CONVERGENCE ANALYSIS OF MACHINE LEARNING ALGORITHMS FOR THE NUMERICAL SOLUTION OF MEAN FIELD CONTROL AND GAMES: I – THE ERGODIC CASE.

RENÉ CARMONA & MATHIEU LAURIÈRE

ABSTRACT. We propose two algorithms for the solution of the optimal control of ergodic McKean-Vlasov dynamics. Both algorithms are based on the approximation of the theoretical solutions by neural networks, the latter being characterized by their architecture and a set of parameters. This allows the use of modern machine learning tools, and efficient implementations of stochastic gradient descent. The first algorithm is based on the idiosyncrasies of the ergodic optimal control problem. We provide a mathematical proof of the convergence of the algorithm, and we analyze rigorously the approximation by controlling the different sources of error. The second method is an adaptation of the deep Galerkin method to the system of partial differential equations issued from the optimality condition.

We demonstrate the efficiency of these algorithms on several numerical examples, some of them being chosen to show that our algorithms succeed where existing ones failed. We also argue that both methods can easily be applied to problems in dimensions larger than what can be found in the existing literature. Finally, we illustrate the fact that, although the first algorithm is specifically designed for mean field control problems, the second one is more general and can also be applied to the partial differential equation systems arising in the theory of mean field games.

1. INTRODUCTION

The purpose of this paper is to develop numerical schemes for the solution of Mean Field Games (MFGs) and Mean Field Control (MFC) problems. The mathematical theory of these problems has attracted a lot of attention in the last decade (see e.g. [23, 15, 9, 17, 18]), and from the numerical standpoint several methods have been proposed, see e.g. [2, 1, 16, 11, 21] and [24, 4, 29, 7] for finite time horizon MFG and MFC respectively, and [6, 14, 12] for stationary MFG. However, despite recent progress, the numerical analysis of these problems is still lagging behind because of their complexity, in particular when the dimension is high. Here, we choose a periodic model to demonstrate that powerful tools developed for machine learning applications can be harnessed to produce efficient numerical schemes performing better than existing technology in the solution of these problems. We derive systematically the mathematical formulation of the optimization problem amenable to the numerical analysis, and we prove rigorously the convergence of a numerical scheme based on feed-forward neural network architectures. Our first method is designed for the optimal control of McKean-Vlasov dynamics, which is the primary purpose of the present work. Besides the intrinsic motivations for this type of problems, a large class of MFGs has a variational structure and can be recast in this form, see e.g. [23, 8]. Furthermore, the second method we present tackles the PDE system characterizing optimality conditions satisfied by the solution, and it can be directly adapted to solve the PDE system arising in MFGs as we shall explain.

In the subsequent analysis of finite horizon mean field control problems, see [19], the thrust of the study will be the numerical solution of Forward-Backward Stochastic Differential Equations (FBSDEs) of the McKean-Vlasov type. Indeed, the well established probabilistic approach to MFGs and MFC

posits that the search for Nash equilibria for MFGs, as well as the search for optimal controls for MFC problems, can be reduced to the solutions of FBSDEs of this type. See for example the books [17, 18] for a comprehensive exposé of this approach. Here, we concentrate on the ergodic problem for which we can provide a direct analytic approach. Our mathematical analysis of the model leads to an infinite dimensional optimization problem for which we can identify and implement numerical schemes capable of providing stable numerical solutions. We prove the theoretical convergence of these approximation schemes and we demonstrate the efficiency of their implementations by comparing their outputs to solutions of benchmark models obtained either by analytical formulas or by a deterministic method for Partial Differential Equations (PDEs).

The reasons for our choice of the ergodic case as a prime testbed for our numerical schemes are twofold. First, the absence of the time variable lowers the complexity of the problem and gives us the opportunity to avoid the use of FBSDEs and to rely on strong approximation results from the theory of feed-forward neural networks which we use in this paper. Second, the objective function can be expressed as an integral over the state space with respect to the invariant measure of the controlled system, leading to a much simpler deterministic optimization problem. Indeed, after proving that the state dynamics at the optimum are given by a gradient diffusion, we postulate the form of the invariant measure and optimize accordingly. Last, the choice of the ergodic case for the first model which we consider is motivated by a forthcoming work on reinforcement learning [20].

As a final remark we emphasize that, while all the results and numerical implementations concern Markovian controls and equilibria, in most cases, both theoretical and numerical results still hold for controls and strategies being feedback functions of the history of the path of the state of the system. The theoretical extensions are straightforward, and the numerical implementations rely on the so-called *recurrent neural networks* instead of the standard feed-forward networks. We refrain from discussing these extensions to avoid the extra technicalities, especially in the notations and the statements of the results.

The paper is structured as follows. In Section 2, we present the framework of ergodic mean field control, derive formally necessary optimality conditions and introduce a setting amenable to numerical computations. To wit, we provide the mathematics that lead to natural introductions of the algorithms and their analyses. The first algorithm is presented in Section 3. We study rigorously its convergence and its accuracy by proving bounds on the approximation and estimation errors (see Theorems 4 and 8 respectively). Section 4 is dedicated to the second of our algorithms. It is based on a variation over the deep Galerkin solver for the PDE system stemming from the aforementioned optimality conditions. Computational results are presented in Section 5. They demonstrate the applicability and the performance of our algorithms. Several test cases are considered. They were chosen because they can be solved either *explicitly* via analytical formulas or numerically by classical PDE system solvers like in the case of ergodic mean field games.

2. Ergodic Mean Field Control

Since we are not aiming at the greatest possible generality, for the sake of definiteness, we work with a standard infinite horizon drift-controlled Itô process:

$$dX_t = b(X_t, \mathcal{L}(X_t), \alpha_t)dt + \sigma dW_t$$

where $\mathbf{W} = (W_t)_{t \geqslant 0}$ is a d-dimensional Wiener process and where we use the notation $\mathcal{L}(X_t)$ for the law of the random variable X_t. We limit ourselves to stationary controls $\boldsymbol{\alpha} = (\alpha_t)_{t \geqslant 0}$ of the form $\alpha_t = \phi(X_t)$ given by deterministic measurable and time-independent feedback functions ϕ taking values in a closed

convex subset A of a Euclidean space $\mathbb{R}^k$. We shall assume that the function b is measurable and bounded on $\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \times A$, and, for notational convenience only, that $\sigma = 1$. The space $\mathcal{P}_2(\mathbb{R}^d)$ is the space of probability measures on $\mathbb{R}^d$ having a finite second moment. We assume that it is equipped with the 2-Wasserstein distance and the corresponding Borel σ-field. Since we consider controls in feedback form, the above controlled state evolution is in fact a stochastic differential equation, but according to Veretennikov's classical result, this equation:

$$(1) \qquad dX_t = b(X_t, \mathcal{L}(X_t), \phi(X_t))dt + \sigma dW_t$$

has a unique strong solution. See for example [32, 33] and [28, Theorem 2]. We say that the feedback control function ϕ is admissible if it is continuous and if the solution $\mathbf{X} = (X_t)_{t \geqslant 0}$ is ergodic in the sense that it has a unique invariant measure which we denote by ν^ϕ and that $\mathcal{L}(X_t)$ converges toward ν^ϕ in $\mathcal{P}_2(\mathbb{R}^d)$. The ergodic theory of McKean-Vlasov stochastic differential equations has recently received a lot of attention. See for example [13, 33, 34] for some specific ergodicity sufficient conditions.

2.1. Ergodic Mean Field Costs.

The goal of the ergodic control problem is to minimize the cost:

$$J(\phi) = \limsup_{T \to \infty} \frac{1}{T} \mathbb{E}\Big[\int_0^T f\big(X_t, \mathcal{L}(X_t), \phi(X_t)\big)dt\Big].$$

For the sake of definiteness, we assume that the running cost function $f : \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \times A \ni (x, \mu, \alpha) \mapsto f(x, \mu, \alpha) \in \mathbb{R}$ is continuous and bounded. The cost can be rewritten in the form:

$$(2) \qquad J(\phi) = \limsup_{T \to \infty} \frac{1}{T} \int_0^T \langle f\big(\cdot, \mu_t, \phi(\cdot)\big), \mu_t \rangle dt, \qquad \mu_t = \mathcal{L}(X_t),$$

if we use the standard notation $\langle \varphi, \nu \rangle$ for the integral of the function φ with respect to the measure ν. When ϕ is admissible, the invariant measure ν^ϕ appears as the limit as $t \to \infty$ of μ_t, and if f is uniformly continuous in the measure argument, uniformly with respect to the other two arguments, then we can take the limit $T \to \infty$ in the formula giving the ergodic cost (2) and obtain:

$$(3) \qquad J(\phi) = \langle f\big(\cdot, \nu^\phi, \phi(\cdot)\big), \nu^\phi \rangle = F(\nu^\phi, \phi)$$

if, for each probability measure $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, and each time-independent A-valued feedback function ϕ on $\mathbb{R}^d$ we use the notation:

$$(4) \qquad F(\mu, \phi) = \int f\big(x, \mu, \phi(x)\big) \, \mu(dx).$$

The controlled process solving (1) being ergodic, we can characterize the unique invariant probability measure as the solutions of the non-linear Poisson equation:

$$(5) \qquad \frac{1}{2}\Delta\nu - \operatorname{div}\big(b(\cdot, \nu, \phi(\cdot))\nu\big) = 0.$$

So the goal of our mean field control problem is to minimize, over the admissible feedback functions ϕ, the quantity:

$$(6) \qquad J(\phi) = F(\nu^\phi, \phi),$$

with F defined above in (4) and ν^ϕ solving the Poisson equation (5).

2.2. **The Adjoint Equation and Optimality Conditions.** In order to characterize the minima of the functional J, we compute its Gateaux derivative. To do so, we assume that the function $b :$ $\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \times A \ni (x, \mu, \alpha) \mapsto b(x, \mu, \alpha) \in \mathbb{R}^d$ is continuously differentiable in the variables $(x, \alpha) \in$ $\mathbb{R}^d \times A \subset \mathbb{R}^d \times \mathbb{R}^k$ and has a continuous functional (i.e. linear) differential in the variable μ when μ is viewed as an element of the (linear) space $\mathcal{M}(\mathbb{R}^d)$ of finite signed measures on $\mathbb{R}^d$. We denote this last derivative as $D_\mu b$. We stress that it is different from the Wasserstein or L-derivative in the sense of Lions.

Let ϕ be fixed and let ψ provide a small perturbation of ϕ. We first compute, at least formally, the derivative of the probability ν^ϕ in the direction ψ, namely:

$$(7) \qquad \delta\nu^{\phi,\psi} = \lim_{\epsilon \searrow 0} \frac{1}{\epsilon}[\nu^{\phi+\epsilon\psi} - \nu^\phi],$$

when we view probability measures as elements of the space $\mathcal{M}(\mathbb{R}^d)$ of finite (signed) measures on $\mathbb{R}^d$. Notice that since $\int \nu^\phi = \int \nu^{\phi+\epsilon\psi} = 1$, we must have $\int \delta\nu^{\phi,\psi} = 0$. The Poisson equation (5) implies:

$$0 = \frac{1}{2}\Delta[\nu^{\phi+\epsilon\psi} - \nu^\phi] - \mathrm{div}\big[\, b(\cdot, \nu^{\phi+\epsilon\psi}, \phi(\cdot) + \epsilon\psi(\cdot))\,[\nu^{\phi+\epsilon\psi} - \nu^\phi]\big]$$

$$- \mathrm{div}\big[\, [b(\cdot, \nu^{\phi+\epsilon\psi}, \phi(\cdot) + \epsilon\psi(\cdot)) - b(\cdot, \nu^{\phi+\epsilon\psi}, \phi(\cdot))]\,\nu^\phi\big]$$

$$- \mathrm{div}\big[\, [b(\cdot, \nu^{\phi+\epsilon\psi}, \phi(\cdot)) - b(\cdot, \nu^\phi \phi(\cdot))]\,\nu^\phi\big]$$

and from this equality, we find that if the directional derivative (7) exists, it must solve the following Partial Differential Equation (PDE):

$$(8)$$
$$0 = \frac{1}{2}\Delta(\delta\nu^{\phi,\psi}) - \mathrm{div}\big[\, b(\cdot, \nu^\phi, \phi(\cdot))\,(\delta\nu^{\phi,\psi})\big] - \mathrm{div}\big[\partial_\alpha b(\cdot, \nu^\phi, \phi(\cdot))\psi(\cdot)\nu^\phi\big] - \mathrm{div}\big[\langle D_\mu b(\cdot, \nu^\phi, \phi(\cdot))\psi(\cdot), \delta\nu^{\phi,\psi}\rangle\nu^\phi\big],$$

just by dividing both sides by ϵ and taking the limit $\epsilon \searrow 0$. Note that the quantity

$$\langle \partial_\mu b(\cdot, \nu^\phi, \phi(\cdot))\psi(\cdot), \delta\nu^{\phi,\psi}\rangle$$

is merely the integral of the function $\partial_\mu b(\cdot, \nu^\phi, \phi(\cdot))\psi(\cdot)$ with respect to the measure $\delta\nu^{\phi,\psi}$.

Before we turn to the objective function J, we introduce the notion of adjoint equation and adjoint function.

Definition 1. *For each admissible feedback function ϕ (and associated solution ν^ϕ of the Poisson equation), we say that the couple (p, λ) where p is a function on the state space and λ is a constant, is a couple of adjoint variables if they satisfy the following linear elliptic PDE:*

$$(9) \qquad \lambda + \frac{1}{2}\Delta p(x) + b(x, \nu^\phi, \phi(x)) \cdot \nabla p(x) = f(x, \nu^\phi, \phi(x)) + \int D_\mu f(\xi, \nu^\phi, \phi(\xi))(x)\, \nu^\phi(d\xi),$$

which we call the adjoint equation. Any solution will be denoted by (p^ϕ, λ^ϕ).

Recall that here, the derivative $D_\mu f$ is the standard linear functional derivative (of smooth functions on the vector space $\mathcal{M}(\mathbb{R}^d)$), which is a function of x.

Proposition 2. *The directional derivative of the cost function J defined in (6) is given by the formula:*

$$(10) \qquad \frac{d}{d\epsilon}J(\phi + \epsilon\psi)\Big|_{\epsilon=0} = \delta^{\phi,\psi}H(\nu^\phi, p^\phi, \phi),$$

where $\delta^{\phi,\psi}$ denotes the functional derivative with respect to ϕ in the direction ψ, and the Hamiltonian H is defined by:

$$(11) \qquad H(\mu, p, \phi) = F(\mu, \phi) + \int p(x)\mathrm{div}[b(\cdot, \mu, \phi(\cdot))\mu](x)dx$$

Proof. Using the definitions (6) and (4) we get:

$$J(\phi + \epsilon\psi) - J(\phi) = \int f(x, \nu^{\phi+\epsilon\psi}, \phi(x) + \epsilon\psi(x))\nu^{\phi+\epsilon\psi}(dx) - \int f(x, \nu^{\phi}, \phi(x))\nu^{\phi}(dx)$$

$$= \int \left[f(x, \nu^{\phi+\epsilon\psi}, \phi(x) + \epsilon\psi(x)) - f(x, \nu^{\phi}, \phi(x) + \epsilon\psi(x)) \right]\nu^{\phi+\epsilon\psi}(dx)$$

$$+ \int \left[f(x, \nu^{\phi}, \phi(x) + \epsilon\psi(x)) - f(x, \nu^{\phi}, \phi(x)) \right]\nu^{\phi+\epsilon\psi}(dx)$$

$$+ \int f(x, \nu^{\phi}, \phi(x))\left[\nu^{\phi+\epsilon\psi} - \nu^{\phi} \right](dx),$$

so that, using Fubini's theorem we have:

$$\frac{d}{d\epsilon}J(\phi + \epsilon\psi)\Big|_{\epsilon=0} = \int\int D_\mu f(x, \nu^{\phi}, \phi(x))(\xi)\,(\delta\nu^{\phi,\psi})(d\xi)\,\nu^{\phi}(dx)$$

$$+ \int \partial_\alpha f(x, \nu^{\phi}, \phi(x))\psi(x)\,\nu^{\phi}(dx) + \int f(x, \nu^{\phi}, \phi(x))\,(\delta\nu^{\phi,\psi})(dx)$$

$$= \int\left[\int D_\mu f(y, \nu^{\phi}, \phi(y))(x)\nu^{\phi}(dy) + f(x, \nu^{\phi}, \phi(x))\right]\,(\delta\nu^{\phi,\psi})(dx)$$

$$+ \int \partial_\alpha f(x, \nu^{\phi}, \phi(x))\psi(x)\,\nu^{\phi}(dx).$$

Now, using the adjoint equation (9) and the fact that the integral of $\delta\nu^{\phi,\psi}$ is 0, we get:

$$\frac{d}{d\epsilon}J(\phi + \epsilon\psi)\Big|_{\epsilon=0} = \int\left[\lambda + \frac{1}{2}\Delta p(x) + b(x, \nu^{\phi}, \phi(x))\cdot\nabla p(x)\right]\,(\delta\nu^{\phi,\psi})(dx)$$

$$+ \int \partial_\alpha f(x, \nu^{\phi}, \phi(x))\psi(x)\,\nu^{\phi}(dx)$$

$$= \int p(x)\frac{1}{2}\Delta(\delta\nu^{\phi,\psi})(x)dx + \int b(x, \nu^{\phi}, \phi(x))\cdot\nabla p(x)\,(\delta\nu^{\phi,\psi})(dx)$$

$$+ \int \partial_\alpha f(x, \nu^{\phi}, \phi(x))\psi(x)\,\nu^{\phi}(dx).$$

Finally, using (8) we get:

$$\frac{d}{d\epsilon}J(\phi + \epsilon\psi)\Big|_{\epsilon=0} = \int p(x)\Big(\mathrm{div}[\partial_\alpha b(\cdot, \phi(\cdot))\psi(\cdot)\nu^{\phi}](x) + \mathrm{div}[\langle D_\mu b(\cdot, \nu^{\phi}, \phi(\cdot))\psi(\cdot), \delta\nu^{\phi,\psi}\rangle\nu^{\phi}](x)\Big)dx$$

$$(12) \qquad\qquad + \int \partial_\alpha f(x, \nu^{\phi}, \phi(x))\psi(x)\,\nu^{\phi}(dx).$$

To complete the proof, we express this directional derivative in terms of the Hamiltonian function defined in (11). The latter can be rewritten as:

$$H(\mu, p, \phi) = F(\mu, \phi) - \int \nabla p(x)b(x, \mu, \phi(x))\mu(dx),$$

and its directional derivative is given by:

$$\delta^{\phi,\psi} H(\mu, p, \phi) = \lim_{\epsilon \searrow 0} \frac{1}{\epsilon} [H(\mu, p, \phi + \epsilon\psi) - H(\mu, p, \phi)]$$

(13)
$$= \int \partial_\alpha f(x, \mu, \phi(x))\psi(x)\mu(dx) - \int \nabla p(x)\partial_\alpha b(x, \mu, \phi(x))\psi(x)\mu(dx)$$

$$= \int \Big[\partial_\alpha f(x, \mu, \phi(x)) - \nabla p(x)\partial_\alpha b(x, \mu, \phi(x))\Big]\psi(x)\mu(dx).$$

Putting together (12) and (13) we get the desired result. $\qquad\square$

So, at least informally, solving the ergodic McKean-Vlasov control problem reduces to the solution of the system:

(14)
$$\begin{cases} 0 = \frac{1}{2}\Delta\nu - \mathrm{div}\big(b(\cdot, \nu, \phi(\cdot))\nu\big) \\ 0 = \lambda + \frac{1}{2}\Delta p(x) + b(x, \nu, \phi(x)) \cdot \nabla p(x) - \int D_\mu f(\xi, \nu, \phi(\xi))(x)\,\nu(d\xi) - f(x, \nu, \phi(x)) \\ 0 = \partial_\alpha f(x, \nu, \phi(x)) - \nabla p(x)\partial_\alpha b(x, \nu, \phi(x)). \end{cases}$$

Note that the third equation guarantees the criticality of the function $\alpha \mapsto f(x, \nu, \alpha) - y \cdot b(x, \nu, \alpha)$, so if we define the minimized Hamiltonian $H^\star$ by:

(15)
$$H^\star(x, \mu, y) = \inf_\alpha \big(f(x, \mu, \alpha) - y \cdot b(x, \mu, \alpha)\big),$$

the above system can be written as:

(16)
$$\begin{cases} 0 = \frac{1}{2}\Delta\nu + \mathrm{div}\big(\partial_y H^\star(\cdot, \nu, \nabla p(\cdot))\nu\big) \\ 0 = \lambda + \frac{1}{2}\Delta p(x) - H^\star(x, \nu, \nabla p(x)) - \int D_\mu H^\star(\xi, \nu, \phi(\xi))(x)\,\nu(d\xi). \end{cases}$$

Both systems should be completed with appropriate boundary conditions when needed (like for example in the next subsection where we use periodic boundary conditions to analyze the system on the torus) and the following condition:

$$\int \nu(x)dx = 1,$$

to which we can add the normalization condition:

$$\int p(x)dx = 0$$

to guarantee uniqueness for p. Indeed, the above equations (16) can only determine p up to an additive constant.

2.3. **A Class of Models Amenable to Numerical Computations.** In general, computing the invariant distribution solving (5) for a given ϕ can be costly. For example, it can be estimated by solving the PDE or by using Monte Carlo simulations for the MKV dynamics (1), see e.g. [10]. To simplify the presentation and focus on the main ingredients of the method proposed here, we shall consider a setting in which the optimal invariant distribution as well as the optimal control can both be expressed directly in terms of an adjoint variable.

From now on we assume that $k = d$ and:

$$b(x, \alpha) = b_0\alpha + \nabla\tilde{b}(x), \qquad \text{and} \qquad f(x, \mu, \alpha) = \frac{1}{2}|\alpha|^2 + \int \tilde{f}(x, \xi)\mu(d\xi)$$

for a constant b_0 and functions $\tilde{b}$ and $\tilde{f}$ satisfying the following assumption.

Assumption: $\tilde{b}$ is of class $\mathcal{C}^1$, and $\nabla\tilde{b}$ and $\tilde{f}$ are Lipschitz in both variables.

Let $(\nu^\star, p^\star, \phi^\star)$ be a solution to the optimality system (14). In this setting, the third equation of (14) gives $\phi^\star(x) = b_0\nabla p^\star(x)$. Substituting in the expression for the drift b and the feedback function $\phi^\star$ into the state equation (1), we see that at the optimum, we are dealing with a *gradient diffusion*:

$$dX_t = \frac{1}{2}\nabla h^\star(X_t)dt + dW_t$$

for the function

$$(17) \qquad h^\star(x) = 2\big(b_0^2 p^\star(x) + \tilde{b}(x)\big).$$

Accordingly, the invariant measure is necessarily of the form:

$$\nu^\star(x) = \frac{e^{h^\star(x)}}{\int e^{h^\star(x)}dx}.$$

Notice that the optimal control is given by

$$(18) \qquad \phi^\star(x) = b_0\nabla p^\star(x) = \frac{1}{b_0}\big(\frac{1}{2}\nabla h^\star(x) - \nabla\tilde{b}(x)\big).$$

Hence minimizing the ergodic cost (3) over controls ϕ under the constraint coming from the Poisson equation (5) can be rephrased as the problem of minimizing the functional:

$$(19) \qquad \tilde{J}(h) = \int\int \widetilde{F}\left(x, y, \nabla h(x), e^{h(x)}, e^{h(y)}, \int e^{h(z)}dz\right)\,dxdy,$$

over functions h, where:

$$(20) \qquad \widetilde{F}(x, y, q, X, Y, Z) = \check{f}(x, y, q)\,XYZ^{-2}$$

with:

$$\check{f}(x, y, q) = \frac{1}{2}\left|\frac{1}{b_0}\big(\frac{1}{2}q - \nabla\tilde{b}(x)\big)\right|^2 + \tilde{f}(x, y).$$

Notice that $F(x, y, q, \alpha X, \alpha Y, \alpha Z) = F(x, y, q, X, Y, Z)$ for all non-zero $\alpha \in \mathbb{R}$. Hence, $\tilde{J}(h + c) = \tilde{J}(h)$ for every constant $c \in \mathbb{R}$. So if $h^\star$ minimizes $\tilde{J}$, so does $h^\star + c$ for any constant $c \in \mathbb{R}$. This is not an issue to guarantee that the optimal value of $\tilde{J}$ is close to the optimal value of the original cost J, but it can lead to numerical difficulties. For this reason it is possible to add a term of the form $|\int\tilde{h}|$ in (19) in order to enforce a normalization condition and hence, uniqueness of the minimizer. The analysis presented below could be adapted to take into account this extra term at the expense of more cumbersome notations, so for the sake of clarity we only consider (19).

From this point on, instead of attempting to solve the system (14) numerically, we search for the right function h in a family of functions $x \mapsto h_\theta(x)$ parameterized by the parameter $\theta \in \Theta$. The desired parameter $\theta^\star$ minimizes the functional:

$$\mathbb{J}(\theta) = \int\int \mathbb{F}_\theta(x, y)dxdy$$

where:

$$\mathbb{F}_\theta(x, y) = \int\int \widetilde{F}\left(x, y, \nabla h_\theta(x), e^{h_\theta(x)}, e^{h_\theta(y)}, \int e^{h_\theta(z)}dz\right)\,dxdy = \int\int \check{f}(x, y, \nabla h_\theta(x))\frac{e^{h_\theta(x)}}{\int e^{h_\theta(x)}dx}\frac{e^{h_\theta(y)}}{\int e^{h_\theta(y)}dy}\,dxdy.$$

One should think of the function $h_\theta(\cdot)$ as a computable approximation of $h(\cdot) = 2\big(b_0^2 p(\cdot) + \tilde{b}(\cdot)\big)$, allowing us to replace the minimization of the ergodic cost (2) by the minimization:

(21) $$\inf_{\theta \in \Theta} \int \int \mathbb{F}_\theta(x,y) dx dy.$$

Notice that the gradient (with respect to the parameter θ) of $\mathbb{F}$ can easily be computed. It reads:

$$\partial_\theta \mathbb{F}_\theta(x,y) = \mathbb{F}_\theta(x,y)\Big(\partial_\theta h_\theta(x) + \partial_\theta h_\theta(y) - 2\frac{\int \partial_\theta h_\theta e^{h_\theta}}{\int e^{h_\theta}} + \partial_\theta \log \check{f}\big(x,y,\nabla h_\theta(x)\big)\Big).$$

In anticipation of the set-up of next section where we consider our optimization problem on the torus, the double integral appearing in (21) can be viewed as an expectation, and its minimization is *screaming* for the use of the Robbins-Monro procedure. Moreover, if we use the family $(h_\theta)_{\theta \in \Theta}$ given by a feed-forward neural network, this minimization can be implemented efficiently with the powerful tools based on the so-called Stochastic Gradient Descent (SGD) developed for the purpose of machine learning.

3. A First Machine Learning Algorithm

We now restrict ourselves to the case of the torus $\mathbb{T}^d = [0, 2\pi]^d$ for the purpose of numerical computations. The admissible feedback functions ϕ being continuous, the drift $\mathbb{T}^d \ni x \mapsto b(x, \phi(x)) \in \mathbb{R}^d$ is a bounded continuous function on the torus and the controlled state process $\mathbf{X} = (X_t)_{t \geqslant 0}$ is a Markov process with infinitesimal generator:

$$L = \frac{1}{2}\Delta + b\big(\cdot, \phi(\cdot)\big)\nabla.$$

The compactness of the state space $\mathbb{T}^d$ and the uniform ellipticity of this generator guarantee that this state process is ergodic and that its invariant probability measure ν^ϕ has a $\mathcal{C}^\infty$ density with respect to the Riemannian measure on $\mathbb{T}^d$ (which we assumed to be normalized to have total mass 1). Note that, because the torus $\mathbb{T}^d$ does not have a boundary, the integration by parts which we used freely in the computations of the above subsection are fully justified in the present situation.

We introduce new notation to define the class of functions $(h_\theta)_{\theta \in \Theta}$ which we use for numerical approximation purposes. We denote by:

$$\mathbf{L}_{d_1, d_2}^\psi = \left\{ \phi : \mathbb{R}^{d_1} \to \mathbb{R}^{d_2} \,\Big|\, \exists \beta \in \mathbb{R}^{d_2}, \exists w \in \mathbb{R}^{d_2 \times d_1}, \forall i \in \{1, \ldots, d_2\},\ \phi(x)_i = \psi\left(\beta_i + \sum_{j=1}^{d_1} w_{i,j} x_j\right) \right\}$$

the set of layer functions with input dimension d_1, output dimension d_2, and activation function $\psi : \mathbb{R} \to \mathbb{R}$. Here, $\circ$ denotes the composition of functions. Building on this notation we define:

$$\mathbf{N}_{d_0, \ldots, d_{\ell+1}}^\psi = \left\{ \varphi : \mathbb{R}^{d_0} \to \mathbb{R}^{d_{\ell+1}} \,\Big|\, \forall i \in \{0, \ldots, \ell-1\}, \exists \phi_i \in \mathbf{L}_{d_i, d_{i+1}}^\psi, \exists \phi_\ell \in \mathbf{L}_{d_\ell, d_{\ell+1}},\ \varphi = \phi_\ell \circ \phi_{\ell-1} \circ \cdots \circ \phi_0 \right\}$$

the set of regression neural networks with ℓ hidden layers and one output layer, the activation function of the output layer being the identity $\psi(x) = x$. Note that as a general rule, we shall not use the superscript ψ in that case. The number ℓ of hidden layers, the numbers $d_0, d_1, \cdots, d_{\ell+1}$ of units per layer, and the activation functions (one single function ψ in the present situation), are what is usually called the architecture of the network. Once it is fixed, the actual network function $\varphi \in \mathbf{N}_{d_0, \ldots, d_{\ell+1}}^\psi$ is determined by the remaining parameters:

$$\theta = (\beta^{(0)}, w^{(0)}, \beta^{(1)}, w^{(1)}, \cdots \cdots, \beta^{(\ell-1)}, w^{(\ell-1)}, \beta^{(\ell)}, w^{(\ell)})$$

defining the functions $\phi_0, \phi_1, \cdots, \phi_{\ell-1}$ and ϕ_ℓ respectively. Their set is denoted by Θ. For each $\theta \in \Theta$, the function φ computed by the network will be denoted by h_θ. As it should be clear from the discussion of the previous section, here, we are interested in the case where $d_0 = d$ and $d_{\ell+1} = 1$.

Our analysis is based on the following algorithm. In practice, instead of having a fixed number of iterations M, one can use a criterion of the form: at iteration m, if $|\nabla \mathbb{J}_S(\theta_m)|$ is small enough, stop; otherwise continue.

Algorithm 1: SGD for ergodic MFC

Data: An initial parameter $\theta_0 \in \Theta$. A sequence $(\alpha_m)_{m \geqslant 0}$ of learning rates.
Result: Parameters $\theta^\star$ such that $h_{\theta^\star}$ approximates $h^\star$
1 **begin**
2   **for** $m = 0, 1, 2, \ldots, M$ **do**
3   Pick $S = (x_\ell, y_\ell)_{\ell=1}^L$ where x_ℓ and y_ℓ are picked i.i.d. uniform in $[0, 2\pi]$
4   Compute the gradient $\nabla \mathbb{J}_S(\theta_m)$ of $\mathbb{J}_S(\theta_m) = \frac{1}{L} \sum_{\ell=1}^L \mathbb{F}_{\theta_m}(x_\ell, y_\ell)$
5   Set $\theta_{m+1} = \alpha_m \theta_m + (1 - \alpha_m) \nabla \mathbb{J}_S(\theta_m)$
6   **return** θ_m

3.1. **The Approximation Estimates.** Our goal is now to analyze the error made by the numerical procedure described in Algorithm 1. We split the error into two parts: the *approximation error* and the *estimation error* (or *generalization error*). The approximation error quantifies the error made by shrinking the class of admissible controls (here we use neural networks of a certain architecture instead of all possible feedback controls). The estimation error quantifies the error made by replacing the integrals by averages over a finite number of Monte Carlo samples.

In this section, $\sigma : \mathbb{R} \to \mathbb{R}$ denotes a $2\pi-$periodic activation function of class $\mathcal{C}^1$ whose Fourier expansion contains 1, i.e.,

$$(22) \qquad 1 \in \left\{ k \in \mathbb{Z} \,\middle|\, \hat{\sigma}(k) := \frac{1}{2\pi} \int_{-\pi}^{\pi} \sigma(x) e^{-ikx} dx \neq 0 \right\}.$$

More general activation functions (such as the hyperbolic tangent) could probably be considered at the expense of additional technicalities. The choice of this class of activation functions is motivated by the fact that we will use it to build a neural network which can approximate a periodic function together with its first order derivatives (namely, $h^\star$ and ∇h^*).

Approximation Error. The proof of our first estimate is based on the following special case of [27, Theorems 2.3 and 6.1].[1] We state it for the sake of completeness. It provides a neural network approximation for a function and its derivative. For positive integers n and m, and a function $g \in \mathcal{C}(\mathbb{T}^m)$, let $E_n^m(g)$ denote the trigonometric degree of approximation of g defined by:

$$E_n^m(g) = \inf_T \|g - T\|_{\mathcal{C}(\mathbb{T}^m)}$$

where the infimum is over trigonometric polynomials of degree at most n in each of its m variables.

---

[1]We use a special case of the *neural networks* considered in [27]. For us, using the notation of Mhaskar and Micchelli, $m_n = \hat{\sigma}(1)$ and $N_n = 1$ for all n.

Theorem 3 (Theorems 2.3 and 6.1 in [27]). *Let $f : \mathbb{T}^d \to \mathbb{R}$ be of class $\mathcal{C}^2$, and let n and N be positive integers. Then there exist $n_{\text{in}} \in O(Nn^d)$ and $\varphi_f \in \mathbf{N}^\sigma_{d,n_{\text{in}},1}$ such that:*

$$
\text{(23)} \qquad \|f - \varphi_f\|_{\mathcal{C}(\mathbb{T}^d)} \leqslant c \left[E_n^d(f) + E_N^1(\sigma) n^{d/2} \|f\|_{\mathcal{C}(\mathbb{T}^d)} \right],
$$

$$
\text{(24)} \qquad \|\partial_i f - \partial_i \varphi_f\|_{\mathcal{C}(\mathbb{T}^d)} \leqslant c \left[E_n^d(\partial_i f) + E_N^1(\sigma') n^{d/2} \|\partial_i f\|_{\mathcal{C}(\mathbb{T}^d)} \right], \quad i = 1, \ldots, d,
$$

where c depends on the activation function through $\hat{\sigma}(1)$ but does not depend on n, N, n_{in}.

The workhorse of our control of the approximation error is the following.

Theorem 4. *Assume that for some integer $K \geqslant 1$, there exists a minimizer over $\mathcal{C}^{K+1}(\mathbb{T}^d)$, say $h^\star$, of the cost function $\widetilde{J}$ defined in (19). Assume that $\sigma \in \mathcal{C}^{K+1}(\mathbb{T}^d)$. Then, for n_{in} large enough we have:*

$$
\widetilde{J}(h^\star) \leqslant \inf_{\varphi \in \mathbf{N}^\sigma_{d,n_{\text{in}},1}} \widetilde{J}(\varphi) \leqslant \widetilde{J}(h^\star) + \epsilon_1(n_{\text{in}})
$$

where

$$
\epsilon_1(n_{in}) \in O\left((n_{in})^{-K/(3d)} \right).
$$

The constants in the above big Bachmann - Landau term $O(\cdot)$ depend only on the data of the problem as well as $\hat{\sigma}(1)$, K, and the $\mathcal{C}^0-$norms of the partial derivatives of σ and $h^\star$ of order up to $K + 1$ (but they do not depend upon n_{in}).

Remark 5. *The exponent in the O term in the statement of the proposition is what is blamed for the so-called curse of dimensionality. In some settings, the constants in the O term can be estimated if bounds on the $\mathcal{C}^0-$norms of the partial derivatives of $h^\star$ of order up to $K + 1$ are known, for instance from a priori estimates on the solution of the PDE system (16).*

Proof of Theorem 4. The first inequality holds by definition of $h^\star$ and because $\mathbf{N}^\sigma_{d,n_{\text{in}},1} \subset \mathcal{C}^{K+1}(\mathbb{T}^d)$. In order to apply the result of Theorem 3 to $f = h^\star$, we bound from above the right hand sides of (23) and (24). We use the fact that the trigonometric degree of approximation of a function of class $\mathcal{C}^r$ is of order $O(n^{-r})$ when using polynomials of degree at most n. More precisely, by [30, Theorem 4.3], if $f : \mathbb{R}^d \to \mathbb{R}$ is an r-times continuously differentiable function which is 2π-periodic in each variable, then for every positive integer n, there exists a trigonometric polynomial T_n of degree at most n such that

$$
|f(x) - T_n(x)| \leqslant C n^{-r}, \qquad x \in [0, 2\pi]^d,
$$

where C depends only on r and on the bounds on the r-th derivatives of f in each direction: $\|\partial_i^{(r)} f\|_{\mathcal{C}^0}$, $i = 1, \ldots, d$. We apply this result, with some integer n to be specified later, to $f = h^\star$ and $f = \nabla h^\star$ with $r = K$, since $h^\star$ is of class $\mathcal{C}^{K+1}$. By [30, Theorem 4.3] again, since σ and σ' are both of class $\mathcal{C}^K$, we obtain that for any integer N there exist trigonometric polynomials $T_N, \tilde{T}_N$ of degree at most N such that

$$
|\sigma(x) - T_N(x)| \leqslant C N^{-r}, \quad |\sigma'(x) - \tilde{T}_N(x)| \leqslant C N^{-r}, \qquad 0 \leqslant x \leqslant 2\pi,
$$

where C depends only on r and on the bounds on the K-th derivatives of σ and σ', namely $\sigma^{(K)}, \sigma^{(K+1)}$. We apply this result with $N = n^{1+d/(2K)}$. Note that $N^{-r} = n^{-K-d/2}$.

So by Theorem 3, we obtain that there exists $n_{\text{in}} \in O(Nn^d)$ and $\varphi_{h^\star} \in \mathbf{N}^\sigma_{d,n_{\text{in}},1}$ such that

$$
\text{(25)} \qquad \|h^\star - \varphi_{h^\star}\|_{\mathcal{C}(\mathbb{T}^d)} + \|\nabla h^\star - \nabla \varphi_{h^\star}\|_{\mathcal{C}(\mathbb{T}^d)} \leqslant C_1 n^{-K},
$$

where the constant C_1 depends on $K, d, \|\partial_i^{(K)} h^\star\|_{\mathcal{C}(\mathbb{T}^d)}, \|\partial_i^{(K+1)} h^\star\|_{\mathcal{C}(\mathbb{T}^d)}, i = 1, \ldots, d, \|\sigma^{(K)}\|_{\mathcal{C}(\mathbb{R})}, \|\sigma^{(K+1)}\|_{\mathcal{C}(\mathbb{R})},$ but not on n or n_{in}. This implies in particular (since $n, K \geqslant 1$) that

$$\|\varphi_{h^\star}\|_{\mathcal{C}(\mathbb{T}^d)} + \|\nabla \varphi_{h^\star}\|_{\mathcal{C}(\mathbb{T}^d)} \leqslant C_2 := \|h^\star\|_{\mathcal{C}(\mathbb{T}^d)} + \|\nabla h^\star\|_{\mathcal{C}(\mathbb{T}^d)} + C_1.$$

Notice that, since $Nn^d = n^{1+d/(2K)+d} = n^{\frac{Kd+K+d/2}{K}} \leqslant n^{3d}$, the number of units in the hidden layer is $n_{\mathrm{in}} \in O(n^{3d})$, hence the right hand side in (25) is of order $O(n_{\mathrm{in}}^{-K/(3d)})$. In other words,

$$(26) \qquad \|h^\star - \varphi_{h^\star}\|_{\mathcal{C}(\mathbb{T}^d)} + \|\nabla h^\star - \nabla \varphi_{h^\star}\|_{\mathcal{C}(\mathbb{T}^d)} \in O\left(n_{\mathrm{in}}^{-K/(3d)}\right),$$

where the constant in the big O might depend on C_1 but is independent of n_{in}.

Going back to the definition (19) of $\widetilde{J}$, we note that, by (25), for all $x \in \mathbb{T}^d$, $h^\star(x)$ and $\varphi_{h^\star}(x)$ both lie in the interval $[-C_2, C_2]$. Since $x \mapsto e^x$ is Lipschitz continuous on this interval with a Lipschitz constant depending only on C_2, we obtain that:

$$|e^{h^\star(x)} - e^{\varphi_{h^\star}(x)}| \leqslant c\|h^\star - \varphi_{h^\star}\|_{\mathcal{C}(\mathbb{T}^d)}, \qquad x \in \mathbb{T}^d,$$

where here and thereafter c denotes a generic constant which depends on the data of the problem as well as K, and bounds on the $\mathcal{C}^0-$norms of the partial derivatives of σ and $h^\star$ up to order $K+1$, and whose exact value might change from line to line. Moreover, $\int e^{h^\star}, \int e^{\varphi_{h^\star}}$ lie in the interval $\left[e^{-C_2}, e^{C_2}\right]$, and $x \mapsto x^{-2}$ is Lipschitz continuous on this interval with a Lipschitz constant depending only on C_2 so we also have:

$$\left| \left(\textstyle\int e^{h^\star}\right)^{-2} - \left(\textstyle\int e^{\varphi_{h^\star}}\right)^{-2} \right| \leqslant c\|h^\star - \varphi_{h^\star}\|_{\mathcal{C}(\mathbb{T}^d)}.$$

Hence, recalling the definition (20) of $\widetilde{F}$, one can check after some calculations that for all $x, y \in \mathbb{T}^d$,

$$\left| \widetilde{F}\left(x, y, \nabla h^\star(x), e^{h^\star(x)}, e^{h^\star(y)}, \int e^{h^\star(z)} dz\right) - \widetilde{F}\left(x, y, \nabla \varphi_{h^\star}(x), e^{\varphi_{h^\star}(x)}, e^{\varphi_{h^\star}(y)}, \int e^{\varphi_{h^\star}(z)} dz\right) \right|$$
$$\leqslant c\|h^\star - \varphi_{h^\star}\|_{\mathcal{C}(\mathbb{T}^d)}.$$

From the definition (19) of $\widetilde{J}$, the considerations above and (26), we deduce that:

$$(27) \qquad \left| \widetilde{J}(h^\star) - \widetilde{J}(\varphi_{h^\star}) \right| \leqslant c\|h^\star - \varphi_{h^\star}\|_{\mathcal{C}(\mathbb{T}^d)} \in O\left(n_{\mathrm{in}}^{-K/d}\right),$$

which completes the proof. $\qquad\qquad\square$

Corollary 6. *If $\sigma \in \mathcal{C}^2$, $\tilde{b} \in \mathcal{C}^2$ and if there exists a classical solution $(\nu^\star, p^\star, \lambda^\star)$ to the optimality system (16), then we have:*

$$\left| \inf_{h \in \mathcal{C}^2} \widetilde{J}(h) - \inf_{\varphi \in \mathbf{N}_{d, n_{\mathrm{in}}, 1}^\sigma} \widetilde{J}(\varphi) \right| \in O\left(n_{\mathrm{in}}^{-1/d}\right).$$

Proof. Indeed, if $\tilde{b} \in \mathcal{C}^2$ and if we have existence of a classical solution $(\nu^\star, p^\star, \lambda^\star)$ to the optimality system (16), in particular if $p^\star \in \mathcal{C}^2$, and $\|p^\star\|_{\mathcal{C}(\mathbb{T}^d)}$, $\|\partial_i p^\star\|_{\mathcal{C}(\mathbb{T}^d)}$ and $\|\partial_{i,j} p^\star\|_{\mathcal{C}(\mathbb{T}^d)}$, $i, j \in \{1, \ldots, d\}$, are bounded by constants depending only on the data of the problem, we obtain that $h^\star$ given by (17) provides a minimizer of $\widetilde{J}$ of class $\mathcal{C}^2$. We can then apply Theorem 4 with $K = 1$. $\qquad\square$

Remark 7. *For mean field games, existence of classical solutions to the ergodic PDE system has been studied in several settings, see e.g. [22, 23]. To the best of our knowledge, corresponding results do not exist yet for the PDE system arising in the ergodic optimal control of MKV dynamics and this question*

will be addressed in a future work. In finite time horizon, existence of classical solutions has been studied e.g. in [3].

Estimation Error. We then turn our attention to the estimation (or *generalization*) error. Let n_{in} be a fixed positive integer. In the numerical implementation, we do not minimize directly $\tilde{J}$ over a set of neural networks with say n_{in} units. Instead, we minimize over empirical versions computed from Monte Carlo samples. To be specific, for a given sample:

$$S = ((x_\ell, y_\ell)_{\ell=1,\dots,L}, (z_q)_{q=1,\dots,Q}) \in (\mathbb{T}^d \times \mathbb{T}^d)^L \times (\mathbb{T}^d)^Q \tag{28}$$

for which the x_ℓ, y_ℓ, z_q are picked independently and uniformly in $[0, 2\pi]$, we minimize:

$$\widehat{J}_S(h) = \frac{1}{L} \sum_{\ell=1}^{L} \widetilde{F}\left(x_\ell, y_\ell, \nabla h(x_\ell), e^{h(x_\ell)}, e^{h(y_\ell)}, \frac{1}{Q} \sum_{q=1}^{Q} e^{h(z_q)}\right), \tag{29}$$

where $\widetilde{F}$ is defined by (20). The intuition is to approximate the double integral over $dxdy$ by an average over L independent Monte Carlo samples (x_ℓ, y_ℓ), and likewise, the integral $\int e^\varphi$ by an empirical average over a sample of points uniformly distributed over $\mathbb{T}^d$. We shall use the following notation. For two positive constants γ_1 and γ_2, we denote by $\mathbf{N}_{d,n_{\text{in}},1}^{\sigma,\gamma_1,\gamma_2}$ the set of functions $\varphi \in \mathbf{N}_{d,n_{\text{in}},1}^{\sigma}$ for which there exist $(\mathbf{w}, \mathbf{u}) \in \mathbb{R}^{n_{in}} \times \mathbb{R}^{n_{in} \times (d+1)}$ satisfying

- $\|\mathbf{w}\|_1 \leqslant \gamma_1$,
- $\|\mathbf{u}_n\|_2 \leqslant \gamma_2$ for all $n \in \{1, \dots, n_{in}\}$,

and such that $\varphi(x) = \sum_{n=1}^{n_{in}} w_n \sigma(\mathbf{u}_n \cdot (x^\top, 1)^\top)$, where the superscript $\top$ denotes the transpose operation. Here, $\|\mathbf{w}\|_1 = \sum_{n=1}^{n_{in}} |w_n|$ and $\|\mathbf{u}_n\|_2 = \sqrt{\sum_{k=1}^{d+1} |u_{n,k}|^2}$.

We are now in a position to prove the following bound on the uniform deviation between $\tilde{J}$ and its empirical counterpart $\widehat{J}$. It is our main insight into the estimation error.

Theorem 8. *Let γ_1, γ_2 be positive constants. We have:*

$$\mathbb{E}_S\left[\sup_{\varphi \in \mathbf{N}_{d,n_{\text{in}},1}^{\sigma,\gamma_1,\gamma_2}} \left|\tilde{J}(\varphi) - \widehat{J}_S(\varphi)\right|\right] \in O\left(\frac{1}{\sqrt{L}} + \frac{1}{\sqrt{Q}}\right),$$

where the expectation is over the samples S as in (28), and the constants in the big Bachmann - Landau term $O(\cdot)$ depend only on the data of the problem and on γ_1 and γ_2, but neither on L nor on Q.

Proof. First, introducing *ghost* Monte Carlo samples $\tilde{S} = ((\tilde{x}_\ell, \tilde{y}_\ell)_\ell, (\tilde{z}_q)_q)$ picked with the same distribution as S, and independent of the latter, we can rewrite (19) as:

$$\tilde{J}(\varphi) = \mathbb{E}_{\tilde{S}}\left[\frac{1}{L} \sum_{\ell=1}^{L} \widetilde{F}\left(\tilde{x}_\ell, \tilde{y}_\ell, \nabla\varphi(\tilde{x}_\ell), e^{\varphi(\tilde{x}_\ell)}, e^{\varphi(\tilde{y}_\ell)}, \int e^{\varphi(z)} dz\right)\right],$$

where the expectation is over the samples $\tilde{S}$. Note that the variables $\tilde{z}_q$ do not appear in this expression. We kept them in the ghost sample for the sake of symmetry. Hence, for each fixed $S = ((x_\ell, y_\ell)_\ell, (z_q)_q)$,

$$\sup_\varphi \left| \tilde{J}(\varphi) - \hat{J}_S(\varphi) \right| \leqslant \mathbb{E}_{\tilde{S}} \sup_\varphi \left| \frac{1}{L} \sum_{\ell=1}^{L} \left[\tilde{F}\left(\tilde{x}_\ell, \tilde{y}_\ell, \nabla\varphi(\tilde{x}_\ell), e^{\varphi(\tilde{x}_\ell)}, e^{\varphi(\tilde{y}_\ell)}, \int e^{\varphi(z)} dz \right) \right. \right.$$
$$\left. \left. - \tilde{F}\left(x_\ell, y_\ell, \nabla\varphi(x_\ell), e^{\varphi(x_\ell)}, e^{\varphi(y_\ell)}, \frac{1}{Q} \sum_{q=1}^{Q} e^{\varphi(z_q)} \right) \right] \right|.$$

Taking expectation over S we get:

$$\mathbb{E}_S \sup_\varphi \left| \tilde{J}(\varphi) - \hat{J}_S(\varphi) \right| \leqslant \mathbb{E}_{S,\tilde{S}} \sup_\varphi \left| \frac{1}{L} \sum_{\ell=1}^{L} \left[\tilde{F}\left(\tilde{x}_\ell, \tilde{y}_\ell, \nabla\varphi(\tilde{x}_\ell), e^{\varphi(\tilde{x}_\ell)}, e^{\varphi(\tilde{y}_\ell)}, \int e^{\varphi(z)} dz \right) \right. \right.$$
$$\left. \left. - \tilde{F}\left(x_\ell, y_\ell, \nabla\varphi(x_\ell), e^{\varphi(x_\ell)}, e^{\varphi(y_\ell)}, \frac{1}{Q} \sum_{q=1}^{Q} e^{\varphi(z_q)} \right) \right] \right|$$

$$\leqslant \mathbb{E}_{S,\tilde{S}} \sup_\varphi \left| \frac{1}{L} \sum_{\ell=1}^{L} \left[\tilde{F}\left(\tilde{x}_\ell, \tilde{y}_\ell, \nabla\varphi(\tilde{x}_\ell), e^{\varphi(\tilde{x}_\ell)}, e^{\varphi(\tilde{y}_\ell)}, \int e^{\varphi(z)} dz \right) \right. \right.$$
$$\left. \left. - \tilde{F}\left(\tilde{x}_\ell, \tilde{y}_\ell, \nabla\varphi(\tilde{x}_\ell), e^{\varphi(\tilde{x}_\ell)}, e^{\varphi(\tilde{y}_\ell)}, \frac{1}{Q} \sum_{q=1}^{Q} e^{\varphi(\tilde{z}_q)} \right) \right] \right|$$

$$+ \mathbb{E}_{S,\tilde{S}} \sup_\varphi \left| \frac{1}{L} \sum_{\ell=1}^{L} \left[\tilde{F}\left(\tilde{x}_\ell, \tilde{y}_\ell, \nabla\varphi(\tilde{x}_\ell), e^{\varphi(\tilde{x}_\ell)}, e^{\varphi(\tilde{y}_\ell)}, \frac{1}{Q} \sum_{q=1}^{Q} e^{\varphi(\tilde{z}_q)} \right) \right. \right.$$
$$\left. \left. - \tilde{F}\left(x_\ell, y_\ell, \nabla\varphi(x_\ell), e^{\varphi(x_\ell)}, e^{\varphi(y_\ell)}, \frac{1}{Q} \sum_{q=1}^{Q} e^{\varphi(z_q)} \right) \right] \right|$$

$$(30) \qquad\qquad = (i) + (ii)$$

and we analyze separately the contributions of the two double expectations to the value of the above right hand side. By definition of $\mathbf{N}_{d,n_{\text{in}},1}^{\sigma,\gamma_1,\gamma_2}$, there exists a constant $C' > 0$ such that for every $\varphi \in \mathbf{N}_{d,n_{\text{in}},1}^{\sigma,\gamma_1,\gamma_2}$ and every sample $x, y, \tilde{z}_1, \ldots, \tilde{z}_Q \in \mathbb{T}^d$, we have:

$$\left(x, y, \nabla\varphi(x), e^{\varphi(x)}, e^{\varphi(y)} \right) \in [-C', C']^{3d+2}, \qquad \int_{\mathbb{T}^d} e^{\varphi(z)} dz \in [\frac{1}{C'}, C'], \qquad \frac{1}{Q} \sum_{q=1}^{Q} e^{\varphi(\tilde{z}_q)} \in [\frac{1}{C'}, C'],$$

and given the assumptions on $\tilde{f}$ and the definitions of $\tilde{F}$ and $\mathbf{N}_{d,n_{\text{in}},1}^{\sigma,\gamma_1,\gamma_2}$, one can find a constant $C > 0$ such that:

$$|\tilde{F}(x, y, q, X, Y, Z) - \tilde{F}(x, y, q, X, Y, Z')| \leqslant C|Z - Z'|$$

for all $(x, y, q, X, Y) \in [-C', C']^{3d+2}$ and Z and Z' in $[1/C', C']$. Notice that the constants C and C' depend upon $\sigma(\cdot)$, γ_1, γ_2, d, and n_{in}, but not on the particular $\varphi \in \mathbf{N}_{d,n_{\text{in}},1}^{\sigma,\gamma_1,\gamma_2}$. Using this Lipschitz bound, we get:

$$(i) \leqslant \mathbb{E}_{\tilde{S}} \sup_\varphi \left| \int e^{\varphi(z)} dz - \frac{1}{Q} \sum_{q=1}^{Q} e^{\varphi(\tilde{z}_q)} \right|.$$

To bound from above the right hand side, we follow a pretty standard strategy. First we notice that:

$$\int e^{\varphi(z)}dz = \frac{1}{Q}\sum_{q=1}^{Q}\mathbb{E}_S e^{\varphi(z_q)}.$$

Moreover, we can introduce a family $\mathbf{r} = (r_q)_{q=1,\cdots,Q}$ of independent Rademacher random variables (i.e. satisfying $\mathbb{P}[r_q = -1] = \mathbb{P}[r_q = 1] = 1/2$), independent of the samples S and $\tilde{S}$. Since the samples $(z_q)_{q=1,\cdots,Q}$ and $(\tilde{z}_q)_{q=1,\cdots,Q}$ are independent and identically distributed, we have

$$(i) \leqslant \mathbb{E}_S\mathbb{E}_{\tilde{S}}\sup_{\varphi}\Big|\frac{1}{Q}\sum_{q=1}^{Q}\Big[e^{\varphi(z_q)} - e^{\varphi(\tilde{z}_q)}\Big]\Big|$$

$$= \mathbb{E}_S\mathbb{E}_{\tilde{S}}\mathbb{E}_{\mathbf{r}}\sup_{\varphi}\Big|\frac{1}{Q}\sum_{q=1}^{Q}r_q\Big[e^{\varphi(z_q)} - e^{\varphi(\tilde{z}_q)}\Big]\Big|$$

$$\leqslant \mathbb{E}_S\mathbb{E}_{\tilde{S}}\mathbb{E}_{\mathbf{r}}\sup_{\varphi}\Big|\frac{1}{Q}\sum_{q=1}^{Q}r_q e^{\varphi(z_q)}\Big| + \mathbb{E}_S\mathbb{E}_{\tilde{S}}\mathbb{E}_{\mathbf{r}}\Big|\frac{1}{Q}\sum_{q=1}^{Q}r_q e^{\varphi(z_q)}\Big|$$

$$= 2\mathbb{E}_S\mathbb{E}_{\mathbf{r}}\sup_{\varphi}\Big|\frac{1}{Q}\sum_{q=1}^{Q}r_q e^{\varphi(z_q)}\Big|$$

$$(31)\qquad\qquad \leqslant C'\frac{1}{\sqrt{Q}},$$

where we used Khintchine inequality to derive the last inequality.

We now turn our attention to the estimation of the term (ii) in (30). Because of the introduction of the ghost samples, for each $\ell \in \{1,\cdots,L\}$, the two terms we compute the difference of are independent and identically distributed, so we can rewrite (ii) using a family $\tau = (\tau_\ell)_{\ell=1,\cdots,L}$ of independent Rademacher random variables independent of the samples S and $\tilde{S}$ in the following way:

$$(ii) = \mathbb{E}_{S,\tilde{S}}\mathbb{E}_\tau\sup_{\varphi}\Big|\frac{1}{L}\sum_{\ell=1}^{L}\tau_\ell\Big[\widetilde{F}\Big(\tilde{x}_\ell,\tilde{y}_\ell,\nabla\varphi(\tilde{x}_\ell),e^{\varphi(\tilde{x}_\ell)},e^{\varphi(\tilde{y}_\ell)},\frac{1}{Q}\sum_{q=1}^{Q}e^{\varphi(\tilde{z}_q)}\Big)$$

$$- \widetilde{F}\Big(x_\ell,y_\ell,\nabla\varphi(x_\ell),e^{\varphi(x_\ell)},e^{\varphi(y_\ell)},\frac{1}{Q}\sum_{q=1}^{Q}e^{\varphi(z_q)}\Big)\Big]\Big|$$

$$\leqslant \mathbb{E}_{S,\tilde{S}}\mathbb{E}_\tau\Big[\sup_{\varphi}\Big|\frac{1}{L}\sum_{\ell=1}^{L}\tau_\ell\widetilde{F}\Big(\tilde{x}_\ell,\tilde{y}_\ell,\nabla\varphi(\tilde{x}_\ell),e^{\varphi(\tilde{x}_\ell)},e^{\varphi(\tilde{y}_\ell)},\frac{1}{Q}\sum_{q=1}^{Q}e^{\varphi(\tilde{z}_q)}\Big)\Big|$$

$$+ \sup_{\varphi}\Big|\frac{1}{L}\sum_{\ell=1}^{L}\tau_\ell\widetilde{F}\Big(x_\ell,y_\ell,\nabla\varphi(x_\ell),e^{\varphi(x_\ell)},e^{\varphi(y_\ell)},\frac{1}{Q}\sum_{q=1}^{Q}e^{\varphi(z_q)}\Big)\Big|\Big]$$

$$(32)\qquad = 2\mathbb{E}_S\mathbb{E}_\tau\sup_{\varphi}\Big|\frac{1}{L}\sum_{\ell=1}^{L}\tau_\ell\widetilde{F}\Big(x_\ell,y_\ell,\nabla\varphi(x_\ell),e^{\varphi(x_\ell)},e^{\varphi(y_\ell)},\frac{1}{Q}\sum_{q=1}^{Q}e^{\varphi(z_q)}\Big)\Big|$$

where we used the fact that S and $\tilde{S}$ are i.i.d. For each fixed $\varphi \in \mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}$ and samples S and τ we have

$$\left| \sum_{\ell=1}^{L} \tau_\ell \widetilde{F} \left(x_\ell, y_\ell, \nabla\varphi(x_\ell), e^{\varphi(x_\ell)}, e^{\varphi(y_\ell)}, \frac{1}{Q} \sum_{q=1}^{Q} e^{\varphi(z_q)} \right) \right|$$

$$\leqslant \left| \sum_{\ell=1}^{L} \tau_\ell \widetilde{F} \left(0,0,0,0,0,1 \right) \right|$$

$$+ \left| \sum_{\ell=1}^{L} \tau_\ell \left[\widetilde{F} \left(x_\ell, y_\ell, \nabla\varphi(x_\ell), e^{\varphi(x_\ell)}, e^{\varphi(y_\ell)}, \frac{1}{Q} \sum_{q=1}^{Q} e^{\varphi(z_q)} \right) - \widetilde{F} \left(0,0,0,0,0,1 \right) \right] \right|.$$

Since $\widetilde{F}(0,0,0,0,0,1)$ is a constant independent of $\varphi \in \mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}$, we denote it momentarily by C'' to ease the notation. Moreover, for each fixed sample $S = (x_\ell, y_\ell, z_q)_{\ell,q}$ we have:

(33)
$$\mathbb{E}_\tau \sup_{\varphi \in \mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}} \left| \sum_{\ell=1}^{L} \tau_\ell \left[\widetilde{F} \left(x_\ell, y_\ell, \nabla\varphi(x_\ell), e^{\varphi(x_\ell)}, e^{\varphi(y_\ell)}, \frac{1}{Q} \sum_{q=1}^{Q} e^{\varphi(z_q)} \right) - C'' \right] \right|$$

$$\leqslant \mathbb{E}_\tau \sup_{\varphi \in \mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}} \sup_{s \in \{-1,+1\}} s \sum_{\ell=1}^{L} \tau_\ell \left[\widetilde{F} \left(x_\ell, y_\ell, \nabla\varphi(x_\ell), e^{\varphi(x_\ell)}, e^{\varphi(y_\ell)}, \frac{1}{Q} \sum_{q=1}^{Q} e^{\varphi(z_q)} \right) - C'' \right]$$

where the variable s is introduced to replace the absolute value. For each $\varphi \in \mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}$ and $s \in \{-1,+1\}$, we define the function ψ_φ^s for $(x,y,Z) \in \mathbb{T}^d \times \mathbb{T}^d \times (\mathbb{T}^d)^Q$ by:

$$\psi_\varphi^s(x,y,(z_q)_{q=1,\ldots,Q}) = \left(x, y, \nabla\varphi(x), e^{\varphi(x)}, e^{\varphi(y)}, \frac{1}{Q} \sum_{q=1}^{Q} e^{\varphi(z_q)}, s \right).$$

By definition of $\mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}$, it is clear that the range of the map ψ_φ^s is contained in a hypercube of the form:

$$\mathcal{D}_{d,n_{\mathrm{in}}}^{\sigma,\gamma_1,\gamma_2} = [-C',C']^{3d+2} \times [\frac{1}{C'}, C'] \times [-1,1] \subset \mathbb{R}^{3d+4}$$

where the constant $C' = C'(\sigma,\gamma_1,\gamma_2,d,n_{\mathrm{in}})$ was introduced earlier. Given the assumptions on $\tilde{f}$ and the definitions of $\widetilde{F}$ and $\mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}$, one can construct a real valued function Φ on $\mathbb{R}^{3d+4}$ which is Lipschitz continuous over the whole space and satisfies:

$$\Phi(x,y,q,X,Y,Z,s) = s \left[\widetilde{F}(x,y,q,X,Y,Z) - \widetilde{F}(0,0,0,0,0,1) \right],$$

for $(x,y,q,X,Y,Z,s) \in \mathcal{D}_{d,n_{\mathrm{in}}}^{\sigma,\gamma_1,\gamma_2}$, and whose Lipschitz constant, say K, depends upon $\sigma(\cdot)$, γ_1, γ_2, d, n_{in} and C'', but not on the particular $\varphi \in \mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}$. Next, we introduce the set of functions:

$$\mathcal{F}_{d,n_{\mathrm{in}}}^{\sigma,\gamma_1,\gamma_2} = \left\{ \psi : \mathbb{T}^d \times \mathbb{T}^d \times (\mathbb{T}^d)^Q \to \mathbb{R}^{3d+4}; \ \exists \varphi \in \mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}, \exists s \in \{-1,+1\}, \psi = \psi_\varphi^s \right\}.$$

We can then rewrite the right hand side of (33) as:

$$\mathbb{E}_\tau \sup_{\psi \in \mathcal{F}_{d,n_{\mathrm{in}}}^{\sigma,\gamma_1,\gamma_2}} \sum_{\ell=1}^{L} \tau_\ell \left[\Phi \left(\psi \left(x_\ell, y_\ell, (z_q)_q \right) \right) \right]$$

By the form of Talagrand's contraction lemma given in Corollary 4 of [26], this quantity is bounded from above by:

$$\sqrt{2}K\,\mathbb{E}_{\tilde{\tau}}\sup_{\psi\in\mathcal{F}_{d,n_{\mathrm{in}}}^{\sigma,\gamma_1,\gamma_2}}\sum_{\ell=1}^{L}\sum_{k=1}^{3d+4}\tilde{\tau}_{\ell,k}\,\psi\left(x_\ell,y_\ell,(z_q)_{q=1,\ldots,Q}\right)_k$$

where, for $\mathbf{z}=(z_q)_{q=1,\ldots,Q}\in(\mathbb{T}^d)^Q$, $\psi(x,y,\mathbf{z})_k$ denotes the k-th component of the vector $\psi(x,y,\mathbf{z})$, and where the family of random variables $\tilde{\tau}=(\tilde{\tau}_{\ell,k})_{\ell=1,\cdots,L,\,k=1,\cdots,3d+4}$ is an independent Rademacher family with one extra index. Accordingly, this quantity is bounded from above by:

$$\sqrt{2}K\sum_{k=1}^{3d+4}\mathbb{E}_{\tilde{\tau}}\sup_{\psi\in\mathcal{F}_{d,n_{\mathrm{in}}}^{\sigma,\gamma_1,\gamma_2}}\sum_{\ell=1}^{L}\tilde{\tau}_{\ell,k}\,\psi\left(x_\ell,y_\ell,\mathbf{z}\right)_k,$$

and we proceed to estimate the $3d+4$ terms of the outer sum one by one. Notice that for $k\leqslant 3d+2$, the term $\psi(x_\ell,y_\ell,\mathbf{z})_k$ does not depend upon $\mathbf{z}$, and we proceed in the following way. The terms corresponding to $k=1,\ldots,d$ (resp. $k=d+1,\ldots,2d$) are easy to control since $\psi(x_\ell,y_\ell,\mathbf{z})_k=(x_\ell)_k$ (resp. $\psi(x_\ell,y_\ell,\mathbf{z})_k=(y_\ell)_{k-d}$) do not depend upon φ or s, rendering the supremum irrelevant. Moreover, since the norms of x_ℓ and y_ℓ in $\mathbb{R}^d$ are bounded by C', Khintchine inequality gives:

$$\mathbb{E}_{\tilde{\tau}}\sum_{\ell=1}^{L}\tilde{\tau}_{\ell,1}\,\|x_\ell\|\leqslant C\sqrt{L},\quad\text{and}\quad\mathbb{E}_{\tilde{\tau}}\sum_{\ell=1}^{L}\tilde{\tau}_{\ell,2}\,\|y_\ell\|\leqslant C\sqrt{L}.$$

For $k=2d+h$ with $h\in\{1,\ldots,d\}$, $\psi(x_\ell,y_\ell,\mathbf{z})_k=\partial_h\varphi(x_\ell)=\sum_{n=1}^{n_{in}}w_n u_{n,h}\sigma'(\mathbf{u}_n\cdot(x_\ell^\top,1)^\top)$, and:

$$\sum_{\ell=1}^{L}\tilde{\tau}_{\ell,k}\left[\sum_{n=1}^{n_{in}}w_n u_{n,h}\sigma'(\mathbf{u}_n\cdot(x_\ell^\top,1)^\top)\right]\leqslant\sum_{n=1}^{n_{in}}|w_n u_{n,h}|\left|\sum_{\ell=1}^{L}\tilde{\tau}_{\ell,k}\left[\sigma'(\mathbf{u}_n\cdot(x_\ell^\top,1)^\top)\right]\right|$$

$$\leqslant\left(\sum_{n=1}^{n_{in}}|w_n u_{n,h}|\right)\sup_{n}\left|\sum_{\ell=1}^{L}\tilde{\tau}_{\ell,k}\left[\sigma'(\mathbf{u}_n\cdot(x_\ell^\top,1)^\top)\right]\right|$$

(34)
$$\leqslant\gamma_1\gamma_2\sup_{n}\left|\sum_{\ell=1}^{L}\tilde{\tau}_{\ell,k}\left[\sigma'(\mathbf{u}_n\cdot(x_\ell^\top,1)^\top)\right]\right|$$

because of the definition of $\varphi\in\mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}$. Consequently, since the above quantity does not depend upon s, the supremum over $\psi\in\mathcal{F}_{d,n_{\mathrm{in}}}^{\sigma,\gamma_1,\gamma_2}$ can be taken over $\varphi\in\mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}$ and we have:

$$\mathbb{E}_{\tilde{\tau}}\sup_{\psi\in\mathcal{F}_{d,n_{\mathrm{in}}}^{\sigma,\gamma_1,\gamma_2}}\sum_{\ell=1}^{L}\tilde{\tau}_{\ell,k}\,\psi(x_\ell,y_\ell,\mathbf{z})_k=\mathbb{E}_{\tilde{\tau}}\sup_{\varphi\in\mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}}\sum_{\ell=1}^{L}\tilde{\tau}_{\ell,k}\,\partial_h\varphi(x_\ell)$$

$$=\mathbb{E}_{\tilde{\tau}}\sup_{\varphi\in\mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}}\sum_{\ell=1}^{L}\tilde{\tau}_{\ell,k}\left[\sum_{n=1}^{n_{in}}w_n u_{n,h}\sigma'(\mathbf{u}_n\cdot(x_\ell^\top,1)^\top)\right]$$

$$\leqslant\gamma_1\gamma_2\mathbb{E}_{\tilde{\tau}}\sup_{\mathbf{u}_n:\|\mathbf{u}_n\|_2\leqslant\gamma_2}\left|\sum_{\ell=1}^{L}\tilde{\tau}_{\ell,k}\,\sigma'(\mathbf{u}_n\cdot(x_\ell^\top,1)^\top)\right|$$

where we used (34). Since the derivative of the activation function σ is Lipschitz (without any loss of generality we use the same constant $K>0$ for its Lipschitz constant), we can use the original version

of Talagrand's contraction lemma to estimate the above right hand side. From [25, Theorem 4.12] with $F(x) = x$, $\varphi_i(t) = \sigma'(t) - \sigma'(0)$, and $T = \{(\mathbf{u} \cdot (x_\ell^\top, 1)^\top)_{\ell=1,\cdots,L}; \|\mathbf{u}\|_2 \leqslant \gamma_2\}$ we get:

$$\mathbb{E}_{\tilde{\tau}} \sup_{\psi \in \mathcal{F}_{d,n_{\mathrm{in}}}^{\sigma,\gamma_1,\gamma_2}} \sum_{\ell=1}^L \tilde{\tau}_{\ell,k}\, \psi(x_\ell, y_\ell, \mathbf{z})_k \leqslant C \mathbb{E}_{\tilde{\tau}} \sup_{\|\mathbf{u}_n\|_2 \leqslant \gamma_2} \Big| \sum_{\ell=1}^L \tilde{\tau}_{\ell,k}[\sigma'(\mathbf{u}_n \cdot (x_\ell^\top, 1)^\top) - \sigma'(0)] \Big| + C\sigma'(0)\mathbb{E}_{\tilde{\tau}} \Big| \sum_{\ell=1}^L \tilde{\tau}_{\ell,k} \Big|$$

$$\leqslant C \left(\mathbb{E}_{\tilde{\tau}} \sup_{\|\mathbf{u}\|_2 \leqslant \gamma_2} \Big| \sum_{\ell=1}^L \tilde{\tau}_{\ell,k} \left[\mathbf{u} \cdot (x_\ell^\top, 1)^\top \right] \Big| + \mathbb{E}_{\tilde{\tau}} \Big| \sum_{\ell=1}^L \tilde{\tau}_{\ell,k} \Big| \right)$$

$$= C \left(\mathbb{E}_{\tilde{\tau}} \sup_{\|\mathbf{u}\|_2 \leqslant \gamma_2} \Big| \mathbf{u} \cdot \sum_{\ell=1}^L \tilde{\tau}_{\ell,k} \left[(x_\ell^\top, 1)^\top \right] \Big| + \mathbb{E}_{\tilde{\tau}} \Big| \sum_{\ell=1}^L \tilde{\tau}_{\ell,k} \Big| \right)$$

$$\leqslant C \left(\mathbb{E}_{\tilde{\tau}} \sup_{\|\mathbf{u}\|_2 \leqslant \gamma_2} \|\mathbf{u}\|_2 \Big\| \sum_{\ell=1}^L \tilde{\tau}_{\ell,k} \left[(x_\ell^\top, 1)^\top \right] \Big\|_2 + \mathbb{E}_{\tilde{\tau}} \Big| \sum_{\ell=1}^L \tilde{\tau}_{\ell,k} \Big| \right)$$

$$\leqslant C \left(\mathbb{E}_{\tilde{\tau}} \Big\| \sum_{\ell=1}^L \tilde{\tau}_{\ell,k} \left[(x_\ell^\top, 1)^\top \right] \Big\|_2 + \mathbb{E}_{\tilde{\tau}} \Big| \sum_{\ell=1}^L \tilde{\tau}_{\ell,k} \Big| \right)$$

$$\leqslant C\sqrt{L},$$

where the value of the constant $C > 0$ changed from line to line, and where we used Cauchy-Schwarz and Khintchine inequalities.

We proceed similarly for the values $k = 3d + 1$ and $k = 3d + 2$ since the exponential function is Lipschitz on the range $[-C', C']$ of the functions $\varphi \in \mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}$.

We now focus on the penultimate term. For $k = 3d + 3$, the term $\psi(x_\ell, y_\ell, \mathbf{z})_k$ is $\frac{1}{Q}\sum_{q=1}^Q e^{\varphi(z_q)}$. It does not depend upon s so the supremum over $\psi \in \mathcal{F}_{d,n_{\mathrm{in}}}^{\sigma,\gamma_1,\gamma_2}$ can be taken over $\varphi \in \mathbf{N}_{d,n_{\mathrm{in}}}^{\sigma,\gamma_1,\gamma_2}$ and we have:

$$\mathbb{E}_{\tilde{\tau}} \sup_{\psi \in \mathcal{F}_{d,n_{\mathrm{in}}}^{\sigma,\gamma_1,\gamma_2}} \sum_{\ell=1}^L \tilde{\tau}_{\ell,k}\, \psi(x_\ell, y_\ell, \mathbf{z})_k = \mathbb{E}_{\tilde{\tau}} \sup_{\varphi \in \mathbf{N}_{d,n_{\mathrm{in}},1}^{\sigma,\gamma_1,\gamma_2}} \sum_{\ell=1}^L \tilde{\tau}_{\ell,k} \frac{1}{Q} \sum_{q=1}^Q e^{\varphi(z_q)}$$

$$\leqslant C' \mathbb{E}_{\tilde{\tau}} \Big| \sum_{\ell=1}^L \tilde{\tau}_{\ell,k} \Big|$$

$$\leqslant C\sqrt{L}$$

because of Khintchine inequality. Finally, the term corresponding to $k = 3d + 4$ can easily be bounded in the same way since $\psi(x_\ell, y_\ell, \mathbf{z})_{3d+4} = s \in \{-1, +1\}$.

This concludes the analysis of (ii), proving that it is bounded from above by a constant times $1/\sqrt{L}$. Combining this with (31) and (30), the proof is complete. $\qquad\square$

4. Application of the Deep Galerkin Method

An alternative way to solve the ergodic mean field control problem is to tackle directly the PDE system (16). In order to do so, we adapt the Deep Galerkin Method (DGM) proposed by Sirignano and Spiliopoulos [31] for a single PDE. The key idea is to rewrite the PDE system as a new minimization problem where the control is the triple (ν, p, λ) and the loss function is the sum of the PDE residuals (plus some terms taking into account the boundary conditions and the normalization conditions). In our setting, this idea can be implemented as follows. To alleviate the notations, we introduce the sets $C_i =$

$\{x_i = 0\}$ where $i \in \{1, \ldots, d\}$ and use the shorthand notation $(x_{-i}, 2\pi)$ for $(x_1, \ldots, x_{i-1}, 2\pi, x_{i+1}, \ldots, x_d)$ and we set

$$(35) \qquad L(\nu, p, \lambda) = L^{(1)}(\nu, p, \lambda) + L^{(2)}(\nu, p, \lambda)$$

where

$$(36) \qquad \begin{aligned} L^{(1)}(\nu, p, \lambda) &= \left\| \frac{1}{2}\Delta\nu + \mathrm{div}\big(\partial_y H^\star(\cdot, \nu, \nabla p(\cdot))\nu\big) \right\|_{L^2(\mathbb{T}^d)} \\ &\quad + \sum_{i=1}^{d} \left(\int_{C_i} |\nu(x) - \nu((x_{-i}, 2\pi))|^2 \, dx \right)^{1/2} + \left| 1 - \int_{\mathbb{T}^d} \nu(x)dx \right| \end{aligned}$$

and

$$(37) \qquad \begin{aligned} L^{(2)}(\nu, p, \lambda) &= \left\| \lambda + \frac{1}{2}\Delta p - H^\star(\cdot, \nu, \nabla p(\cdot)) - \int D_\mu H^\star(\xi, \nu, \nabla p(\xi))(\cdot)\, \nu(d\xi) \right\|_{L^2(\mathbb{T}^d)} \\ &\quad + \sum_{i=1}^{d} \left(\int_{C_i} |p(x) - p((x_{-i}, 2\pi))|^2 \, dx \right)^{1/2} + \left| \int_{\mathbb{T}^d} p(x)dx \right|. \end{aligned}$$

Each function encodes one of the two PDEs of the optimality system (16) and contains one term for the residual of the PDE, one term for the periodicity condition, and one term for the normalization condition. These terms can be weighted to adjust their relative importance. In any case, note that $L(\nu, p, \lambda) = 0$ if (ν, p, λ) solves the PDE system (16). Since our primary motivation is the optimal control of MKV dynamics, we present the method in this setting. However the same ideas can be readily applied to other PDE systems by designing differently the loss function. For instance, to solve the PDE system arising in the corresponding stationary MFG, one simply needs to remove the term $\int D_\mu H^\star(\xi, \nu, \nabla p(\xi))(\cdot)\, \nu(d\xi)$ in (37). For the sake of illustration, we present an example below, see Test case 3 in the next section.

We then look for ν and p in the form of neural networks, say ν_{θ_1} and p_{θ_2} with fixed architectures and parameterized by θ_1 and θ_2 respectively. The unknown λ is replaced by a variable coefficient $\theta_3 \in \mathbb{R}$ which is learnt along the way. As in the method discussed in the previous sections, the integrals are interpreted as expectations with respect to a random variable with uniform distribution over $\mathbb{T}^d$, and one uses SGD to minimize the total loss function. More precisely, for a given $\mathbf{S} = (S, (S_i)_{i \in \{1, \ldots, d\}})$ where $S \subset [0, 1]$ is a finite set of points and S_i is a finite set of points in C_i for every $i \in \{1, \ldots, d\}$, we define the empirical loss function as follows: for $\theta = (\theta_1, \theta_2, \theta_3)$,

$$(38) \qquad L_{\mathbf{S}}(\theta) = L_{\mathbf{S}}^{(1)}(\theta) + L_{\mathbf{S}}^{(2)}(\theta)$$

where

$$\begin{aligned} L_{\mathbf{S}}^{(1)}(\theta) &= \left(\sum_{x \in S} \left| \frac{1}{2}\Delta\nu_{\theta_1}(x) + \mathrm{div}\big(\partial_y H^\star(\cdot, \nu_{\theta_1}, \nabla p_{\theta_2}(\cdot))\nu_{\theta_1}\big)(x) \right|^2 \right)^{1/2} \\ &\quad + \sum_{i=1}^{d} \left(\sum_{x \in S_i} |\nu_{\theta_1}(x) - \nu_{\theta_1}((x_{-i}, 2\pi))|^2 \right)^{1/2} + \left| 1 - \sum_{x \in S} \nu_{\theta_1}(x) \right| \end{aligned}$$

and

$$L_{\mathbf{S}}^{(2)}(\theta) = \left(\sum_{x \in S} \left| \theta_3 + \frac{1}{2}\Delta p_{\theta_2}(x) - H^{\star}(x, \nu_{\theta_1}, \nabla p_{\theta_2}(x)) - \int D_\mu H^{\star}(\xi, \nu_{\theta_1}, \nabla p_{\theta_2}(\xi))(x)\, \nu_{\theta_1}(d\xi) \right|^2 \right)^{1/2}$$

$$+ \sum_{i=1}^{d} \left(\sum_{x \in S_i} |p_{\theta_2}(x) - p_{\theta_2}((x_{-i}, 2\pi))|^2 \right)^{1/2} + \left| \sum_{x \in S} p_{\theta_2}(x) \right|.$$

One can use SGD to minimize the loss function (38). The approximation power of this method has been discussed in [31] using a universal approximation theorem. However, this type of results does not give any rate of convergence. More precise convergence results could be obtained by the techniques presented in Section 3. In particular, the approximation error can be bounded by combining again Theorems 2.3 and 6.1 in [27]. For instance, if the PDE system (16) has a solution (ν, p, λ) such that $p, \nu \in \mathcal{C}^3(\mathbb{T}^d)$, then there exist neural networks $\varphi_p, \varphi_\nu \in \mathbf{N}_{d,n_{\text{in}},1}^\sigma$ such that $\|p - \varphi_p\|_{\mathcal{C}^2(\mathbb{T}^d)}$ and $\|\nu - \varphi_\nu\|_{\mathcal{C}^2(\mathbb{T}^d)}$ are in $O\left(n_{\text{in}}^{-2/(3d)} \right)$. In turn, this property leads to bounds on both the loss function of the algorithm and the error on the value function of the control problem. The detailed analysis is left for future work. Let us also note that a similar method has recently been used in [5] to solve numerically a time-dependent MFG.

5. NUMERICAL RESULTS

In this section we present numerical results obtained using implementation of the methods described in the previous sections. Algorithm 1 refers to the method based on minimization of the cost functional introduced in Section 3. Algorithm 2 refers to the DGM method described in Section 4. We have used feed-forward neural networks implemented in `TensorFlow` with at most 3 hidden layers, each layer having at most 20 units, with the exception of the the last test case (see Test Case 5 below). We have used Adam procedure for the gradient-based optimization. The results are presented on the unit torus (i.e., $[0,1]^d$ with periodic boundary conditions) instead of $\mathbb{T}^d = [0, 2\pi]^d$ as in the previous sections.

5.1. **Examples in Dimension 1.** For ease of visualization, we start with univariate examples. We first consider models without explicit solutions, and we compare the solutions computed by the two algorithms introduced in the prequel with a benchmark solution computed by a deterministic method based on a finite difference scheme for the PDE system [2].

Test case 1: For the sake of illustration we include a model without mean field interaction, say

$$b(x, \mu, \phi) = \phi, \qquad f(x, \mu, \phi) = \frac{1}{2}|\phi|^2 + \tilde{f}(x),$$

with

(39) $$\tilde{f}(x) = 50\Big(0.1\cos(2\pi x) + \cos(4\pi x) + 0.1\sin\big(2\pi\big(x - \tfrac{\pi}{8}\big)\big) \Big)$$

which is displayed in Figure 1. The solution computed with the first algorithm is presented in Figure 2.

Test case 2: Next, we add a mean field interaction term in the cost

(40) $$b(x, \mu, \phi) = \phi, \qquad f(x, \mu, \phi) = \frac{1}{2}|\phi|^2 + \tilde{f}(x) + |\mu(x)|^2,$$

with $\tilde{f}$ given by (39). Here $\mu(x)$ stands for the density of the measure μ at $x \in [0,1]$. The results are presented in Figure 3. Comparing with the first test case, one sees that due to the mean field term
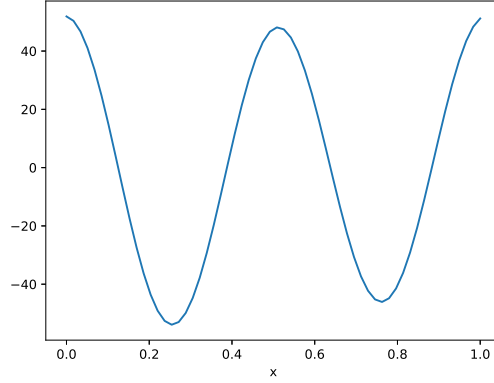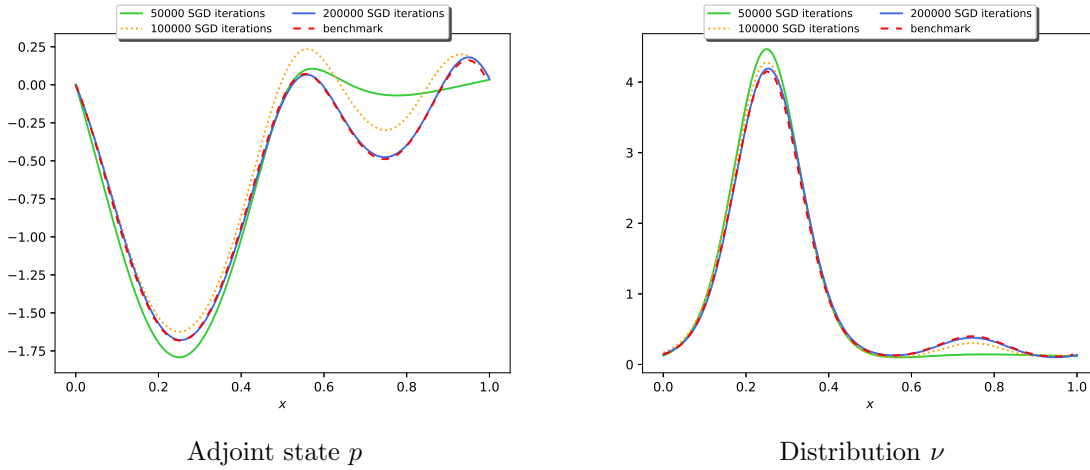
FIGURE 1. Cost $\tilde{f}$ defined by (39)

Adjoint state p Distribution ν

FIGURE 2. Test case 1. Solution computed by Algorithm 1 and benchmark solution from deterministic method (dashed red line).

$|\mu(x)|^2$ in the cost function, the distribution is less concentrated around the global minimum and part of the mass is transferred to the second local minimum.

Test case 3: The DGM method can be used to solve the previous examples, but can also be used to solve other PDE systems, such as the one arising from mean field games. In the MFG setting, the PDE system for the optimality condition takes the following form [22]:

$$(41) \qquad \left\{ \begin{array}{l} 0 = \frac{1}{2}\Delta\nu + \operatorname{div}\big(\partial_y H^\star(\cdot, \nu, \nabla p(\cdot))\nu\big) \\ 0 = \lambda + \frac{1}{2}\Delta p(x) - H^\star(x, \nu, \nabla p(x)), \end{array} \right.$$

with normalization and boundary conditions, and where the minimized Hamiltonian $H^\star$ is defined in (15). Notice that this PDE system (41) is different from the PDE system (16) for mean field control.
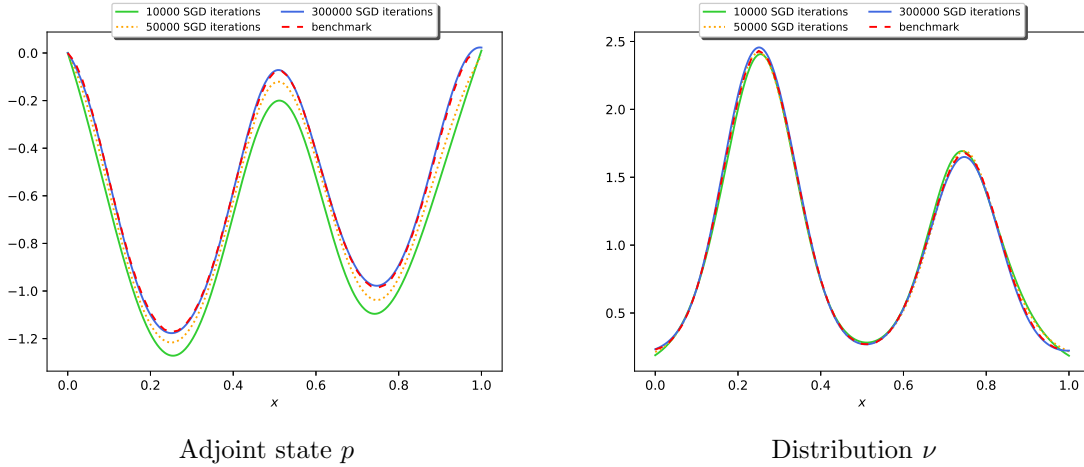
Adjoint state p Distribution ν

FIGURE 3. Test case 2. Solution computed by Algorithm 1 and benchmark solution from deterministic method (dashed red line).

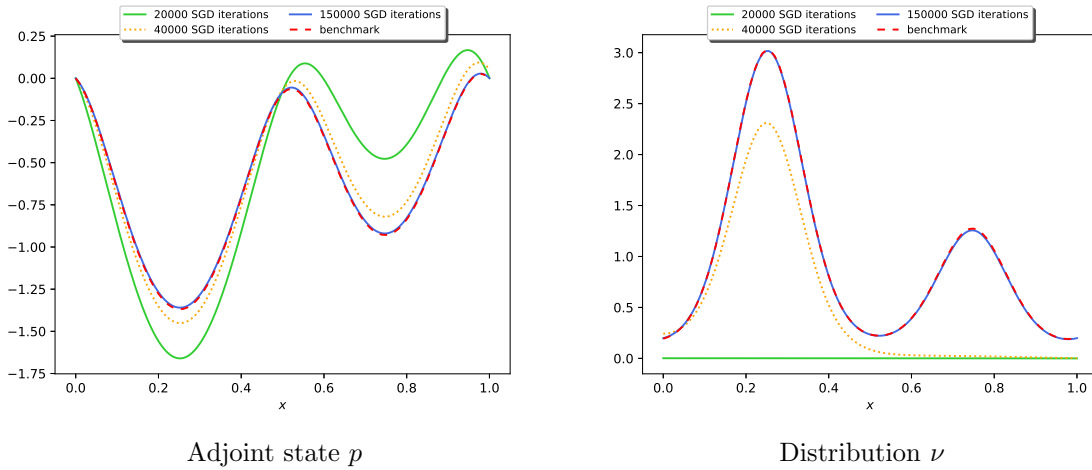Adjoint state p Distribution ν

FIGURE 4. Test case 3. Solution computed by Algorithm 2 (DGM) and benchmark solution from deterministic method (dashed red line).

Taking b and f as in the previous test, namely (40), yields the solution displayed in Figure 4 (to be compared with the corresponding curves for the MFC model of Test case 2, see Figure 3). Recall that with the DGM method, both p and ν are approximated using two separate neural networks. In particular, we see on Figure 4 that after 20000 iterations of SGD, the neural network for p has already roughly learnt the shape of the optimum, whereas the neural network for ν is still almost flat.

5.2. **Multivariate Examples with Explicit Solution.** To assess the quality of the proposed algorithms in higher dimension, we introduce simple toy models which can be solved explicitly. These

models are very much in the spirit of examples considered in [6]. Let us take:

$$b(x, \alpha) = b(\alpha) = \alpha, \qquad f(x, \mu, \alpha) = \frac{1}{2}|\alpha|^2 + \tilde{f}(x) + \ln(\mu(x)),$$

Then, the minimizer $\alpha^\star$ entering the definition of $H^\star(x, \mu, y)$ is given by:

$$\alpha^\star = \alpha^\star(y) = y.$$

So $H^\star(x, \mu, y) = -\frac{1}{2}|y|^2 + \tilde{f}(x) + \ln(\mu(x))$ and $\int D_\mu H^\star(\xi, \nu, \nabla p(\xi))(x)\,\nu(d\xi) = 1$. The PDE system (16) rewrites:

$$(42) \qquad \begin{cases} 0 = \frac{1}{2}\Delta\nu - \mathrm{div}\big(\nabla p\nu\big) \\ 0 = \lambda + \frac{1}{2}\Delta p(x) + \frac{1}{2}|\nabla p(x)|^2 - \tilde{f}(x) - \left(\ln(\nu(x)) + 1\right). \end{cases}$$

Assuming the existence of a smooth enough solution (ν, p, λ), the first equation allows us to express ν in terms of p as follows:

$$(43) \qquad \nu(x) = \frac{e^{2p(x)}}{\int e^{2p(x')}dx'}.$$

The second equation in (42) rewrites

$$\nu(x) = \frac{e^{\frac{1}{2}(\Delta p(x) + |\nabla p(x)|^2) - \tilde{f}(x)}}{e^{1-\lambda}}.$$

In this case, the PDE system (42) is solved provided the above equation and the second equation in (42) are satisfied, which means that (p, λ) solves:

$$2p(x) = \frac{1}{2}(\Delta p(x) + |\nabla p(x)|^2) - \tilde{f}(x), \qquad \lambda = 1 - \ln\left(\int e^{2p}\right).$$

We consider two specific instances of $\tilde{f}$ for which we are able to obtain closed-form expressions for p.

Test case 4: Let $\tilde{f}$ be given by

$$\tilde{f}(x) = 2\pi^2\left[-\sum_{i=1}^d \sin(2\pi x_i) + \sum_{i=1}^d |\cos(2\pi x_i)|^2\right] - 2\sum_{i=1}^d \sin(2\pi x_i),$$

then the solution is given by $p(x) = \sum_{i=1}^d \sin(2\pi x_i)$ and $\lambda = 1 - \ln(\int e^{2\sum_{i=1}^d \sin(2\pi\xi_i)}d\xi)$.

We have solved numerically this problem in dimension $d = 4$. The convergence of the approximation p_θ learnt by our first algorithm towards the analytical solution p is presented in Figure 5. This figure shows the relative L^2-error, which is defined as

$$\left(\frac{\|p - p_\theta\|_2^2}{\|p\|_2^2}\right)^{1/2} = \sqrt{\left(\int_{\mathbb{T}^d} |p(x) - p_\theta(x)|^2 dx\right) \Big/ \left(\int_{\mathbb{T}^d} |p(x)|^2 dx\right)}.$$

In the implementation, this quantity is estimated with 10^5 Monte Carlo samples for each integral. The figure corresponds to one run of SGD and illustrates the fact that the algorithm can be stuck in a local minimum for a certain number of iterations (between roughly iterations 10^5 and 2×10^5 on this example) before finding its way out to a better solution. The distribution ν is deduced from p using the formula (43), which explains why the two convergence curves have the same shape.

For the DGM method, numerical convergence is presented in Figure 6. As in the previous test case, the convergence rate of p and ν is quite different because they are approximated by distinct neural
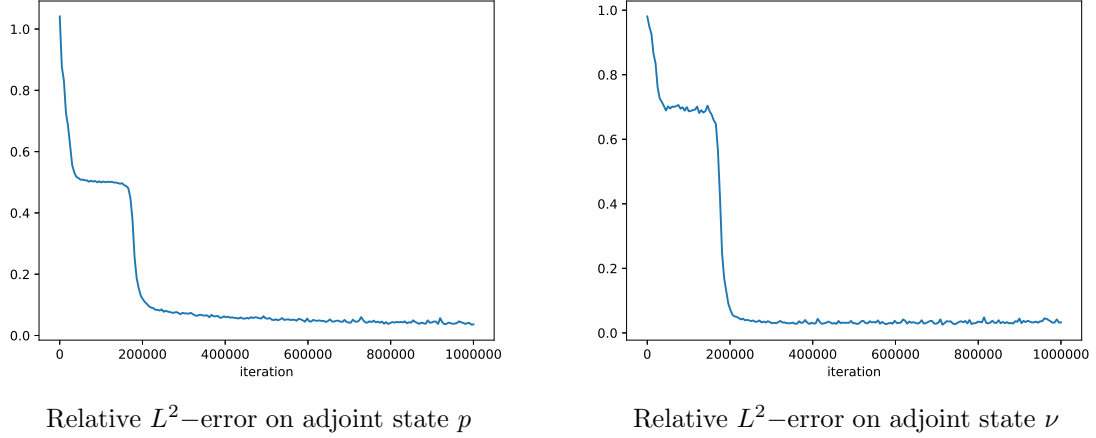
Relative L^2-error on adjoint state p Relative L^2-error on adjoint state ν

FIGURE 5. Test case 4. Relative L^2-error by Algorithm 1.

Relative L^2-error on adjoint state p Relative L^2-error on distribution ν
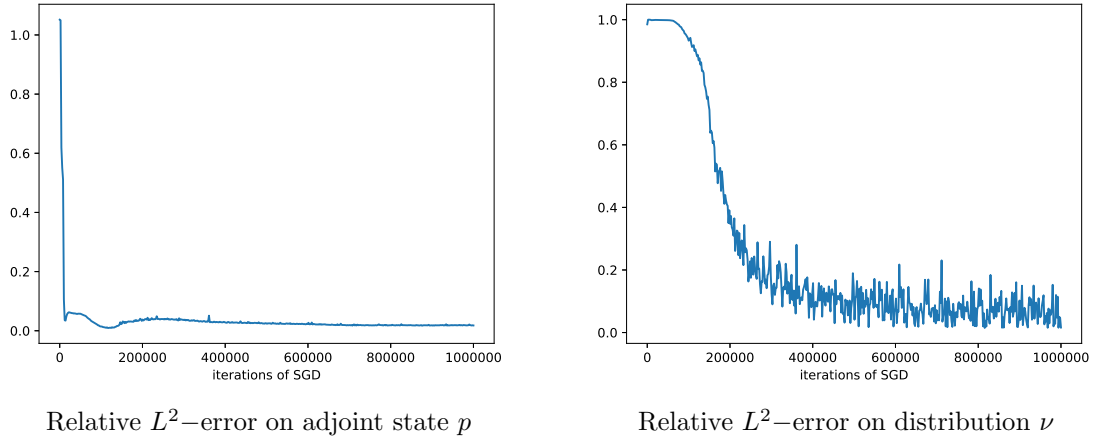
FIGURE 6. Test case 4. Relative L^2-error by Algorithm 2 (DGM).

networks. In particular, the error on ν decreases at a lower rate and suffers from a larger noise, which could be due to the form of the solution, see (43).

Test case 5: We consider a variant of the previous test case where $\tilde{f}$ is chosen such that

$$p(x) = \prod_{i=1}^{d} \sin(2\pi x_i)^2 - \int_{\mathbb{T}^d} \prod_{i=1}^{d} \sin(2\pi x_i)^2 dx.$$

We use this example to study the influence of the number of hidden units and the number of samples in the population on the approximation p_θ found by the algorithm. For simplicity and to be consistent with the theoretical bounds provided in the prequel, we consider here neural networks with a single hidden layer. Figure 7 illustrates the dependence on the number of hidden units. As seen on Figure 7B,
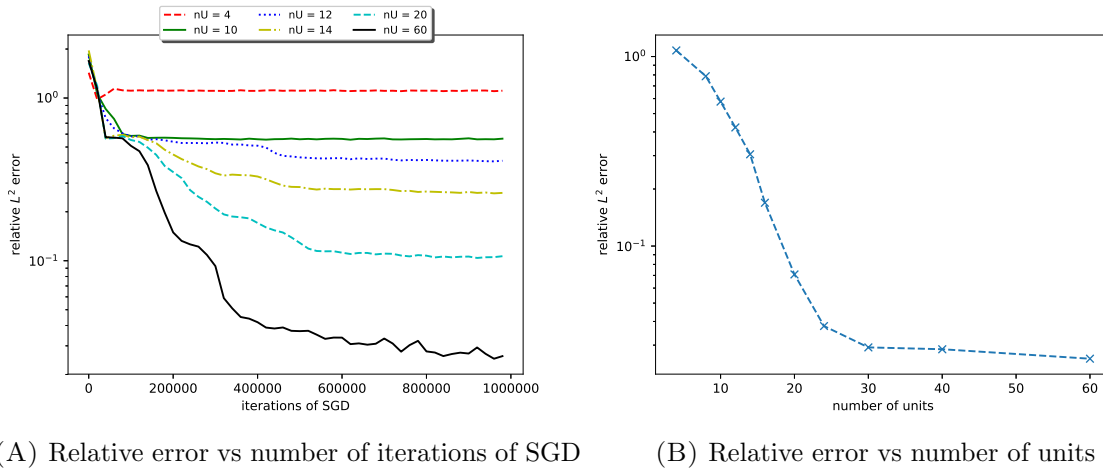
(A) Relative error vs number of iterations of SGD   (B) Relative error vs number of units

FIGURE 7. Test case 5. Dependence of the relative L^2 error on the number of hidden units (Algorithm 1). The number of samples in the population is 10^5. The number of units is indicated by "nU" for the figure on the left. On the right, relative L^2 error after 10^6 iterations.

Relative error vs number of iterations of SGD   Relative error vs number of samples
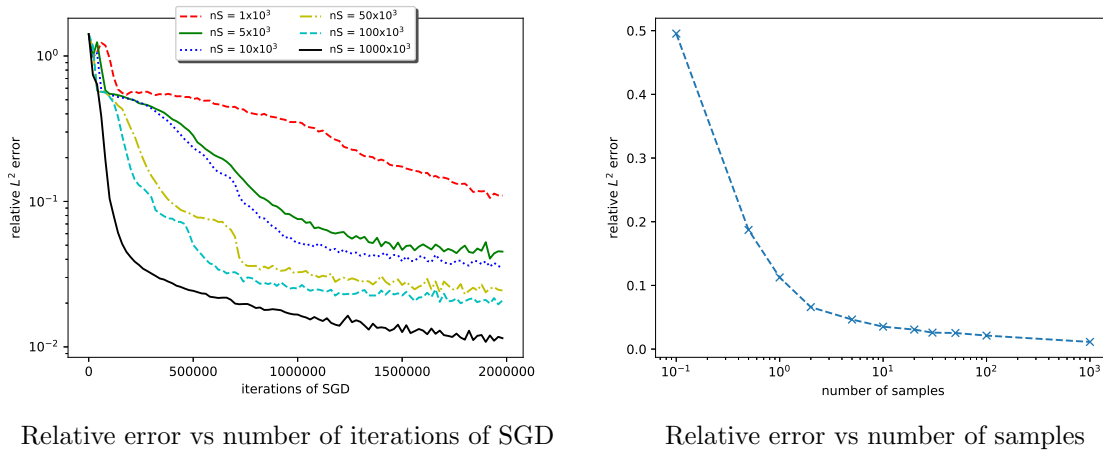
FIGURE 8. Test case 5. Dependence of the relative L^2 error on the number of samples in a population (Algorithm 1). The number of hidden units it 60 for all curves. The number of samples is indicated by "nS" for the figure on the left. On the right, relative L^2 error after 10^6 iterations.

the error decreases quickly as the number of units grows until 30. However, for a number of units larger than 30, the error almost stagnates. This is due to the fact that the number of samples in the population drawn at each iteration of SGD is kept fixed to 10^5. The dependence on this number of samples is illustrated in Figure 8, while keeping the number of units fixed to 60. These numerical results were obtained by averaging over 10 runs of SGD.

6. Conclusion

In this paper, we introduced two numerical algorithms for the solution of the optimal control of ergodic McKean-Vlasov dynamics also known as ergodic mean field control problems. We approximated the theoretical solutions by functions given by neural networks, the latter being determined by their architectures and suitable sets of parameters. This allowed the use of modern machine learning tools, and efficient implementations of stochastic gradient descent.

The first algorithm is based on the specific structure of the ergodic optimal control problem. We provided a mathematical proof of the convergence of the algorithm, and we analyzed rigorously the numerical scheme by controlling both the approximation and the estimation error. The second method is an adaptation of the deep Galerkin method to the system of partial differential equations issued from the optimality conditions.

We demonstrated the efficiency of these algorithms on several numerical examples, some of them being chosen to show that our methods succeed where existing ones failed. We also argued that both methods can easily be applied to problems in dimension larger than 3, which is not the case with the existing technology. Finally, we illustrated the fact that, although the first algorithm is specifically designed for mean field control problems, the second one is more general and can also be applied to the partial differential equation systems arising in the theory of mean field games.

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