rho_l dx = 0, \quad (11)$$

for each vector field $\zeta \in L^2(\mathbb{R}^d; \rho_{l-1})$.

- (ii) If $M(\rho | \rho_{l-1}) = \frac{1}{2} W_2^2(\rho | \rho_{l-1})$, the Wasserstein distance defined in (7), then ρ_l satisfies

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} (y-x) \cdot \zeta(y) p(dx dy) + \Delta t_l \int \nabla h \cdot \zeta \rho_l dx = 0, \quad (12)$$

for each vector field $\zeta \in L^2(\mathbb{R}^d; \rho_{l-1})$. Here, $p \in \mathbb{P}$ is the infimizer in the definition of $W_2^2(\rho_{l-1} | \rho_l)$ (see (7)).

We are now prepared to state the main theorem concerning $\rho^{(L)}(x, t)$, which was obtained from an interpolation of the minimizers $\{\rho_l\}_{l=0}^L$. The proof appears in Appendix B.

Theorem 1: Let $\{\rho_l\}_{l=0}^L$ be the sequence of minimizers of the time-stepping procedure (5) and $\rho^{(L)}(x, t)$ be the interpolated density defined in (9). Denote $\rho(x, t)$ as the limiting density of $\rho^{(L)}(x, t)$, as $\Delta t_l \rightarrow 0$ (We assume that such a density exists). Then,

- (i) If $M = D$, the K-L divergence, the density $\rho(x, t)$ is a weak solution of the replicator equation:

$$\frac{\partial \rho}{\partial t}(x, t) = -(h(x) - \hat{h}_t) \rho(x, t), \quad (13)$$

where $\hat{h}_t := \int h(x) \rho(x, t) dx$.

- (ii) If $M = \frac{1}{2} W_2^2$, the Wasserstein metric, the density ρ obtained in (i) is a weak solution of the Fokker-Planck equation,

$$\frac{\partial \rho}{\partial t}(x, t) = \nabla \cdot (\rho(x, t) \nabla h(x)). \quad (14)$$

Corollary 1: Suppose M is a convex combination of the K-L divergence and the Wasserstein metrics (see (8)) with a fixed $\varepsilon \in (0, 1)$. Denote $p^*(x, t) := \rho(x, t)$, the limiting density described in Theorem 1. Then $p^*(x, t)$ is a weak solution of the evolution equation,

$$\frac{\partial p^*}{\partial t}(x, t) = \varepsilon \nabla \cdot (p^*(x, t) \nabla h(x)) - (1 - \varepsilon)(h(x) - \hat{h}_t) p^*(x, t) \quad (15)$$

where now $\hat{h}_t = \int h(x) p^*(x, t) dx$.

B. Convergence

Next we analyze the convergence of the density evolution in (15). The dynamics can be interpreted as the *gradient flow* of the energy $E(p^*)$ with respect to a pseudo-metric which, in this case, is a convex combination of the Wasserstein distance and the K-L divergence. Hence, it is natural to set $E(p^*)$ as the Lyapunov function for (15). The related result is summarized in the next theorem; the proof appears in Appendix C.

Theorem 2: Let the density $p^*(x, t)$ satisfy (15), then:

$$\int h(x) p^*(x, t) dx \rightarrow h(\bar{x}) \text{ as } t \rightarrow \infty. \quad (16)$$

If the global minimizer \bar{x} is unique, this implies that the density $p^*(x, t)$ asymptotically concentrates at the global minimizer \bar{x} .

IV. PARTICLE SYSTEM

A. Particle dynamics and control architecture

The particle system is comprised of N coupled stochastic processes $\{X_t^i\}_{i=1}^N$, whose dynamics evolve according to,

$$dX_t^i = -\varepsilon \nabla h(X_t^i) dt + (1 - \varepsilon) u(X_t^i, t) dt, \quad (17)$$

where the control function $u(x, t) \in \mathbb{R}^d$. The initial conditions $\{X_0^i\}_{i=1}^N$ are i.i.d. and drawn from the initial distribution $p^*(x, 0)$.

We denote the distribution of X_t^i as $p(x, t)$, and impose an admissibility requirement on the control:

Definition 1 (Admissible control): The control input $u(X_t^i, t)$ is *admissible* if the random variable $u(x, t)$ satisfies: $E[|u|^2] := E[\sum_{i=1}^d |u_i(x, t)|^2] < \infty$, for all $t \in [0, T]$.

Note that there are two types of distributions of interest in our analysis:

- 1) $p^*(x, t)$: The desired distribution, evolving according to (15).
- 2) $p(x, t)$: The distribution of X_t^i .

The control function $u(x, t)$ is said to be *optimal* if $p^* \equiv p$. That is, given $p^*(\cdot, 0) = p(\cdot, 0)$, our goal is to choose u in the particle dynamics so that these distributions coincide. The forward equation for $p^*(x, t)$ is given by (15). The forward equation for $p(x, t)$ is the Fokker-Planck equation for the particle dynamics (17):

$$\frac{\partial p}{\partial t}(x, t) = \varepsilon \nabla \cdot (p(x, t) \nabla h(x)) - (1 - \varepsilon) \nabla \cdot (p(x, t) u(x, t)). \quad (18)$$

B. Optimal control and consistency

The optimal control input is chosen by inspection. In particular, comparison of (15) and (18) suggests the choice,

$$u(x, t) = \nabla \phi(x, t),$$

where $\phi(x, t)$ is the solution of the Poisson equation:

$$\begin{aligned} \nabla \cdot (p(x, t) \nabla \phi(x, t)) &= (h(x) - \hat{h}) p(x, t), \\ \int \phi(x, t) p(x, t) dx &= 0. \end{aligned} \quad (19)$$

The normalization $\int \phi(x, t) p(x, t) dx = 0$ is for convenience: if ϕ^o is a solution to the Poisson equation above, we get the desired normalization by subtracting its mean.

For the purposes of both analysis and numerics, it is useful to introduce the weak formulation of the BVP (19). Denote

$$H_0^1(\mathbb{R}^d; p) := \{\phi \in H^1(\mathbb{R}^d; p) \mid \int \phi p dx = 0\}.$$

A function $\phi \in H_0^1(\mathbb{R}^d; p)$ is said to be a weak solution of the BVP (19) if

$$\int \nabla \phi(x, t) \cdot \nabla \psi(x) p(x, t) dx = - \int (h(x) - \hat{h}) \psi(x) p(x, t) dx, \quad (20)$$

for all $\psi \in H^1(\mathbb{R}^d; p)$.

Denoting $E[\cdot] := \int \cdot p(x, t) dx$, the weak form of the BVP (19) can also be expressed as

$$E[\nabla \phi \cdot \nabla \psi] = -E[(h - \hat{h}) \psi], \quad \forall \psi \in H^1(\mathbb{R}^d; p). \quad (21)$$

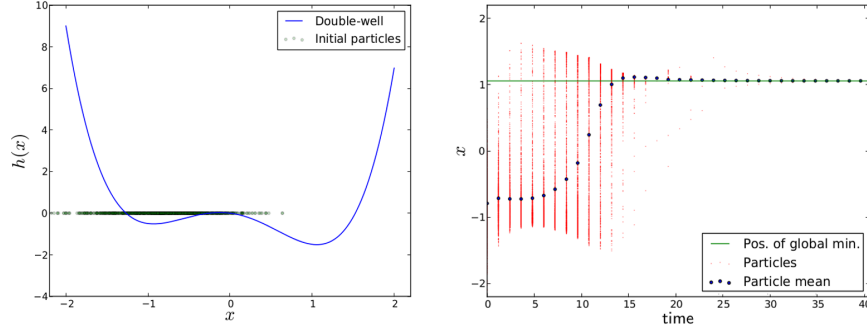


Fig. 1. (a) The Double-well function and the initial distribution of particles. (b) Particles (scattered vertically at each time) concentrate at the global minimizer quickly.

This representation is useful for the numerical algorithm described in Sec. IV-C.

The proof of the following consistency theorem appears in Appendix D. The main part of the proof is to show that the control function, obtained by solving BVP (19), is admissible.

Theorem 3: Consider the two distributions $p^*(x, t)$ and $p(x, t)$ evolving according to (15) and (18), respectively. Suppose Assumptions (A1)-(A2) hold, and the control $u(x, t)$ is chosen based on (19). Then, provided $p^*(\cdot, 0) = p(\cdot, 0)$, we have for all $t \geq 0$,

$$p^*(\cdot, t) = p(\cdot, t).$$

C. Galerkin method for solving the BVP

In this section, a Galerkin algorithm is described to construct an approximate solution of (19). The time t is fixed. For notational ease, the explicit dependence on time is suppressed (That is, $p(x, t)$ is denoted as $p(x)$, $\phi(x, t)$ as $\phi(x)$, $u(x, t)$ as $u(x)$ etc.).

The function ϕ is approximated as,

$$\phi(x) = \sum_{k=1}^K \alpha_k \psi_k(x),$$

where $\{\psi_k(x)\}_{k=1}^K$ are *basis functions*.

The finite-dimensional approximation of (21) is to choose constants $\{\alpha_k\}_{k=1}^K$ such that

$$\sum_{k=1}^K \alpha_k E[\nabla \psi_k \cdot \nabla \psi] = -E[(h - \hat{h})\psi], \quad \forall \psi \in S, \quad (22)$$

where $S := \text{span}\{\psi_1, \psi_2, \dots, \psi_K\} \subset H^1(\mathbb{R}^d; p)$.

Denoting $[A]_{mk} = E[\nabla \psi_k \cdot \nabla \psi_m]$, $b_k = -E[(h - \hat{h})\psi_k]$, $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_K)^T$, the finite-dimensional approximation (22) is expressed as a linear matrix equation:

$$A\alpha = b. \quad (23)$$

The matrix A and vector b are approximated by using only the particles:

$$[A]_{mk} = E[\nabla \psi_k \cdot \nabla \psi_m] \approx \frac{1}{N} \sum_{i=1}^N \nabla \psi_k(X_t^i) \cdot \nabla \psi_m(X_t^i),$$

$$b_k = -E[(h - \hat{h})\psi_k] \approx -\frac{1}{N} \sum_{i=1}^N (h(X_t^i) - \hat{h})\psi_k(X_t^i),$$

where recall $\hat{h} \approx N^{-1} \sum_{i=1}^N h(X_t^i) =: \hat{h}^{(N)}$.

The important point to note is that the control function can be expressed in terms of certain averages taken over the population.

V. NUMERICAL EXPERIMENTS

Consider the minimization problem for the double-well function

$$h(x) = -2x^2 + x^4 - 0.5x,$$

depicted in Fig. 1 (a). The global minimizer $\bar{x} = 1.057$ while $x \approx -1$ is a local minimizer.

In the numerical simulation, the initial condition of the particles is sampled from the Gaussian distribution $\mathcal{N}(-0.8, 0.5^2)$. The sample size $N = 1000$. The particles are also depicted in Fig. 1 (a). Note that there are relatively more particles close to the local minimizer at -1 than to the global minimizer \bar{x} .

The control function is approximated by using the Galerkin procedure with the Fourier basis functions,

$$\left\{ x, \cos\left(\frac{2\pi}{4}x\right), \sin\left(\frac{2\pi}{4}x\right) \right\}.$$

The parameter $\varepsilon = 0.02$.

Fig. 1 (b) depicts the convergence of particles to the global minimizer \bar{x} .

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APPENDIX

A. Proof of Lemma 1

We follow the approach proposed in [6] and introduce a flux $\{\Phi_\tau\}_{\tau \geq 0}$ to generate the first variation of the minimizer ρ_l for the functional (5): At time τ define $\rho_\tau := \Phi_\tau^\# \rho_l$ as the *push forward* of ρ_l . Φ_τ is generated by a vector field $\varsigma: \mathbb{R}^d \rightarrow \mathbb{R}^d$,

$$\frac{d}{d\tau} \Phi_\tau = \varsigma(\Phi_\tau), \quad \Phi_0(x) = x \quad (24)$$

where for now we assume $\varsigma \in C_c^1$. Thus for an arbitrary function f ,

$$\int f(z) \rho_\tau(z) dz = \int f(\Phi_\tau(x)) \rho_l(x) dx, \quad (25)$$

$$|D\Phi_\tau(x)| \rho_\tau(\Phi_\tau(x)) = \rho_l(x), \quad (26)$$

where $D\cdot$ denotes the Jacobian of a map and $|\cdot|$ denotes the determinant of a matrix. Denote $i(\tau) = I_l(\rho_\tau)$, then the first-order optimality condition reads,

$$\left. \frac{d}{d\tau} i(\tau) \right|_{\tau=0} = 0. \quad (27)$$

We evaluate the left hand side term by term according to (5).

(i) $M(\rho | \rho_{l-1}) = D(\rho | \rho_{l-1})$,

$$i(\tau) = \int \rho_\tau \ln \rho_\tau dz - \int \rho_{l-1} \ln \rho_{l-1} dz + \Delta t_l \int h \rho dz. \quad (28)$$

For the first integral, using (25) and (26),

$$\begin{aligned} \int \rho_\tau(z) \ln \rho_\tau(z) dz &= \int \ln[\rho_\tau(\Phi_\tau(x))] \rho_l(x) dx \\ &= C - \int \ln[|D\Phi_\tau(x)|] \rho_l(x) dx, \end{aligned}$$

where $C = \int \rho_l(x) \ln \rho_l(x) dx$ is independent of τ . Then

$$\begin{aligned} \left. \frac{d}{d\tau} \int \rho_\tau(z) \ln \rho_\tau(z) dz \right|_{\tau=0} \\ = - \int \left. \frac{d}{d\tau} \ln[|D\Phi_\tau(x)|] \right|_{\tau=0} \rho_l(x) dx = - \int \nabla \cdot \varsigma(x) \rho_l(x) dx. \end{aligned}$$

Here the interchange of differentiation and integration is justified because ς has compact support, $\Phi_\tau(x) = \Phi_0(x) = x$ outside this support and the difference quotient

$$\frac{1}{\tau} \left(\ln[|\nabla \Phi_\tau(x)|] - \ln[|\nabla \Phi_0(x)|] \right)$$

converges uniformly to $\left. \frac{d}{d\tau} \ln[|\nabla \Phi_\tau(x)|] \right|_{\tau=0} = \nabla \cdot \varsigma(x)$, as $\tau \downarrow 0$.

Calculations for the remaining terms in (28) are similar and thus omitted. On substituting these results into (27) we obtain (11). Finally, to extend the E-L equation to an arbitrary vector field ς in $L^2(\mathbb{R}^d; \rho_{l-1})$, it suffices to approximate ς by a sequence of smooth, compactly supported vector fields. (ii) For derivation of (12) with $M(\rho | \rho_{l-1}) = \frac{1}{2} W_2^2(\rho | \rho_{l-1})$, see [6]. ■

B. Proof of Theorem 1

(i) For the case $M(\rho | \rho_{l-1}) = D(\rho | \rho_{l-1})$, we begin with some preliminaries:

Under Assumption (A1) (see Sec. II), the density ρ_0 is known to satisfy a logarithmic Sobolev inequality for some constant $\lambda_0 > 0$. That is, for all functions f on \mathbb{R}^d with $\int f^2 \rho_0 dx = 1$,

$$\int f^2 \ln f^2 \rho_0 dx \leq \frac{1}{2\lambda_0} \int |\nabla f|^2 \rho_0 dx. \quad [\text{LSI}(\lambda_0)]$$

Furthermore, the following lemma asserts that all minimizers ρ_l satisfy a uniform logarithmic Sobolev inequality. The proof is omitted.

Lemma 2: For $\{\rho_l\}_{l=0}^L$ obtained in (10), under Assumption (A1)-(A2), we have

- 1) ρ_l is of the form $\rho_l = e^{-\mathcal{G}_l}$ where $\mathcal{G}_l \in C^2$, $\nabla \mathcal{G}_l = O(|x|)$ as $|x| \rightarrow \infty$, and $D^2 \mathcal{G}_l \in L^\infty$.
- 2) There is $\bar{\lambda} > 0$ such that ρ_l satisfies $\text{LSI}(\bar{\lambda})$ for all l .
- 3) If $g \in L^2(\mathbb{R}^d; \rho_{l-1})$, then $g \in L^2(\mathbb{R}^d; \rho_l)$ with

$$\int |g|^2 \rho_l dx \leq \exp(2\Delta t_l \|h\|_\infty) \int |g|^2 \rho_{l-1} dx. \quad (29)$$

Equation (29) implies that, if $\rho_{l-1} \in \mathcal{P}$, then $\rho_l \in \mathcal{P}$ (take $g(x) = x$). By induction, $\rho_l \in \mathcal{P}$ if $\rho_0 \in \mathcal{P}$ for all l .

Now we derive the result in (i). First, (11) can be compactly written as,

$$\int \frac{\rho_l}{\rho_{l-1}} \nabla \cdot (\rho_{l-1} \varsigma) dx - \Delta t_l \int \nabla h \cdot \varsigma \rho_l dx = 0. \quad (30)$$

Given a test function $f \in C_c^0$, $f \in L^2(\mathbb{R}^d; \rho_l)$ for all $l \in \{0, 1, 2, \dots, L\}$, with a uniform bound,

$$\|f\|_{L^2(\mathbb{R}^d; \rho_l)} \leq C_0. \quad (31)$$

Let $\xi_l \in L^2(\mathbb{R}^d; \rho_{l-1})$ be the solution of

$$\nabla \cdot (\rho_{l-1} \xi_l) = (f - \hat{f}_{l-1}) \rho_{l-1} \quad (32)$$

where $\hat{f}_{l-1} := \int f \rho_{l-1} dx$. The existence and uniqueness of such a solution is proved in [11], where the following apriori bound is also shown:

$$\int |\xi_l|^2 \rho_{l-1} dx \leq (\text{const.}) \int |f - \hat{f}_{l-1}|^2 \rho_{l-1} dx \leq C_0. \quad (33)$$

Substituting (32) into (30) with $\varsigma = \xi_l$, we obtain

$$\hat{f}_l - \hat{f}_{l-1} = \Delta t_l \int \nabla h \cdot \xi_l \rho_l dx, \quad (34)$$

On summing,

$$\hat{f}_L = \hat{f}_0 + \Delta t_l \sum_{l=1}^L \int \nabla h \cdot \xi_l \rho_l dx. \quad (35)$$

The integral of the summand is well-defined since $\xi_l \in L^2(\mathbb{R}^d; \rho_l)$ (by Lemma 2-(3)) and $\nabla h \in L^\infty$.

Now let $\eta_l \in L^2(\mathbb{R}^d; \rho_{l-1})$ be a solution of

$$\nabla \cdot (\rho_{l-1} \eta_l) = (\nabla h \cdot \xi_l - \int \nabla h \cdot \xi_l \rho_{l-1} dx) \rho_{l-1}. \quad (36)$$

By repeating the arguments now for η_l , the fact $\nabla h \in L^\infty$ and relation (33) imply

$$\int |\eta_l|^2 \rho_{l-1} dx \leq C_1, \quad (37)$$

where the constant C_1 is independent of l .

Employing (30) once more with $\varsigma = \eta_l$,

$$\Delta t_l \int \nabla h \cdot \xi_l \rho_l dx = \Delta t_l \int \nabla h \cdot \xi_l \rho_{l-1} dx + \mathcal{E}_l, \quad (38)$$

and $\mathcal{E}_l = -(\int \nabla h \cdot \eta_l \rho_l dx) \Delta t_l^2$. Integrating by part and using (32), the first integral on the right hand side becomes,

$$\int \nabla h \cdot \xi_l \rho_{l-1} dx = - \int h(f - \hat{f}_{l-1}) \rho_{l-1} dx. \quad (39)$$

Substituting (38) and (39) into (35), we have,

$$\hat{f}_L = \hat{f}_0 - \sum_{l=1}^L \int h(f - \hat{f}_{l-1}) \rho_{l-1} dx + \sum_{l=1}^L \mathcal{E}_l. \quad (40)$$

To pass to the limit $\Delta t_l \downarrow 0$ (i.e. $L \rightarrow \infty$), we claim that $\sum_{l=1}^L |\mathcal{E}_l| \rightarrow 0$. Indeed, the uniform bound in (37), in conjunction with Lemma 2-(3) and the assumption $\nabla h \in L^\infty$, leads to,

$$\begin{aligned} |\mathcal{E}_l| &\leq \left(\int |\nabla h|^2 \rho_l dx \right)^{1/2} \left(\int |\eta_l|^2 \rho_l dx \right)^{1/2} \Delta t_l^2 \\ &\leq C_2 \exp(\Delta t_l \|h\|_\infty) \Delta t_l^2 \end{aligned}$$

for some C_2 independent of l .

Now denote

$$\rho(x, t) := (\text{const.}) \exp(-h(x)t) p_0^*(x),$$

where (const.) is some normalization constant (see (10)). Then as $\Delta t_l \downarrow 0$, $\rho^{(L)}(x, t) \rightarrow \rho(x, t)$ a.s. and by (40),

$$\begin{aligned} \hat{f}_t &= \hat{f}_0 - \int_0^t \int h(x)(f(x) - \hat{f}_s) \rho(x, s) dx ds \\ &= \hat{f}_0 - \int_0^t \int (h(x) - \hat{h}_s) f(x) \rho(x, s) dx ds \end{aligned}$$

for all $f \in C_c^0$, showing that $\rho(x, t)$ is a weak solution of the replicator equation (13).

For (ii), cf., [6]. ■

C. Proof of Theorem 2

Central to the proof is constructing a Lyapunov function that decreases over time. A natural choice is $E(p^*) = \int h p^* dx$. A direct calculation shows:

$$\begin{aligned} \frac{d}{dt} E(p^*) &= \int h \frac{\partial}{\partial t} p^* dx \\ &\stackrel{(15)}{=} \varepsilon \int h \nabla \cdot (p^* \nabla h) - (1 - \varepsilon) \int h(h - \hat{h}) p^* dx \\ &= - \int p^* [\varepsilon |\nabla h|^2 + (1 - \varepsilon)(h - \hat{h})^2] dx, \end{aligned}$$

which is strictly negative for all distribution $p^* > 0$. Moreover, $E(p^*)$ is bounded below:

$$E(p^*) = \int h p^* dx \geq \int h(\bar{x}) p^* dx \geq h(\bar{x}).$$

As a consequence, we have $E(p^*) \rightarrow h(\bar{x})$ as $t \rightarrow \infty$. ■

D. Proof of Theorem 3

If $u(\cdot, t)$ is admissible, the consistency is straightforward: substitute the first equality in (19) into (18) with $u(x, t) = \nabla \phi(x, t)$, we get precisely the same evolution dynamics as (15).

It remains to show uniqueness and admissibility of $u(x, t)$. By Assumption (A1)-(A2), Lemma 2 and Theorem 1, we have for all time t , $p = e^{-\mathcal{G}(x, t)}$ where $\mathcal{G} \in C^2$, $\nabla \mathcal{G} = O(|x|)$ as $|x| \rightarrow \infty$ and $D^2 \mathcal{G} \in L^\infty$. Moreover, there is some $\lambda > 0$ such that p satisfies LSI(λ) uniformly in t . Then p is known to admit a spectral gap (or Poincaré inequality) with some

constant $\tilde{\lambda} > 0$, and as shown in [11], equation (19) has a unique solution $\phi \in H_0^1(\mathbb{R}^d; p)$ satisfying

$$\int |\nabla \phi|^2 p dx \leq \frac{1}{\tilde{\lambda}} \int |h - \hat{h}|^2 p dx, \quad (41)$$

which implies

$$E[|u|^2] = \int |\nabla \phi|^2 p dx \leq \frac{1}{\tilde{\lambda}} \int |h - \hat{h}|^2 p dx \leq \frac{1}{\tilde{\lambda}} \int |h|^2 p dx. \quad (42)$$

If we assume $h \in L^2(\mathbb{R}^d; p_0^*)$, then Lemma 2 (iii) and (42) ensure that the control $u(x, t)$ obtained from (19) is admissible. ■

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