AN INTERACTING PARTICLE CONSENSUS METHOD FOR CONSTRAINED GLOBAL OPTIMIZATION

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ABSTRACT. This paper presents a particle-based optimization method designed for addressing minimization problems with equality constraints, particularly in cases where the loss function exhibits non-differentiability or non-convexity. The proposed method combines components from consensus-based optimization algorithm with a newly introduced forcing term directed at the constraint set. A rigorous mean-field limit of the particle system is derived, and the convergence of the mean-field limit to the constrained minimizer is established. Additionally, we introduce a stable discretized algorithm and conduct various numerical experiments to demonstrate the performance of the proposed method.

1. INTRODUCTION

In this paper, we are concerned with the following minimization problem with m equality constraints,

$$\min_{v \in \mathbb{R}^d} \ \mathcal{E}(v) \text{s.t.} \ g_1(v) = 0, \ g_2(v) = 0, \ \dots, \ g_m(v) = 0.$$

The above optimization problems have widespread application across various domains. For example, in supply chain optimization, equality constraints play a pivotal role in maintaining a balance between demand and supply [26]; astronomers employ constrained optimization to calculate spacecraft trajectories, adhering to the laws of physics and orbital equations [8, 38]; in structural design, engineers optimize dimensions of beams, columns, or trusses while ensuring that the structural equilibrium equations are satisfied as equality constraints [20]. In this paper we deal with the cases when the objective function can be *non-convex* and *non-differentiable*.

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Traditional algorithms like the Lagrange Multipliers [32] and the Alternating Direction Method of Multipliers (ADMM) [37] lack guarantees of converging to the global constrained minimizer when dealing with non-convex or non-differentiable loss functions $\mathcal{E}(v)$. A new framework is required to effectively handle such cases, and recently, a class of gradient-free methods called consensus-based optimization (CBO) methods [5, 29, 36] have emerged as promising approaches for handling non-convex and non-differentiable loss functions. Motivated by the well-known Laplace's principle [3, 10, 27], they are decentralized and gradient-free algorithms that leverage the power of information sharing and cooperation among individual particles. However, it is important to highlight that much of the existing work has focused on the unconstrained case such as [5, 6, 9, 15, 17, 18, 22, 23, 24, 25, 30, 31, 34]. We refer the readers to survey articles [7, 21, 35] for a more detailed and complete summary.

Limited work has been done for the constrained case. The primary challenge lies in reconciling the CBO model's tendency to drive agents towards the global minimizer with the need for agents to remain within the constraint set and converge to the constrained minimizer. Currently, there are mainly two approaches. One involves projection onto the hypersurface [12, 13, 14]. However, this method is restricted to sphere constraints, and its applicability to general constraints or multiple equality constraints remains unclear. Another method introduces constraints as a penalized term in the objective function [4, 7], transforming it into an unconstrained problem for CBO. However, the convergence is sensitive to the landscape of the objective function and the penalization constant, which makes it difficult to achieve high accuracy.

In this paper, we introduce a third strategy for constrained CBO along with convergence analysis and numerical experiments. Instead of performing projection onto the constraint set or adding penalty terms, we propose a novel approach that combines the classical unconstrained CBO algorithm with gradient descent on the function $G(v) = \sum_{i=1}^{m} g_i^2(v)$, serving as a forcing term to the constraint set. Importantly, we do not require the differentiability of the target function \mathcal{E} and only need a mild differentiability condition on G. Compared with the other two constrained CBO methods, our method applies to general equality constraints, achieves faster convergence, and has consistently more stable performance as shown in Figures 1 and 2.

1.1. Contributions. Our main contributions are three folds. Firstly, we introduce a new CBO-based method for solving constrained optimization problems, with possibly nonconvex and non-differentiable objective functions. This method can accommodate a wide range of equality constraints, including the ability to handle multiple constraints concurrently. Secondly, we provide rigorous theoretical guarantees for the continuous-in-time model of the proposed method. Specifically, we establish the mean-field limit of the method and conduct a thorough analysis of its convergence behavior within this limit. Thirdly, we present a stable discretized algorithm designed to approximate the dynamics of the continuous-in-time model efficiently. Notably, this algorithm handles the stiff term of order $O(\epsilon^{-1})$ without requiring the time step to approach zero as ϵ tends to zero. 1.2. **Organizations.** The paper is structured as follows. Section 2 provides an introduction to the continuous-in-time stochastic differential equations, which serves as the model for the proposed method. Following that, Section 3 studies the well-posedness of the introduced SDEs and explores their mean-field limit. In Section 4, we analyze the convergence properties of the method by establishing the long-time behavior of the mean-field limit. This includes demonstrating, under appropriate assumptions, the convergence of the meanfield limit model to the constrained minimizer. Section 5 details the implementation of the algorithm, accompanied by a series of numerical experiments showcasing its performance. Finally, Section 6 offers a comprehensive summary of the findings presented in this paper.

1.3. Notations. We use $\mathcal{C}_b^k(\mathbb{R}^d)$ and $\mathcal{C}_c^k(\mathbb{R}^d)$ to denote the space of k-times continuous differentiable functions defined on \mathbb{R}^d that are bounded and compactly supported respectively. The space \mathcal{C}_*^2 is defined as

$$\mathcal{C}^2_*(\mathbb{R}^d) := \left\{ \phi \in \mathcal{C}^2(\mathbb{R}^d) | \ |\partial_{x_k} \phi(x)| \le C(1+|x_k|) \text{ and } \sup_{x \in \mathbb{R}^d} |\partial_{x_k x_k} \phi(x)| < \infty \text{ for all } k = 1, 2, ..., d \right\}.$$

When X and Y are topological spaces, we use $\mathcal{C}(X,Y)$ to denote the space of continuous functions mapping from X to Y. When X is a topological space, $\mathcal{P}(X)$ denotes the space of all the Borel probability measure, which is equipped with the Levy-Prokhorov metric. Given $1 \leq p < \infty$, $\mathcal{P}_p(\mathbb{R}^d)$ is the collection of all probability measures on \mathbb{R}^d with finite p-th moment, which is equipped with the Wasserstein-p distance, denoted by $W_p(\cdot, \cdot)$. If ρ is a probability measure, $\rho^{\otimes N}$ denotes the probability space obtained by coupling ρ independently N times.

 $\|\cdot\|_p$ denotes the usual l^p vector norm in the Euclidean space, $\|\cdot\|_{L^1\rho}$ denotes L^1 norm of a function with respect to ρ and $|\cdot|$ denotes the absolute value of a real number. $B^{\infty}(x,r)$ denotes the closed l^{∞} ball centered at x with radius r. \mathbb{I}_d denotes the $d \times d$ identity matrix. When u is a vector, diag(u) denotes the diagonal matrix with u being the diagonal.

Throughout this paper, we use the symbols C and L to represent generic positive uniform constants. It is important to note that these constants may take on different values in different sections or parts of this paper.

2. The dynamics of the constrained consensus-based optimization Algorithm

In this section, we carry out the continuous-in-time dynamics of our method. The practical discretized algorithm will be introduced in Section 5.

Consider the following constrained optimization problem,

$$\min_{v \in \mathbb{R}^d} \quad \mathcal{E}(v) \text{s.t.} \quad g_1(v) = 0, \ g_2(v) = 0, \ \dots, \ g_m(v) = 0.$$
 (1)

Here, we require the function $g_i(x)$ is first-order differentiable and assume that v^* is the unique solution to the optimization problem (1). It is noteworthy that Problem (1) can be reformulated equivalently as follows:

$$\min_{v \in \mathbb{R}^d} \quad \mathcal{E}(v) \\ \text{s.t.} \quad G(v) = 0,$$
 (2)

where $G(v) = \sum_{i=1}^{m} g_i^2(v)$. Our method will be based on formulation (2). To start with, we take N particles $V^{1,N}, V^{2,N}, ..., V^{N,N}$, which are independently sampled from a common initial law ρ_0 at initialization. Here we use $V_t^{i,N}$ for the location of the i-th particle at time t. Now we introduce the following empirical mean measure:

$$d\hat{\rho}_t^N(v) = \frac{1}{N} \sum_{i=1}^N \delta_{V_t^{i,N}}(v).$$

The goal of the dynamics is to encourage the measure $d\hat{\rho}_t^N$ to converge to the measure δ_{v^*} , which is the Dirac measure at the solution of the constrained optimization problem (2). Now we propose the dynamics of the *i*-th particle, which follows the below stochastic differential equation:

$$dV_t^{i,N} = -\lambda \left(V_t^{i,N} - v_\alpha(\hat{\rho}_t^N) \right) dt - \frac{1}{\epsilon} \nabla G(V_t^{i,N}) dt + \sigma D_t^{i,N} dB_t^{i,N},$$

$$V_0^{i,N} \sim \rho_0,$$
(3)

where

$$v_{\alpha}(\hat{\rho}_t^N) = \int v \cdot \frac{\omega_{\alpha}(v)}{\|\omega_{\alpha}\|_{L^1(\hat{\rho}_t^N)}} d\hat{\rho}_t^N.$$
(4)

The dynamics are driven by three distinct terms. The first and third terms are inherited from classical consensus-based optimization methods, while the second term is crafted as a forcing term to enforce the constraint. We will now explain each of them in sequence.

The first drift term $-\lambda (V_t^{i,N} - v_\alpha(\hat{\rho}_t)) dt$ is formulated to guide all particles toward the consensus point $v_{\alpha}(\hat{\rho}_t^N)$. This consensus point is strategically chosen as a location where the function is likely to achieve a small value. It is defined through a Gibbs-type distribution (4) where the weight ω_{α} is defined as

$$\omega_{\alpha}(v) = e^{-\alpha \mathcal{E}(v)}.$$

Here λ controls the force magnitude driving the particles towards the consensus point $v_{\alpha}(\hat{\rho}_t).$

The choice of the consensus point is inspired by the well-known Laplace's principle [3, 10, 27]. According to this principle, for any absolutely continuous probability measure ρ on \mathbb{R}^d , one has

$$\lim_{\alpha \to \infty} \left(-\frac{1}{\alpha} \log \left(\int \omega_{\alpha}(v) \, d\rho(v) \right) \right) = \inf_{v \in \operatorname{supp}(\rho)} \mathcal{E}(v).$$

It is expected that the consensus point $v_{\alpha}(\hat{\rho}_t^N)$ serves as a reasonable approximation of $\operatorname{argmin}_{i=1,\ldots,N} \mathcal{E}(V_t^{i,N})$ when α is sufficiently large. Consequently, the particles are gathered to a location where $\mathcal{E}(v)$ attains a small value.

The diffusion term $\sigma D_t^{i,N} dB_t^{i,N}$ encourages particles to explore the landscape of $\mathcal{E}(v)$, where $D_t^{i,N}$ is a $d \times d$ matrix function that determines the way in which particles explore the landscape and $\{B_t^{i,N}\}_{i=1,\dots,N}$ are independent Wiener processes. There are different choices for the matrix function $D_t^{i,N}$. One option is isotropic exploration [29], in which $D_t^{i,N}$ is defined as:

$$D_t^{i,N} = \|V_t^{i,N} - v_\alpha(\hat{\rho}_t^N)\|_2 \mathbb{I}_d,$$
(5)

where the norm used above is the usual L^2 norm of vectors in \mathbb{R}^d . Another option is anisotropic exploration, first introduced in [6] to address the curse of dimensionality, in which $D_t^{i,N}$ reads

$$D_t^{i,N} = \operatorname{diag}\left(V_t^{i,N} - v_\alpha(\hat{\rho}_t^N)\right).$$
(6)

In this paper, we use (6) for its advantage in high-dimensional scenarios as illustrated in [6, 14, 16].

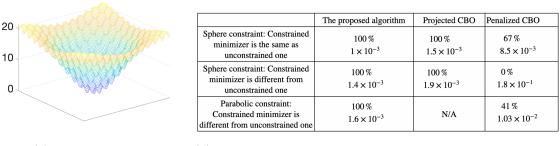
The two terms introduced above are consistent with classical Consensus-Based Optimization (CBO) methods. Now we introduce a third term:

$$-\frac{1}{\epsilon}\nabla G(V_t^{i,N})\,dt,$$

which addresses the constraint $\{G = 0\}$. Since 0 is the minimum of the non-negative function G(v), finding the constraint $\{G(v) = 0\}$ is the same as minimizing G(v). Therefore, we propose the third term as a gradient descent of G(v), allowing G(v) to be minimized during the algorithm's progression. Here $\epsilon > 0$ is a parameter that controls the magnitude of this term. When ϵ is small, this term will encourage particles to concentrate around $\{G = 0\}$.

Before we proceed to the theoretical analysis of the model, we first present a comparison result in Figures 1 and 2 to illustrate the superior performance of the proposed interacting particle system (3) compared to the projected CBO system [12] and the penalized CBO system [4]. We defer algorithmic formulation to Section 5, and details of the experiments to Appendix H.1, respectively.

We conducted tests on a two-dimensional Ackley function (shown in Figure 1), which is a highly nonconvex optimization problem with constraints on a circular domain or parabolic curve. The success rate of finding the unconstrained minimizer v^* and the averaged distance to v^* over 100 simulations are presented in the table shown in Figure 1. Additionally, the evolution of the averaged distance to the true minimizer is depicted in Figure 2. Our method achieves a 100% success rate in finding the unconstrained minimizer and demonstrates the fastest convergence rate in all experiments. The projected CBO performs similarly to our method when the constraint is a circle, but it is not applicable to parabolic curves. In contrast, the Penalized CBO exhibits a significantly lower success rate due to two main reasons: First, when the constrained minimizer is not a local minimizer of the objective function, the global minimizer v_p^* of the penalized objective function usually differs from the constrained minimizer v^* . Second, although it is possible to increase the



(a) Ackley function.

(b) The success rate and averaged Euclidean distance to the constrained minimizer.

Figure 1. Objective function and success rate of three constrained CBO methods.

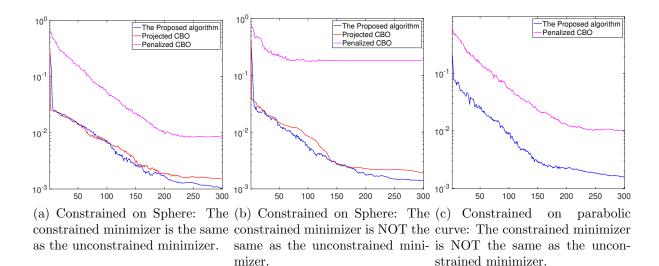


Figure 2. The averaged distance to the true constrained minimizer over 100 simulations.

penalty sufficiently to reduce the distance $||v_p^* - v^*||_2$, the landscape is dominated by the penalized term, making the objective function resemble a minor perturbation around the penalty. Consequently, it becomes more challenging for the optimization method to locate the global minimizer, and leads to a longer time for CBO to converge.

3. Well-posedness and Mean-field limit

In this section we study some theoretical properties of the particle system described by Equation (3). We consider anisotropic diffusion (6) in both Section 3 and Section 4. Consequently, the system defined by Equation (3) transforms into the following form:

$$dV_t^{i,N} = -\lambda \left(V_t^{i,N} - v_\alpha(\hat{\rho}_t^N) \right) dt - \frac{1}{\epsilon} \nabla G(V_t^{i,N}) dt + \sigma \operatorname{diag} \left(V_t^{i,N} - v_\alpha(\hat{\rho}_t^N) \right) dB_t^{i,N},$$

$$V_0^{i,N} \sim \rho_0,$$
(7)

where i = 1, ..., N.

When the number of particles N is large enough, one could study the mean-field limit as $N \to \infty$. This limit yields an equation that characterizes the macroscopic behavior of the particles, specifically their density distribution. The investigation of the mean-field equation reveals the long-term dynamics of the particle system, which is related to the convergence of the particle system or the optimization method. However, prior to this analysis in Section 4, it is necessary to establish the existence of the mean-field limit. In this section, we establish the well-posedness of Equation (7), its mean-field limit, and the well-posedness of the resultant mean-field model.

Throughout this section, we make the following assumptions.

Assumption 1. (1) The loss function \mathcal{E} is bounded with $\inf \mathcal{E} = \underline{\mathcal{E}}$ and $\sup \mathcal{E} = \overline{\mathcal{E}}$. (2) There exist positive numbers L and C such that for $\forall u, v \in \mathbb{R}^d$,

$$\begin{aligned} \|\mathcal{E}(u) - \mathcal{E}(v)\|_2 &\leq L(\|u\|_2 + \|v\|_2) \|u - v\|_2, \\ \mathcal{E}(u) - \underline{\mathcal{E}} &\leq C(1 + \|u\|_2^2), \end{aligned}$$

(3) There exists L > 0 such that for $\forall u, v \in \mathbb{R}^d$,

$$\|\nabla G(u) - \nabla G(v)\|_2 \le L \|u - v\|_2,$$

(4) There exists C > 0 such that for $\forall u \in \mathbb{R}^d$,

$$\|\nabla G(u)\|_2 \le C \|v\|_2.$$

Briefly speaking, in Assumption 1 (1) and (2), we assume the loss function \mathcal{E} is bounded, locally Lipschitz and with at most quadratic growth. In Assumption 1 (3) and (4), we assume the gradient of the function G is globally Lipschitz and with at most linear growth.

3.1. Well-posedness of the microscopic model. In this subsection, we establish the well-posedness of the interacting particle system (7), as presented in the following theorem.

Theorem 3.1. For any $N \in \mathbb{N}$, the stochastic differential equation (7) has a unique strong solution $\left\{V_t^{i,N} | t \ge 0\right\}_{i=1}^N$ for any initial condition $V_0^{i,N}$ satisfying $\mathbb{E}\left[\|V_0^{i,N}\|_2^2\right] < \infty$. *Proof.* See Appendix A.1.

3.2. The mean-field limit and its well-posedness. By letting the number of agents $N \to \infty$ in the model (7), the mean-field limit of the model is formally given by the following SDE

$$d\bar{V}_t = -\lambda \left(\bar{V}_t - v_\alpha(\rho_t)\right) dt - \frac{1}{\epsilon} \nabla G \, dt + \sigma \operatorname{diag}\left(\bar{V}_t - v_\alpha(\rho_t)\right) dB_t.$$
(8)

Then the corresponding Fokker-Planck equation is

$$\partial_t \rho_t = \lambda \operatorname{div}\left(\left(v - v_\alpha(\rho_t) + \frac{1}{\epsilon}\nabla G\right)\rho_t\right) + \frac{\sigma^2}{2}\sum_{k=1}^d \partial_{x_k x_k}\left(\left(v - v_\alpha(\rho_t)\right)_k^2 \rho_t\right).$$
(9)

Next, we will prove the above equations (8), (9) are well-posed, and they model the mean-field limit.

For the corresponding Fokker-Planck equation, we in particular study its weak solution, which is defined as follows.

Definition 3.2. We say $\rho_t \in \mathcal{C}([0,T], \mathcal{P}_4(\mathbb{R}^d))$ is a weak solution to (9) if (i) The continuity in time is in \mathcal{C}'_b topology:

$$\left\langle \phi, d\rho_{t_n} \right\rangle \to \left\langle \phi, d\rho_t \right\rangle$$

for $\forall \phi \in \mathcal{C}_b(\mathbb{R}^d)$ and $t_n \to t$. (ii) One of the following two equivalent equations holds for $\forall \phi \in \mathcal{C}_c^2(\mathbb{R}^d)$:

$$\frac{d}{dt} \left\langle \phi, d\rho_t \right\rangle = -\lambda \left\langle \left(v - v_\alpha(\rho_t) \right) \cdot \nabla \phi(v), d\rho_t \right\rangle - \frac{1}{\epsilon} \left\langle \nabla G(v) \cdot \nabla \phi(v), d\rho_t \right\rangle \\ + \frac{\sigma^2}{2} \left\langle \sum_{k=1}^d \left(v - v_\alpha(\rho_t) \right)_k^2 \partial_{kk} \phi(v), d\rho_t \right\rangle$$

or

$$0 = \left\langle \phi, d\phi_t \right\rangle - \left\langle \phi, d\rho_0 \right\rangle + \lambda \int_0^t \left\langle \left(v - v_\alpha(\rho_\tau) \right) \cdot \nabla \phi(v), d\rho_\tau \right\rangle d\tau + \frac{1}{\epsilon} \int_0^t \left\langle \nabla G(v) \cdot \nabla \phi(v), d\rho_\tau \right\rangle d\tau - \frac{\sigma^2}{2} \int_0^t \left\langle \sum_{k=1}^d \left(v - v_\alpha(\rho_\tau) \right)_k^2 \partial_{kk} \phi(v), d\rho_\tau \right\rangle d\tau.$$

Remark 1. In the Definition 3.2 (ii), the test function space is $C_c^2(\mathbb{R}^d)$. We could extend $C_c^2(\mathbb{R}^d)$ to a larger space $C_*^2(\mathbb{R}^d)$ as explained in Appendix C, which will be used in the proof later. $C_*^2(\mathbb{R}^d)$ is defined below.

$$\mathcal{C}^2_*(\mathbb{R}^d)$$

:= $\{\phi \in \mathcal{C}^2(\mathbb{R}^d) | |\partial_k \phi(x)| \le C(1+|x_k|) \text{ and } \sup_{x \in \mathbb{R}^d} |\partial_{kk} \phi(x)| < \infty \text{ for all } k = 1, 2, ..., d\}.$

In other words, if $\rho_t \in \mathcal{C}([0,T], \mathcal{P}_4(\mathbb{R}^d))$ solves equation (9) in the weak sense as in Definition 3.2, then the two equalities in Definition 3.2 will hold for any test function $\phi \in \mathcal{C}^2_*(\mathbb{R}^d)$.

Now we state the well-posedness result of (8) and (9).

Theorem 3.3. Let \mathcal{E} satisfy Assumption 1 and $\rho_0 \in \mathcal{P}_4(\mathbb{R}^d)$. Then there exists a unique nonlinear process $\overline{V} \in \mathcal{C}([0,T],\mathbb{R}^d)$, T > 0 satisfying (8) with initial distribution $\overline{V}_0 \sim \rho_0$

in the strong sense, and $\rho_t = Law(\bar{V}_t) \in \mathcal{C}([0,T],\mathcal{P}_4(\mathbb{R}^d))$ satisfies the corresponding Fokker-Planck equation (9) in the weak sense with $\lim_{t\to 0} \rho_t = \rho_0$.

Proof. See Appendix A.2.

Then we present the result showing that (8), (9) indeed characterize the mean-field limit of the particle system.

Theorem 3.4. Let \mathcal{E} satisfy Assumption 1 and $\rho_0 \in \mathcal{P}_4(\mathbb{R}^d)$. For any $N \geq 2$, assume that $\{(V_t^{i,N})\}_{i=1}^N$ is the unique solution to (7) with $\rho_0^{\otimes N}$ distributed initial data $\{V_0^{i,N}\}_{i=1}^N$. Then the limit (denoted by ρ_t) of the sequence $\{\hat{\rho}_t^N\}_{N\in\mathbb{N}}$, as $N \to \infty$ exists. Moreover, ρ_t is deterministic and it is the unique weak solution to the corresponding Fokker-Planck equation (9) of the mean-field model.

Proof. Please see Appendix A.3.

4. Convergence to the constrained minimizer in the mean-field limit

In this section, we will analyze the behavior of the weak solution of the Fokker-Planck equation (9). Recall that v^* is the unique solution of Problem (2). Our primary goal is to establish a key result: under suitable assumptions and the selection of appropriate parameters, the particles will concentrate around v^* with arbitrary closeness. This confirms the effectiveness of the method in the mean-field limit.

For simplicity and without loss of generality, we assume $\mathcal{E}(v^*) = 0$. Throughout this section, we use ρ_t to represent the solution of Equation (9) as defined in Definition 3.2.

4.1. Main Results. To study the convergence of ρ_t to v^* , we define the following energy functional

$$\mathcal{V}(\rho_t) := \frac{1}{2} \int \|v - v^*\|_2^2 \, d\rho_t(v). \tag{10}$$

The above defined quantity $\mathcal{V}(\rho_t)$ provides a measure of the distance between the distribution of the particles ρ_t and the Dirac measure at v^* , denoted as δ_{v^*} . Specifically, we have the relationship

$$2\mathcal{V}(\rho_t) = W_2^2(\rho_t, \delta_{v^*}),$$

where $W_2(\rho_t, \delta_{v^*})$ denotes the Wasserstein-2 distance between ρ_t and δ_{v^*} . The diminishing behavior of $\mathcal{V}(\rho_t)$ indicates that ρ_t is approaching δ_{v^*} , implying that particles are concentrating around v^* . In this paper, we establish the following main theorem concerning the decay of $\mathcal{V}(\rho_t)$.

Theorem 4.1. Suppose G and \mathcal{E} are well-behaved. Fix any $\tau \in (0,1)$ and parameters $\lambda, \sigma > 0$ with $2\lambda > \sigma^2$. There exists a function $I : \mathbb{R} \to \mathbb{R}$ such that for any error tolerance

 $\delta \in (0, \mathcal{V}(\rho_0))$, as long as $\rho_0(B(v^*, r)) > 0$ for all r > 0 and $\int G d\rho_0(v) \leq I(\delta)$, then one can find α and ϵ so that

$$\min_{t \in [0,T^*]} \mathcal{V}(\rho_t) \le \delta,\tag{11}$$

where

$$T^* = \frac{1}{(1-\tau)(2\lambda - \sigma^2)} \log\left(\frac{\mathcal{V}(\rho_0)}{\delta}\right).$$
(12)

Furthermore, until $\mathcal{V}(\rho_t)$ reaches the prescribed accuracy δ , the following exponential decay holds:

$$\mathcal{V}(\rho_t) \le \mathcal{V}(\rho_0) \exp\left(-(1-\tau)(2\lambda-\sigma^2)t\right).$$
(13)

Remark 2. In the above theorem, the function I only depends on G, \mathcal{E} and parameters τ, λ, σ . It does not depend on δ . The choice of α, ϵ will depend on δ as described in (24) and (70) respectively. Roughly speaking, when δ is fixed, we select a sufficiently large α , and subsequently, based on this chosen α , we select a small enough ϵ . Additionally, it is worth noting that the selection of λ and σ remains independent of the dimension d, as the only requirement is $2\lambda > \sigma^2$. However, α will exhibit a logarithmic dependence on d as illustrated in (24).

4.2. Assumption. In this subsection, we define clearly what it means by "being well**behaved**". G and \mathcal{E} are well-behaved if the following Assumption 2 is satisfied. It is worth noting that Assumption 2 in this section is independent of Assumption 1. In other words, for the proofs in this section, Assumption 1 is not required.

Assumption 2. A. Assumptions on \mathcal{E} :

- (A1) \mathcal{E} is bounded: $\underline{\mathcal{E}} \leq \mathcal{E} \leq \overline{\mathcal{E}}$.
- (A2) \mathcal{E} is locally Hölder continuous around v^* , i.e. there exists $r_0 > 0$ such that for $\forall v_1, v_2 \in B^{\infty}(v^*, r_0),$

$$|\mathcal{E}(v_1) - \mathcal{E}(v_2)| \le C ||v_1 - v_2||_{\infty}^{\beta}$$

for some C > 0 and $\beta > 0$.

B. Assumptions on G:

(B1)
$$\langle \nabla G(v), v - v^* \rangle \geq 0$$
 holds for any $v \in \mathbb{R}^d$

- (B2) $G(v) \in \mathcal{C}^2_*(\mathbb{R}^d)$ and there exists C > 0 such that $G(v) \leq C \|\nabla G(v)\|_2^2$ for $\forall v \in \mathbb{R}^d$. (B3) $\nabla G(v) \neq 0$ for $\forall v \in \{G(v) \in (0, u_0)\}$ and $\int_{G(v) \in (0, u_0)} \frac{1}{\|\nabla G(v)\|_2} dv < \infty$ for some $u_0 > 0$ small enough.

Remark 3. Assumption 2 (B1) is related to the convexity of function G but is less stringent than the convexity condition. If it is not satisfied, similar to other gradient descent algorithms, there is a possibility for some particles to get trapped in the local minimizers \hat{v} of G, i.e. $\nabla q(\hat{v}) = 0$. Nevertheless, provided the function values $\mathcal{E}(v)$ at those local minimizers of G do not fall below $\mathcal{E}(v^*)$, a condition attainable by adding a positive scalar

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multiple of G to \mathcal{E} without altering the solution v^* , it won't affect the convergence of the consensus point to the constrained minimizer v^* , as evidenced in the experiments detailed in Section 5.2.1, Figure 5. It is noteworthy that this slight adjustment on $\mathcal{E}(v)$ differs from the penalization method outlined in [4]. Here, there is no necessity for the penalty parameter to approach infinity, as the convergence is enforced through the dynamics rather than penalization. The introduction of a positive scalar multiple of G to \mathcal{E} is to avoid the extreme case. Thus a mild penalization would suffice.

Assumption 2 (B2) is primarily technical in nature. Assumption 2 (B3) guarantees that the gradient of G around the constraint $\{G = 0\}$ does not vanish too rapidly.

C. Assumptions on the coupling of \mathcal{E} and G: The following holds for $\forall u \in [0, u_0]$ where $u_0 > 0$ is a small constant.

(C1) There exist $v_u \in \mathbb{R}^d, \mathcal{E}_u \in \mathbb{R}$ such that

$$v_u = \underset{v \in \{G(v)=u\}}{\operatorname{arg\,min}} \mathcal{E}(v) \text{ and } \underline{\mathcal{E}}_u = \mathcal{E}(v_u).$$

Moreover, there exists a non-negative increasing function $\tau_1(x)$ from \mathbb{R} to \mathbb{R} with $\lim_{x\to 0} \tau_1(x) = 0$ such that

$$\|v_u - v^*\|_{\infty} \le \tau_1(u) \text{ and}$$
$$\partial B^{\infty}(v_u, r) \cap \{v \mid G(v) = u\} \neq \emptyset.$$

(C2) There exist $\eta > 0$, $\mu > 0$, $R_0 > 0$ and $\mathcal{E}_{\infty} > 0$ such that

$$\|v - v_u\|_{\infty} \le \frac{1}{\eta} \left(\mathcal{E}(v) - \underline{\mathcal{E}}_u \right)^{\prime}$$

for
$$\forall v \in B^{\infty}(v_u, R_0) \cap \{G(v) = u\}$$
 and
 $\mathcal{E}_{\infty} < \mathcal{E}(v) - \underline{\mathcal{E}_u}$
for $\forall v \in B^{\infty}(v_u, R_0)^c \cap \{G(v) = u\}.$

Remark 4. The above Assumption 2 (C1) ensures the geometry of \mathcal{E} on the set $\{G = u\}$ is similar among small enough u, i.e., on sets $\{G = u\}$, the constrained minimizers v_u and constrained minimums $\mathcal{E}(v_u)$ are close among small enough values for u. To illustrate, if this condition is not met, as depicted in Figure 3 (a), the desired constrained minimizer v^* (depicted as a solid green pentagon) is considerably distant from the minimizer v_u on a nearby level set $\{G = u\}$ (depicted as a solid orange circle) for all sufficiently small u. Consider an extreme case where we assume $\mathcal{E}(v_u)$ is significantly smaller than $\mathcal{E}(v^*)$ for all positive but sufficiently small u. Due to the nature of gradient descent on G for each particle, which may not precisely enforce each particle to remain on the constraint $\{G = 0\}$, these particles will tend to remain in a neighborhood of $\{G = 0\}$. Consequently, numerous particles will cluster around $\{G = u\}$ for sufficiently small u, as illustrated in Figure 3 (a). Given that numerous particles are near v_u , where the function value is significantly small, the algorithm computes the consensus point around v_u rather than v^* . Consequently, the consensus point will gradually lead particles to concentrate around v_u rather than v^* ,

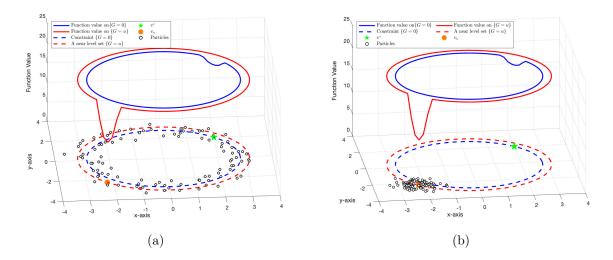


Figure 3. The blue curves represent function values on the constraint set $\{G = 0\}$ and the red curves on the level set $\{G = u\}$. Dashed lines represent corresponding constraint sets. The green pentagon denotes the constrained minimizer v^* , and the orange circle represents the minimizer v_u on the nearby level set G = u. Empty circles represent particles.

as illustrated in Figure 3 (b), which leads to a failure in this extreme scenario. To avoid the occurrence of such extreme cases, we proposed Assumption 2 (C1). In conjunction with other assumptions, the similarity of the local geometry of \mathcal{E} on the set $\{G = u\}$ for sufficiently small values of u is guaranteed as established in Lemma B.1.

The Assumption 2 (C2) ensures that the constrained minimizer is distinguishable from other points, i.e., on each adjacent level set $\{G = u\}$, there is a unique minimizer v_u and $\mathcal{E}(v)$ behaves like $||v - v_u||_{\infty}^{1/\mu}$ near the v_u .

4.3. Sketch of the Proof. In this subsection, we layout the strategy of the proof. The forthcoming subsections (4.4, 4.5, 4.6, 4.7, and 4.8) will introduce needed lemmas, propositions, and the complete proof of Theorem 4.1.

Initiating our analysis with Lemma 4.2 in Subsection 4.4, we plug $\frac{1}{2} ||v - v^*||_2^2$ into Definition 3.2. This yields the following differential inequality:

$$\frac{d}{dt}\mathcal{V}(\rho_t) \leq -(2\lambda - \sigma^2)\mathcal{V}(\rho_t) + \sqrt{2}(\lambda + \sigma^2)\sqrt{\mathcal{V}(\rho_t)} \|v_\alpha(\rho_t) - v^*\|_2 + \frac{\sigma^2}{2}\|v_\alpha(\rho_t) - v^*\|_2^2.$$

It is noteworthy that if $||v_{\alpha}(\rho_t) - v^*||_2$ could be bounded by a suitable scalar multiple of $\sqrt{\mathcal{V}(\rho_t)}$, we would then obtain the inequality:

$$\frac{d}{dt}\mathcal{V}(\rho_t) \le \left(-(1-\tau)(2\lambda-\sigma^2)\right)\mathcal{V}(\rho_t),\tag{14}$$

to which Gronwall's inequality can be applied, ensuring exponential decay. Consequently, in Proposition 1 in Subsection 4.5, we establish the following inequality:

$$\begin{aligned} \|v_{\alpha}(\rho_{t}) - v^{*}\|_{2} &\leq 2\sqrt{d} \cdot \frac{\left(q + \mathcal{E}_{r}^{0} + \tau_{2}(u) + \tau_{4}(\max\{u, r\})\right)^{\mu}}{\eta} \\ &+ \frac{\sqrt{d}e^{-\alpha\left(q - \tau_{3}(\max\{u, r\})\right)}}{\rho_{t}\left(B^{\infty}(v^{*}, r)\right)} \int_{\{G \in (0, u)\}} \|v - v_{G(v)}\|_{2} d\rho_{t}(v) \\ &+ \frac{\sqrt{d}e^{-\alpha\left(q - \tau_{3}(r)\right)}}{\rho_{t}\left(B^{\infty}(v^{*}, r)\right)} \int_{\{G = 0\}} \|v - v^{*}\|_{2} d\rho_{t}(v) \\ &+ \sqrt{d}\tau_{1}(u) \\ &+ \int_{\{G(v) \geq u\}} \frac{\|v - v^{*}\|_{2}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha\mathcal{E}(v)} d\rho_{t}(v). \end{aligned}$$

where q, u, r are parameters to be determined. It is observed that with an appropriate choice of q, u, r, provided $\rho_t(B(v^*, r))$ is suitably bounded from below, as proven in Lemma 4.5 in Subsection 4.6, letting α be sufficiently large will make the first four terms above small enough. Concerning the last term, it is related to $\int G d\rho_t(v)$, which can be controlled by Lemma 4.6 in Subsection 4.7.

Consequently, we can control $||v_{\alpha}(\rho_t) - v^*||_2$ in such a way that (14) holds, thereby ensuring exponential decay.

4.4. Dynamics of $\mathcal{V}(\rho_t)$. In this subsection, we present the dynamics of the energy functional $\mathcal{V}(\rho_t)$.

Lemma 4.2. Let $\mathcal{V}(\rho_t)$ be the energy functional defined in (10). Under Assumption 2,

$$\frac{d}{dt}\mathcal{V}(\rho_t) \leq -(2\lambda - \sigma^2)\mathcal{V}(\rho_t) + \sqrt{2}(\lambda + \sigma^2)\sqrt{\mathcal{V}(\rho_t)} \|v_{\alpha}(\rho_t) - v^*\|_2 + \frac{\sigma^2}{2}\|v_{\alpha}(\rho_t) - v^*\|_2^2 - \frac{1}{\epsilon} \int \left\langle \nabla G, v - v^* \right\rangle d\rho_t(v).$$
roof. See Appendix D.

Proof. See Appendix D.

4.5. Laplace's Principle. One can notice, in the dynamics proved in the last subsection, there is an unknown quantity $||v_{\alpha}(\rho_t) - v^*||_2$. As mentioned in Subsection 4.3, if $\|v_{\alpha}(\rho_t) - v^*\|_2$ could be bounded by a suitable scalar multiple of $\sqrt{\mathcal{V}(\rho_t)}$, we can apply Gronwall's inequality. In this subsection, we deduce a quantitative Laplace principle to bound $||v_{\alpha}(\rho_t) - v^*||_2$. One can first prove the following two lemmas.

Lemma 4.3. Fix $r \in (0, R_0)$ small enough. For $\forall q > 0$ with $q + \mathcal{E}_r^0 < \mathcal{E}_{\infty}$,

$$\int_{\{G=0\}} \frac{\|v-v^*\|_2}{\|\omega_\alpha\|_{L^1(\rho_t)}} e^{-\alpha \mathcal{E}(v)} \, d\rho_t(v) \le \frac{\sqrt{d}(q+\mathcal{E}_r^0)^{\mu}}{\eta} + \frac{\sqrt{d}e^{-\alpha}(q-\tau_3(r))}{\rho_t(B^{\infty}(v^*,r))} \int_{\{G=0\}} \|v-v^*\|_2 \, d\rho_t(v).$$

Here, \mathcal{E}_r^0 , \mathcal{E}_{∞} and τ_3 are quantities defined in Assumption 2 (C) and Lemma B.1.

Proof. See Appendix E.1

Lemma 4.4. Fix $0 < u < u_0$ and r > 0 small. For $\forall q > 0$ satisfying the condition that $q + \mathcal{E}_r^{\tilde{u}} - \underline{\mathcal{E}}_{\tilde{u}} < \mathcal{E}_{\infty}$ is true for $\forall \tilde{u} \in (0, u)$, then

$$\int_{\{G\in(0,u)\}} \frac{\|v-v^*\|_2}{\|\omega_\alpha\|_{L^1(\rho_t)}} e^{-\alpha\mathcal{E}(v)} d\rho_t(v) \leq \frac{\sqrt{d} \left(q + \mathcal{E}_r^0 + \tau_2(u) + \tau_4(\max\{u,r\})\right)^{\mu}}{\eta} \\
+ \frac{\sqrt{d} e^{-\alpha \left(q - \tau_3(\max\{u,r\})\right)}}{\rho_t \left(B^{\infty}(v^*,r)\right)} \int_{\{G\in(0,u)\}} \|v-v_{G(v)}\|_2 d\rho_t(v) \\
+ \sqrt{d} \tau_1(u).$$

Here, $v_{G(v)} = \arg\min_{v' \in \{G(v') = G(v)\}} \mathcal{E}(v')$, $\underline{\mathcal{E}}_{\tilde{u}}$ and τ_1 are defined in Assumption 2 (C1), $\mathcal{E}_r^{\tilde{u}}$, τ_3 and τ_4 are quantities defined in Lemma B.1.

Proof. See Appendix E.2

Now we are ready to prove a quantitative Laplace principle.

Proposition 1 (A Quantitative Laplace Principle). Fix r > 0 small enough and u > 0 small enough. q > 0 is a constant such that $q + \mathcal{E}_r^{\tilde{u}} - \underline{\mathcal{E}}_{\tilde{u}} < \mathcal{E}_{\infty}$ is true for $\forall \tilde{u} \in [0, u)$. Then

$$\begin{aligned} \|v_{\alpha}(\rho_{t}) - v^{*}\|_{2} &\leq 2\sqrt{d} \cdot \frac{\left(q + \mathcal{E}_{r}^{0} + \tau_{2}(u) + \tau_{4}(\max\{u, r\})\right)^{\mu}}{\eta} \\ &+ \frac{\sqrt{d}e^{-\alpha\left(q - \tau_{3}(\max\{u, r\})\right)}}{\rho_{t}\left(B^{\infty}(v^{*}, r)\right)} \int_{\{G \in (0, u)\}} \|v - v_{G(v)}\|_{2} d\rho_{t}(v) \\ &+ \frac{\sqrt{d}e^{-\alpha\left(q - \tau_{3}(r)\right)}}{\rho_{t}\left(B^{\infty}(v^{*}, r)\right)} \int_{\{G = 0\}} \|v - v^{*}\|_{2} d\rho_{t}(v) \\ &+ \sqrt{d}\tau_{1}(u) \\ &+ \int_{\{G(v) \geq u\}} \frac{\|v - v^{*}\|_{2}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha\mathcal{E}(v)} d\rho_{t}(v). \end{aligned}$$

Proof. By the definition of the consensus point $v_{\alpha}(\rho_t)$, one has

$$\begin{aligned} \|v_{\alpha}(\rho_{t}) - v^{*}\|_{2} &= \|\int v \cdot \frac{e^{-\alpha \mathcal{E}(v)}}{\|\omega_{\alpha}\|_{1}} \, d\rho_{t}(v) - v^{*}\|_{2} \\ &= \|\int (v - v^{*}) \cdot \frac{e^{-\alpha \mathcal{E}(v)}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} \, d\rho_{t}(v)\|_{2} \leq \int \frac{\|v - v^{*}\|_{2}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha \mathcal{E}(v)} \, d\rho_{t}(v), \end{aligned}$$

where we used Minkowski's inequality. Then we can compute:

$$\begin{aligned} \|v_{\alpha}(\rho_{t}) - v^{*}\|_{2} &\leq \int \frac{\|v - v^{*}\|_{2}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha \mathcal{E}(v)} \, d\rho_{t}(v) \\ &= \int_{\{G=0\}} \frac{\|v - v^{*}\|_{2}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha \mathcal{E}(v)} \, d\rho_{t}(v) + \int_{\{G\in(0,u)\}} \frac{\|v - v^{*}\|_{2}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha \mathcal{E}(v)} \, d\rho_{t}(v) \\ &+ \int_{\{G\geq u\}} \frac{\|v - v^{*}\|_{2}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha \mathcal{E}(v)} \, d\rho_{t}(v). \end{aligned}$$

For the first term, we can upper bound it using Lemma 4.3:

$$\begin{split} \int_{\{G=0\}} \frac{\|v-v^*\|_2}{\|\omega_{\alpha}\|_{L^1(\rho_t)}} e^{-\alpha \mathcal{E}(v)} \, d\rho_t(v) &\leq \frac{\sqrt{d}(q+\mathcal{E}_r^0)^{\mu}}{\eta} + \frac{\sqrt{d}e^{-\alpha}(q-\tau_3(r))}{\rho_t(B^{\infty}(v^*,r))} \int_{\{G=0\}} \|v-v^*\|_2 \, d\rho_t(v) \\ &\leq \frac{\sqrt{d}(q+\mathcal{E}_r^0+\tau_2(u)+\tau_4(\max\{u,r\}))^{\mu}}{\eta} \\ &+ \frac{\sqrt{d}e^{-\alpha}(q-\tau_3(r))}{\rho_t(B^{\infty}(v^*,r))} \int_{\{G=0\}} \|v-v^*\|_2 \, d\rho_t(v). \end{split}$$

For the second term, we can upper bound it using Lemma 4.4:

$$\int_{\{G\in(0,u)\}} \frac{\|v-v^*\|_2}{\|\omega_{\alpha}\|_{L^1(\rho_t)}} e^{-\alpha \mathcal{E}(v)} d\rho_t(v) \leq \frac{\sqrt{d} \left(q + \mathcal{E}_r^0 + \tau_2(u) + \tau_4(\max\{u, r\})\right)^{\mu}}{\eta} \\
+ \frac{\sqrt{d} e^{-\alpha \left(q - \tau_3(\max\{u, r\})\right)}}{\rho_t \left(B^{\infty}(v^*, r)\right)} \int_{\{G\in(0,u)\}} \|v - v_{G(v)}\|_2 d\rho_t(v) \\
+ \sqrt{d} \tau_1(u).$$

Finally, We leave the third term unchanged. Combining the estimates for the above three terms, we can finish the proof. $\hfill \Box$

4.6. Lower bound for $\rho_t(B^{\infty}(v^*, r))$. In this subsection, we establish a lower bound for $\rho_t(B^{\infty}(v^*, r))$, a crucial element for our subsequent application of the Laplace principle. We first define the mollifier $\phi_r(v)$ as follows

$$\phi_r(v) = \begin{cases} \prod_{k=1}^d \exp\left(1 - \frac{r^2}{r^2 - (v - v^*)_k^2}\right), & \text{if } \|v - v^*\|_\infty < r, \\ 0, & \text{else.} \end{cases}$$
(15)

Lemma 4.5. Let $B = \sup_{t \in [0,T]} \|v_{\alpha}(\rho_t) - v^*\|_{\infty}$. Then for all $t \in [0,T]$,

$$\rho_t \left(B^{\infty}(v^*, r) \right) \ge \left(\int \phi_r \, d\rho_0(v) \right) e^{-at},$$

for $a = 2d \max \left\{ \frac{\lambda(\sqrt{cr} + B)\sqrt{c}}{(1-c)^2 r} + \frac{\sigma^2(cr^2 + B^2)(2c+1)}{(1-c)^4 r^2}, \frac{2\lambda^2}{(2c-1)\sigma^2} \right\},$

where $c \in (\frac{1}{2}, 1)$ is some constant satisfying

$$(2c-1)c \ge (1-c)^2$$

Proof. See Applendix F.

4.7. Dynamics of $\int G d\rho_t(v)$. In Lemma 4.2, we have gained control over $\|v_\alpha(\rho_t) - v^*\|_2$, yet the dynamics of the last term

$$-\frac{1}{\epsilon} \int \left\langle \nabla G, v - v^* \right\rangle d\rho_t(v)$$

remains to be studied, which we do now.

Lemma 4.6. Assume $\sup_{t\in[0,T]} \|v_{\alpha}(\rho_t) - v^*\|_2 < \infty$ and $\sup_{t\in[0,T]} \mathcal{V}(\rho_t) < \infty$. Then for $\epsilon > 0$ small enough,

$$\int G \, d\rho_t(v) \le \int G \, d\rho_0(v)$$

for $\forall t \in [0, T]$.

Proof. See Appendix G.

4.8. **Proof of Theorem 4.1.** In this subsection, we present the complete proof of Theorem 4.1.

For simplicity, in the following, we assume $\tau_1(u) = \tau_2(u) = \tau_3(u) = \tau_4(u) = u$, where $\tau_1, \tau_2, \tau_3, \tau_4$ are defined in Assumption 2 (C) and Lemma B.1. We point out that the proof technique remains valid for any choice of τ_i that is an increasing function and converges to 0 as u approaches 0.

Now we are ready to prove Theorem 4.1.

Proof of Theorem 4.1. First we use Lemma 4.2 to derive the dynamics of $\mathcal{V}(\rho_t)$:

$$\frac{d}{dt}\mathcal{V}(\rho_t) \le -(2\lambda - \sigma^2)\mathcal{V}(\rho_t) + \sqrt{2}(\lambda + \sigma^2)\sqrt{\mathcal{V}(\rho_t)} \|v_\alpha(\rho_t) - v^*\|_2 + \frac{\sigma^2}{2} \|v_\alpha(\rho_t) - v^*\|_2^2,$$

where the last term on the right-hand-side of Lemma 4.2 is omitted because of its nonpositivity due to Assumption 2 (B1).

Now we define C(t) as follows,

$$C(t) = \min\left\{\frac{\tau}{2}\frac{(2\lambda - \sigma^2)}{\sqrt{2}(\lambda + \sigma^2)}, \sqrt{\tau \frac{(2\lambda - \sigma^2)}{\sigma^2}}\right\}\sqrt{\mathcal{V}(\rho_t)},$$

and $T_{\alpha,\epsilon}$ as

$$T_{\alpha,\epsilon} = \sup \left\{ t \ge 0 | \mathcal{V}(\rho_{t'}) > \delta, \| v_{\alpha}(\rho_{t'}) - v^* \|_2 \le C(t') \text{ for all } t' \in [0,t] \right\}.$$

As long as $||v_{\alpha}(\rho_{t'}) - v^*||_2 \leq C(t')$ is true, it is straightforward to verify that

$$\frac{d}{dt}\mathcal{V}(\rho_{t'}) \leq -(1-\tau)(2\lambda-\sigma^2)\mathcal{V}(\rho_{t'}).$$

Thus by Gronwall's inequality, if $t \leq T_{\alpha,\epsilon}$, one has

$$\mathcal{V}(\rho_t) \leq \mathcal{V}(\rho_0) \exp\left(-(1-\tau)(2\lambda-\sigma^2)t\right)$$

Different choices of (α, ϵ) will result in different cases as follows.

Case 1 $(T_{\alpha,\epsilon} \ge T^*)$.

Notice that $\mathcal{V}(\rho_{T^*}) \leq \mathcal{V}(\rho_0) \exp\left(-(1-\tau)(2\lambda-\sigma^2)t\right) = \delta$. So we have $\min_{t \in [0,T^*]} \mathcal{V}(\rho_t) \leq \delta$. This completes the proof.

Case 2
$$(T_{\alpha,\epsilon} < T^* \text{ and } \mathcal{V}(\rho_{T_{\alpha,\epsilon}}) = \delta).$$

In this case, it clear that $\min_{t \in [0,T^*]} \mathcal{V}(\rho_t) \leq \mathcal{V}(\rho_{T_{\alpha,\epsilon}}) = \delta$, which completes the proof. Case $\Im \Big(T_{\alpha,\epsilon} < T^*, \, \mathcal{V}(\rho_{T_{\alpha,\epsilon}}) > \delta$ and $\| v_\alpha(\rho_{T_{\alpha,\epsilon}}) - v^* \|_2 = C(T_{\alpha,\epsilon}) \Big).$

Case 3 is the only non-trivial case. We now show that suitable choices of α and ϵ will make Case 3 impossible.

We pick

$$q = \min\left\{\frac{1}{4} \left(\eta \frac{C(T_{\alpha,\epsilon})}{8\sqrt{d}}\right)^{1/\mu}, \frac{1}{2\sqrt{d}} \mathcal{E}_{\infty}\right\},$$
$$r = \min\left\{\max_{s\in(0,R_0)} \{s \mid \mathcal{E}_s^0 \le \frac{1}{4}q\}, \frac{q}{4}\right\},$$
$$u = \min\left\{\frac{1}{4} \left(\eta \frac{C(T_{\alpha,\epsilon})}{8\sqrt{d}}\right)^{1/\mu}, \frac{q}{4}, \frac{C(T_{\alpha,\epsilon})}{4\sqrt{d}}\right\}.$$

One can verify that this choice of q, r and u will satisfy the assumptions of Proposition 1, i.e., $q + \mathcal{E}_r^{\tilde{u}} - \underline{\mathcal{E}}_{\tilde{u}} < \mathcal{E}_{\infty}$. To see this, firstly, by the choice of q, r, u, for any $\tilde{u} \in [0, u)$:

$$|\underline{\mathcal{E}_{\tilde{u}}}| \leq \tilde{u} < u \leq \frac{1}{4}q$$

and

$$\mathcal{E}_{r}^{\tilde{u}} = \mathcal{E}_{r}^{0} + (\mathcal{E}_{r}^{\tilde{u}} - \mathcal{E}_{r}^{0}) \le \frac{1}{4}q + \max\{\tilde{u}, r\} \le \frac{1}{4}q + \max\{u, r\} \le \frac{1}{4}q + \frac{1}{4}q = \frac{1}{2}q.$$

Here the first inequality is due to the definition of r and Lemma B.1. Thus, one has

$$q + \mathcal{E}_r^{\tilde{u}} - \underline{\mathcal{E}}_{\tilde{u}} \le q + \frac{1}{2}q + \frac{1}{4}q = \frac{7}{4}q \le \frac{7}{8}\mathcal{E}_{\infty} < \mathcal{E}_{\infty}.$$

This verifies the assumptions in Proposition 1.

Next, in Case 3, one has $\mathcal{V}(\rho_{T_{\alpha,\epsilon}}) > \delta$. Thus

$$C(T_{\alpha,\epsilon}) = \min\left\{\frac{\tau}{2} \frac{(2\lambda - \sigma^2)}{\sqrt{2}(\lambda + \sigma^2)}, \sqrt{\tau \frac{(2\lambda - \sigma^2)}{d\sigma^2}}\right\} \sqrt{\mathcal{V}(\rho_{T_{\alpha,\epsilon}})}$$
$$> \min\left\{\frac{\tau}{2} \frac{(2\lambda - \sigma^2)}{\sqrt{2}(\lambda + \sigma^2)}, \sqrt{\tau \frac{(2\lambda - \sigma^2)}{\sigma^2}}\right\} \sqrt{\delta}.$$

The last inequality above, will be utilized later, is Denoted

$$C_{\delta} \coloneqq \min\left\{\frac{\tau}{2} \frac{(2\lambda - \sigma^2)}{\sqrt{2}(\lambda + \sigma^2)}, \sqrt{\tau \frac{(2\lambda - \sigma^2)}{\sigma^2}}\right\} \sqrt{\delta}.$$
(16)

Then one can see that q, r and u are bounded below by

$$\min\left\{\frac{1}{4}\left(\eta\frac{C_{\delta}}{8\sqrt{d}}\right)^{1/\mu}, \frac{1}{2\sqrt{d}}\mathcal{E}_{\infty}\right\}, \quad \min\left\{\max_{s\in(0,R_0)}\{s\mid \mathcal{E}_s^0\leq\frac{1}{4}q(\delta)\}, \frac{q(\delta)}{4}\right\}$$

and

$$\min\left\{\frac{1}{4}\left(\eta\frac{C_{\delta}}{8\sqrt{d}}\right)^{1/\mu}, \frac{q(\delta)}{4}, \frac{C_{\delta}}{4\sqrt{d}}\right\}$$

respectively. We use $q(\delta)$, $r(\delta)$ and $u(\delta)$ to denote them. We now apply Proposition 1 to $\rho_{T_{\alpha,\epsilon}}$ to get

$$\begin{aligned} \|v_{\alpha}(\rho_{T_{\alpha,\epsilon}}) - v^{*}\|_{2} &\leq 2\sqrt{d} \cdot \frac{\left(q + \mathcal{E}_{r}^{0} + \tau_{2}(u) + \tau_{4}(\max\{u, r\})\right)^{\mu}}{\eta} \\ &+ \frac{\sqrt{d}e^{-\alpha\left(q - \tau_{3}(\max\{u, r\})\right)}}{\rho_{T_{\alpha,\epsilon}}\left(B^{\infty}(v^{*}, r)\right)} \int_{\{G \in (0, u)\}} \|v - v_{G(v)}\|_{2} d\rho_{T_{\alpha,\epsilon}}(v) \\ &+ \frac{\sqrt{d}e^{-\alpha\left(q - \tau_{3}(r)\right)}}{\rho_{T_{\alpha,\epsilon}}\left(B^{\infty}(v^{*}, r)\right)} \int_{\{G = 0\}} \|v - v^{*}\|_{2} d\rho_{T_{\alpha,\epsilon}}(v) \\ &+ \sqrt{d}\tau_{1}(u) \\ &+ \int_{\{G(v) \geq u\}} \frac{\|v - v^{*}\|_{2}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{T_{\alpha,\epsilon}})}} e^{-\alpha\mathcal{E}(v)} d\rho_{T_{\alpha,\epsilon}}(v). \end{aligned}$$

Each of the five terms on the right-hand side of the above inequality will be individually bounded.

For the first term, one can use the definition of q, r and u to get

$$2\sqrt{d} \cdot \frac{\left(q + \mathcal{E}_r^0 + \tau_2(u) + \tau_4(\max\{u, r\})\right)^{\mu}}{\eta} \le 2\sqrt{d} \cdot \frac{\left(4 \cdot \frac{1}{4} \cdot \left(\eta \frac{C(T_{\alpha, \epsilon})}{8\sqrt{d}}\right)^{1/\mu}\right)^{\mu}}{\eta} = \frac{C(T_{\alpha, \epsilon})}{4},$$
(17)

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where the inequality above is because each term in the sum on the numerator is bounded above by $\frac{1}{4} \cdot \left(\eta \frac{C(T_{\alpha,\epsilon})}{8\sqrt{d}}\right)^{1/\mu}$ as determined by the choice of q, r and u. For the second term, with the chosen values of u and r, one can first verify

 $q - \tau_3(\max\{u, r\}) = q - \max\{u, r\} \ge q - \frac{q}{4} > \frac{q}{2}.$ (18)

Then

$$\frac{\sqrt{d}e^{-\alpha\left(q-\tau_{3}(\max\{u,r\})\right)}}{\rho_{T_{\alpha,\epsilon}}\left(B^{\infty}(v^{*},r)\right)} \int_{\{G\in(0,u)\}} \|v-v_{G(v)}\|_{2} d\rho_{T_{\alpha,\epsilon}}(v)$$

$$\leq \frac{\sqrt{d}}{\int \phi_{r(\delta)} d\rho_{0}} \cdot e^{a(\delta)T^{*}} \cdot e^{-\alpha q/2} \left(\int_{\{G\in(0,u)\}} \|v-v^{*}\|_{2} + \|v^{*}-v_{G(v)}\|_{2} d\rho_{T_{\alpha,\epsilon}}(v)\right)$$

$$\leq \frac{\sqrt{d}}{\int \phi_{r(\delta)} d\rho_{0}} \cdot e^{a(\delta)T^{*}} \cdot e^{-\alpha q/2} \left(\sqrt{2\mathcal{V}(\rho_{0})} + \int_{\{G\in(0,u)\}} \sqrt{d}\tau_{1}(u) d\rho_{T_{\alpha,\epsilon}}(v)\right)$$

$$\leq \frac{\sqrt{d}}{\int \phi_{r(\delta)} d\rho_{0}} \cdot e^{a(\delta)T^{*}} \cdot e^{-\alpha q/2} \left(\sqrt{2\mathcal{V}(\rho_{0})} + \sqrt{d}\tau_{1}(u)\right)$$

$$\leq \frac{\sqrt{d}}{\int \phi_{r(\delta)} d\rho_{0}} \cdot e^{a(\delta)T^{*}} \cdot e^{-\alpha q/2} \left(\sqrt{2\mathcal{V}(\rho_{0})} + \mathcal{E}_{\infty}\right),$$
(19)

where

$$a(\delta) = 2d \max\left\{\frac{\lambda(\sqrt{cR_0 + C(0)})\sqrt{c}}{(1-c)^2 r(\delta)} + \frac{\sigma^2(cR_0^2 + C(0)^2)(2c+1)}{(1-c)^4 r(\delta)^2}, \frac{2\lambda^2}{(2c-1)\sigma^2}\right\}.$$

In the first inequality above, we used (18), the fact that $T_{\alpha,\epsilon} < T^*$ and Lemma 4.5 with parameter $B = \sup_{t \in [0,T_{\alpha,\epsilon}]} \|v_{\alpha}(\rho_t) - v^*\|_{\infty} \leq \sup_{t \in [0,T_{\alpha,\epsilon}]} \|v_{\alpha}(\rho_t) - v^*\|_2 \leq \sup_{t \in [0,T_{\alpha,\epsilon}]} C(t) \leq C(0)$. In the second inequality above, we used the Cauchy inequality. Assumption 2 (C1) was used to deduce $\|v - v_{G(v)}\|_2 \leq \sqrt{d}\|v - v_{G(v)}\|_{\infty} \leq \sqrt{d}\tau_1(G(v)) \leq \sqrt{d}\tau_1(u)$. In the last inequality above, we used the definition of u to deduce that $u \leq \frac{\mathcal{E}_{\infty}}{\sqrt{d}}$.

For the third term, similarly, one has

$$\frac{\sqrt{d}e^{-\alpha\left(q-\tau_3(r)\right)}}{\rho_{T_{\alpha,\epsilon}}\left(B(v^*,r)\right)} \int_{\{G=0\}} \|v-v^*\|_2 \, d\rho_{T_{\alpha,\epsilon}}(v) \le \frac{\sqrt{d}}{\int \phi_{r(\delta)} \, d\rho_0} \cdot e^{a(\delta)T^*} \cdot e^{-\alpha q/2} \left(\sqrt{2\mathcal{V}(\rho_0)}\right). \tag{20}$$

For the fourth term, one has

$$\sqrt{d\tau_1(u)} = \sqrt{du} \le \frac{C(T_{\alpha,\epsilon})}{4}.$$
(21)

Combining (17, 19, 20, 21), we can get the following estimate:

$$|v_{\alpha}(\rho_{T_{\alpha,\epsilon}}) - v^*||_2 \leq \frac{C(T_{\alpha,\epsilon})}{2} + 2 \cdot \frac{\sqrt{d}}{\int \phi_{r(\delta)} d\rho_0} \cdot e^{a(\delta)T^*} \cdot e^{-\alpha q/2} \left(\sqrt{2\mathcal{V}(\rho_0)} + \mathcal{E}_{\infty}\right) + \int_{\{G(v) \geq u\}} \frac{\|v - v^*\|_2}{\|\omega_{\alpha}\|_{L^1(\rho_{T_{\alpha,\epsilon}})}} e^{-\alpha \mathcal{E}(v)} d\rho_{T_{\alpha,\epsilon}}(v).$$

$$(22)$$

Now we pick α so that

$$2 \cdot \frac{\sqrt{d}}{\int \phi_{r(\delta)} \, d\rho_0} \cdot e^{a(\delta)T^*} \cdot e^{-\alpha q/2} \left(\sqrt{2\mathcal{V}(\rho_0)} + \mathcal{E}_\infty \right) \le \frac{1}{4} C(T_{\alpha,\epsilon}). \tag{23}$$

It turns out that if one picks α to be

$$\alpha(\delta) = \frac{2}{q(\delta)} \log\left(\frac{8\sqrt{d}e^{a(\delta)T^*}\left(\sqrt{2\mathcal{V}(\rho_0) + \mathcal{E}_{\infty}}\right)}{C_{\delta}\int\phi_{r(\delta)}d\rho_0}\right),\tag{24}$$

then

LHS of (23)
$$\leq 2 \cdot \frac{\sqrt{d}}{\int \phi_{r(\delta)} d\rho_0} \cdot e^{a(\delta)T^*} \cdot e^{-\alpha q(\delta)/2} \left(\sqrt{2\mathcal{V}(\rho_0)} + \mathcal{E}_\infty\right) \leq \frac{1}{4}C_\delta \leq \frac{1}{4}C(T_{\alpha,\epsilon}),$$

where in the first and third inequalities, we used the facts that $q \ge q(\delta)$ and $C(T_{\alpha,\epsilon}) > C_{\delta}$. We remark here that $\alpha(\delta)$ is fixed once δ is fixed. With this choice of α , we have

$$\|v_{\alpha}(\rho_{T_{\alpha,\epsilon}}) - v^*\|_2 \le \frac{3}{4}C(T_{\alpha,\epsilon}) + \int_{\{G(v)\ge u\}} \frac{\|v - v^*\|_2}{\|\omega_{\alpha}\|_{L^1(\rho_{T_{\alpha,\epsilon}})}} e^{-\alpha\mathcal{E}(v)} \, d\rho_{T_{\alpha,\epsilon}}(v).$$
(25)

Then we can go back to estimate the last term of (22). We can deduce

$$\int_{\{G(v)\geq u\}} \frac{\|v-v^*\|_2}{\|\omega_{\alpha}\|_{L^1(\rho_{T_{\alpha,\epsilon}})}} e^{-\alpha\mathcal{E}(v)} d\rho_{T_{\alpha,\epsilon}}(v) \leq e^{\alpha(\delta)(\overline{\mathcal{E}}-\underline{\mathcal{E}})} \int_{\{G\geq u\}} \|v-v^*\|_2 d\rho_{T_{\alpha,\epsilon}}(v) \\ \leq e^{\alpha(\delta)(\overline{\mathcal{E}}-\underline{\mathcal{E}})} \sqrt{2\mathcal{V}(\rho_0)} \cdot \sqrt{\rho_{T_{\alpha,\epsilon}}(\{G\geq u\})} \\ \leq e^{\alpha(\delta)(\overline{\mathcal{E}}-\underline{\mathcal{E}})} \sqrt{2\mathcal{V}(\rho_0)} \cdot \frac{1}{\sqrt{u}} \cdot \sqrt{\int G d\rho_{T_{\alpha,\epsilon}}(v)} \\ \leq e^{\alpha(\delta)(\overline{\mathcal{E}}-\underline{\mathcal{E}})} \sqrt{2\mathcal{V}(\rho_0)} \cdot \frac{1}{\sqrt{u(\delta)}} \cdot \sqrt{\int G d\rho_{T_{\alpha,\epsilon}}(v)},$$
(26)

where in the second inequality, we used the Cauchy inequality, in the third inequality, we used the Markov inequality and in the last inequality, we used the fact that $u \ge u(\delta)$. Thus by applying Lemma 4.6 with B = C(0) and $\tilde{B} = \mathcal{V}(\rho_0)$, when ϵ is small enough, the following holds:

$$\int G \, d\rho_{T_{\alpha,\epsilon}}(v) \le \int G \, d\rho_0(v). \tag{27}$$

Thus combining (26) and (27) gives

$$\int_{\{G(v)\geq u\}} \frac{\|v-v^*\|_2}{\|\omega_{\alpha}\|_{L^1(\rho_{T_{\alpha,\epsilon}})}} e^{-\alpha\mathcal{E}(v)} \, d\rho_{T_{\alpha,\epsilon}}(v) \leq e^{\alpha(\delta)(\overline{\mathcal{E}}-\underline{\mathcal{E}})} \sqrt{2\mathcal{V}(\rho_0)} \cdot \frac{1}{\sqrt{u(\delta)}} \cdot \sqrt{\int G \, d\rho_0(v)}.$$
(28)

Now we pick the function I(x) to be

$$\frac{1}{128\mathcal{V}(\rho_0)}C_x^2 e^{-2\alpha(x)(\overline{\mathcal{E}}-\underline{\mathcal{E}})}u^2(x),$$

where C_x and $\alpha(x)$ are defined in (16) and (24) respectively. As long as

$$\int G \, d\rho_0(v) \le I(\delta),\tag{29}$$

combining (28) and (29) yield

$$\int_{\{G(v)\geq u\}} \frac{\|v-v^*\|_2}{\|\omega_\alpha\|_{L^1(\rho_{T_{\alpha,\epsilon}})}} e^{-\alpha\mathcal{E}(v)} d\rho_{T_{\alpha,\epsilon}}(v) \leq e^{\alpha(\delta)(\overline{\mathcal{E}}-\underline{\mathcal{E}})} \sqrt{2\mathcal{V}(\rho_0)} \cdot \frac{1}{\sqrt{u(\delta)}} \cdot \sqrt{\int G d\rho_0(v)} \leq \frac{1}{8} C_\delta \leq \frac{1}{8} C(T_{\alpha,\epsilon}).$$

By plugging the above inequality back to (25), one gets

$$\|v_{\alpha}(\rho_{T_{\alpha,\epsilon}}) - v^*\|_2 \leq \frac{3}{4}C(T_{\alpha,\epsilon}) + \frac{1}{8}C(T_{\alpha,\epsilon}) = \frac{7}{8}C(T_{\alpha,\epsilon}) < C(T_{\alpha,\epsilon}),$$

which contradicts with the assumption $||v_{\alpha}(T_{\alpha,\epsilon}) - v^*||_2 = C(T_{\alpha,\epsilon})$ as stated in Case 3. Therefore, we have demonstrated that under the assumptions of Theorem 4.1, if one selects α to be $\alpha(\delta)$ and chooses ϵ to be sufficiently small, Case 3 will not occur.

Thus we have proved that if all the conditions in Theorem 4.1 are satisfied, the desired decay can be achieved with the specified choices of α and ϵ .

5. Numerical Experiments

In this section, we present the discretized algorithm of the continuous model (3). Throughout this section, we use the anisotropic version (6) as it is more efficient in solving highdimensional optimization problems.

5.1. Algorithm. First, one notices that in the time-continuous model (3), the forcing term $\frac{1}{\epsilon}\nabla G$ needs to be relatively large for the particles to remain near the constraint set. However, a straightforward explicit scheme of the dynamics requires the time step γ to be of the same order as ϵ . This implies that as ϵ approaches zero, the algorithm becomes expensive. On the other hand, making the stiff term $\frac{1}{\epsilon}\nabla G(V_{k+1}^i)$ implicit enhances numerical stability, but it becomes computationally challenging for complex constraints. To address this, we introduce an algorithm with better stability for any equality constraints.

The key idea is to employ Taylor expansion to approximate the term $\nabla G(V_{k+1}^i)$ in the implicit algorithm with its first-order approximation.

$$V_{k+1}^j = V_k^j - \lambda \gamma (V_k^j - v_\alpha(\hat{\rho}_k)) - \left(\frac{\gamma}{\epsilon} \nabla G(V_k^j) + \frac{\gamma}{\epsilon} \nabla^2 G(V_k^j) (V_{k+1}^j - V_k^j)\right) - \sigma \sqrt{\gamma} (V_k^j - \bar{v}_k) \odot z_k,$$

which leads to the following constrained CBO algorithm,

$$V_{k+1}^{j} = V_{k}^{j} - \left[I + \frac{\gamma}{\epsilon} \nabla^{2} G(V_{k}^{j})\right]^{-1} \left(\lambda \gamma (V_{k}^{j} - v_{\alpha}(\hat{\rho}_{k})) + \frac{\gamma}{\epsilon} \sum_{i=1}^{m} g_{i}(V_{k}^{j}) \nabla g_{i}(V_{k}^{j}) + \sigma \sqrt{\gamma} (V_{k}^{j} - \bar{v}_{k}) \odot z_{k}\right),$$
(30)

where $\nabla^2 G(v)$ represents the Hessian of G(v), i.e., $\nabla^2 G(v) = \sum_{i=1}^m (\nabla g_i)^\top \nabla g_i + g_i \nabla^2 g_i$ and γ is the time step, and \odot is a point-wise multiplication, i.e., the i-th component of $x \odot y$ is $x_i y_i$. Here V_k^j approximates the space location of the *j*-th particle at time $t = k\gamma$, and z_k is a *d*-dimensional random variable following a standard normal distribution $\mathcal{N}(0, \mathbb{I}_d)$. During different steps, z_k is sampled independently. The complete algorithm is formulated as in Algorithm 1.

The preliminary results shown in Figure 2 (a) are obtained using the above scheme with $\epsilon = 0.01$ and $\gamma = 0.1$, which demonstrates the stability of the algorithm.

We propose an alternative algorithm when the dimensionality is high, where we introduce independent noise after the particles concentrate. This algorithm introduces additional noises to help the particles explore the landscape better, which is necessary when the dimension of the optimization problem is high. The complete algorithm is formulated as in Algorithm 2.

Algorithm 1 Constrained CBO Algorithm

Initialization: Choose hyperparameters ϵ , α , time step γ , stopping threshold ϵ_{stop} , and sample size N. Sample N particles V^j from distribution $\rho_0(v)$.

1: while
$$\frac{1}{dN} \sum_{j=1}^{N} ||V^{j} - v_{\alpha}(\hat{\rho})||^{2} > \epsilon_{\text{stop}} \text{ do}$$

2: Calculate $v_{\alpha}(\hat{\rho})$:
 $v_{\alpha}(\hat{\rho}) = \frac{1}{Z} \sum_{j=1}^{N} \mu_{j} V^{j}, \text{ with } Z = \sum_{j=1}^{N} e^{-\alpha \mathcal{E}(V^{j})}, \quad \mu_{j} = e^{-\alpha \mathcal{E}(V^{j})}$
3: Update each particle's position $\{V^{j}\}_{j=1}^{N}$:
 $V^{j} \leftarrow V^{j} - \left[I + \frac{\gamma}{\epsilon} \sum_{i=1}^{m} \nabla^{2} \left[g_{i}^{2}(V^{j})\right]\right]^{-1} \left(\lambda \gamma (V^{j} - v_{\alpha}(\hat{\rho})) + \frac{\gamma}{\epsilon} \sum_{i=1}^{m} \nabla \left[g_{i}^{2}(V^{j})\right] + \sigma \sqrt{\gamma} (V^{j} - v_{\alpha}(\hat{\rho})) \odot z\right)$

where $z \sim \mathcal{N}(0, \mathbb{I}_d)$.

- 4: end while
- 5: Output $v_{\alpha}(\hat{\rho}), \mathcal{E}(v_{\alpha}(\hat{\rho}))$

5.2. Numerical examples.

Algorithm 2 Constrained CBO Algorithm with Independent Noise

Initialization: Choose suitable hyper-parameters ϵ, α , and time step γ , stopping threshold $\epsilon_{\text{stop}}, \epsilon_{\text{indep}}$, independent noise σ_{indep} . Sample N particles V^j following distribution $\rho_0(v)$ and set \mathcal{E}^* to be a large constant.

1: while $|\mathcal{E}(v_{\alpha}(\hat{\rho})) - \mathcal{E}^{\star}| \geq \epsilon_{\text{indep}} \operatorname{\mathbf{do}}$

2: while
$$\frac{1}{dN} \sum_{j=1}^{N} \|V^j - v_\alpha(\hat{\rho})\|^2 > \epsilon_{\text{stop}} \operatorname{do}$$

3: Calculate $v_{\alpha}(\hat{\rho})$:

$$v_{\alpha}(\hat{\rho}) = \frac{1}{Z} \sum_{j=1}^{N} \mu_j V^j, \quad \text{with} \quad Z = \sum_{j=1}^{N} e^{-\alpha \mathcal{E}(V^j)}, \quad \mu_j = e^{-\alpha \mathcal{E}(V^j)}$$

4: Update each particle's position $\{V^j\}_{j=1}^N$:

$$V^{j} \leftarrow V^{j} - \left[I + \frac{\gamma}{\epsilon} \sum_{i=1}^{m} \nabla^{2} \left[g_{i}^{2}(V^{j})\right]\right]^{-1} \left(\lambda \gamma (V^{j} - v_{\alpha}(\hat{\rho})) + \frac{\gamma}{\epsilon} \sum_{i=1}^{m} \nabla \left[g_{i}^{2}(V^{j})\right] + \sigma \sqrt{\gamma} (V^{j} - v_{\alpha}(\hat{\rho})) \odot z\right),$$
where $\gamma \in \mathcal{N}(0, \mathbb{T}_{*})$

where $z \sim \mathcal{N}(0, \mathbb{I}_d)$.

- 5: end while
- 6: **if** $\mathcal{E}(v_{\alpha}(\hat{\rho})) < \mathcal{E}^{\star}$ **then**
- 7:

9:

$$\mathcal{E}^{\star} = \mathcal{E}(v_{\alpha}(\hat{\rho})), \quad v_{\alpha}(\hat{\rho})^{\star} = v_{\alpha}(\hat{\rho})$$

8: end if

Each particle does an independent move:

$$V^j \leftarrow V^j + \sigma_{\text{indep}} \sqrt{\gamma} z$$
, for $1 \le j \le N$,

where $z \sim \mathcal{N}(0, \mathbb{I}_d)$. 10: **end while** 11: Output $v_{\alpha}(\hat{\rho})^{\star}, \mathcal{E}^{\star}$.

5.2.1. A simple example. We first test the algorithm on a 2-dimensional example,

$$\min_{(v_1, v_2) \in \mathbb{R}^2} v_1^2 + v_2^2 \tag{31}$$

We test two difference types of constraints. The first case is an ellipse,

$$g(v) = \frac{(v_1 + 1)^2}{2} + v_2^2 - 1 = 0.$$
(32)

The second case is a line,

$$g(v) = v_1 + v_2 - 3 = 0. (33)$$

The exact minimizers are,

Ellipse:
$$v^* = (\sqrt{2} - 1, 0);$$
 Line: $v^* = (3/2, 3/2).$

We use Algorithm 1 with

$$N = 50, \ \alpha = 50, \ \epsilon = 0.01, \ \lambda = 1, \ \sigma = 5, \ \gamma = 0.1, \ \epsilon_{\text{stop}} = 10^{-14},$$

and the particles are initially set to follow a uniform distribution in the range of [-3,3] for both dimensions. We consider our search for the constrained minimizer successful if, when the algorithm finishes, $||v_{\alpha}(\hat{\rho}) - v^*||_{\infty} \leq 0.1$. The success rate and the average distance are shown in Table 1, where the average distance to v^* in the table is measured using the following norm

$$D(v, v^*) = \frac{1}{\sqrt{d}} \|v - v^*\| = \sqrt{\frac{1}{d} \sum_{i=1}^d (v - v^*)_i^2}.$$
(34)

In Figure 4, we show the evolution of the objective function value $\mathcal{E}(v_{\alpha}(\hat{\rho}))$, the constraint value $g(v_{\alpha}(\hat{\rho}))$, and the distance $D(v_{\alpha}(\hat{\rho}), v^*)$ over 100 simulations. It is evident that the consensus point converges within 10 steps for all simulations.

In Figure 5, the evolution of all the particles and the consensus point are shown in time steps k = 0, 5, 50, 100. In all cases, after 5 steps, most of the particles are driven to the constraints by the strong constraint term $\frac{1}{\epsilon}\nabla G(v)$ and stay there consistently. It is worth noting that in the case of the ellipse, not all particles converge around the consensus point. Some particles remain at the point \tilde{v} where $\nabla g(\tilde{v}) = 0$ instead of satisfying g(v) = 0. This happens when $G(v) = g^2(v)$ does not satisfy Assumption 2 (B1). However, it will not affect the convergence of the consensus point as long as the loss function value at \tilde{v} is not significantly small compared to the constrained minimum. (See Remark 3 for more explanation.)

Table 1. The result of Algorithm 1 on (31) with constraints (32) or (33)

	success rate	average distance to v^*
ellipse constraint	100%	0.0147
line constraint	100%	0.0157

5.2.2. Ackley function. We now test the proposed algorithms on a highly non-convex objective function. Consider the following Ackley function,

$$\min_{v} \quad -A \exp\left(-a\sqrt{\frac{b^2}{d} \|v - \hat{v}\|_2^2}\right) - \exp\left(\frac{1}{d}\sum_{i=1}^d \cos(2\pi b(v_i - \hat{v}_i))\right) + e^1 + A, \quad (35)$$

where b = 1, A = 20, a = 0.1, and \hat{v} is the global minimum of the unconstrained problem. The above function in two-dimension is shown in Figure 1. Here we consider three different

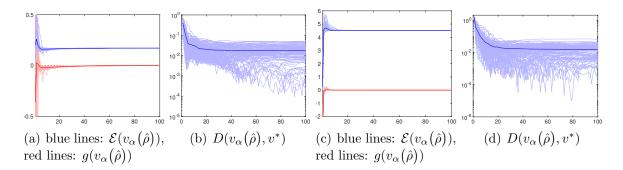


Figure 4. The first line is the result for the optimization problem (31) with ellipse constraint (32), while the second line is for the line constraint (33). The left column is the evolution of the objective function value and constraint value, while the right column is the evolution of the distance between the consensus point and the exact minimizer, where the distance is defined in (34). The light lines are results from 100 simulations, while the dark lines are the average values.

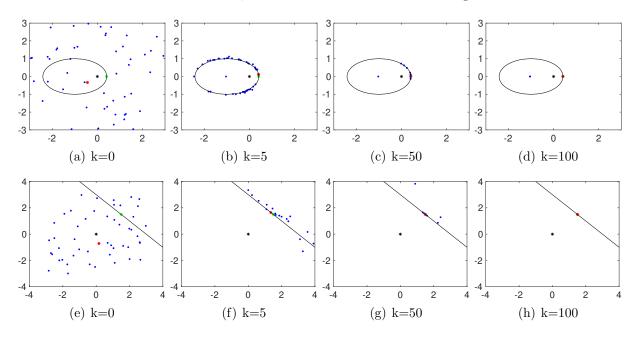


Figure 5. The evolution of all the particles (in blue) and its consensus point (in red) in 2-dimensional plane when solving for the constrained problem (31) with the ellipse constraint (32) (the first line) and the line constraint (33) (the second line). The constrained line is plotted in black, the black point is the global minimizer of the objective function, while the green point is the constrained minimizer v^* .

constraints,

Case 1.
$$||v||_2^2 - 1 = 0.$$
 (36)

Case 2.
$$\sum_{i=1}^{d-1} v_i^2 - v_d = 0.$$
 (37)

Case 3.
$$\sum_{i=1}^{d} v_i - 1 = 0, \quad 2\sum_{i=1}^{d-1} v_i - \frac{1}{2}v_d - \frac{1}{2} = 0.$$
 (38)

We set $\hat{v} = (0.4, \dots, 0.4)$, s.t. the unconstrained minimizer is not the same as the constrained minimizer. The constrained minimizers for the three-dimensional cases are

Case 1.
$$v^* = 1/\sqrt{3(1,1,1)}$$
; Case 2. $v^* = (0.4283, 0.4283, 0.3669)$; Case 3. $v^* = (0.2, 0.2, 0.6)$

The constrained minimizers for the 20-dimensional case are

Case 1.
$$v_i^* = 1/\sqrt{20}, \ 1 \le i \le 20;$$
 Case 2. $v_i^* = 0.3542, \ 1 \le i \le 19, \ v_{20}^* = 2.3839$

For the 3-dimensional Ackley function, we use Algorithm 1 with

$$N = 100, \ \alpha = 50, \ \epsilon = 0.01, \ \lambda = 1, \ \sigma = 1, \ \gamma = 0.1, \ \epsilon_{\text{stop}} = 10^{-14}.$$

For the 20-dimensional Ackley function, we use Algorithm 2 with

$$N = 100, \ \alpha = 50, \ \epsilon = 0.01, \ \lambda = 1, \ \sigma = 1, \ \gamma = 0.1, \ \epsilon_{\text{indep}} = 10^{-5},$$

Case 1. & Case 3. $\epsilon_{\text{min}} = 0.01, \ \sigma_{\text{indep}} = 0.3;$
Case 2. $\epsilon_{\text{indep}} = 0.001, \ \sigma_{\text{indep}} = 1;$

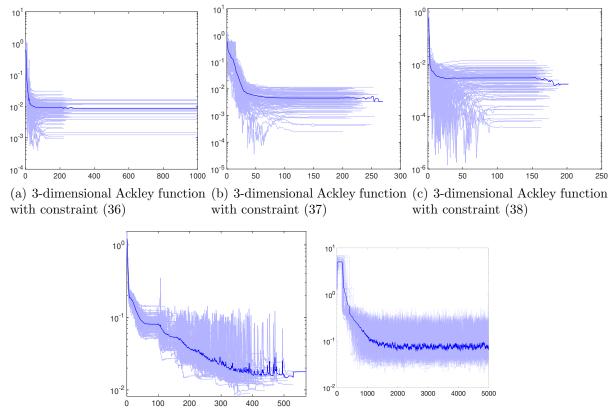
and all the particles initially follow $V^j \sim \text{Unif}[-3,3]^d$.

The evolution of the distance $D(v_{\alpha}(\hat{\rho}), v^*)$ between the consensus point and the accurate solution is shown in Figure 6, where one can see that the consensus point converges to the true minimizer within 100 steps. Besides, The success rate, averaged distance for the output consensus point v^* , and the averaged total steps are stated in Table 2. We consider the simulation to be successful if $\max_k |v_{\alpha}(\hat{\rho})_k - v_k^*| \leq 0.1$, and the distance to v^* is measured in $D(v_{\alpha}(\hat{\rho}), v^*)$ and averaged over 100 simulations. One can see that except for the 20-dimensional case 2, the algorithm can find the exact minimizer within 400 steps with 100% success rate. Even for the 20-dimensional case 2, although the success rate is a bit less than 100%, the average distance to v^* is less than 0.05, which means that they are all relatively close to the exact minimizer v^* .

The reason for the nonsmoothness in the later stage of the average line is due to the limited number of samples for the larger steps. In most simulations, the algorithm typically concludes its iterations around the average total steps in the table. As it is hard to find the exact minimizer for 20-dimensional Ackley function with the constraints (38), so we only plot the result for case 3 in 3-dimension.

Table 2. The result of Algorithm 1 on 3-dimensional Ackley function and Algorithm 2 for 20-dimensional Ackley function.

		success rate	average distance to v^*	average total steps
case 1	d=3	100%	8×10^{-3}	295
	d=20	100%	1.56×10^{-2}	390
case 2	d=3	100%	4.5×10^{-3}	213
	d=20	96%	3.13×10^{-2}	4288
case 3	d=3	100%	2.8×10^{-3}	163



(d) 20-dimensional Ackley func- (e) 20-dimensional Ackley function with constraint (36) tion with constraint (37)

Figure 6. The evolution of the distance $D(v_{\alpha}(\hat{\rho}), v^*)$ between the consensus point and the exact minimizer. The light lines are the results from 100 simulations, while the dark lines are the average values.

5.2.3. Thomson's Problem. The Thomson problem involves determining the positions for k electrons on a sphere in a way that minimizes the electrostatic interaction energy between each pair of electrons with equal charges. The associated constrained optimization problem

is formulated as follows,

min
$$\mathcal{E}(v_1, ..., v_k) = \frac{1}{k} \sum_{i < j} \frac{1}{\|v_i - v_j\|_2}$$

s.t. $\|v_i\|_2^2 - 1 = 0$, for $i = 1, \cdots, k$.

We use Algorithm 2 with

 $N = 50, \ \alpha = 50, \ \epsilon = 0.01, \ \lambda = \sigma = 1, \ \gamma = 0.1, \ \epsilon_{\text{indep}} = 10^{-14}, \ \epsilon_{\text{min}} = 0.01, \ \sigma_{\text{indep}} = 0.3,$

and all the particle initially follow $V^j \sim \text{Unif}[-1, 1]^{3k}$.

We run the above algorithm for k = 2, 3, 8, 15, 56, 470, which is equivalent to conducting a 3k-dimensional optimization problem with k constraints. The success rate, averaged relative error, averaged constraints value (value of $\sum_{i=1}^{m} g_i(v_{\alpha}(\hat{\rho}))$) and averaged total steps are summarized in Table 3. We define

relative error =
$$\frac{|\mathcal{E}(v_{\alpha}(\hat{\rho})) - \mathcal{E}(v^*)|}{\mathcal{E}(v^*)}$$
(39)

and consider a simulation to be successful if both inequalities are satisfied for the output $v_{\alpha}(\hat{\rho})$,

relative error
$$\leq 0.05$$
, $\sum_{i=1}^{k} (|\|v_i\|_2^2 - 1|) \leq 10^{-3}$.

In Figure 7, the evolution of the relative error across 100 simulations and their average values are depicted, illustrating that all experiments converge to the optimal minimizer within 2000 steps. The nonsmoothness of the average lines is due to the fewer samples in large steps. For k = 56,470, corresponding to an optimization problem of dimensions 168 and 1410 with 56,470 constraints, the success rate is not 100%. However, it remains above 90%. Besides, the relative error and constraints value in the third and fourth columns of Table 3 are over the success simulations, which are very small. This verifies our algorithm has an excellent performance in high dimensions.

Table 3. The result of Algorithm 2 on Thomson problem.

	success rate	relative error	constraints value	total steps
k = 2, (d = 6)	100%	4.4×10^{-3}	3.8×10^{-11}	382
k = 3, (d = 9)	100%	9.9×10^{-3}	1.4×10^{-10}	407
k = 8, (d = 24)	100%	1.78×10^{-2}	2.3×10^{-10}	567
k = 15, (d = 45)	100%	1.57×10^{-2}	3.4×10^{-10}	895
k = 56, (d = 168)	97%	1.44×10^{-2}	2.91×10^{-6}	1610
k = 470, (d = 1410)	93%	1.95×10^{-2}	4.03×10^{-6}	1960

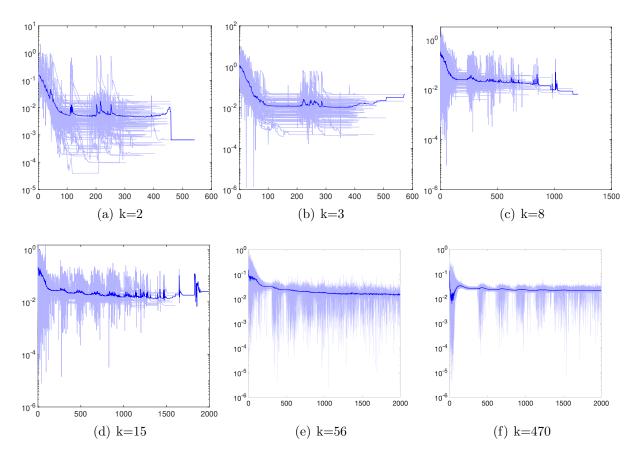


Figure 7. Thomson Problem: the decay of the relative error over 100 simulation and its mean.

6. Conclusions

In this paper, we propose a new CBO-based method for solving constrained non-convex minimization problem with equality constraints and potentially non-differentiable loss functions. Specifically, we augment the original CBO framework with a new forcing term designed to guide particles toward the constraint set. On the theoretical side, we conduct a rigorous analysis of the mean-field limit for the proposed model (7), deriving the corresponding macroscopic model (8) and establishing well-posedness results for both the microscopic and macroscopic models. To demonstrate the convergence of the method, we study the long-time behavior of the macroscopic model (8) through an analysis of the associated Fokker-Planck equation (9). Our results establish that, under Assumption 2 and with a proper choice of parameters, particles converge to the constrained minimizer v^* with arbitrary closeness. Notably, Assumption 2 (C) fits well with the basic nature of the algorithm, while Assumption 2 (B) serves as a technical requirement needed by our proof technique, which might be relaxed further with an alternative proof technique, as suggested by the performance exhibited in numerical experiments where Assumption 2 (B) may not be strictly satisfied. On the practical side, we proposed a stable algorithm based the continuous-in-time model. In Section 5, the algorithm's performance is illustrated through a series of experiments, including challenging high-dimensional problems.

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Appendix A. Some details in the Proofs of Well-posedness and Mean-field limit

A.1. **Proof of Theorem 3.1.** Consider the microscopic model, which is governed by the following equation:

$$dV_t^{i,N} = -\lambda \left(V_t^{i,N} - v_\alpha(\hat{\rho}_t^N) \right) dt - \frac{1}{\epsilon} \nabla G \left(V_t^{i,N} \right) dt + \sigma \operatorname{diag} \left(V_t^{i,N} - v_\alpha(\hat{\rho}_t^N) \right) dB_t^{i,N},$$
$$V_0^{i,N} \sim \rho_0,$$

where i = 1, ..., N. We can concantenate $\left\{V_t^{i,N}\right\}_{i=1}^N$ into one vector and put them in one equation. To be specific, we define

$$V_t = \left(\left(V_t^{1,N} \right)^T, ..., \left(V_t^{N,N} \right)^T \right)^T$$

Then V_t is a vector in \mathbb{R}^{Nd} for each fixed t and it will satisfy the following equation:

$$dV_t = -\lambda F_N(V_t) dt - \frac{1}{\epsilon} L_N(V_t) dt + \sigma M_N(V_t) dB_t^{(N)}.$$
(40)

Here $B^{(N)}$ is the standard Wiener process in \mathbb{R}^{Nd} ,

$$L_N(V_t) = \left(\left(\nabla G(V_t^{1,N}) \right)^T, ..., \left(\nabla G(V_t^{N,N}) \right)^T \right)^T \in \mathbb{R}^{Nd},$$
$$M_N(V_t) = \operatorname{diag}\left(F_N^1(V_t), ..., F_N^N(V_t) \right) \in \mathbb{R}^{Nd \times Nd}$$

and

$$F_N(V_t) = \left(\left(F_N^1(V_t) \right)^T, ..., \left(F_N^N(V_t) \right)^T \right)^T \in \mathbb{R}^{Nd},$$

where

$$F_N^i(V_t) = \frac{\sum_{j \neq i} \left(V_t^{i,N} - V_t^{j,N} \right) \omega_\alpha(V_t^{j,N})}{\sum_j \omega_\alpha(V_t^{j,N})} \in \mathbb{R}^d.$$

Thus it suffices to prove the well-posedness result of equation (40), which is the following theorem.

Theorem A.1. For each $n \in \mathbb{N}$, the stochastic differential equation (40) has a unique strong solution $\{V_t | t \ge 0\}$ for any initial condition V_0 satisfying $\mathbb{E}[\|V_0\|^2] < \infty$.

Proof. Following the same steps in Theorem 2.1 [5], we obtain

$$-2\lambda V \cdot F_N(V) \le 2\lambda \sqrt{N} ||V||^2$$
, and $\operatorname{trace}(M_N M_N^T)(V) = ||F_N(V)||^2 \le 4N ||V||^2$.

Thus

$$-2\lambda V \cdot F_N(V) + \sigma^2 \operatorname{trace}(M_N M_N^T)(V) \le b_N \|V\|^2,$$

where b_N is a positive number that depends only on λ, σ, d and N. Also, we notice that for $X \in \mathbb{R}^d$

$$-\frac{2}{\epsilon}X\cdot\nabla G(X) \leq \frac{2}{\epsilon}\|X\|\cdot\|\nabla G(X)\| \leq \frac{2}{\epsilon}\|X\|\cdot\|X\| = \frac{2}{\epsilon}\|X\|^2,$$

where we used Assumption 1 (4). Thus,

$$-\frac{2}{\epsilon}V \cdot L_N(V) \le \frac{2}{\epsilon} \left\|V\right\|^2.$$

This implies that

$$2V \cdot \left(-\lambda F_N(V) - \frac{1}{\epsilon}L_N(V)\right) + \sigma^2 \operatorname{trace}(M_N M_N^T)(V) \le \tilde{b}_N \|V\|^2,$$

where \tilde{b}_N is some positive number that depends only on $\lambda, \sigma, d, \epsilon$ and N. Then we apply Theorem 3.1 in [11] to finish the proof.

A.2. Proof of Theorem 3.3. Below is Lemma 3.2 from [5]

Lemma A.2. Let \mathcal{E} satisfy Assumption 1 and $\mu, \hat{\mu} \in \mathcal{P}_2(\mathbb{R}^d)$ with

$$\int \left\| v \right\|^4 d\mu, \int \left\| \hat{v} \right\| d\hat{\mu} \le K.$$

Then the following stability estimate holds

$$\left\| v_{\alpha}(\mu) - v_{\alpha}(\hat{\mu}) \right\| \le c_0 W_2(\mu, \hat{\mu}),$$

for a constant $c_0 > 0$ depending only on α , L and K, where $W_2(\mu, \hat{\mu})$ is the Wasserstein 2-distance between μ and $\hat{\mu}$.

Also, we recall Theorem 11.3 in [19].

Theorem A.3. Let T be a compact mapping of a Banach space \mathcal{B} into itself, and suppose there exists a constant M such that

 $\|x\|_{\mathcal{B}} < M$

for all $x \in \mathcal{B}$ and $\sigma \in [0, 1]$ satisfying $x = \sigma T x$. Then T has a fixed point.

Proof of Theorem 3.3. Step 1 (construct a map T): Let us fix $u_t \in C[0, T]$. By Theorem 6.2.2 in [1], there is a unique solution to

$$dV_t = -\lambda(V_t - u_t) dt - \frac{1}{\epsilon} \nabla G dt + \sigma \operatorname{diag}(V_t - u_t) dB_t,$$

$$V_0 \sim \rho_0,$$
(41)

We use ρ_t to denote the corresponding law of the unique solution. Using ρ_t , one can compute $v_{\alpha}(\rho_t)$, which is uniquely determined by u_t and is in $\mathcal{C}[0,T]$. Thus one can construct a map from $\mathcal{C}[0,T]$ to $\mathcal{C}[0,T]$ which maps u_t to $v_{\alpha}(\rho_t)$. Step 2 (*T* is compact):

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Firstly, by referencing Chapter 7 in [1], we obtain the following inequality for the solution V_t to equation (41):

$$\mathbb{E}\left[\left\|V_{t}\right\|\right]^{4} \leq \left(1 + \mathbb{E}\left[\left\|V_{0}\right\|\right]^{4}\right)e^{ct}$$

where c > 0. Thus one can deduce

$$\mathbb{E}[\|V_t\|^4] \lesssim 1 \text{ and } \mathbb{E}[\|V_t\|^2] \lesssim 1.$$
(42)

Now it suffices to prove that ImT is in $\mathcal{C}^{1/2}[0,T]$, which is compactly embedded into $\mathcal{C}[0,T]$.

By Lemma A.2, one obtains

$$\left\| v_{\alpha}(\rho_t) - v_{\alpha}(\rho_s) \right\| \le c_0 W_2(\rho_t, \rho_s).$$
(43)

For $W_2(\rho_t, \rho_s)$, it holds that

$$W_2^2(\rho_t, \rho_s) \le \mathbb{E}[||V_t - V_s||^2].$$
 (44)

Further we can deduce

$$V_t - V_s = \int_s^t -\lambda(V_\tau - u_\tau) - \frac{1}{\epsilon} \nabla G(V_\tau) \, d\tau + \sigma \int_s^t \operatorname{diag}(V_\tau - u_\tau) \, dB_\tau.$$

Thus

$$\mathbb{E}\left[\left\|V_{t}-V_{s}\right\|^{2}\right] \lesssim \mathbb{E}\left[\left\|\int_{s}^{t} \left(V_{\tau}-u_{\tau}\right) d\tau\right\|^{2}\right] + \mathbb{E}\left[\left\|\int_{s}^{t} \nabla G(V_{\tau}) d\tau\right\|^{2}\right] + \mathbb{E}\left[\left\|\int_{s}^{t} \operatorname{diag}\left(V_{\tau}-u_{\tau}\right) dB_{\tau}\right\|^{2}\right].$$
(45)

Now we bound from above the three terms on the right hand side respectively. For the first term, we have

$$\mathbb{E}\left[\left\|\int_{s}^{t} (V_{\tau} - u_{\tau}) d\tau\right\|^{2}\right] \leq \mathbb{E}\left[\left(\int_{s}^{t} \left\|V_{\tau} - u_{\tau}\right\| d\tau\right)^{2}\right] \\
\leq |t - s| \mathbb{E}\left[\int_{s}^{t} \left\|V_{\tau} - u_{\tau}\right\|^{2} d\tau\right] \\
\lesssim |t - s| \left(\int_{s}^{t} \mathbb{E}\left[\left\|V_{\tau}\right\|^{2}\right] d\tau + \int_{s}^{t} \left\|u_{\tau}\right\|^{2} d\tau\right) \lesssim |t - s|,$$
(46)

where in the second inequality we used Cauchy's inequality and in the last inequality, we used (42) and the fact that u_t is continuous thus bounded in [0, T].

For the second term, we have

$$\mathbb{E}\left[\left\|\int_{s}^{t} \nabla G(V_{\tau}) d\tau\right\|^{2}\right] \leq \mathbb{E}\left[\left(\int_{s}^{t} \left\|\nabla G(V_{\tau})\right\| d\tau\right)^{2}\right]$$

$$\leq \mathbb{E}\left[\left(\int_{s}^{t} \left\|V_{\tau}\right\| d\tau\right)^{2}\right]$$

$$\leq |t-s|\mathbb{E}\left[\int_{s}^{t} \left\|V_{\tau}\right\|^{2} d\tau\right] \lesssim |t-s|,$$
(47)

where in the second inequality, we used Assumption 1 (4) and in the last inequality, we used (42).

For the third term in (45), we have the following estimation:

$$\mathbb{E}\left[\left\|\int_{s}^{t} \operatorname{diag}(V_{\tau}-u_{\tau}) dB_{\tau}\right\|^{2}\right] = \mathbb{E}\left[\int_{s}^{t} \left\|\operatorname{diag}(V_{\tau}-u_{\tau})\right\|_{F}^{2} d\tau\right] \\
\leq |t-s|\mathbb{E}\left[\int_{s}^{t} \left\|V_{\tau}-u_{\tau}\right\|^{4} d\tau\right] \\
\lesssim |t-s|(\mathbb{E}\left[\int_{s}^{t} \left\|V_{\tau}\right\|^{4} d\tau\right] + \int_{s}^{t} \left\|u_{\tau}\right\|^{4} d\tau) \lesssim |t-s|,$$
(48)

where the first equality comes from Itô's Isometry, while in the first inequality, we used Cauchy's inequality and in the last inequality, we used (42) and the fact that u_t is bounded.

Finally, we combine (43), (44), (45), (46), (47) and (48) to deduce

$$\left\| v_{\alpha}(\rho_t) - v_{\alpha}(\rho_s) \right\| \lesssim |t-s|^{1/2},$$

which implies that $v_{\alpha}(\rho_t) \in \mathcal{C}^{0,1/2}[0,T]$. Thus, T is compact. Step 3 (Existence):

We make use of Theorem A.3. Let us take u_t satisfying $u_t = \theta T u_t$ for $\theta \in [0, 1]$. We now try to prove $||u_t||_{\infty} \leq q$ for some finite q > 0. First, one has

$$\left\|u_{t}\right\|^{2} = \theta^{2} \left\|v_{\alpha}\left(\rho_{t}\right)\right\|^{2} \leq \theta^{2} e^{\alpha(\overline{\mathcal{E}}-\underline{\mathcal{E}})} \int \left\|v\right\|^{2} d\rho_{t}.$$
(49)

Then, to bound u_t , we try to bound $\int ||v||^2 d\rho_t$. Since ρ_t is a weak solution to the corresponding Fokker-Planck equation (9), one has

$$\frac{d}{dt} \int \left\| v \right\|^2 d\rho_t = \int \sigma^2 \left\| v - u_t \right\|^2 - 2\lambda(v - u_t) \cdot v - \frac{2}{\epsilon} \nabla G(v) \cdot v \, d\rho_t$$
$$= \int (\sigma^2 - 2\lambda) \left\| v \right\|^2 + 2(\lambda - \sigma^2) v \cdot u_t + d\sigma^2 \left\| u_t \right\|^2 - \frac{2}{\epsilon} \nabla G(v) \cdot v \, d\rho_t.$$

Since

$$\int v \cdot u_t \, d\rho_t \le \int \|v\| \cdot \|u_t\| \, d\rho_t \lesssim \int \|v\|^2 \, d\rho_t + \int \|u_t\|^2 \, d\rho_t = \int \|v\|^2 \, d\rho_t + \|u_t\|^2$$

and

$$\left\|\nabla G(v)\right\| \lesssim \|v\|,$$

one can further deduce

$$\frac{d}{dt} \int \left\| v \right\|^2 d\rho_t \lesssim \int \left\| v \right\|^2 d\rho_t + \left\| u_t \right\|^2 \lesssim \int \left\| v \right\|^2 d\rho_t$$

where in the last inequality, we used (49). Applying Gronwall's inequality yields that $\int \|v\|^2 d\rho_t$ is bounded and from the above inequality, the bound does not depend on u_t itself. Thus we' have shown that $\|u_t\|_{\infty}$ is bounded by a uniform constant q. Theorem A.3 then gives the existence.

Step 4 (Uniqueness):

Suppose we are given two fixed points of T: u_t and \hat{u}_t . We use V_t and \hat{V}_t respectively to represent the solutions of equation (41) with u_t and \hat{u}_t plugged in. We also assume that V_t and \hat{V}_t are defined in the same probability space. From the steps above, there exist constants q > 0 and K > 0 such that

$$\left\| u_t \right\|_{\infty}, \left\| \hat{u}_t \right\|_{\infty} < q \tag{50}$$

and

$$\sup_{t \in [0,T]} \int \|v\|^4 \, d\rho_t, \sup_{t \in [0,T]} \int \|v\|^4 \, d\hat{\rho}_t < K,\tag{51}$$

where ρ_t and $\hat{\rho}_t$ are the distributions of V_t and \hat{V}_t respectively. Let us consider $Z_t = V_t - \hat{V}_t$. One has

$$Z_t = Z_0 - \lambda \int_0^t Z_\tau \, d\tau + \lambda \int_0^t (u_\tau - \hat{u}_\tau) \, d\tau - \frac{1}{\epsilon} \int_0^t \left(\nabla G(V_\tau) - \nabla G(\hat{V}_\tau) \right) \, d\tau \\ + \sigma \int_0^t \operatorname{diag} \left(\left(V_\tau - u_\tau \right) - \left(\hat{V}_\tau - \hat{u}_\tau \right) \right) \, dB_\tau.$$

Thus

$$\mathbb{E}\left[\left\|Z_{t}\right\|^{2}\right] \\
\lesssim \mathbb{E}\left[\left\|Z_{0}\right\|^{2}\right] + \mathbb{E}\left[\left(\int_{0}^{t}\left\|Z_{\tau}\right\| d\tau\right)^{2}\right] + \mathbb{E}\left[\left(\int_{0}^{t}\left\|u_{\tau} - \hat{u}_{\tau}\right\| d\tau\right)^{2}\right] \\
+ \mathbb{E}\left[\left(\int_{0}^{t}\left\|\nabla G(V_{\tau}) - \nabla G(\hat{V}_{\tau})\right\| d\tau\right)^{2}\right] \mathbb{E}\left[\left\|\int_{0}^{t} \operatorname{diag}\left(\left(V_{\tau} - u_{\tau}\right) - \left(\hat{V}_{\tau} - \hat{u}_{\tau}\right)\right) dB_{\tau}\right\|^{2}\right].$$
(52)

For $\mathbb{E}[(\int_0^t || Z_\tau || d\tau)^2]$, we have that

$$\mathbb{E}\left[\left(\int_{0}^{t} \left\|u_{\tau} - \hat{u}_{\tau}\right\| d\tau\right)^{2}\right] = \mathbb{E}\left[\left(\int_{0}^{t} \left\|v_{\alpha}(\rho_{\tau}) - v_{\alpha}(\hat{\rho}_{\tau})\right\| d\tau\right)^{2}\right] \le t\mathbb{E}\left[\int_{0}^{t} \left\|v_{\alpha}(\rho_{\tau}) - v_{\alpha}(\hat{\rho}_{\tau})\right\|^{2} d\tau\right],\tag{53}$$

where in the inequality, we used the fact that u_t and \hat{u}_t are fixed points. For $\mathbb{E}[(\int_0^t \|\nabla G(V_\tau) - \nabla G(\hat{V}_\tau)\| d\tau)^2]$, one has

$$\mathbb{E}\left[\left(\int_{0}^{t} \left\|\nabla G(V_{\tau}) - \nabla G(\hat{V}_{\tau})\right\| d\tau\right)^{2}\right] \lesssim \mathbb{E}\left[\left(\int_{0}^{t} \left\|V_{\tau} - \hat{V}_{\tau}\right\| d\tau\right)^{2}\right] \\
= \mathbb{E}\left[\left(\int_{0}^{t} \left\|Z_{\tau}\right\| d\tau\right)^{2}\right] \leq t \cdot \mathbb{E}\left[\int_{0}^{t} \left\|Z_{\tau}\right\|^{2} d\tau\right].$$
(54)

Here we used the Lipschitz property of ∇G . For $\mathbb{E}[\|\int_0^t \operatorname{diag}\left((V_{\tau}-u_{\tau})-(\hat{V}_{\tau}-\hat{u}_{\tau})\right) dB_{\tau}\|^2]$. Then

$$\mathbb{E}\left[\left\|\int_{0}^{t} \operatorname{diag}\left(\left(V_{\tau}-u_{\tau}\right)-\left(\hat{V}_{\tau}-\hat{u}_{\tau}\right)\right) dB_{\tau}\right\|^{2}\right] \\
=\mathbb{E}\left[\int_{0}^{t}\left\|\operatorname{diag}\left(\left(V_{\tau}-u_{\tau}\right)-\left(\hat{V}_{\tau}-\hat{u}_{\tau}\right)\right)\right\|_{F}^{2} d\tau\right] \\
\lesssim \mathbb{E}\left[\int_{0}^{t}\left\|V_{\tau}-\hat{V}_{\tau}\right\|^{2} d\tau\right] + \mathbb{E}\left[\int_{0}^{t}\left\|u_{\tau}-\hat{u}_{\tau}\right\|^{2} d\tau\right] \\
=\mathbb{E}\left[\int_{0}^{t}\left\|Z_{\tau}\right\|^{2} d\tau\right] + \mathbb{E}\left[\int_{0}^{t}\left\|v_{\alpha}(\rho_{\tau})-v_{\alpha}(\hat{\rho}_{\tau})\right\|^{2} d\tau\right],$$
(55)

where in the first equality, we used Itô's Isometry. Thus combining (52), (53), (54) and (55) yield

$$\mathbb{E}\left[\left\|Z_{t}\right\|^{2}\right] \lesssim \mathbb{E}\left[\left\|Z_{0}\right\|^{2}\right] + \int_{0}^{t} \mathbb{E}\left[\left\|Z_{\tau}\right\|^{2}\right] d\tau + \mathbb{E}\left[\int_{0}^{t}\left\|v_{\alpha}(\rho_{\tau}) - v_{\alpha}(\hat{\rho}_{\tau})\right\|^{2} d\tau\right]$$

We further notice that by Lemma A.2,

$$\left\| v_{\alpha}(\rho_{\tau}) - v_{\alpha}(\hat{\rho}_{\tau}) \right\| \lesssim W_{2}(\rho_{\tau}, \hat{\rho}_{\tau}) \leq \sqrt{\mathbb{E}\left[\left\| V_{\tau} - \hat{V}_{\tau} \right\|^{2} \right]} = \sqrt{\mathbb{E}\left[\left\| Z_{\tau} \right\|^{2} \right]}.$$

So we can deduce

$$\mathbb{E}\left[\left\|Z_{t}\right\|^{2}\right] \lesssim \mathbb{E}\left[\left\|Z_{0}\right\|^{2}\right] + \int_{0}^{t} \mathbb{E}\left[\left\|Z_{\tau}\right\|^{2}\right] d\tau + \mathbb{E}\left[\int_{0}^{t} \mathbb{E}\left[\left\|Z_{\tau}\right\|^{2}\right] d\tau\right]$$
$$\lesssim \mathbb{E}\left[\left\|Z_{0}\right\|^{2}\right] + \int_{0}^{t} \mathbb{E}\left[\left\|Z_{\tau}\right\|^{2}\right] d\tau.$$

Then applying Gronwall's inequality with the fact that $\mathbb{E}[||Z_0||^2] = 0$ gives the uniqueness result.

A.3. Proof of Theorem 3.4. We first prove the following lemma.

Lemma A.4. Let \mathcal{E} satisfy Assumption 1 and $\rho_0 \in \mathcal{P}_4(\mathbb{R}^d)$. For any $N \geq 2$, assume that $\{(V_t^{i,N})_{t\in[0,T]}\}_{i=1}^N$ is the unique solution to the particle system (7) with $\rho_0^{\otimes N}$ distributed initial data $\{V_0^{i,N}\}_{i=1}^N$. Then there exists a constant K > 0 independent of N such that

$$\sup_{i=1,\dots,N} \left\{ \sup_{t \in [0,T]} \mathbb{E} \Big[\left\| V_t^{i,N} \right\|^2 + \left\| V_t^{i,N} \right\|^4 \Big] + \sup_{t \in [0,T]} \mathbb{E} \Big[\left\| v_\alpha(\hat{\rho}_t^N) \right\|^2 + \left\| v_\alpha(\hat{\rho}_t^N) \right\|^4 \Big] \right\} \le K.$$

Proof. For each i, we have

$$dV_t^{i,N} = -\lambda \left(V_t^{i,N} - v_\alpha(\hat{\rho}_t) \right) dt - \frac{1}{\epsilon} \nabla G(V_t^i) dt + \sigma \operatorname{diag} \left(V_t^{i,N} - v_\alpha(\hat{\rho}_t^i) \right) dB_t^i,$$
$$V_0^i \sim \rho_0.$$

Now we pick p = 1 or p = 2. Then

$$\mathbb{E} \|V_{t}^{i,N}\|^{2p} \lesssim \mathbb{E} \|V_{0}^{i,N}\|^{2p} + \mathbb{E} (\int_{0}^{t} \|V_{\tau}^{i,N}\| d\tau)^{2p} + \mathbb{E} (\int_{0}^{t} \|v_{\alpha}(\hat{\rho}_{\tau}^{N})\| d\tau)^{2p} + \mathbb{E} \|\int_{0}^{t} \operatorname{diag} (V_{\tau}^{i,N}) dB_{\tau}^{i}\|^{2p} + \mathbb{E} \|\int_{0}^{t} \operatorname{diag} (v_{\alpha}(\hat{\rho}_{\tau}^{N})) dB_{\tau}^{i}\|^{2p}.$$

Here, we used Assumption 1 (4). Now by Cauchy's inequality,

$$\mathbb{E}\left(\int_0^t \left\|V_{\tau}^{i,N}\right\| d\tau\right)^{2p} \le t^p \cdot \mathbb{E}\left(\int_0^t \left\|V_{\tau}^{i,N}\right\|^2 d\tau\right)^p$$

and

$$\mathbb{E}\left(\int_0^t \left\| v_\alpha(\hat{\rho}_\tau^N) \right\| d\tau\right)^{2p} \le t^p \cdot \mathbb{E}\left(\int_0^t \left\| v_\alpha(\hat{\rho}_\tau^N) \right\|^2 d\tau\right)^p.$$

Also, by Itô Isometry,

$$\mathbb{E} \left\| \int_0^t \operatorname{diag}(V_{\tau}^{i,N}) \, dB_{\tau}^i \right\|^{2p} = \mathbb{E} \left(\int_0^t \left\| V_{\tau}^{i,N} \right\|^2 d\tau \right)^p$$

and

$$\mathbb{E} \Big\| \int_0^t \operatorname{diag} \left(v_\alpha(\hat{\rho}_\tau^N) \right) dB_\tau^i \Big\|^{2p} = \mathbb{E} \left(\int_0^t \left\| v_\alpha(\hat{\rho}_\tau^N) \right\|^2 d\tau \right)^p.$$

Thus

$$\mathbb{E} \left\| V_t^{i,N} \right\|^{2p} \lesssim \mathbb{E} \left\| V_0^{i,N} \right\|^{2p} + \mathbb{E} \left(\int_0^t \left\| V_\tau^{i,N} \right\|^2 d\tau \right)^p + \mathbb{E} \left(\int_0^t \left\| v_\alpha \left(\hat{\rho}_\tau^N \right) \right\|^2 d\tau \right)^p.$$

Further, by Hölder inequality,

$$\mathbb{E}\left(\int_{0}^{t} \left\|V_{\tau}^{i,N}\right\|^{2} d\tau\right)^{p} \leq \mathbb{E}\int_{0}^{t} \left\|V_{\tau}^{i,N}\right\|^{2p} d\tau \text{ and } \mathbb{E}\left(\int_{0}^{t} \left\|v_{\alpha}\left(\hat{\rho}_{\tau}^{N}\right)\right\|^{2} d\tau\right)^{p} \leq \mathbb{E}\int_{0}^{t} \left\|v_{\alpha}\left(\hat{\rho}_{\tau}^{N}\right)\right\|^{2p} d\tau.$$

So we can deduce

$$\mathbb{E} \|V_t^{i,N}\|^{2p} \lesssim \mathbb{E} \|V_0^{i,N}\|^{2p} + \mathbb{E} \int_0^t \|V_\tau^{i,N}\|^{2p} d\tau + \mathbb{E} \int_0^t \|v_\alpha(\hat{\rho}_\tau^N)\|^{2p} d\tau.$$

Thus

$$\mathbb{E} \int \left\| v \right\|^{2p} d\hat{\rho}_t^N \lesssim \mathbb{E} \int \left\| v \right\|^{2p} d\hat{\rho}_0^N + \int_0^t (\mathbb{E} \int \left\| v \right\|^{2p} d\hat{\rho}_\tau^N) d\tau + \int_0^t (\mathbb{E} \left\| v_\alpha \left(\hat{\rho}_\tau^N \right) \right\|^{2p}) d\tau.$$
(56)

Now by Lemma 3.3 in [5], one has

$$\int \left\| v \right\|^2 \frac{\omega_{\alpha}(v)}{\left\| \omega_{\alpha} \right\|_{L^1(\tilde{\rho}_{\tau}^N)}} d\hat{\rho}_{\tau}^N \le b_1 + b_2 \int \left\| v \right\|^2 d\hat{\rho}_{\tau}^N.$$
(57)

Then we can calculate

$$\begin{aligned} \left\| v_{\alpha}(\hat{\rho}_{\tau}^{N}) \right\|^{2p} &= \left\| \int v \cdot \frac{\omega_{\alpha}(v)}{\left\| \omega_{\alpha} \right\|_{L^{1}(\bar{\rho}_{\tau}^{N})}} d\hat{\rho}_{\tau}^{N} \right\|^{2p} \\ &\leq \left(\int \left\| v \right\| \cdot \frac{\omega_{\alpha}(v)}{\left\| \omega_{\alpha} \right\|_{L^{1}(\bar{\rho}_{\tau}^{N})}} d\hat{\rho}_{\tau}^{N} \right)^{2p} \\ &\leq \left(\int \left\| v \right\|^{2} \cdot \frac{\omega_{\alpha}(v)}{\left\| \omega_{\alpha} \right\|_{L^{1}(\bar{\rho}_{\tau}^{N})}} \cdot \frac{\omega_{\alpha}(v)}{\left\| \omega_{\alpha} \right\|_{L^{1}(\bar{\rho}_{\tau}^{N})}} d\hat{\rho}_{\tau}^{N} \right)^{p} \\ &\leq \left(\int \left\| v \right\|^{2} \cdot \frac{\omega_{\alpha}(v)}{\left\| \omega_{\alpha} \right\|_{L^{1}(\bar{\rho}_{\tau}^{N})}} d\hat{\rho}_{\tau}^{N} \right)^{p} \leq \left(b_{1} + b_{2} \int \left\| v \right\|^{2} d\hat{\rho}_{\tau}^{N} \right)^{p} \lesssim 1 + \int \left\| v \right\|^{2p} d\hat{\rho}_{\tau}^{N}, \end{aligned}$$

where in the second inequality, we used Cauchy's inequality and in the fourth inequality, we used (57) and in the last inequality, we used Hölder inequality. Combine the above inequality and (56) leads to

$$\mathbb{E} \int \left\| v \right\|^{2p} d\hat{\rho}_t^N \lesssim \mathbb{E} \int \left\| v \right\|^{2p} d\hat{\rho}_0^N + \int_0^t \left(\mathbb{E} \int \left\| v \right\|^{2p} d\hat{\rho}_\tau^N \right) d\tau + 1.$$

By applying Gronwall's inequality, it follows that $\mathbb{E} \int |v|^{2p} d\hat{\rho}_t^N$ is bounded for $t \in [0, T]$, and the bound does not depend on N. Also, we know that

$$\left\|v_{\alpha}\left(\hat{\rho}_{\tau}^{N}\right)\right\|^{2p} \lesssim 1 + \int \left\|v\right\|^{2p} d\hat{\rho}_{\tau}^{N},$$

which implies that

$$\mathbb{E} \left\| v_{\alpha}(\hat{\rho}_{\tau}^{N}) \right\|^{2p} \lesssim 1 + \mathbb{E} \int \left\| v \right\|^{2p} d\hat{\rho}_{t}^{N}.$$

So $\mathbb{E} \| v_{\alpha}(\hat{\rho}_t^N) \|^{2p}$ is bounded for $t \in [0, T]$ and the bound does not depend on N.

As in [24], we then make the following definition.

Definition A.5. Fix $\phi \in \mathcal{C}^2_c(\mathbb{R}^d)$. Define functional $F_\phi : \mathcal{P}(\mathcal{C}[0,T];\mathbb{R}^d) \to \mathbb{R}$:

$$F_{\phi}(d\mu_{t}) = \left\langle \phi, d\mu_{t} \right\rangle - \left\langle \phi, d\mu_{0} \right\rangle + \lambda \int_{0}^{t} \left\langle \left(v - v_{\alpha}(\rho_{\tau}) \right) \cdot \nabla \phi(v), d\mu_{\tau} \right\rangle d\tau \\ + \frac{1}{\epsilon} \int_{0}^{t} \left\langle \nabla G(v) \cdot \nabla \phi(v), d\mu_{\tau} \right\rangle d\tau - \frac{\sigma^{2}}{2} \int_{0}^{t} \left\langle \sum_{k=1}^{d} \left(v - v_{\alpha}(\rho_{\tau}) \right)_{k}^{2} \partial_{kk} \phi(v), d\mu_{\tau} \right\rangle d\tau.$$

We can then prove the following proposition about the functional F_{ϕ} defined above.

Proposition 2. Let \mathcal{E} satisfy Assumption 1 and $\rho_0 \in \mathcal{P}_4(\mathbb{R}^d)$. For any $N \geq 2$, assume that $\{(V_t^{i,N})\}_{i=1}^N$ is the unique solution to (7) with $\rho_0^{\otimes N}$ distributed initial data $\{V_0^{i,N}\}_{i=1}^N$. There exists a constant C > 0 depending only on σ, K, T and $\|\nabla \phi\|_{\infty}$ such that

$$\mathbb{E}\big[|F_{\phi}(\hat{\rho}_t^N)|^2\big] \le \frac{C}{N}.$$

Proof. First we compute

$$\begin{split} F_{\phi}(\hat{\rho}_{t}^{N}) = & \frac{1}{N} \sum_{i=1}^{N} \phi(V_{t}^{i,N}) - \frac{1}{N} \sum_{i=1}^{N} \phi(V_{0}^{i,N}) + \lambda \int_{0}^{t} \frac{1}{N} \sum_{i=1}^{N} \left(V_{\tau}^{i,N} - v_{\alpha}(\hat{\rho}_{\tau}^{N}) \right) \cdot \nabla \phi(V_{\tau}^{i,N}) \, d\tau \\ & + \frac{1}{\epsilon} \int_{0}^{t} \sum_{i=1}^{N} \nabla G(V_{\tau}^{i,N}) \cdot \nabla \phi(V_{\tau}^{i,N}) \, d\tau \\ & - \frac{\sigma^{2}}{2} \int_{0}^{t} \frac{1}{N} \sum_{i=1}^{N} \sum_{k=1}^{d} \left(V_{\tau}^{i,N} - v_{\alpha}(\hat{\rho}_{\tau}^{N}) \right)_{kk}^{2} \partial_{kk} \phi(V_{\tau}^{i,N}) \, d\tau. \end{split}$$

On the other hand, the Itô-Doeblin formula gives

$$\begin{split} \phi(V_t^{i,N}) &- \phi(V_0^{i,N}) = -\lambda \int_0^t \left(V_\tau^{i,N} - v_\alpha(\hat{\rho}_\tau^N) \right) \cdot \nabla \phi(V_\tau^{i,N}) \, d\tau - \frac{1}{\epsilon} \int_0^t \nabla G(V_\tau^{i,N}) \cdot \nabla \phi(V_\tau^{i,N}) \, d\tau \\ &+ \sigma \int_0^t \left(\nabla \phi(V_\tau^{i,N}) \right)^T \left(\operatorname{diag} \left(V_\tau^{i,N} - v_\alpha(\hat{\rho}_\tau^N) \right) \, dB_\tau^i \right) \\ &+ \frac{\sigma^2}{2} \int_0^t \sum_{k=1}^d \left(V_\tau^{i,N} - v_\alpha(\hat{\rho}_\tau^N) \right)_k^2 \partial_{kk} \phi(V_\tau^{i,N}) \, d\tau. \end{split}$$

Then one gets

$$F_{\phi}(\hat{\rho}_t^N) = \frac{\sigma}{N} \int_0^t \sum_{i=1}^N \left(\nabla \phi(V_{\tau}^{i,N}) \right)^T \left(\operatorname{diag} \left(V_{\tau}^{i,N} - v_{\alpha} \left(\hat{\rho}_{\tau}^N \right) \right) dB_{\tau}^i \right).$$

Finally, we can compute

$$\begin{split} \mathbb{E}\Big[|F_{\phi}(\hat{\rho}_{t}^{N})|^{2}\Big] &= \frac{\sigma^{2}}{N^{2}} \sum_{i=1}^{N} \mathbb{E}\Big[\Big|\int_{0}^{t} \sum_{i=1}^{N} \left(\nabla\phi(V_{\tau}^{i,N})\right)^{T} \operatorname{diag}\left(V_{\tau}^{i,N} - v_{\alpha}\left(\hat{\rho}_{\tau}^{N}\right)\right) dB_{\tau}^{i}\Big|\Big]^{2} \\ &= \frac{\sigma^{2}}{N^{2}} \sum_{i=1}^{N} \mathbb{E}\Big[\int_{0}^{t} \sum_{i=1}^{N} \left\|\left(\nabla\phi(V_{\tau}^{i,N})\right)^{T} \operatorname{diag}\left(V_{\tau}^{i,N} - v_{\alpha}\left(\hat{\rho}_{\tau}^{N}\right)\right)\right\|_{2}^{2} d\tau\Big] \\ &\leq \frac{\sigma^{2}}{N^{2}} \left\|\nabla\phi\right\|_{\infty}^{2} \sum_{i=1}^{N} \int_{0}^{t} \mathbb{E}\Big[\left\|V_{\tau}^{1,N} - v_{\alpha}\left(\hat{\rho}_{\tau}^{N}\right)\right\|_{2}^{2}\Big] d\tau \\ &\lesssim \frac{\sigma^{2}}{N^{2}} \left\|\nabla\phi\right\|_{\infty}^{2} \sum_{i=1}^{N} \int_{0}^{t} K d\tau = \frac{\sigma^{2}}{N^{2}} \left\|\nabla\phi\right\|_{\infty}^{2} \sum_{i=1}^{N} tK \leq T \frac{\sigma^{2}K}{N} \left\|\nabla\phi\right\|_{\infty}, \end{split}$$

where in the second equality, we used Itô's isometry and in the third inequality, we used Lemma A.4. This completes the proof. $\hfill \Box$

We recall the Aldous criteria ([2], Section 34.3), which could prove the tightness of a sequence of distributions:

Lemma A.6 (The Aldous criteria). Let $\{V^n\}_{n\in\mathbb{N}}$ be a sequence of random variables defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and valued in $\mathcal{C}([0, T]; \mathbb{R}^d)$. The sequence of probability distributions $\{\mu_{V^n}\}_{n\in\mathbb{N}}$ of $\{V^n\}_{n\in\mathbb{N}}$ is tight on $\mathcal{C}([0, T]; \mathbb{R}^d)$ if the following two conditions hold.

(Con1) For all $t \in [0,T]$, the set of distributions of V_t^n , denoted by $\{\mu_{V^n}\}_{n \in \mathbb{N}}$, is tight as a sequence of probability measures on \mathbb{R}^d .

(Con2) For all $\epsilon > 0$, $\eta > 0$, there exists $\delta_0 > 0$ and $n_0 \in \mathbb{N}$ such that for all $n \ge n_0$ and for all discrete-valued $\sigma(V_{\tau}^n; \tau \in [0, T])$ -stopping times β with $0 \le \beta + \delta_0 \le T$, it holds that

$$\sup_{\delta \in [0,\delta_0]} \mathbb{P}\Big(\big\| V_{\beta+\delta}^n - V_{\beta}^n \big\| \ge \eta \Big) \le \epsilon.$$

Now we use the above lemma to prove the tightness of $\{\mathcal{L}(\hat{\rho}^N)\}_{N\geq 2}$.

Theorem A.7. Under the same assumption as in Lemma A.4, the sequence $\{\mathcal{L}(\hat{\rho}^N)\}_{N\geq 2}$ is tight in $\mathcal{P}(\mathcal{P}(\mathcal{C}([0,T];\mathbb{R}^d)))$.

Proof. It suffices to prove that $\{\mathcal{L}(V^{1,N})\}_{N\geq 2}$ is tight in $\mathcal{P}(\mathcal{C}([0,T];\mathbb{R}^d))$ due to Proposition 2.2(ii) in [33]. By Lemma A.6, one only needs to verify the two conditions in it. For condition 1, let us fix $\epsilon > 0$. Now we consider the compact set $U_{\epsilon} = \{\|v\|^2 \leq K/\epsilon\}$, where K is the constant in Lemma A.4. Then by Markov's inequality,

$$\mathcal{L}(V_t^{1,N})(U_\epsilon^c) = \mathbb{P}\Big(\left\| V_t^{1,N} \right\| > \frac{\epsilon}{K} \Big) \le \frac{\epsilon \mathbb{E}\Big[\left\| V_t^{1,N} \right\|^2 \Big]}{K} \le \epsilon$$

for any $N \ge 2$, where in the last inequality we used Lemma A.4. Thus condition 1 is verified.

For condition 2, we fix $\epsilon > 0$ and $\eta > 0$. Notice that

$$V_{\beta+\delta}^{1,N} - V_{\beta}^{1,N} = -\lambda \int_{\beta}^{\beta+\delta} \left(V_{\tau}^{1,N} - v_{\alpha}(\hat{\rho}_{\tau}^{N}) \right) d\tau + \sigma \int_{\beta}^{\beta+\delta} \operatorname{diag} \left(V_{\tau}^{1,N} - v_{\alpha}(\hat{\rho}_{\tau}^{N}) \right) dB_{\tau}^{1} - \frac{1}{\epsilon} \int_{\beta}^{\beta+\delta} \nabla G(V_{\tau}^{1,N}) d\tau.$$
(58)

Following the same steps in the proof of Lemma 2.1 in [24],

$$\mathbb{E}\Big[\left\|\lambda \int_{\beta}^{\beta+\delta} \left(V_{\tau}^{1,N} - v_{\alpha}(\hat{\rho}_{\tau}^{N})\right) d\tau\right\|^{2}\Big] \le 2TK\lambda^{2}\delta$$
(59)

and

$$\mathbb{E}\Big[\left\|\sigma\int_{\beta}^{\beta+\delta}\operatorname{diag}\left(V^{1,N}-v_{\alpha}\left(\hat{\rho}_{\tau}^{N}\right)\right)dB_{\tau}^{1}\right\|^{2}\Big] \leq \sigma^{2}\sqrt{8\delta TK}.$$
(60)

Also, we can compute

$$\begin{split} \left\|\frac{1}{\epsilon}\int_{\beta}^{\beta+\delta} \nabla G(V_{\tau}^{1,N}) \, d\tau\right\|^2 &\leq \frac{1}{\epsilon^2}\int_{\beta}^{\beta+\delta} \left\|\nabla G(V_{\tau}^{1,N})\right\| \, d\tau \\ &\lesssim \left(\int_{\beta}^{\beta+\delta} \left\|V_{\tau}^{i,N}\right\| \, d\tau\right)^2 \leq \delta \int_{\beta}^{\beta+\delta} \left\|V_{\tau}^{i,N}\right\|^2 \, d\tau, \end{split}$$

where in the second inequality we used Assumption 1 (4). Thus

$$\mathbb{E}\Big[\left\| \frac{1}{\epsilon} \int_{\beta}^{\beta+\delta} \nabla G(V_{\tau}^{1,N}) \, d\tau \right\|^2 \Big] \lesssim \delta \mathbb{E}\Big[\int_{\beta}^{\beta+\delta} \left\| V_{\tau}^{i,N} \right\|^2 d\tau \Big] \\ = \delta \int_{\beta}^{\beta+\delta} \mathbb{E} \left\| V_{\tau}^{i,N} \right\|^2 d\tau \lesssim \delta \int_{\beta}^{\beta+\delta} d\tau = \delta^2$$

where we used Lemma A.4. Combining the above inequality and (58), (59) and (60), we can conclude

$$\mathbb{E}\Big[\big\|V_{\beta}^{1,N} - V_{\beta+\delta}^{1,N}\big\|^2\Big] \lesssim O(\sqrt{\delta}).$$

Then one can deduce

$$\mathbb{P}(\left\|V_{\beta}^{1,N} - V_{\beta+\delta}^{1,N}\right\| > \eta) \le \frac{\mathbb{E}\left[\left\|V_{\beta}^{1,N} - V_{\beta+\delta}^{1,N}\right\|^{2}\right]}{\eta} \lesssim \frac{O(\sqrt{\delta})}{\eta}.$$

Choose δ_0 small enough finishes the proof.

By Shorokhod's lemma, for every convergent subsequence of $\{\hat{\rho}_t^N\}_{N \in \mathbb{N}}$, which is denoted by the sequence itself for simplicity and has ρ_t as limit, one can find a probability space space $(\Omega, \mathcal{F}, \mathbb{P})$ on which $\hat{\rho}_t^N$ converges to ρ_t as random variables valued in $\mathcal{P}(\mathcal{C}[0, T]; \mathbb{R}^d)$. We use V_N to denote the corresponding random variable of $\hat{\rho}_t^N$ and V to denote the corresponding random variable of ρ_t . Moreover, by the dominated convergence theorem, one has

$$\left\langle \phi, d\hat{\rho}_t^N - d\rho_t \right\rangle \to 0$$
 (61)

almost surely for fixed $t \in [0, T]$ and $\phi \in \mathcal{C}_b(\mathbb{R}^d)$.

After all these preparations, we now prove Theorem 3.4.

Proof of Theorem 3.4. We first show that every convergent sequence converges to a solution of (9). Now suppose we have a convergent subsequence of $\{\hat{\rho}_t^N\}_{N\in\mathbb{N}}$, which is denoted by the sequence itself for simplicity and has ρ_t as limit. Also, we use V_N and V to denote the corresponding random variables generated by Shorokhod's lemma as mentioned above. We verify that ρ_t is a solution to the Fokker-Planck equation (9).

For continuity, we have that for any $\phi \in \mathcal{C}^2_c(\mathbb{R}^d)$ and $t_n \to t$:

$$\left\langle \phi, d\rho_{t_n} \right\rangle = \int \phi \left(V(t_n) \right) d\mathbb{P} \to \int \phi \left(V(t) \right) d\mathbb{P} = \left\langle \phi, d\rho_t \right\rangle.$$

To prove ρ_t satisfies the Fokker-Planck equation (9), we first prove the following four limits:

$$(1) \mathbb{E}\left[\left(\left\langle\phi,\hat{\rho}_{t}^{N}\right\rangle-\left\langle\phi,d\hat{\rho}_{0}\right\rangle\right)-\left(\left\langle\phi,d\rho_{t}\right\rangle-\left\langle\phi,d\rho_{0}\right\rangle\right)\right] \text{ converges to 0 as } N\to\infty.$$

$$(2) \mathbb{E}\left[\int_{0}^{t}\left\langle\left(v-v_{\alpha}(\hat{\rho}_{\tau}^{N})\right)\cdot\nabla\phi(v),d\hat{\rho}_{\tau}^{N}\right\rangle d\tau-\int_{0}^{t}\left\langle\left(v-v_{\alpha}(\hat{\rho}_{\tau}^{N})\right)\cdot\nabla\phi(v),d\rho_{\tau}\right\rangle d\tau\right] \text{ converges to 0 as } N\to\infty.$$

$$(3) \mathbb{E}\left[\int_{0}^{t}\left\langle\sum_{k=1}^{d}\left(v-v_{\alpha}(\hat{\rho}_{\tau}^{N})\right)_{k}^{2}\partial_{kk}\phi(v),d\hat{\rho}_{\tau}^{N}\right\rangle d\tau-\int_{0}^{t}\left\langle\sum_{k=1}^{d}\left(v-v_{\alpha}(\rho_{\tau})\right)_{k}^{2}\partial_{kk}\phi(v),d\rho_{\tau}\right\rangle d\tau\right] \text{ converges to 0 as } N\to\infty.$$

$$(4) \mathbb{E}\left[\int_{0}^{t}\left\langle\nabla G(v)\cdot\nabla\phi(v),d\hat{\rho}_{\tau}^{N}\right\rangle d\tau-\int_{0}^{t}\left\langle\nabla G(v)\cdot\nabla\phi(v),d\rho_{\tau}\right\rangle d\tau\right] \text{ converges to 0 as } N\to\infty.$$

The first three limits can be proved using the same methods as in Theorem 3.3 in [24] and the last one is a direct result of (61). Combining the above four limits gives

$$\mathbb{E}\left[F_{\phi}(\rho_t) - F_{\phi}(\hat{\rho}_t^N)\right] = 0.$$

Then we can deduce

$$\left| \mathbb{E} \left[F_{\phi}(\rho_t) \right] \right| \leq \lim_{N \to \infty} \left| \mathbb{E} \left[F_{\phi}(\rho_t) - F_{\phi}(\hat{\rho}_t^N) \right] \right| + \left| \mathbb{E} \left[F_{\phi}(\hat{\rho}_t^N) \right] \right| \leq 0 + \lim_{N \to \infty} \sqrt{\frac{C}{N}} = 0,$$

where in the last inequality, we used Proposition 2. Thus $F_{\phi}(\rho_t) = 0$ almost surely, which implies that ρ_t is a solution to the corresponding Fokker-Planck equation (9).

Then we utilize Lemma A.9 to establish that every convergent subsequence converges to the same limit: the unique solution to (9). Combining with Theorem A.7, we deduce that $\{\hat{\rho}_t^N\}_{N\in\mathbb{N}}$ converges and the limit is exactly the solution to (9).

A.4. Some auxiliary results used in the proof of Theorem 3.4.

Theorem A.8. For $\forall T > 0$, let $b_t \in \mathcal{C}([0,T]; \mathbb{R}^d)$ and $\rho_0 \in \mathcal{P}_2(\mathbb{R}^d)$. The following linear PDE

$$\partial_t \rho_t = \lambda \nabla \cdot \left(\left((v - b_t) + \frac{1}{\epsilon} \nabla G(v) \right) \rho_t \right) + \frac{\sigma^2}{2} \sum_{k=1}^d \partial_{x_k x_k} \left((v - b_t)_k^2 \rho_t \right)$$
(62)

has a unique weak solution $\rho_t \in \mathcal{C}([0,T]; \mathcal{P}_2(\mathbb{R}^d)).$

Proof. We can obtain a solution to (62) as the law of the solution to the associated linear SDE to (62). Thus we have the existence result. For uniqueness, let us fix $t_0 \in [0, T]$ and $\psi \in \mathcal{C}^{\infty}_c(\mathbb{R}^d)$. We then can solve the following backward PDE

$$\partial_t h_t = \left(\lambda(v - b_t) + \frac{1}{\epsilon}\nabla G(v)\right) \cdot \nabla h_t - \frac{\sigma^2}{2} \sum_{k=1}^d (v - b_t)_k^2 \partial_{x_k x_k} h_t,$$
$$(t, v) \in [0, t_0] \times \mathbb{R}^d; h_{t_0} = \psi.$$

It has a classical solution:

$$h_t = \mathbb{E}\left[\psi(V_{t_0}^{t,v})\right], t \in [0, t_0]$$

where $(V_{\tau}^{t,x})_{0 \le t \le s \le t_0}$ is the strong solution to

$$dV_{\tau}^{t,v} = -\left(\lambda(V_{\tau}^{t,v} - b_{\tau}) + \frac{1}{\epsilon}\nabla G(V_{\tau}^{t,v})\right)d\tau + \sigma \operatorname{diag}\left(V_{\tau}^{t,v} - b_{\tau}\right)dB_{\tau}, V_{t}^{t,v} = v.$$

Suppose ρ^1 and ρ^2 are two weak solutions to (62). Consider $\delta \rho = \rho^1 - \rho^2$. Then

$$\left\langle h_{t_0}, \delta \rho_{t_0} \right\rangle = \int_0^{t_0} \left\langle \partial_\tau h_\tau, \delta \rho_\tau \right\rangle d\tau - \lambda \int_0^{t_0} \left\langle (v - b_\tau) \nabla h_\tau, \delta \rho_\tau \right\rangle d\tau - \frac{1}{\epsilon} \int_0^{t_0} \left\langle \nabla G \cdot \nabla h_\tau, \delta \rho_\tau \right\rangle d\tau + \frac{\sigma^2}{2} \int_0^{t_0} \left\langle \sum_{k=1}^d (v - b_\tau)_k^2 \partial_{kk} h_\tau, \delta \rho_\tau \right\rangle d\tau = \int_0^{t_0} \left\langle \partial_\tau h_\tau, \delta \rho_\tau \right\rangle d\tau + \int_0^{t_0} \left\langle -\partial_\tau h_\tau, \delta \rho_\tau \right\rangle d\tau = 0.$$

This implies that $\int \psi \delta \rho_{t_0} = 0$ for any chosen $\psi \in \mathcal{C}_c^{\infty}(\mathbb{R}^d)$ and $t_0 \in [0, T]$. Thus $\delta \rho_t = 0$. This proves the uniqueness.

Lemma A.9. Assume that $\rho^1, \rho^2 \in \mathcal{C}([0,T]; \mathcal{P}_2(\mathbb{R}^d))$ are two weak solutions to PDE (9) in the sense of Definition 3.2 with the same initial data ρ_0 . Then it holds that

$$\sup_{t \in [0,T]} W_2(\rho_t^1, \rho_t^2) = 0,$$

where W_2 is the 2-Wasserstein distance.

Proof. Given ρ^1 and ρ^2 , we first solve the following two linear SDEs

$$d\tilde{V}_t^i = -\lambda \left(\tilde{V}_t^i - v_\alpha(\rho_t^i) \right) dt - \frac{1}{\epsilon} \nabla G \, dt + \sigma \operatorname{diag} \left(\tilde{V}_t^i - v_{\alpha(\rho_t^i)} \right) dB_t,$$
$$\hat{V}_0^i \sim \rho_0$$

for i = 1, 2. We use $\tilde{\rho}_t^i$ to denote the law of \tilde{V}_t^i for i = 1, 2. Thus $\tilde{\rho}_t^i$ solves

$$\partial_t \tilde{\rho}_t^i = \lambda \operatorname{div} \left((v - v_\alpha(\rho_t^i) + \frac{1}{\epsilon} \nabla G) \tilde{\rho}_t^i \right) + \frac{\sigma^2}{2} \sum_{k=1}^d \partial_{x_k x_k} \left(\left\| v - v_\alpha(\rho_t^i) \right\|^2 \tilde{\rho}_t^i \right), \\ \tilde{\rho}_0^i = \rho_0$$

in the weak sense for i = 1, 2. Moreover, ρ^i solves the above PDE since we assumed that ρ^i solves (9). But from Theorem A.9, the solution to the above PDE is unique for i = 1, 2. This implies that $\tilde{\rho}_t^i = \rho_t^i$ for i = 1, 2. As a result, \tilde{V}_t^1 and \tilde{V}_t^2 both solve (8). By Theorem 3.3, it holds that

$$\sup_{t \in [0,T]} \mathbb{E} \left[|\tilde{V}_t^1 - \tilde{V}_t^2|^2 \right] = 0.$$

Then one has

$$\sup_{t \in [0,T]} W_2(\rho^1, \rho^2) = \sup_{t \in [0,T]} W_2(\tilde{\rho}^1, \tilde{\rho}^2) \le \sup_{t \in [0,T]} \mathbb{E}\left[|\tilde{V}_t^1 - \tilde{V}_t^2|^2\right] = 0$$

This completes the proof.

APPENDIX B. LEMMA B.1

Lemma B.1. There exist non-negative increasing function $\tau_2(x)$, $\tau_3(x)$ and $\tau_4(x)$ mapping from \mathbb{R} to \mathbb{R} with $\lim_{x\to 0} \tau_i(x) = 0$ for i = 2, 3, 4 so that the following hold for $\forall u, r \ge 0$ small enough:

$$\begin{aligned} |\underline{\mathcal{E}}_{\underline{u}}| &= |\mathcal{E}(v_u)| \le \tau_2(u); \\ |\mathcal{E}_r^u - \mathcal{E}_r| \le \tau_3(\max\{u, r\}); \\ |\mathcal{E}_r^u - \mathcal{E}_r^0| \le \tau_4(\max\{u, r\}), \end{aligned}$$

where

$$\mathcal{E}_r^u = \max_{v \in B^\infty(v_u, r) \cap \{G(v)=u\}} \mathcal{E}(v)$$

and

$$\mathcal{E}_r = \max_{v \in B^{\infty}(v^*, r)} \mathcal{E}(v).$$

Proof. We first prove the existence of τ_2 . To begin with, one deduces

$$|\underline{\mathcal{E}}_{u}| = |\mathcal{E}(v_{u})| = |\mathcal{E}(v_{u}) - 0| = |\mathcal{E}(v_{u}) - \mathcal{E}(v^{*})| \le C ||v_{u} - v^{*}||_{\infty}^{\beta} \le C\tau_{1}^{\beta}(u),$$

where the first inequality comes from Assumption 2 (A2) and the second inequality comes from Assumption 2 (C1). Then by taking $\tau_2(x)$ to be $\tau_1^{\beta}(x)$ will finish the proof of the existence of τ_2 .

For the existence of τ_3 , we can first pick $v_1 \in B^{\infty}(v_u, r) \cap \{G(v) = u\}, v_2 \in B^{\infty}(v^*, r)$ and then do the following calculation:

$$\begin{aligned} |\mathcal{E}(v_1) - \mathcal{E}(v_2)| &\leq C \|v_1 - v_2\|_{\infty}^{\beta} \\ &\lesssim (\|v_1 - v_u\|_{\infty}^{\beta} + \|v_u - v^*\|_{\infty}^{\beta} + \|v^* - v_2\|_{\infty}^{\beta}) \\ &\leq (r^{\beta} + \tau_1(u)^{\beta} + r^{\beta}) \\ &\leq (\max\{u, r\}^{\beta} + \tau_1(\max\{u, r\})^{\beta} + \max\{u, r\}^{\beta}), \end{aligned}$$

where in the first inequality, we used Assumption 2 (A2) and in the third inequality, we used Assumption 2 (C1). Then one has

$$\sup_{\substack{v_1 \in B(v_u, r) \cap \{G(v)=u\}, \\ v_2 \in B(v^*, r)}} |\mathcal{E}(v_1) - \mathcal{E}(v_2)| \lesssim \left(\max\{u, r\}^{\beta} + \tau_1(\max\{u, r\})^{\beta} + \max\{u, r\}^{\beta}\right).$$

 So

$$|\mathcal{E}_r^u - \mathcal{E}_r| \lesssim \left(\max\{u, r\}^\beta + \tau_1(\max\{u, r\})^\beta + \max\{u, r\}^\beta \right).$$

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Therefore, selecting $\tau_3(x)$ as a scalar multiple of $2x^{\beta} + \tau_1^{\beta}(x)$ will suffice. One can apply the same method to prove the existence of $\tau_4(x)$.

APPENDIX C. EXPLANATIONS FOR EXPANDING THE TEST FUNCTION SPACE

We follow the same argument as in [15]. To start with, for any $\phi \in \mathcal{C}^2_*(\mathbb{R}^d)$, one apply Ito's formula to \bar{V}_t to get

$$d\phi(\bar{V}_t) = \nabla\phi(\bar{V}_t) \cdot \left(\left(-\lambda(\bar{V}_t - v_\alpha(\rho_t)) - \frac{1}{\epsilon}\nabla G(\bar{V}_t) \right) dt \right) \\ + \frac{1}{2}\sigma^2 \sum_{k=1}^d \partial_{kk}\phi(\bar{V}_t) \left(\bar{V}_t - v_\alpha(\rho_t) \right)_k^2 dt + \sigma\nabla\phi(\bar{V}_t)^T \operatorname{diag}\left(\bar{V}_t - v_\alpha(\rho_t) \right) dB_t.$$

Note that $\mathbb{E} \int_0^t \sigma \nabla \phi(\bar{V}_t)^T \operatorname{diag}(\bar{V}_t - v_\alpha(\rho_t)) dB_t = 0$ by applying Theorem 3.2.1 (iii) in [28] due to the facts that $\phi \in \mathcal{C}^2_*(\mathbb{R}^d)$ and $\rho_t \in \mathcal{C}([0,T], \mathcal{P}_4(\mathbb{R}^d))$. Taking the expectation and applying Fubini's theorem gives

$$\frac{d}{dt}\mathbb{E}\phi(\bar{V}_t) = -\lambda\mathbb{E}\nabla\phi(\bar{V}_t)\cdot\left(-\lambda(\bar{V}_t - v_\alpha(\rho_t)) - \frac{1}{\epsilon}\nabla G(\bar{V}_t)\right) \\ + \frac{1}{2}\sigma^2\mathbb{E}\sum_{k=1}^d \partial_{kk}\phi(\bar{V}_t)\left(\bar{V}_t - v_\alpha(\rho_t)\right)_k^2,$$

which is exactly the first expression in Definition 3.2 (ii) with ϕ being a function in $\mathcal{C}^2_*(\mathbb{R}^d)$.

Appendix D. Proof of Lemma 4.2

Proof. Substituting $\phi(v) = \frac{1}{2} ||v - v^*||^2$ into Definition 3.2 gives

$$\frac{d}{dt}\mathcal{V}(\rho_t) = -\lambda \int \left\langle v - v_\alpha(\rho_t), v - v^* \right\rangle d\rho_t - \frac{1}{\epsilon} \int \left\langle \nabla G, v - v^* \right\rangle d\rho_t + \frac{\sigma^2}{2} \int \|v - v(\rho_t)\|^2 d\rho_t.$$
(63)

Notice that

$$-\lambda \int \left\langle v - v_{\alpha}(\rho_{t}), v - v^{*} \right\rangle d\rho_{t}(v)$$

= $-\lambda \int \left\langle v - v^{*}, v - v^{*} \right\rangle d\rho_{t}(v) + \lambda \int \left\langle v - v^{*}, v_{\alpha}(\rho_{t}) - v^{*} \right\rangle d\rho_{t}(v)$
= $-2\lambda \mathcal{V}(\rho_{t}) + \lambda \left\langle \int (v - v^{*}) d\rho_{t}(v), v_{\alpha}(\rho_{t}) - v^{*} \right\rangle.$

Then one can deduce

$$-\lambda \int \left\langle v - v_{\alpha}(\rho_{t}), v - v^{*} \right\rangle d\rho_{t}(v) \leq -2\lambda \mathcal{V}(\rho_{t}) + \lambda \| \int (v - v^{*}) d\rho_{t}(v) \|_{2} \cdot \|v_{\alpha}(\rho_{t}) - v^{*}\|_{2}$$

$$\leq -2\lambda \mathcal{V}(\rho_{t}) + \lambda \int \|(v - v^{*})\|_{2} d\rho_{t}(v) \cdot \|v_{\alpha}(\rho_{t}) - v^{*}\|_{2}$$

$$\leq -2\lambda \mathcal{V}(\rho_{t}) + \lambda \sqrt{2\mathcal{V}(\rho_{t})} \cdot \|v_{\alpha}(\rho_{t}) - v^{*}\|_{2},$$
(64)

where the first and third inequalities come from Cauchy's inequality and the second inequality is a consequence of Minkowski's inequality.

For the last term on the right-hand side of (63), we can do the following estimate,

$$\frac{\sigma^{2}}{2} \int \|v - v(\rho_{t})\|_{2}^{2} d\rho_{t}(v)
= \frac{\sigma^{2}}{2} \left(\int \|v - v^{*}\|_{2}^{2} d\rho_{t}(v) - 2 \left\langle \int (v - v^{*}) d\rho_{t}(v), v_{\alpha}(\rho_{t}) - v^{*} \right\rangle + \|v_{\alpha}(\rho_{t}) - v^{*}\|_{2}^{2} \right)
\leq \sigma^{2} \left(\mathcal{V}(\rho_{t}) + \int \|v - v^{*}\|_{2} d\rho_{t}(v) \cdot \|v_{\alpha}(\rho_{t}) - v^{*}\|_{2} + \frac{1}{2} \|v_{\alpha}(\rho_{t}) - v^{*}\|_{2}^{2} \right)
\leq \sigma^{2} \left(\mathcal{V}(\rho_{t}) + \sqrt{2\mathcal{V}(\rho_{t})} \|v_{\alpha}(\rho_{t}) - v^{*}\|_{2} + \frac{1}{2} \|v_{\alpha}(\rho_{t}) - v^{*}\|_{2}^{2} \right),$$
(65)

where in the first inequality, we use Cauchy's inequality and Minkowski's inequality and in the second inequality, we use Cauchy's inequality again. Plugging (64) and (65) back into (63) finishes the proof. \Box

APPENDIX E. LEMMAS USED IN LAPLACE'S PRINCIPLE

E.1. Proof of Lemma 4.3.

Proof. Let $\tilde{r} = \frac{(q + \mathcal{E}_r^0)^{\mu}}{\eta}$. One can verify that (1) $\tilde{r} \ge r$ (2) $\mathcal{E}(v) - \mathcal{E}_r^0 \ge q$ for $\forall v \in \{G = 0\} \cap B^{\infty}(v^*, \tilde{r})^c$.

For (1), we begin by computing directly:

$$\tilde{r} = \frac{(q + \mathcal{E}_r^0)^{\mu}}{\eta} \ge \frac{(\mathcal{E}_r^0)^{\mu}}{\eta} = \frac{(\mathcal{E}_r^0 - \underline{\mathcal{E}}_0)^{\mu}}{\eta},$$

where the last equality is because $\underline{\mathcal{E}}_0 = \mathcal{E}(v^*) = 0$. Then for any $v \in B^{\infty}(v^*, r) \cap \{G = 0\}$, by the definition of \mathcal{E}_r^0 , in Lemma B.1, one has

$$\frac{(\mathcal{E}_r^0 - \underline{\mathcal{E}}_0)^{\mu}}{\eta} \geq \frac{(\mathcal{E}(v) - \underline{\mathcal{E}}_0)^{\mu}}{\eta}$$

Then we use Assumption 2 (C2) to get

$$\tilde{r} \ge \frac{(\mathcal{E}(v) - \underline{\mathcal{E}}_0)^{\mu}}{\eta} \ge \left\| v - v^* \right\|_{\infty}.$$

By Assumption 2 (C1), $\partial B^{\infty}(v^*, r) \cap \{G = 0\} \neq \emptyset$, which leads to

$$\sup_{v\in B^{\infty}(v^*,r)\cap\{G=0\}}\left\|v-v^*\right\|_{\infty}=r.$$

Since the above inequality holds for $\forall v \in B^{\infty}(v^*, r) \cap \{G = 0\}$, one then has $\tilde{r} \ge r$, which completes the proof of the first one. And for (2), for all $v \in \{G = 0\} \cap B^{\infty}(v^*, r)^c$, we can compute:

$$\begin{aligned} \mathcal{E}(v) - \mathcal{E}_r^0 &= \mathcal{E}(v) - \underline{\mathcal{E}_0} - (\mathcal{E}_r^0 - \underline{\mathcal{E}_0}) \\ &\geq (\eta \| v - v^* \|_{\infty})^{1/\mu} - (\mathcal{E}_r^0 - \underline{\mathcal{E}_0}) \geq (\eta \tilde{r})^{1/\mu} - (\mathcal{E}_r^0 - \underline{\mathcal{E}_0}) = q + \underline{\mathcal{E}_0} = q, \end{aligned}$$

where the first inequality comes from Assumption 2 (C2), the second inequality is due to $v \in B^{\infty}(v^*, \tilde{r})^c$, the third inequality is because of the definition of \tilde{r} and the last equality is because we assumed $\mathcal{E}(v^*) = 0$. This completes the proof of the second one.

Then we have

$$\begin{split} \int_{\{G=0\}} \frac{\|v-v^*\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha \mathcal{E}(v)} \, d\rho_{t}(v) &= \int_{\{G=0\} \cap B^{\infty}(v^*,\tilde{r})} \frac{\|v-v^*\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha \mathcal{E}(v)} \, d\rho_{t}(v) \\ &+ \int_{\{G=0\} \cap B^{\infty}(v^*,\tilde{r})^{c}} \frac{\|v-v^*\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha \mathcal{E}(v)} \, d\rho_{t}(v). \end{split}$$

For the former term, we have the following estimate

$$\int_{\{G=0\}\cap B^{\infty}(v^{*},\tilde{r})} \frac{\|v-v^{*}\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha\mathcal{E}(v)} d\rho_{t}(v) \leq \tilde{r} \int_{\{G=0\}\cap B^{\infty}(v^{*},\tilde{r})} \frac{1}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha\mathcal{E}(v)} d\rho_{t}(v) \leq \tilde{r}.$$
(66)

For the latter term, we first notice that

$$\begin{aligned} \left\|\omega_{\alpha}\right\|_{L^{1}(\rho_{t})} &= \int e^{-\alpha \mathcal{E}(v)} \, d\rho_{t}(v) \geq \int_{B^{\infty}(v^{*},r)} e^{-\alpha \mathcal{E}(v)} \, d\rho_{t}(v) \geq \int_{B^{\infty}(v^{*},r)} e^{-\alpha \mathcal{E}_{r}} \, d\rho_{t}(v) \\ &= e^{-\alpha \mathcal{E}_{r}} \rho_{t} \left(B^{\infty}(v^{*},r)\right). \end{aligned}$$

Here the second inequality is because of the definition of \mathcal{E}_r in Lemma B.1. So

$$\left\|\omega_{\alpha}\right\|_{L^{1}(\rho_{t})} \ge e^{-\alpha \mathcal{E}_{r}} \rho_{t} \left(B^{\infty}(v^{*}, r)\right)$$
(67)

holds true for any choice of α and r. Then one can deduce

$$\int_{\{G=0\}\cap B^{\infty}(v^{*},\tilde{r})^{c}} \frac{\|v-v^{*}\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha\mathcal{E}(v)} d\rho_{t}(v)
\leq \int_{\{G=0\}\cap B^{\infty}(v^{*},\tilde{r})^{c}} \frac{\|v-v^{*}\|_{\infty}}{\rho_{t}(B^{\infty}(v^{*},r))} e^{-\alpha\left(\mathcal{E}(v)-\mathcal{E}_{r}\right)} d\rho_{t}(v)
\leq \int_{\{G=0\}\cap B^{\infty}(v^{*},\tilde{r})^{c}} \frac{\|v-v^{*}\|_{\infty}}{\rho_{t}(B^{\infty}(v^{*},r))} e^{-\alpha\left(\mathcal{E}(v)-\mathcal{E}_{r}^{0}-\tau_{3}(r)\right)} d\rho_{t}(v)
\leq \int_{\{G=0\}} \frac{\|v-v^{*}\|_{\infty}}{\rho_{t}(B^{\infty}(v^{*},r))} e^{-\alpha\left(q-\tau_{3}(r)\right)} d\rho_{t}(v),$$

where in the second inequality, we used Lemma B.1 and in the third third inequality, we used the fact (2) that $\mathcal{E}(v) - \mathcal{E}_r^0 \ge q$ for $\forall v \in \{G = 0\} \cap B^{\infty}(v^*, \tilde{r})^c$. Thus

$$\int_{\{G=0\}\cap B^{\infty}(v^*,\tilde{r})^c} \frac{\|v-v^*\|_{\infty}}{\|\omega_{\alpha}\|_{L^1(\rho_t)}} e^{-\alpha\mathcal{E}(v)} \, d\rho_t(v) \le \int_{\{G=0\}} \frac{\|v-v^*\|_{\infty}}{\rho_t(B^{\infty}(v^*,r))} e^{-\alpha\left(q-\tau_3(r)\right)} \, d\rho_t(v).$$

Combining the above inequality and (66), we can get

$$\int_{\{G=0\}} \frac{\|v-v^*\|_{\infty}}{\|\omega_{\alpha}\|_{L^1(\rho_t)}} e^{-\alpha \mathcal{E}(v)} \, d\rho_t(v) \le \frac{(q+\mathcal{E}_r^0)^{\mu}}{\eta} + \frac{e^{-\alpha \left(q-\tau_3(r)\right)}}{\rho_t \left(B^{\infty}(v^*,r)\right)} \int_{\{G=0\}} \|v-v^*\|_{\infty} \, d\rho_t(v).$$

Since $\|\cdot\|_{\infty} \leq \|\cdot\|_2 \leq \sqrt{d} \|\cdot\|_2$, we have

$$\int_{\{G=0\}} \frac{\|v-v^*\|_2}{\|\omega_{\alpha}\|_{L^1(\rho_t)}} e^{-\alpha \mathcal{E}(v)} d\rho_t(v) \le \frac{\sqrt{d}(q+\mathcal{E}^0_r)^{\mu}}{\eta} + \frac{\sqrt{d}e^{-\alpha(q-\tau_3(r))}}{\rho_t(B^{\infty}(v^*,r))} \int_{\{G=0\}} \|v-v^*\|_2 d\rho_t(v).$$

This completes the proof.

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This completes the proof.

E.2. Proof of Lemma 4.4.

Proof. We first can deduce

$$\begin{split} \int_{\{G\in(0,u)\}} \frac{\|v-v^*\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha\mathcal{E}(v)} \, d\rho_{t}(v) &= \int_{\{G\in(0,u)\}} \frac{\|v-v^*\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} \|\nabla G\|_{2} e^{-\alpha\mathcal{E}(v)} \|\nabla G\|_{2} \rho_{t} \, dv \\ &= \int_{0}^{u} d\tilde{u} \int_{\{G(v)=\tilde{u}\}} \frac{\|v-v^*\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha\mathcal{E}(v)} \rho_{t} \, dH_{d-1}(v). \end{split}$$

Here, the first equality is because of Assumption 2 (B3) that $\nabla G \neq 0$ and the second equality comes from the co-area formula. $dH_{d-1}(v)$ is the (d-1) dimensional Hausdorff measure.

Now we fix $0 < \tilde{u} < u$ and study the inner integral. We pick $\tilde{r}_{\tilde{u}} = \frac{(q + \mathcal{E}_{r}^{\tilde{u}} - \underline{\mathcal{E}}_{\tilde{u}})^{\mu}}{\eta}$. One can easily use Assumption 2 (C2) to verify the following facts:

(1)
$$\tilde{r}_{\tilde{u}} \geq r$$
.
(2) $\mathcal{E}(v) - \mathcal{E}_{r}^{\tilde{u}} \geq q$ for $v \in B^{\infty}(v_{\tilde{u}}, \tilde{r}_{\tilde{u}})^{c} \cap \{G(v) = \tilde{u}\}$.
(3) $\tilde{r}_{\tilde{u}} \leq \tilde{r} = \frac{\left(q + \mathcal{E}_{r}^{0} + \tau_{2}(u) + \tau_{4}(\max\{u, r\})\right)^{\mu}}{\eta}$.

For the proof of the first two facts, one can use the same method we used at the beginning of the proof of Lemma 4.3 and details are omitted. For (3), one can prove it as follows:

$$\begin{split} \tilde{r}_{\tilde{u}} &= \frac{\left(q + \mathcal{E}_{r}^{\tilde{u}} - \underline{\mathcal{E}}_{\tilde{u}}\right)^{\mu}}{\eta} \\ &= \frac{\left(q + \mathcal{E}_{r}^{0} + (\mathcal{E}_{r}^{\tilde{u}} - \mathcal{E}_{r}^{0}) - \underline{\mathcal{E}}_{\tilde{u}}\right)^{\mu}}{\eta} \\ &\leq \frac{\left(q + \mathcal{E}_{r}^{0} + \tau_{4}(\max\{\tilde{u}, r\}) - \tau_{2}(\tilde{u})\right)^{\mu}}{\eta} \leq \frac{\left(q + \mathcal{E}_{r}^{0} + \tau_{4}(\max\{u, r\}) - \tau_{2}(u)\right)^{\mu}}{\eta}, \end{split}$$

where the two inequalities are because of Assumption 2 (C2) and Lemma B.1.

Then by the triangle inequality, one obtains

$$\leq \int_{\{G(v)=\tilde{u}\}} \frac{\|v-v^*\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} \|\nabla G\|_{2} e^{-\alpha \mathcal{E}(v)} \rho_{t} dH_{d-1}(v)$$

$$\leq \int_{\{G(v)=\tilde{u}\}\cap B^{\infty}(v_{\tilde{u}},\tilde{r}_{\tilde{u}})} \frac{\|v-v_{\tilde{u}}\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} \|\nabla G\|_{2} e^{-\alpha \mathcal{E}(v)} \rho_{t} dH_{d-1}(v)$$

$$+ \int_{\{G(v)=\tilde{u}\}\cap B^{\infty}(v_{\tilde{u}},\tilde{r}_{\tilde{u}})^{c}} \frac{\|v-v_{\tilde{u}}\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} \|\nabla G\|_{2} e^{-\alpha \mathcal{E}(v)} \rho_{t} dH_{d-1}(v)$$

$$+ \int_{\{G(v)=\tilde{u}\}} \frac{\|v^*-v_{\tilde{u}}\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} \|\nabla G\|_{2} e^{-\alpha \mathcal{E}(v)} \rho_{t} dH_{d-1}(v).$$

Thus one needs to bound the above three terms. For the first one,

$$\begin{split} &\int_{\{G(v)=\tilde{u}\}\cap B^{\infty}(v_{\tilde{u}},\tilde{r}_{\tilde{u}})} \frac{\|v-v_{\tilde{u}}\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} \|\nabla G\|_{2} e^{-\alpha \mathcal{E}(v)} \rho_{t} \, dH_{d-1}(v) \\ &\leq \tilde{r}_{\tilde{u}} \int_{\{G(v)=\tilde{u}\}} \frac{1}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} \|\nabla G\|_{2} e^{-\alpha \mathcal{E}(v)} \rho_{t} \, dH_{d-1}(v) \\ &\leq \tilde{r} \int_{\{G(v)=\tilde{u}\}} \frac{1}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} \|\nabla G\|_{2} e^{-\alpha \mathcal{E}(v)} \rho_{t} \, dH_{d-1}(v). \end{split}$$

For the second one,

$$\begin{split} &\int_{\{G(v)=\tilde{u}\}\cap B^{\infty}(v_{\tilde{u}},\tilde{r}_{\tilde{u}})^{c}} \frac{\left\|v-v_{\tilde{u}}\right\|_{\infty}}{\left\|\omega_{\alpha}\right\|_{1}\left\|\nabla G\right\|_{2}} e^{-\alpha\mathcal{E}(v)}\rho_{t} \, dH_{d-1}(v) \\ &\leq \int_{\{G(v)=\tilde{u}\}\cap B^{\infty}(v_{\tilde{u}},\tilde{r}_{\tilde{u}})^{c}} \frac{\left\|v-v_{\tilde{u}}\right\|_{\infty}}{\rho_{t}\left(B^{\infty}(v^{*},r)\right)\left\|\nabla G\right\|_{2}} e^{-\alpha\left(\mathcal{E}(v)-\mathcal{E}_{r}^{\tilde{u}}-\tau_{3}(\max\{\tilde{u},r\})\right)}\rho_{t} \, dH_{d-1}(v) \\ &\leq \int_{\{G(v)=\tilde{u}\}\cap B^{\infty}(v_{\tilde{u}},\tilde{r}_{\tilde{u}})^{c}} \frac{\left\|v-v_{\tilde{u}}\right\|_{\infty}}{\rho_{t}\left(B^{\infty}(v^{*},r)\right)\left\|\nabla G\right\|_{2}} e^{-\alpha\left(\mathcal{E}(v)-\mathcal{E}_{r}^{\tilde{u}}-\tau_{3}(\max\{\tilde{u},r\})\right)}\rho_{t} \, dH_{d-1}(v) \\ &\leq \int_{\{G(v)=\tilde{u}\}\cap B^{\infty}(v_{\tilde{u}},\tilde{r}_{\tilde{u}})^{c}} \frac{\left\|v-v_{\tilde{u}}\right\|_{\infty}}{\rho_{t}\left(B^{\infty}(v^{*},r)\right)\left\|\nabla G\right\|_{2}} e^{-\alpha\left(\mathcal{E}(v)-\mathcal{E}_{r}^{\tilde{u}}-\tau_{3}(\max\{u,r\})\right)}\rho_{t} \, dH_{d-1}(v) \\ &\leq \int_{\{G(v)=\tilde{u}\}\cap B^{\infty}(v_{\tilde{u}},\tilde{r}_{\tilde{u}})^{c}} \frac{\left\|v-v_{\tilde{u}}\right\|_{\infty}}{\rho_{t}\left(B^{\infty}(v^{*},r)\right)\left\|\nabla G\right\|_{2}} e^{-\alpha\left(q-\tau_{3}(\max\{u,r\})\right)}\rho_{t} \, dH_{d-1}(v) \\ &\leq \int_{\{G(v)=\tilde{u}\}\cap B^{\infty}(v_{\tilde{u}},\tilde{r}_{\tilde{u}})^{c}} \frac{\left\|v-v_{\tilde{u}}\right\|_{\infty}}{\rho_{t}\left(B^{\infty}(v^{*},r)\right)\left\|\nabla G\right\|_{2}} e^{-\alpha\left(q-\tau_{3}(\max\{u,r\})\right)}\rho_{t} \, dH_{d-1}(v) \\ &\leq \int_{\{G(v)=\tilde{u}\}\cap B^{\infty}(v_{\tilde{u}},\tilde{r}_{\tilde{u}})^{c}} \frac{\left\|v-v_{\tilde{u}}\right\|_{\infty}}{\rho_{t}\left(B^{\infty}(v^{*},r)\right)\left\|\nabla G\right\|_{2}} e^{-\alpha\left(q-\tau_{3}(\max\{u,r\})\right)}\rho_{t} \, dH_{d-1}(v) \end{aligned}$$

where in the first inequality above, we used (67) and in the second and third inequalities above, we used Lemma B.1 that $|\mathcal{E}_r^u - \mathcal{E}_r| \leq \tau_3(\max\{u, r\})$ and the assumption that τ_3 is an increasing function. In the fourth inequality, we used the fact (2) that $\mathcal{E}(v) - \mathcal{E}_r^{\tilde{u}} \geq q$ for $v \in B(v_{\tilde{u}}, \tilde{r}_{\tilde{u}})^c \cap \{G(v) = \tilde{u}\}$.

For the third term,

$$\begin{split} &\int_{\{G(v)=\tilde{u}\}} \frac{\left\|v^{*}-v_{\tilde{u}}\right\|_{\infty}}{\left\|\omega_{\alpha}\right\|_{L^{1}(\rho_{t})}} \left\|\nabla G\right\|_{2}} e^{-\alpha \mathcal{E}(v)} \rho_{t} \, dH_{d-1}(v) \\ &= \left\|v^{*}-v_{\tilde{u}}\right\|_{\infty} \int_{\{G(v)=\tilde{u}\}} \frac{1}{\left\|\omega_{\alpha}\right\|_{L^{1}(\rho_{t})}} \left\|\nabla G\right\|_{2}} e^{-\alpha \mathcal{E}(v)} \rho_{t} \, dH_{d-1}(v) \\ &\leq \tau_{1}(\tilde{u}) \int_{\{G(v)=\tilde{u}\}} \frac{1}{\left\|\omega_{\alpha}\right\|_{L^{1}(\rho_{t})}} \left\|\nabla G\right\|_{2}} e^{-\alpha \mathcal{E}(v)} \rho_{t} \, dH_{d-1}(v) \\ &\leq \tau_{1}(u) \int_{\{G(v)=\tilde{u}\}} \frac{1}{\left\|\omega_{\alpha}\right\|_{L^{1}(\rho_{t})}} \left\|\nabla G\right\|_{2}} e^{-\alpha \mathcal{E}(v)} \rho_{t} \, dH_{d-1}(v), \end{split}$$

where in the first and second inequalities, we used Assumption 2 (C1) that $||v_u - v^*|| \le \tau_1(u)$ and the fact that τ_1 is an increasing function. Thus

$$\leq \int_{\{G(v)=\tilde{u}\}} \frac{\|v-v^*\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} \|\nabla G\|_{2} e^{-\alpha \mathcal{E}(v)} \rho_{t} dH_{d-1}(v)$$

$$\leq \tilde{r} \int_{\{G(v)=\tilde{u}\}} \frac{1}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} \|\nabla G\|_{2} e^{-\alpha \mathcal{E}(v)} \rho_{t} dH_{d-1}(v)$$

$$+ \frac{e^{-\alpha \left(q-\tau_{3}(\max\{u,r\})\right)}}{\rho_{t} \left(B^{\infty}(v^*,r)\right)} \int_{\{G(v)=\tilde{u}\}} \frac{\|v-v_{\tilde{u}}\|_{\infty}}{\|\nabla G\|_{2}} \rho_{t} dH_{d-1}(v)$$

$$+ \tau_{1}(u) \int_{\{G(v)=\tilde{u}\}} \frac{1}{\|\omega_{\alpha}\|_{1}} \|\nabla G\|_{2} e^{-\alpha \mathcal{E}(v)} \rho_{t} dH_{d-1}(v).$$

We can integrate the above inequality with respect to \tilde{u} from 0 to u to get

$$\int_{\{G\in(0,u)\}} \frac{\|v-v^*\|_{\infty}}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} e^{-\alpha\mathcal{E}(v)} d\rho_{t}(v)$$

$$\leq \qquad \left(\tilde{r}+\tau_{1}(u)\right) \int_{0}^{u} d\tilde{u} \int_{\{G(v)=\tilde{u}\}} \frac{1}{\|\omega_{\alpha}\|_{L^{1}(\rho_{t})}} \|\nabla G\|_{2} e^{-\alpha\mathcal{E}(v)} \rho_{t} dH_{d-1}(v)$$

$$+ \frac{e^{-\alpha\left(q-\tau_{3}(\max\{u,r\})\right)}}{\rho_{t}\left(B^{\infty}(v^{*},r)\right)} \int_{0}^{u} d\tilde{u} \int_{\{G(v)=\tilde{u}\}} \frac{\|v-v_{\tilde{u}}\|_{\infty}}{\|\nabla G\|_{2}} \rho_{t} dH_{d-1}(v)$$

$$= \qquad \tilde{r}+\tau_{1}(u) + \frac{e^{-\alpha\left(q-\tau_{3}(\max\{u,r\})\right)}}{\rho_{t}\left(B^{\infty}(v^{*},r)\right)} \int_{\{G\in(0,u)\}} \|v-v_{G(v)}\|_{\infty} d\rho_{t}(v),$$

where in the equality, we used the co-area formula again and the definition of ω_{α} . Then combining with the fact that $\|\cdot\|_{\infty} \leq \|\cdot\|_2 \leq \sqrt{d} \|\cdot\|_2$ finishes the proof.

Appendix F. The Complete Proof of Lemma 4.5

Proof. Since $\phi_r \leq 1$, one can show that

$$\rho_t(B(v^*,r)) \ge \int \phi_r(v) \, d\rho_t(v).$$

So it suffices to find a lower bound for $\int \phi_r(v) d\rho_t(v)$. To do this, since $\phi_r \in \mathcal{C}^2_*(\mathbb{R}^d)$, one can plug ϕ_r into the Definition (3.2) to get that

$$\frac{d}{dt}\int\phi_r(v)\,d\rho_t(v)=\int\left(T_1(v)+T_2(v)+T_3(v)\right)d\rho_t(v),$$

where

$$T_1(v) = -\lambda \left(v - v_\alpha(\rho_t) \right) \cdot \nabla \phi_r(v),$$

$$T_2(v) = \frac{\sigma^2}{2} \sum_{k=1}^d \left(v - v_\alpha(\rho_t) \right)_k^2 \partial_{kk} \phi_r(v)$$

and

$$T_3(v) = -\frac{1}{\epsilon} \int \left\langle \nabla G, \nabla \phi \right\rangle.$$

One can calculate directly that

$$\nabla \phi_r(v) = -2r^2 \frac{v - v^*}{\left(r^2 - \left\|v - v^*\right\|^2\right)^2} \phi_r(v),$$

$$\partial_{kk} \phi_r(v) = 2r^2 \left(\frac{2\left(2(v - v^*)_k^2 - r^2\right)(v - v^*)_k^2 - d\left(r^2 - (v - v^*)_k^2\right)^2}{\left(r^2 - (v - v^*)_k^2\right)^4}\right) \phi_r(v).$$

By the expression of $\nabla \phi_r$, one knows that $T_3 \ge 0$ because of Assumption 2 (B1). Thus wone only has to find the lower bound of T_1 and T_2 . The details of bounding them are exactly the same as [16] Proposition 2. Following the same steps, it turns out

$$\int (T_1(v) + T_2(v)) d\rho_t(v) \ge -a \int \phi_r(v) d\rho_t(v),$$

where a is the constant defined in the statement of Theorem 4.5. Thus

$$\frac{d}{dt} \int \phi_r(v) \, d\rho_t(v) \\ = \int \left(T_1(v) + T_2(v) + T_3(v) \right) \, d\rho_t(v) \ge \int \left(T_1(v) + T_2(v) \right) \, d\rho_t(v) \ge -a \int \phi_r(v) \, d\rho_t(v).$$

Then applying Gronwall's inequality will finish the proof.

Appendix G. Proof of Lemma 4.6

Proof. Let $B = \sup_{t \in [0,T]} \|v_{\alpha}(\rho_t) - v^*\|_2$ and $\tilde{B} = \sup_{t \in [0,T]} \mathcal{V}(\rho_t)$. Also, because of Assumption 2 (B2) that $G(v) \in C^2_*(\mathbb{R}^d)$ and $G(v) \lesssim \|\nabla G(v)\|_2^2$, one can find some positive constant \tilde{c} such that

$$\left|\partial_{kk}G(v)\right| \le \tilde{c}, \left\|\nabla G(v)\right\| \le \tilde{c}\left(1 + \left\|v - v^*\right\|\right)$$
(68)

and

$$G(v) \le \tilde{c} \|\nabla G(v)\|^2.$$
⁽⁶⁹⁾

Plug G into Definition 3.2 gives

$$\frac{d}{dt} \int G \, d\rho_t(v) = -\lambda \int \left\langle v - v_\alpha(\rho_t), \nabla G \right\rangle d\rho_t(v) + \frac{\sigma^2}{2} \int \sum_{k=1}^d \left(v - v_\alpha(\rho_t) \right)_k^2 \partial_{kk} G \, d\rho_t(v)
- \frac{1}{\epsilon} \int \left\| \nabla G \right\|_2^2 d\rho_t(v)
\leq -\lambda \int \left\langle v - v^*, \nabla G \right\rangle d\rho_t(v) - \lambda \int \left\langle v^* - v_\alpha(\rho_t), \nabla G \right\rangle d\rho_t(v)
+ \sigma^2 \int \sum_{k=1}^d \left((v - v^*)_k^2 + \left(v^* - v_\alpha(\rho_t) \right)_k^2 \right) \partial_{kk} G \, d\rho_t(v) - \frac{1}{\epsilon} \int \left\| \nabla G \right\|_2^2 d\rho_t(v)$$

The first term is non-positive because of Assumption 2 (B1) and the second term can be bounded as follows

$$\begin{aligned} -\lambda \int \left\langle v^* - v_{\alpha}(\rho_t), \nabla G \right\rangle d\rho_t(v) &\leq \lambda \int \left\| v^* - v_{\alpha}(\rho_t) \right\| \left\| \nabla G \right\| d\rho_t(v) \\ &\leq \lambda \int B \left\| \nabla G \right\| d\rho_t(v) \\ &\leq \lambda B \tilde{c} \int \left(1 + \left\| v - v^* \right\| \right) d\rho_t(v) \\ &\leq \lambda B \tilde{c} \left(1 + \sqrt{2\tilde{B}} \right), \end{aligned}$$

where the third inequality above is due to (68). The third term is bounded above by $\tilde{c}\sigma^2(\tilde{B} + B^2)$ and the fourth term is upper bounded by $-\frac{1}{\tilde{c}\epsilon}\int G\,d\rho_t(v)$ because of (69). Thus one has

$$\frac{d}{dt} \int G \, d\rho_t(v) \le \lambda B\tilde{c} \left(1 + \sqrt{2\tilde{B}}\right) + \tilde{c}\sigma^2 \left(\tilde{B} + B^2\right) - \frac{1}{\epsilon\tilde{c}} \int G \, d\rho_t(v).$$

We use D to denote $\lambda B\tilde{c}\left(1+\sqrt{2\tilde{B}}\right)+\tilde{c}\sigma^{2}(\tilde{B}+B^{2}).$

Now consider f satisfying

$$\frac{d}{dt}f = D - \frac{1}{\tilde{c}\epsilon}f$$

with initial condition $f(0) = \int G d\rho_0(v)$. By the comparison theorem, one knows that before T, $\int G d\rho_t(v)$ is dominated by f, i.e. $\int G d\rho_t(v) \leq f(t)$. And one has an explicit expression for f:

$$f(t) = \tilde{c}\epsilon D + (\int G d\rho_0(v) - \tilde{c}\epsilon D)e^{-(1/\tilde{c}\epsilon)t}$$

When ϵ is small enough, i.e.,

$$\epsilon < \frac{\int G \, d\rho_0(v)}{\tilde{c}D},\tag{70}$$

one can deduce

$$f(t) = \tilde{c}\epsilon D + \left(\int G \,d\rho_0(v) - \tilde{c}\epsilon D\right) e^{-(1/\tilde{c}\epsilon)t} \leq \tilde{c}\epsilon D + \left(\int G \,d\rho_0(v) - \tilde{c}\epsilon D\right) = \int G \,d\rho_0(v).$$

Thus for $t \in [0,T]$,

$$\int G \, d\rho_t(v) \le \int G \, d\rho_0(v)$$

This completes the proof.

APPENDIX H. DETAILS OF THE NUMERICAL EXPERIMENTS

H.1. Figures 1 and Figure 2. The objective function $\mathcal{E}(v)$ is the similar to (35)

$$\min_{v} -A \exp\left(-a\sqrt{\frac{b^2}{d}\|v-\hat{v}\|_2^2}\right) - \exp\left(\frac{1}{d}\sum_{i=1}^d \cos(2\pi b(v-\hat{v})_i)\right) + e^1 + A;$$

with b = 3, A = 20, a = 0.2. The circular constraint reads,

$$g_1(v) = \|v\|_2^2 - 1;$$

and the parabolic constraint reads,

$$g_2(v) = v_1^2 - v_2.$$

The first case is a circular constraint, and the unconstrained minimizer is the same as the constrained minimizer.

$$\hat{v} = v^* = \frac{1}{\sqrt{2}}(1, -1).$$

the second case is a circular constraint, and the unconstrained minimizer is different from the constrained minimizer. Therefore,

$$\hat{v} = (1/2, 1/3), \quad v^* = (0.781475; \sqrt{1 - 0.781475^2}).$$

The third case is a parabolic constraint, and the unconstrained minimizer is different from the constrained minimizer. Therefore,

$$\hat{v} = (1/2, 1/3), \quad v^* = (0.5428; 0.5428^2).$$

We use Algorithm 1 with

$$N = 50, \ \alpha = 30, \ \epsilon = 0.01, \ \lambda = 1, \ \sigma = 1, \ \gamma = 0.01, \ \epsilon_{\text{stop}} = 0.$$
(71)

We set ϵ_{stop} to be 0 to see the iteration evolves until it reaches 300 steps. All the particles initially follow Unif $[-3,3]^2$. We consider the algorithm successful in finding the constrained minimizer v^* if the distance between the consensus point v_{α} and v^* satisfies $||v^* - v_{\alpha}||_{\infty} < 0.01$. The distance is measured in terms of (34).

We use Algorithm 1 in [13] for the projected CBO method. For the penalized CBO method, we set the penalty as $\frac{1}{\epsilon}G(v)$, and then apply the CBO algorithm to the following unconstrained optimization problem,

$$\mathcal{E}^{\epsilon}(v) = \mathcal{E}(v) + \frac{1}{\epsilon}G(v).$$

We use the same parameters as (71) for the two alternative algorithms.

References

- [1] L. Arnold. Stochastic Differential Equations: Theory and Applications. Wiley, New York, 1974.
- [2] R. F. Bass. Stochastic Processes. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge University Press, 2011.
- [3] C. M. Bender and S. A. Orszag. Advanced mathematical methods for scientists and engineers I: Asymptotic methods and perturbation theory, volume 1. Springer, New York, 1999.
- [4] G. Borghi, M. Herty, and L. Pareschi. Constrained consensus-based optimization. SIAM Journal on Optimization, 33(1):211–236, 2023.
- [5] J. A. Carrillo, Y.-P. Choi, C. Totzeck, and O. Tse. An analytical framework for consensus-based global optimization method. *Mathematical Models and Methods in Applied Sciences*, 28(06):1037–1066, 2018.
- [6] J. A. Carrillo, S. Jin, L. Li, and Y. Zhu. A consensus-based global optimization method for high dimensional machine learning problems. *ESAIM: Control, Optimisation and Calculus of Variations*, 27:S5, 2021.
- [7] J. A. Carrillo, C. Totzeck, and U. Vaes. Consensus-based optimization and ensemble kalman inversion for global optimization problems with constraints. In *Modeling and Simulation for Collective Dynamics*, pages 195–230. World Scientific, 2023.
- [8] R. Chai, S. Chai A. Savvaris, A. Tsourdos, and Y. Xia. A review of optimization techniques in spacecraft flight trajectory design. *Progress in Aerospace Sciences*, 109:100543, 2019.
- [9] J. Chen, S. Jin, and L. Lyu. A consensus-based global optimization method with adaptive momentum estimation. *Communications in Computational Physics*, 31(4):1296–1316, 2022.
- [10] A. Dembo and O. Zeitouni. Large deviations techniques and applications, volume 38. Springer Berlin, Heidelberg, 2009.
- [11] R. Durrett. Stochastic Calculus: A Practical Introduction. Probability and Stochastics Series. CRC Press, 1996.
- [12] M. Fornasier, H. Huang, L. Pareschi, and P. Sünnen. Consensus-based optimization on hypersurfaces: Well-posedness and mean-field limit. *Mathematical Models and Methods in Applied Sciences*, 30(14):2725–2751, 2020.
- [13] M. Fornasier, H. Huang, L. Pareschi, and P. Sünnen. Consensus-based optimization on the sphere: Convergence to global minimizers and machine learning. *The Journal of Machine Learning Research*, 22(1):10722–10776, 2021.
- [14] M. Fornasier, H. Huang, L. Pareschi, and P. Sünnen. Anisotropic diffusion in consensus-based optimization on the sphere. SIAM Journal on Optimization, 32(3):1984–2012, 2022.
- [15] M. Fornasier, T. Klock, and K. Riedl. Consensus-based optimization methods converge globally. arXiv preprint arXiv:2103.15130, 2021.
- [16] M. Fornasier, T. Klock, and K. Riedl. Convergence of anisotropic consensus-based optimization in mean-field law. In Juan Luis Jiménez Laredo, J. Ignacio Hidalgo, and Kehinde Oluwatoyin Babaagba, editors, *Applications of Evolutionary Computation*, pages 738–754. Springer International Publishing, 2022.
- [17] M. Fornasier, P. Richtárik, K. Riedl, and L. Sun. Consensus-based optimization with truncated noise. arXiv preprint arXiv:2310.16610, 2023.
- [18] N. J. Gerber, F. Hoffmann, and U. Vaes. Mean-field limits for consensus-based optimization and sampling. arXiv preprint arXiv:2312.07373, 2023.
- [19] D. Gilbarg and N.S. Trudinger. Elliptic Partial Differential Equations of Second Order. Classics in Mathematics. Springer Berlin, Heidelberg, 2001.
- [20] R. V. Grandhi and V. B. Venkayya. Structural optimization with frequency constraints. AIAA Journal, 26(7):858–866, 1988.

- [21] S. Grassi, H. Huang, L. Pareschi, and J. Qiu. Mean-field particle swarm optimization. In *Modeling and Simulation for Collective Dynamics*, pages 127–193. World Scientific, 2023.
- [22] S. Grassi and L. Pareschi. From particle swarm optimization to consensus based optimization: stochastic modeling and mean-field limit. *Mathematical Models and Methods in Applied Sciences*, 31(08):1625– 1657, 2021.
- [23] S.-Y. Ha, S. Jin, and D. Kim. Convergence and error estimates for time-discrete consensus-based optimization algorithms. *Numerische Mathematik*, 147:255–282, 2021.
- [24] H. Huang and J. Qiu. On the mean-field limit for the consensus-based optimization. Mathematical Methods in the Applied Sciences, 45(12):7814–7831, 2022.
- [25] H. Huang, J. Qiu, and K. Riedl. Consensus-based optimization for saddle point problems. arXiv preprint arXiv:2212.12334, 2022.
- [26] M.T. Melo, S. Nickel, and F. Saldanha da Gama. Facility location and supply chain management a review. European Journal of Operational Research, 196(2):401–412, 2009.
- [27] P. D. Miller. Applied asymptotic analysis, volume 75. American Mathematical Soc., 2006.
- [28] B. Oksendal. Stochastic differential equations: an introduction with applications. Springer Berlin, Heidelberg, 2013.
- [29] R. Pinnau, C. Totzeck, O. Tse, and S. Martin. A consensus-based model for global optimization and its mean-field limit. *Mathematical Models and Methods in Applied Sciences*, 27(01):183–204, 2017.
- [30] K. Riedl. Leveraging memory effects and gradient information in consensus-based optimisation: On global convergence in mean-field law. *European Journal of Applied Mathematics*, page 1–32, 2023.
- [31] K. Riedl, T. Klock, C. Geldhauser, and M. Fornasier. Gradient is all you need? arXiv preprint arXiv:2306.09778, 2023.
- [32] R. T. Rockafellar. Lagrange multipliers and optimality. SIAM Review, 35(2):183–238, 1993.
- [33] A. Sznitman. Topics in propagation of chaos. In Ecole d'Eté de Probabilités de Saint-Flour XIX 1989, pages 165–251. Springer Berlin, Heidelberg, 1991.
- [34] Claudia T. and Marie-Therese W. Consensus-based global optimization with personal best. Mathematical Biosciences and Engineering, 17(5):6026–6044, 2020.
- [35] C. Totzeck. Trends in consensus-based optimization. In Active Particles, Volume 3: Advances in Theory, Models, and Applications, pages 201–226. Springer, 2021.
- [36] C. Totzeck, R. Pinnau, S. Blauth, and S. Schotthöfer. A numerical comparison of consensus-based global optimization to other particle-based global optimization schemes. *Proceedings in Applied Mathematics and Mechanics*, 18:1–2, 12 2018.
- [37] E. Wei and A. Ozdaglar. Distributed alternating direction method of multipliers. In 2012 IEEE 51st IEEE Conference on Decision and Control (CDC), pages 5445–5450, 2012.
- [38] W. Yao, X. Chen, W. Luo, M. van Tooren, and J. Guo. Review of uncertainty-based multidisciplinary design optimization methods for aerospace vehicles. *Progress in Aerospace Sciences*, 47(6):450–479, 2011.

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