IDENTIFICATION OF MEAN-FIELD DYNAMICS USING TRANSFORMERS

Anonymous authors

Paper under double-blind review

Abstract

This paper investigates the use of transformer architectures to approximate the mean-field dynamics of interacting particle systems exhibiting collective behavior. Such systems are fundamental in modeling phenomena across physics, biology, and engineering, including gas dynamics, opinion formation, biological networks, and swarm robotics. The key characteristic of these systems is that the particles are indistinguishable, leading to permutation-equivariant dynamics. We demonstrate that transformers, which inherently possess permutation equivariance, are well-suited for approximating these dynamics. Specifically, we prove that if a finite-dimensional transformer can effectively approximate the finite-dimensional vector field governing the particle system, then the expected output of this transformer provides a good approximation for the infinite-dimensional mean-field vector field. Leveraging this result, we establish theoretical bounds on the distance between the true mean-field dynamics and those obtained using the transformer. We validate our theoretical findings through numerical simulations on the Cucker-Smale model for flocking, and the mean-field system for training two-layer neural networks.

025 026 027

004

006

008 009

010 011

012

013

014

015

016

017

018

019

021

023

1 INTRODUCTION

028 The identification of dynamical system models for physical processes is a fundamental application 029 of machine learning (ML). Of particular interest are systems of particles exhibiting collective behaviors-such as swarming, flocking, opinion dynamics, and consensus-are of significant interest. 031 These systems involve a large number of particles or agents that follow identical dynamics, which are independent of the particles' identities and are permutation-equivariant. Examples include biological 033 entities (Lopez et al., 2012), robots (Elamvazhuthi & Berman, 2019), traffic flow (Piccoli et al., 034 2009; Siri et al., 2021), and parameters in two-layer neural networks (Mei et al., 2019). A common approach to simplifying the analysis of such systems is to consider the continuum limit as the number of particles $n \to \infty$, resulting in *mean-field models* rooted in statistical physics. Instead of specifying the dynamics of each agent, the particles are modeled using probability measures. This paper learns 037 the mean-field dynamics of particles via particle trajectories using transformers.

There have been several works on learning mean-field dynamics using machine learning. For example,
recent works have utilized classical approaches. Pham & Warin (2023) constructed two different
types of neural network based function approximators for mean-field mappings and proved their
approximation capabilities. The works Feng et al. (2021); Lu et al. (2019) present a kernel-based
method for identifying dynamics of interacting particle systems Miller et al. (2023) employed kernelbased methods. The work Messenger & Bortz (2022) presents a weak form of the SINDy algorithm
Brunton et al. (2016) for identifying mean-field dynamics of interacting particle systems.

This paper explores the use of transformers to approximate the dynamical systems governing the collective behavior of interacting particles with permutation-equivariant dynamics. We define a new transformer architecture for mean-field or measure-dependent vector fields by taking the expectation of a finite-dimensional transformer with respect to a product measure, which we refer to as the *expected transformer*. This approach differs from recent works Vuckovic et al. (2020); Geshkovski et al. (2023); Furuya et al. (2024a); Adu & Gharesifard (2024) that express transformers as maps on the space of probability measures by defining a continuous version of attention.

053 Encoding permutation equivariance into the function class or model used for identifying such systems is potentially advantageous due to the benefits of the inductive bias in learning. This raises

the question of which classes of functions guarantee approximation and learning benefits while
 possessing permutation equivariance. Transformers Vaswani et al. (2017), which have achieved
 state-of-the-art performance in many learning applications involving sequence-to-sequence mappings,
 are one such model class.

058 In this work, we analyze the approximation capabilities of the expected transformer and establish 059 rates of approximation of the expected transformer as a function of the approximation error achieved 060 by the finite-dimensional transformer and the sequence length used. Using this approximation result, 061 we demonstrate that the solution of the *continuity equation*—which describes the mean-field behavior 062 of interacting particle systems—can be approximated by approximating the vector fields using the 063 expected transformer model. We validate our theoretical findings through numerical simulations and 064 comparisons with established benchmarks, specifically on the Cucker-Smale model for swarming, and the mean-field system for training two-layer neural networks. 065

066 067

To summarize, our main **contributions** are as follows:

- We define a continuum version of the transformer as an expectation of finite-dimensional transformers (see Equation 7). This is distinct from prior work such as Geshkovski et al. (2023) that define neural networks on infinite dimensional spaces directly. Instead, we lift a finite-dimensional model into infinite-dimensional space.
- 071 10.000 minute-dimensional space.
 2. We establish approximation rates of measure-valued maps by this expected transformer (see Theorem 3).
 073 3. We show that the solution of the continuity equation can be approximated by approximating the
- 3. We show that the solution of the continuity equation can be approximated by approximating the vector fields using the expected transformer (see Theorem 4).

076 **Other related work** Universal approximation of functions by neural networks has a long history. 077 One of the prominent earlier results Hornik et al. (1989) proved that continuous functions can be 078 well approximated by using neural networks of bounded depth but arbitrary width. For the standard 079 activation functions, the complementary result for bounded width but arbitrary depth has also been shown in Telgarsky (2016); Yarotsky (2018). For bounded width and depth, Maiorov & Pinkus (1999) 080 provided such a result for special activation functions. Recent results such as Kidger & Lyons (2020); 081 Shen et al. (2022) have investigated bounded width and depth for more standard network architectures. The capabilities of bounded width but arbitrary depth residual networks for approximating solutions 083 of the continuity equation, such as those arising in normalizing flows, has been studied in Ruiz-Balet 084 & Zuazua (2023); Elamvazhuthi et al. (2022). 085

Significant work has been done using ML to approximate solutions to differential equations, par-086 ticularly solutions to partial differential equations (PDEs). Specifically, Physics Informed Neural 087 Networks (PINN) were introduced by Raissi et al. (2019) as a method for solving PDEs using neural 088 networks. PINNs have been successfully used in Cai et al. (2021); Weinan & Yu (2017); Bhatnagar 089 et al. (2019). The idea here is to use the differential equation as the loss function for the neural 090 network. Other works have also investigated the problem of approximating the solution operator 091 to PDEs on a mesh (Guo et al., 2016; Zhu & Zabaras, 2018; Adler & Öktem, 2017; Bhatnagar 092 et al., 2019). Building on this, (Kovachki et al., 2021; Li et al., 2020a;b) developed neural operators 093 defined on infinite-dimensional spaces to solve PDES, and Furuya et al. (2024b) provide universal 094 approximation results. Additionally, Li et al. (2023) provide quantitative results for approximating 095 eigenfunctions of the Laplace equation on manifolds.

096 097 098

2 NOTATION

In this section, we present the notation used throughout the paper. Let \mathbb{R}^d denote the *d*-dimensional Euclidean space, and let \mathbb{Z}_+ denote the set of positive integers. The diameter of a subset $A \subset \mathbb{R}^d$ is defined as diam $(A) := \sup\{||x - y|| : x, y \in A\}$ and the closed ball of radius r > 0 centered at $z \in \mathbb{R}^d$ is denoted by $B_r(z)$.

We denote by $\mathcal{P}(\mathbb{R}^d)$ the set of all Borel probability measures on \mathbb{R}^d . The subset of probability measures with finite *p*-th moments is denoted by

- 106
- 107

$$\mathcal{P}_p(\mathbb{R}^d) := \left\{ \nu \in \mathcal{P}(\mathbb{R}^d) : M_p(\mu) := \left(\int_{\mathbb{R}^d} \|x\|^p \, d\mu(x) \right)^{1/p} < \infty \right\}.$$

108 We denote by $\mathcal{P}_c(\mathbb{R}^d)$ the set of probability measures with compact support. The set of empirical 109 measures formed by finite sums of n Dirac-delta measures is denoted by 110

$$\mathcal{D}^{n}(\mathbb{R}^{d}) := \left\{ \nu \in \mathcal{P}(\mathbb{R}^{d}) : \nu = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_{i}}, \ x_{i} \in \mathbb{R}^{d} \right\}$$

For $\nu \in \mathcal{P}(\mathbb{R}^d)$, the *n*-fold product measure on $(\mathbb{R}^d)^n$ is denoted by $\nu^{\otimes n} := \underbrace{\nu \times \cdots \times \nu}$. The 113 114 115

support of a measure $\nu \in \mathcal{P}(\mathbb{R}^d)$, denoted by $\operatorname{supp}(\nu)$, is the smallest closed set $S \subset \mathbb{R}^d$ such that 116 $\mu(\mathbb{R}^d \setminus S) = 0$. The qth moment of a measure ν is denoted by $M_q(\nu)$. Given a measurable map 117 $X: \mathbb{R}^d \to \mathbb{R}^d$ and a measure $\mu \in \mathcal{P}(\mathbb{R}^d)$, the pushforward measure $X_{\#}\mu \in \mathcal{P}(\mathbb{R}^d)$ is defined by 118

$$(X_{\#}\mu)(A) := \mu \left(X^{-1}(A) \right)$$

120 for every Borel measurable set $A \subset \mathbb{R}^d$. 121

Boldface letters, such as z, denote elements in $\mathbb{R}^{n \times d}$, representing collections of n vectors in \mathbb{R}^d . 122 For a vector $y \in \mathbb{R}^d$, the *i*-th component is denoted by $(y)_i$. We denote by $L^p(\mathbb{R}^d, \mu)$ the space of 123 measurable functions $f : \mathbb{R}^d \to \mathbb{R}$ such that 124

$$||f||_{L^p(\mu)} := \left(\int_{\mathbb{R}^d} |f(x)|^p \, d\mu(x)\right)^{1/p} < \infty$$

The space of essentially bounded measurable functions is denoted by $L^{\infty}(\mathbb{R}^d, \mu)$, with the essential supremum norm

134 135

136

137 138 139

140

144 145

147

150

151

125 126 127

128

111 112

119

 $||f||_{L^{\infty}(\mu)} := \operatorname{ess\,sup}_{x \in \mathbb{R}^d} |f(x)|.$

131 A function $f: (\mathbb{R}^d)^n \to (\mathbb{R}^d)^n$ is permutation equivariant if for any permutation $\sigma \in S_n$, where S_n 132 is the symmetric group on n elements, and for any $\mathbf{x} = (x_1, \dots, x_n) \in (\mathbb{R}^d)^n$, we have 133

$$f(x_{\sigma(1)},\ldots,x_{\sigma(n)}) = \left(f_{\sigma(1)}(\mathbf{x}),\ldots,f_{\sigma(n)}(\mathbf{x})\right),\,$$

where $f_i(\mathbf{x})$ denotes the *i*-th component of the output. We denote by $C^k(\mathbb{R}^d)$ the space of k-times continuously differentiable functions on \mathbb{R}^d . The space of continuous functions with compact support is denoted by $C_c(\mathbb{R}^d)$.

3 PROBLEM FORMULATION

141 Let $\Omega \subset \mathbb{R}^d$. Consider a vector field $\mathcal{F} : \Omega \times \mathcal{P}(\Omega) \to \mathbb{R}^d$. The following equation describes the 142 general mean-field behavior of interacting particles evolving on Ω , 143

$$\frac{dz}{dt} = \mathcal{F}(z,\mu), \, z(0) = z_0 \sim \mu_0,$$
(1)

where $z \in \Omega$ denotes the state of a particle, $\mu \in \mathcal{P}(\Omega)$ is the distribution of the particles at time t, 146 and μ_0 is the initial distribution. The inter-particle interactions are modeled through μ ; specifically, the dynamics of each particle are influenced by the distribution of all particles. 148

Corresponding to Equation 1, the *continuity equation* describes the evolution of the distribution μ : 149

$$\frac{\partial \mu}{\partial t} + \nabla_z \cdot \left(\mathcal{F}(z,\mu)\mu \right) = 0, \ \mu(0) = \mu_0.$$
⁽²⁾

152 For a finite final time $\tau > 0$, we denote by $\mu^{\mathcal{F}} : [0,\tau] \to \mathcal{P}(\Omega)$ the solution of the continuity 153 Equation 2 over the time interval $[0, \tau]$. In this paper, we propose to use transformers to approximate 154 the maps in Equation 1 and Equation 2. 155

3.1 LIFTING TRANSFORMERS TO THE SPACE OF MEASURES

158 Traditionally, transformers are defined on sequences of vectors in \mathbb{R}^d . However, the map we wish to 159 approximate, \mathcal{F} , is defined on $\Omega \times \mathcal{P}(\Omega)$. Therefore, we lift the standard transformer to operate on $\Omega \times \mathcal{P}(\Omega)$ via an expectation operation. Before we do this, we briefly review the standard transformer 160 architecture; the following definitions are adapted from Alberti et al. (2023). The core component of 161 the transformer is the multi-head self-attention mechanism.

165

169 170 171

172

173

174 175

177

178 179 180

181

182

183

184 185

187

192

193 194 195

203

207 208

211

212

Definition 1 (Multi-Headed Self-Attention). Let $X \in \mathbb{R}^{n \times d}$ be a matrix whose rows are n data points in \mathbb{R}^d . Let $W_Q, W_K, W_V \in \mathbb{R}^{d \times d}$ be learnable weight matrices. Define the query, key, and value matrices by

$$Q = XW_Q, \quad K = XW_K, \quad V = XW_V.$$

166 Let softmax denote the softmax function applied row-wise to a matrix. The self-attention head 167 function AttHead : $\mathbb{R}^{n \times d} \to \mathbb{R}^{n \times d}$ is defined as

$$\operatorname{AttHead}(X) := \operatorname{softmax}\left(\frac{QK^{\top}}{\sqrt{d}}\right)V.$$
(3)

Let $h \in \mathbb{Z}_+$ be the number of attention heads. Let $AttHead_1, \ldots, AttHead_h$ be attention heads with their own weight matrices, and let $W_0 \in \mathbb{R}^{hd \times d}$ be a learnable weight matrix. The multi-head self-attention layer $Att : \mathbb{R}^{n \times d} \to \mathbb{R}^{n \times d}$ is defined as

$$Att(X) := [AttHead_1(X), AttHead_2(X), \dots, AttHead_h(X)] W_0,$$
(4)

where $[\cdot]$ denotes concatenation along the feature dimension.

Definition 2 (Transformer Network). A transformer block $Block : \mathbb{R}^{n \times d} \to \mathbb{R}^{n \times d}$ is defined as

$$Block(X) := X + FC(X + Att(X)),$$
(5)

where FC are feed-forward layers (position-wise fully connected layers), and ReLU is the rectified linear unit activation function. The addition operations represent residual connections. Let $L \in \mathbb{Z}_+$, and let $\operatorname{Block}_1, \ldots, \operatorname{Block}_L$ be transformer blocks. A transformer network $T : \mathbb{R}^{n \times d} \to \mathbb{R}^{n \times k}$ is defined as a composition of transformer blocks followed by an output network:

$$T(X) := \operatorname{FC}_{out}\left(\operatorname{Block}_{L} \circ \operatorname{Block}_{L-1} \circ \cdots \circ \operatorname{Block}_{1}(X)\right),\tag{6}$$

186 where $FC_{out} : \mathbb{R}^{n \times d} \to \mathbb{R}^{n \times k}$ is a fully connected neural network applied position-wise.

Next, we introduce the *expected transformer* \mathcal{T}_n , which allows us to lift any transformer $T : \Omega^{n+1} \to \mathbb{R}^{(n+1)\times d}$ to a model $\mathcal{T}_n : \Omega \times \mathcal{P}(\Omega) \to \mathbb{R}^d$.

Definition 3 (Expected Transformer). Given a transformer $T : \Omega^{n+1} \to \mathbb{R}^{n+1 \times d}$ and a prescribed sequence length n, define the expected transformer $\mathcal{T}_n : \Omega \times \mathcal{P}(\Omega) \to \mathbb{R}^d$ by

$$\mathcal{T}_{n}(x,\mu) := \mathbb{E}_{\mathbf{z}\sim\mu^{\otimes n}} \left[\left(T\left([x; \mathbf{z}] \right) \right)_{1} \right],$$

$$= \int_{\Omega^{n}} \left(T\left([x; z_{1}, \dots, z_{n}] \right) \right)_{1} d\mu(z_{1}) \cdots d\mu(z_{n}),$$
(7)

where $[x; \mathbf{z}]$ denotes the concatenation of x and $\mathbf{z} = (z_1, ..., z_n)$ to form an input sequence of length n + 1, and $(T([x; \mathbf{z}]))_1$ denotes the first output vector.

Remark 1 (Computing $\mathcal{T}_n(x, \mu)$). Given a finite dimensional transformer T, \mathcal{T}_n can be approximated empirically. In particular, let the data tensor be of size $B \times n \times d$, where B is the batch size, and the sequence size $n \times d$ are sampled from $\mu^{\otimes n}$. Then, given a point, x, we add it to each sequence, process the whole batch at once, and compute the mean. In this manner, inference with the expected transformer is straightforward.

Some prior works Geshkovski et al. (2023); Furuya et al. (2024a) have defined transformers \hat{T} : $\Omega \times \mathcal{P}(\Omega) \to \mathbb{R}^d$ through a continuous version of self-attention Γ . For $x \in \Omega$ and $\mu \in \mathcal{P}(\Omega)$, Γ is defined as

$$\Gamma(x,\mu) := x + \frac{1}{Z(x,\mu)} \int_{\Omega} \operatorname{Att}\left([x;\ y]\right) \, d\mu(y),\tag{8}$$

where $Z(x, \mu)$ is a normalization factor. Then the transformer \hat{T} in Geshkovski et al. (2023); Furuya et al. (2024a) is defined as

 $\hat{T}(x,\mu) := \mathrm{FC}_{\xi_L} \circ \Gamma_{\theta_L} \circ \dots \circ \mathrm{FC}_{\xi_1} \circ \Gamma_{\theta_1}(x), \tag{9}$

where Γ_{θ_j} and FC_{ξ_j} are attention and feed-forward layers with parameters θ_j and ξ_j , respectively. When μ is an empirical measure (a sum of Dirac deltas), this formulation reduces to the standard transformer definition 6. However, due to the nested expectations, computing, or even approximating, $\hat{T}(x,\mu)$ is not straightforward. 220 221 222

225

226 227

228

229

230

231

232

233

234 235 236

243

244 245 246

247

255 256 257

258

262 263

268

269

Goals Our objectives are twofold. First, in Theorem 3, we show that, given a vector field \mathcal{F} as in Equation 1, we can approximate it by the expected transformer \mathcal{T}_n as defined in Equation 7 in a suitable sense. Second, we wish to approximate the solution of the continuity equation 2. Towards this goal, we define an approximate continuity equation using \mathcal{T}_n :

$$\frac{\partial \mu}{\partial t} + \nabla_z \cdot (\mathcal{T}_n(z,\mu)\mu) = 0, \ \mu(0) = \mu_0.$$
(10)

Let $\mu^{\mathcal{F}}(t)$ be the solution to Equation 2, and let $\mu^{\mathcal{T}_n}(t)$ be the solution to Equation 10. In Theorem 4, we will prove that $\mu^{\mathcal{T}_n}(t)$ approximates $\mu^{\mathcal{F}}(t)$ in a suitable sense.

3.2 UNIVERSAL APPROXIMATION OF TRANSFORMERS

At the heart of our argument is the approximation result for finite dimensional transformers can be lifted to approximation results for the expected transformer. Universal approximation of functions on $\mathbb{R}^{d \times n}$ by transformers was first proved in Yun et al. (2020). The approximation was proved under the $L^p(\mathbb{R}^{d \times n})$ norm. The recent work by Alberti et al. (2023), stated below, improves this prior result by proving approximation under the uniform norm.

Theorem 1 (Universal Approximation by Transformer Alberti et al. (2023)). Let $f : \mathbb{R}^{d \times n} \to \mathbb{R}^{d \times n}$ be a permutation equivariant function, for each $\varepsilon < 0$, there exists a transformer T such that,

$$\sup_{X \in \mathbb{R}^{d \times n}} \left\| f(X) - T(X) \right\|_{\infty} < \varepsilon.$$

The concurrent work Furuya et al. (2024a) proves the following approximation result for continuous maps \mathcal{F} by the continuum version of the transformer \hat{T} (equation 9).

Theorem 2. Let $\Omega \subset \mathbb{R}^d$ be a compact set and $F^* : \Omega \times \mathcal{P}(\mathbb{R}^d) \to \mathbb{R}^d$ be continuous, where $\mathcal{P}(\mathbb{R}^d)$ is endowed with the weak* topology. Then for all $\varepsilon > 0$, there exist l and parameters $(\theta_j, \xi_j)_{j=1}^l$ such that

$$\|\hat{T}(\mu, x) - F^*(\mu, x)\| \le \varepsilon, \ \forall (\mu, x) \in \Omega \subset \mathcal{P}(\mathbb{R}^d)$$

where the parameters θ_j, ξ_j depend linearly on the dimension d.

4 THEORETICAL RESULTS

To state the result, we require some assumptions on the map \mathcal{F} . One key assumption we make is that \mathcal{F} is Lipschitz continuous with respect to its second argument, the probability measure. To formalize this, we require a metric on the space of probability measures $\mathcal{P}(\Omega)$. A commonly used metric is the *p*-Wasserstein distance.

Definition 4 (*p*-Wasserstein Distance). *Given two probability measures* $\mu, \nu \in \mathcal{P}_p(\Omega)$ *on a metric* space (Ω, d) , where d is the metric on Ω , the p-Wasserstein distance between μ and ν is defined as

$$\mathcal{W}_p(\mu,\nu) := \left(\inf_{\gamma \in \Pi(\mu,\nu)} \int_{\Omega \times \Omega} d(x,y)^p, d\gamma(x,y)\right)^{1/p},\tag{11}$$

where $\Pi(\mu,\nu)$ denotes the set of all couplings (transport plans) γ on $\Omega \times \Omega$ with marginals μ and ν .

259 When Ω is compact, the *p*-Wasserstein distance metrizes the weak convergence of probability 260 measures (Theorem 6.9 in Villani (2008)). That is, if $\mu_n \in \mathcal{P}_p(\Omega)$ is a sequence of measures such 261 that $\mu_n \to \mu$ weakly if and only if

 $\mathcal{W}_p(\mu_n, \mu) \to 0.$

Additionally, since Ω is compact, convergence in \mathcal{W}_p implies convergence in \mathcal{W}_q , for all q < p.

We now state the main assumptions required for our analysis.

Assumption 1 (Regularity and Growth Conditions). Assume that the vector field $\mathcal{F} : \Omega \times \mathcal{P}_p(\Omega) \rightarrow \mathbb{R}^d$ satisfies the following conditions:

a) (Lipschitz Continuity) There exists a constant \mathcal{L} such that for all $x, y \in \Omega$ and $\mu, \nu \in \mathcal{P}_p(\Omega)$,

$$\|\mathcal{F}(x,\mu) - \mathcal{F}(y,\nu)\|_{L_{\infty}} \le \mathscr{L}\left(\|x-y\|_{L_{\infty}} + \mathcal{W}_{p}(\mu,\nu)\right),$$

b) (*Linear Growth*) There exists a constant $\mathcal{M} > 0$ such that for all $x \in \Omega$ and $\mu \in \mathcal{P}_p(\Omega)$,

$$\|\mathcal{F}(x,\mu)\|_{L_1} \le \mathscr{M} \left(1 + \|x\|_{L_1} + M_1(\mu)\right),$$

where $M_1(\mu) := \int_{\Omega} |y| d\mu(y)$ is the first moment of μ .

c) (Smoothness) For each $\mu \in \mathcal{P}_p(\Omega)$, the function $x \mapsto \mathcal{F}(x, \mu)$ is continuously differentiable on Ω ; that is, $\mathcal{F}(\cdot, \mu) \in C^1(\Omega)$.

Remark 2. Note that Assumption 1a) implies Assumption 1b).

These assumptions are standard in the analysis of mean-field models and are satisfied by many classical systems, such as the Cucker-Smale flocking model (Cucker & Smale, 2007). Theorem 2 of Piccoli et al. (2015) shows that the model satisfies the conditions of Assumption 1. In Section 5, we provide numerical simulations based on this model. To establish our approximation results for functions $\mathcal{H}: \Omega \times \mathcal{P}(\Omega) \to \mathbb{R}^d$, we define the following norm.

Definition 5. Given a function $\mathcal{H} : \Omega \times \mathcal{P}(\Omega) \to \mathbb{R}^d$, we define its norm by

$$\|\mathcal{H}\| := \sup x \in \Omega \sup_{\mu \in \mathcal{P}(\Omega)} \|\mathcal{H}(x,\mu)\|_{L_{\infty}}.$$
(12)

4.1 Approximating the Vector Field \mathcal{F}

We begin by considering the finite-dimensional approximation of the model (equation 1) via a particlelevel system defined on Ω . Specifically, let the state of each particle $i \in \{1, ..., n\}$ be represented by $z_i \in \Omega$. We assume that each z_i is independently sampled from the distribution $\mu \in \mathcal{P}(\Omega)$. Let $\mathbf{z} = (z_1, ..., z_n) \in \Omega^n$ denote the collection of particle states. The empirical distribution of the *n*-particle system is then given by

$$\nu_{\mathbf{z}}^{n} := \frac{1}{n} \sum_{i=1}^{n} \delta_{z_{i}} \in \mathcal{D}^{n}(\Omega).$$
(13)

The particle-level dynamics on \mathbb{R}^d according to the map defined in equation 1 can be written as

$$\dot{z}_i = \mathcal{F}(z_i, \nu_z^n). \tag{14}$$

Note that the collection of random variables (z_i) is permutation equivariant because the joint distribution of (z_i) is invariant under any permutation of the indices. To approximate the vector field \mathcal{F} , we define, for a fixed n, the finite-dimensional map $F_n : \Omega^n \to \mathbb{R}^{d \times n}$ as

$$F_n(\mathbf{z}) := [\mathcal{F}(z_1, \nu_{\mathbf{z}}^n) \quad \dots \quad \mathcal{F}(z_n, \nu_{\mathbf{z}}^n)]$$
(15)

We now state our main result regarding the universal approximation of the mean-field vector field \mathcal{F} by the expected transformer \mathcal{T}_n .

Theorem 3 (Universal Approximation). Let $\varepsilon > 0$. Let $\Omega \subset \mathbb{R}^d$ be a compact set containing 0. Let $\mathcal{F}: \Omega \times \mathcal{P}(\Omega) \to \mathbb{R}^d$ satisfy Assumption 1a) for a given p. Suppose that there exists a transformer network $T: \Omega^{n+1} \to \mathbb{R}^{(n+1) \times d}$ such that

$$\sup_{\dots, z_{n+1} \in \Omega} \|T(z_1, \dots, z_{n+1}) - F_{n+1}(z_1, \dots, z_{n+1})\|_{\infty} \le \varepsilon.$$
(16)

Then, for any q > p there exists a constant C(p,q,d), depending only on p, q, and d, such that for all $n \ge 1$, the corresponding continuum version $\mathcal{T}_n : \Omega \times \mathcal{P}(\Omega) \to \mathbb{R}^d$ (equation 7) satisfies

$$\|\mathcal{T}_n - \mathcal{F}\| \le \varepsilon + C\mathscr{L}diam(\Omega)^p \left(\frac{1}{n^{\frac{q-p}{q}}} + \begin{cases} n^{-1/2} & p > d/2, \ q \ne 2p \\ n^{-1/2}\log(n+1) & p = d/2, \ q \ne 2p \\ n^{-p/d} & p < d/2, \ q \ne d/(d-p) \end{cases}\right).$$

318 319

272 273

274

275

283 284 285

287

288

289

290

291

292

293

295 296 297

298 299 300

301

302

303 304 305

306

307

311 312 313

314

315 316 317

320 *Proof Sketch.* The main steps of the proof are as follows. For a given measure $\mu \in \mathcal{P}(\Omega)$, consider 321 its empirical approximation $\nu_{\mathbf{z}}^n$, where $\mathbf{z} = (z_1, \ldots, z_n)$ are i.i.d. samples from μ . First, using 322 Assumption 1*a*), we show that for any $x \in \Omega$, the difference $\|\mathcal{F}(x,\mu) - \mathcal{F}(x,\nu_{\mathbf{z}}^n)\|$ can be bounded 323 in terms of $\mathcal{W}_p(\mu, \nu_{\mathbf{z}}^n)$. We then bound the distance between μ and $\nu_{\mathbf{z}}^n$ by using Theorem 1 from 324 Fournier & Guillin (2015). 324 Second, we define the finite-dimensional map $F_{n+1}(x, z)$ as Equation 15, and using the Lipschitz 325 continuity of \mathcal{F} , show that the first component $(F_{n+1}(x, \mathbf{z}))_1$ approximates $\mathcal{F}(x, \nu^n \mathbf{z})$ well. 326

Third, since the transformer T approximates F_{n+1} uniformly within ε , we conclude that $\mathcal{T}_n(x,\mu)$, 327 which is defined as the expected value of $(T(x, \mathbf{z}))_1$ over $\mathbf{z} \sim \mu^{\otimes n}$, approximates $\mathcal{F}(x, \mu)$ within the 328 stated bound. 329

330 In Theorem 3, we have shown that finite-dimensional transformers can approximate maps on infinite-331 dimensional spaces under the uniform norm (Equation 12). In particular, we see that the approximation 332 depends on two quantities. First, the approximation depends on how well the finite dimensional 333 transformer T approximates our finite dimensional map F_n , which itself is an approximation of \mathcal{F} . 334 This corresponds to the ε term in the bound. In particular, any universal approximation rates for 335 transformers instantly lifts to expect transformer.

336 Second it depends on the convergence rates of $\mathcal{W}_p(\mu, \nu_{\mathbf{z}}^n)$. We obtain these rates from Theorem 1 of 337 Fournier & Guillin (2015), which depend on n, p, q, and d. Fournier & Guillin (2015) showed that 338 these rates are tight. Furthermore, we see that the stronger regularity the map \mathcal{F} has, i.e., the larger 339 the value of p, the easier it is to approximate. The best rates are obtained for $p = \lfloor \frac{d}{2} + 1 \rfloor$. Thus, 340 if we better approximate F_n or use longer sequences, we obtain an improved approximation of the 341 vector-field \mathcal{F} .

343 Comparison with Result From Furuya et al. (2024a): To compare with Theorem 2, we state the 344 following corollary to Theorem 3.

Corollary 1. Let $\varepsilon > 0$ and n > 1. Let $\Omega \subset \mathbb{R}^d$ be a compact set containing 0. Let $\mathcal{F} : \Omega \times \mathcal{P}(\Omega) \to \mathcal{P}(\Omega)$ 346 \mathbb{R}^d satisfy Assumption 1a) for a given p. Then there exists a transformer T with depth $\Theta(1)$, one attention layer with width $\Theta(d)$ such that the expected transformer \mathcal{T}_n satisfies

$$\|\mathcal{T}_n - \mathcal{F}\| \le \varepsilon + C\mathscr{L}diam(\Omega)^p \left(\frac{1}{n^{\frac{q-p}{q}}} + \begin{cases} n^{-1/2} & p > d/2, \ q \ne 2p\\ n^{-1/2}\log(n+1) & p = d/2, \ q \ne 2p\\ n^{-p/d} & p < d/2, \ q \ne d/(d-p) \end{cases}\right).$$

Proof. We use Theorem 4.3 from Alberti et al. (2023) to construct the transformer T that satisfies the assumptions for Theorem 3.

While Corollary 1 and Theorem 2 are about two different models, they share notable similarities while exhibiting key differences. Both results feature $\Theta(d)$ width for the attention layers, independent of ε and n, and neither provides bounds for the width of feedforward layers. However, our work establishes a bound on network depth, which Furuya et al. (2024a) does not. Moreover, we note that providing a bound on the feedforward network, in our case, is straightforward, owing to recent developments that provide bounds on both width and depth Augustine (2024). Lastly, we note that Furuya et al. (2024a) impose weaker assumptions for the map \mathcal{F} .

363 4.2 APPROXIMATING THE MEAN FIELD DYNAMICS 364

365 In this section, we build upon our previous approximation results to show that solutions of the continuity equation 2 can be approximated by approximating the vector field \mathcal{F} using a transformer 366 \mathcal{T}_n . To formalize this, we first introduce an appropriate notion of a solution to the continuity equation. 367 368 **Definition 6.** A measure-valued function $\mu \in C([0, \tau]; \mathcal{P}_n(\mathbb{R}^d))$ is called a Lagrangian solution of 369 the continuity equation 2 if there exists $X : [0, \tau] \times \mathbb{R}^d \to \mathbb{R}^d$, referred to as the flow map, satisfying

$$X(t,x) = x + \int_0^t \mathcal{F}(X(s,x),\mu(s))ds \tag{17}$$

371 372 373

370

342

345

347

353

354 355

356

357

358

359

360

361

362

for all $x \in \mathbb{R}^d$ and $\mu(t) = X(t, \cdot)_{\#} \mu_0$ for all $t \in [0, \tau]$. 374

375 Under Assumption 1a, it is known that there is a unique Lagrangian solution corresponding to 2. See Proposition 4.8 in Cavagnari et al. (2022). However, a transformer might not be globally Lipschitz as 376 required in Assumption 1a). Hence, the transformer continuity equation 10 may not have a unique 377 Lagrangian solution. For this reason we also need the following assumption.

378 **Assumption 2.** The vector field \mathcal{T}_n is such that there exists a unique Lagrangian solution $\mu^{\mathcal{T}_n} \in$ 379 $C([0,\tau]; \mathcal{P}_p(\mathbb{R}^d))$ to the continuity equation 380

$$\frac{\partial \mu}{\partial t} + \nabla_z \cdot (\mathcal{T}_n(z,\mu)\mu) = 0,$$
(18)

with initial condition $\mu(0) = \mu_0$.

We are now ready to state our main theorem regarding the approximation of mean-field dynamics using transformers.

Theorem 4 (Mean Field Dynamics Approximation Using Transformers). Let $\delta > 0$ and $n \ge 1$. 387 Suppose \mathcal{F} satisfies Assumption 1 for some p and Assumption 2 for $\mu_0 \in \mathcal{P}_c(\mathbb{R}^d)$. If $\operatorname{supp} \mu_0 \subseteq B_R(0)$ 388 for some R > 0, and $K \in \mathbb{R}$ is such that $K > (R + 2\mathcal{M}\tau e^{3(\mathcal{M}\tau)})$. \mathcal{T}_n satisfies for all $z \in \bar{B}_K(0)$ 389 and $\mu \in \mathcal{P}(\bar{B}_K(0))$ 390 $\|\mathcal{T}_n(x,\mu) - \mathcal{F}(z,\mu)\|_{L_{\infty}} < \delta$

391 392

381 382

384

385

386

Then we have that 393

 $W_n(\mu^{\mathcal{F}}(t), \mu^{\mathcal{T}_n}(t)) < \delta \cdot 2^p t \exp(2^p \mathscr{L} t)$ (19)

394 where $\mu^{\mathcal{F}}$ and $\mu^{\mathcal{T}_n}$ are the solutions to equation 2 and equation 10, respectively, and the constants 395 are independent of $\mu_0 \in \mathcal{P}(B_R(0))$. 396

Theorem 4 shows that if \mathcal{T}_n approximates \mathcal{F} well then we can use \mathcal{T}_n to simulate the dynamics 397 equation 2 over any time interval. We observe that the error bound 19 grows exponentially. Therefore, 398 small approximation error for the vector field implies small approximation error for the solution of 399 the continuity equation only for small time horizons. However, we note that bound also depends on 400 the regularity of \mathcal{F} , namely p and \mathcal{L} . Therefore, the more regular the vector-field \mathcal{F} , i.e., larger p and 401 smaller \mathcal{L} , the better the bound 19. 402

We can combine Theorem 3 and Theorem 4 to obtain the following corollary. 403

Corollary 2. Suppose \mathcal{F} satisfies Assumption 1 for some p and Assumption 2 for $\mu_0 \in \mathcal{P}_c(\mathbb{R}^d)$. If 405 $\sup \mu_0 \subseteq B_R(0)$ for some R > 0, and $K \in \mathbb{R}$ is such that $K > (R + 2\mathcal{M}\tau e^{3(\mathcal{M}\tau)})$. Then, for all 406 $\varepsilon > 0$ small enough and $n \in \mathbb{Z}_+$ large enough, there exists a transformer network $T : \mathbb{R}^{d \times (n+1)} \to \mathbb{R}^{d \times (n+1)}$ $\mathbb{R}^{d \times (n+1)}$, with its corresponding continuum version $\mathcal{T}_n : \mathbb{R}^d \times \mathcal{P}(\mathbb{R}^d) \to \mathbb{R}^d$ such that 407

$$W_p(\mu^{\mathcal{F}}(t), \mu^{\mathcal{T}_n}(t)) < 2^p(\varepsilon + \delta(n, K))t\exp(2^p\mathscr{L}t)$$

where

$$\delta(n,K) = \mathscr{L}(2K)^p \left(\frac{1}{n^{\frac{q-p}{q}}} + \begin{cases} n^{-1/2} & p > d/2, q \neq 2p \\ n^{-1/2}\log(n+1) & p = d/2, q \neq 2p \\ n^{-p/d} & p < d/2, q \neq d/(d-p) \end{cases} \right).$$

414 415 416

417

404

408 409 410

411 412 413

5 NUMERICAL SIMULATIONS

418 While Corollary 1 establishes the existence of a transformer network that approximates the vector field, 419 it does not provide a method for determining the model weights. This section presents experiments where we train transformers to approximate the finite-dimensional vector fields and then use them 420 to simulate solutions. To proceed, suppose that we have N training data points that correspond to 421 input-output pairs $\{(\mathbf{p}_{\mathbf{z}}^{n})^{(j)}, (F_{n}(\mathbf{z}))^{(j)}\}_{i=1,\dots,N}$. We train the transformer T on this data using the 422 mean squared loss. We will consider two examples of mean-field systems. The first is a synthetic 423 example where we construct the data from the Cucker-Smale (Cucker & Smale, 2007). The second is 424 the mean-field dynamics of training two-layer neural networks (Mei et al., 2019). 425

Cucker-Smale The first example we consider is the well-studied 2-dimensional Cucker-Smale 427 equation that models consensus of a N-agent system Cucker & Smale (2007). In the equation below, 428 $x \in \mathbb{R}^2$ and $v \in \mathbb{R}^2$ denote the position and velocity of each agent, respectively. Hence, in this setup, 429 d = 4. The vector field $\mathcal{F} : \mathbb{R}^4 \times \mathcal{P}(\mathbb{R}^4) \to \mathbb{R}^4$ is given by 430

431

$$\mathcal{F}(x,v,\mu) = \begin{bmatrix} v \\ -\int_{\mathbb{R}^4} \phi(\|x-y\|)(v-u)d\mu(y,u) \end{bmatrix}, \ \phi(r) = \frac{H}{(s^2+r^2)^b}.$$



Figure 1: Figure comparing training a two-layer neural network using gradient descent to update the weights and using a transformer to update the weights. The solid line is the median value over 100 trials, while the shaded region is the interquartile range (25th-75th percentile). Left: evolution of the training error during training. Center: evolution of the test error during training. Right: difference between the parameters learned by gradient descent and the transformer.

Here, ϕ , a non-negative function, is the interaction potential that determines the inter-agent interaction, and H, s, b are parameters (here set to 1). We also consider the particle version of the system.

0

$$\frac{dx_i}{dt} = v_i, \ 0 \le i \le N \tag{20}$$

$$\frac{dv_i}{dt} = \frac{1}{N} \sum_{j=1}^{N} \phi(\|x_i - x_j\|)(v_j - v_i)$$
(21)

457 To generate the data, we compute the trajectory for 500 different initial conditions. Each initial 458 condition $(x_0^{(j)}, v_0^{(j)})$ is chosen uniformly at random from $\Omega = [0, 1] \times [0, 1]$. For each initial 459 condition, we generate solution trajectories for N = 20 agents over a time horizon [0, 100] using 460 SciPy's solve_ivp using the BDF method. Hence, for each initial condition, we get T_i time steps 461 $t_1^{(j)}, \ldots, t_T^{(j)}$ and for each time step, the method gives us the position and velocities at those time 462 points. Hence, we use a transformer to approximate the $\begin{vmatrix} x \\ v \end{vmatrix}$ $\begin{vmatrix} \dot{x} \\ \dot{v} \end{vmatrix}$ 463 \mapsto . We need to compute \dot{v} for each 464 training point. We could have used the true equation to simulate \dot{v} , but to align better with real-world 465 scenarios, we compute \dot{v} using the centered difference method, ignoring the points at the boundary. 466 This gives a total of 16834 data points. 467

Training 2-Layer Neural Network Consider a two-layer network $f(x) = \sum_{i=1}^{N} a_i \sigma(x^T w_i)$. Let $\theta_i = (a_i, w_i)$ be the parameters. In this model, we consider each θ_i as a particle, and its distribution evolves as we train the model. Mei et al. (2019) showed that the following continuity equation can model the dynamics in the $N \to \infty$ limit.

$$\dot{\mu} = 2\xi(t)\nabla_{\theta} \cdot (\mu\nabla_{\theta}\Psi(\theta,\rho))$$

474 where $\xi(t)$ depends on the learning rate schedule and

ļ

$$\Phi(\theta) = (a, w), \mu) := -\mathbb{E}_{x, y} \left[ya\sigma(x^T w) \right] + \int \mathbb{E}_{x, y} \left[a\hat{a}\sigma(x^T w)\sigma(x^T \hat{w}) \right] d\mu(\hat{a}, \hat{w})$$

478 Here, the vector field we wish to approximate by the transformer is $\mathcal{F}(\theta, \mu) = 2\xi(t)\nabla_{\theta}\Psi(\theta, \mu)$. To 479 generate data, we fix a two-layer teacher network with sigmoid activation and use isotropic Gaussian 480 inputs. We set N = 100 and use an input dimension of 10. Since the sigmoid is 1-Lipschitz, the 481 above equations satisfy our assumptions.

482 483

484

473

475 476 477

442

443

444

445

446

447 448

449

450 451

452 453

- 5.1 Results
- 485 Figure 1 illustrates the training and test loss as we train the model. The blue line represents





Figure 2: Figure comparing the true dynamics of the Cucker-Smaler versus those obtained from a transformer. The solid line is the median value over 100 trials, while the shaded region is the interquartile range (25th-75th percentile).

503 the model trained using SGD, while the orange line corresponds to the model trained with the 504 transformer. Note that the transformer model 505 does not compute any gradients. We trained 506 models with one hundred different random ini-507 tializations. The solid lines indicate the me-508 dian, and the shaded regions represent the in-509 terquartile range. The transformer-trained mod-510 els exhibit favorable training and test loss perfor-511 mance. The rightmost plot in Figure 1 shows the 512 Frobenius norm of the difference between the pa-513 rameters learned using SGD and the transformer. The figure demonstrates that the maximum norm 514

of the difference is at most 5×10^{-5} , even after

516 500 iterations.

517 Next, we simulate the Cucker-Smale flocking dynamics. Each particle is represented by a point in two-518 dimensional space. Figure 3 shows the evolution of ten particles using the Cucker-Smale equations 519 equation 20-equation 21 along with the transformer approximation. Notably, the transformer tracks 520 the true solution quite well. Figure 2 plots the L_2 distance between the positions coordinates x, yand velocities u, v. The figure indicates that the error is generally quite small (< 10⁻⁴), although it 521 increases over time. This increase appears to be linear for the position coordinates, while the error in 522 the velocity seems to plateau and even decrease slightly. Additionally, the initial interquartile range is 523 small, but it grows over time. 524

525 526

527 528

498

499

500 501 502

6 CONCLUSION

In conclusion, this paper demonstrated the efficacy of transformer architectures in approximating the mean-field dynamics of interacting particle systems. We showed that finite-dimensional transformer models can be lifted to approximate the infinite-dimensional mean-field dynamics. Through theoretical results on approximations of the vector field and solution to the continuity equation, as well as numerical simulations, we established that transformers can be powerful tools for modeling and learning the collective behavior of particle systems. In the future, we would like to investigate if transformers can be used to for mean-field control.

535 536

538

537 REFERENCES

Jonas Adler and Ozan Öktem. Solving ill-posed inverse problems using iterative deep neural networks. *Inverse Problems*, 33(12):124007, 2017. 559

564

565

566 567

578

579

580 581

- Daniel Owusu Adu and Bahman Gharesifard. Approximate controllability of continuity equation of transformers. *IEEE Control Systems Letters*, 2024.
- Silas Alberti, Niclas Dern, Laura Thesing, and Gitta Kutyniok. Sumformer: Universal approximation
 for efficient transformers. In *Topological, Algebraic and Geometric Learning Workshops 2023*, pp. 72–86. PMLR, 2023.
- Midhun T Augustine. A survey on universal approximation theorems. arXiv preprint arXiv:2407.12895, 2024.
- Saakaar Bhatnagar, Yaser Afshar, Shaowu Pan, Karthik Duraisamy, and Shailendra Kaushik. Prediction of aerodynamic flow fields using convolutional neural networks. *Computational Mechanics*, 64:525–545, 2019.
- Steven L Brunton, Joshua L Proctor, and J Nathan Kutz. Discovering governing equations from data by sparse identification of nonlinear dynamical systems. *Proceedings of the national academy of sciences*, 113(15):3932–3937, 2016.
- Shengze Cai, Zhiping Mao, Zhicheng Wang, Minglang Yin, and George Em Karniadakis. Physics informed neural networks (pinns) for fluid mechanics: A review. *Acta Mechanica Sinica*, 37(12):
 1727–1738, 2021.
- Giulia Cavagnari, Stefano Lisini, Carlo Orrieri, and Giuseppe Savaré. Lagrangian, eulerian and kantorovich formulations of multi-agent optimal control problems: Equivalence and gamma-convergence. *Journal of Differential Equations*, 322:268–364, 2022. ISSN 0022-0396. doi: https://doi.org/10.1016/j.jde.2022.03.019. URL https://www.sciencedirect.com/science/article/pii/S0022039622001978.
 - Felipe Cucker and Steve Smale. Emergent behavior in flocks. *IEEE Transactions on automatic control*, 52(5):852–862, 2007.
- Karthik Elamvazhuthi and Spring Berman. Mean-field models in swarm robotics: A survey. *Bioinspiration & Biomimetics*, 15(1):015001, 2019.
- Karthik Elamvazhuthi, Bahman Gharesifard, Andrea L Bertozzi, and Stanley Osher. Neural ode
 control for trajectory approximation of continuity equation. *IEEE Control Systems Letters*, 6: 3152–3157, 2022.
- Jinchao Feng, Yunxiang Ren, and Sui Tang. Data-driven discovery of interacting particle systems using gaussian processes. *arXiv e-prints*, pp. arXiv–2106, 2021.
- 576 Nicolas Fournier and Arnaud Guillin. On the rate of convergence in wasserstein distance of the
 577 empirical measure. *Probability theory and related fields*, 162(3):707–738, 2015.
 - Takashi Furuya, Maarten V de Hoop, and Gabriel Peyré. Transformers are universal in-context learners. *arXiv preprint arXiv:2408.01367*, 2024a.
- Takashi Furuya, Michael Puthawala, Matti Lassas, and Maarten V de Hoop. Globally injective and bijective neural operators. *Advances in Neural Information Processing Systems*, 36, 2024b.
- Borjan Geshkovski, Cyril Letrouit, Yury Polyanskiy, and Philippe Rigollet. A mathematical perspective on transformers. *arXiv preprint arXiv:2312.10794*, 2023.
- Xiaoxiao Guo, Wei Li, and Francesco Iorio. Convolutional neural networks for steady flow approximation. In *Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining*, KDD '16, pp. 481–490. Association for Computing Machinery, 2016. ISBN 9781450342322.
- Kurt Hornik, Maxwell Stinchcombe, and Halbert White. Multilayer feedforward networks are universal approximators. *Neural Networks*, 2(5):359–366, 1989. ISSN 0893-6080. doi: https://doi.org/10.1016/0893-6080(89)90020-8. URL https://www.sciencedirect.com/science/article/pii/0893608089900208.

594 595	Patrick Kidger and Terry Lyons. Universal approximation with deep narrow networks. In <i>Conference on learning theory</i> , pp. 2306–2327. PMLR, 2020.
597 598 599	Nikola Kovachki, Zongyi Li, Burigede Liu, Kamyar Azizzadenesheli, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. Neural operator: Learning maps between function spaces. <i>arXiv</i> preprint arXiv:2108.08481, 2021.
600 601	Chenghui Li, Rishi Sonthalia, and Nicolas Garcia Trillos. Spectral neural networks: Approximation theory and optimization landscape. <i>arXiv preprint arXiv:2310.00729</i> , 2023.
603 604	Zongyi Li, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. Fourier neural operator for parametric partial differential equations. <i>arXiv preprint arXiv:2010.08895</i> , 2020a.
606 607 608	Zongyi Li, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. Neural operator: Graph kernel network for partial differential equations. <i>arXiv preprint arXiv:2003.03485</i> , 2020b.
609 610	Ugo Lopez, Jacques Gautrais, Iain D Couzin, and Guy Theraulaz. From behavioural analyses to models of collective motion in fish schools. <i>Interface focus</i> , 2(6):693–707, 2012.
612 613 614	Fei Lu, Ming Zhong, Sui Tang, and Mauro Maggioni. Nonparametric inference of interaction laws in systems of agents from trajectory data. <i>Proceedings of the National Academy of Sciences</i> , 116(29): 14424–14433, 2019.
615 616	Vitaly Maiorov and Allan Pinkus. Lower bounds for approximation by mlp neural networks. <i>Neuro-computing</i> , 25(1-3):81–91, 1999.
617 618 619 620	Song Mei, Theodor Misiakiewicz, and Andrea Montanari. Mean-field theory of two-layers neural networks: dimension-free bounds and kernel limit. In <i>Conference on learning theory</i> , pp. 2388–2464. PMLR, 2019.
621 622	Daniel A Messenger and David M Bortz. Learning mean-field equations from particle data using wsindy. <i>Physica D: Nonlinear Phenomena</i> , 439:133406, 2022.
623 624 625	Jason Miller, Sui Tang, Ming Zhong, and Mauro Maggioni. Learning theory for inferring interaction kernels in second-order interacting agent systems. <i>Sampling Theory, Signal Processing, and Data Analysis</i> , 21(1):21, 2023.
627 628	Huyên Pham and Xavier Warin. Mean-field neural networks: learning mappings on wasserstein space. <i>Neural Networks</i> , 168:380–393, 2023.
629 630	Benedetto Piccoli, Andrea Tosin, et al. Vehicular traffic: A review of continuum mathematical models. Encyclopedia of complexity and systems science, 22:9727–9749, 2009.
632 633	Benedetto Piccoli, Francesco Rossi, and Emmanuel Trélat. Control to flocking of the kinetic cucker- smale model. <i>SIAM Journal on Mathematical Analysis</i> , 47(6):4685–4719, 2015.
634 635 636	Maziar Raissi, Paris Perdikaris, and George E Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. <i>Journal of Computational Physics</i> , 378:686–707, 2019.
637 638 639	Domenec Ruiz-Balet and Enrique Zuazua. Neural ode control for classification, approximation, and transport. <i>SIAM Review</i> , 65(3):735–773, 2023.
640 641	Zuowei Shen, Haizhao Yang, and Shijun Zhang. Optimal approximation rate of relu networks in terms of width and depth. <i>Journal de Mathématiques Pures et Appliquées</i> , 157:101–135, 2022.
642 643 644	Silvia Siri, Cecilia Pasquale, Simona Sacone, and Antonella Ferrara. Freeway traffic control: A survey. <i>Automatica</i> , 130:109655, 2021.
645 646 647	Matus Telgarsky. benefits of depth in neural networks. In Vitaly Feldman, Alexander Rakhlin, and Ohad Shamir (eds.), 29th Annual Conference on Learning Theory, volume 49 of Proceedings of Machine Learning Research, pp. 1517–1539, Columbia University, New York, New York, USA, 23–26 Jun 2016. PMLR.

648 649 650	Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. <i>Advances in neural information processing systems</i> , 30, 2017.
651 652 653	Cédric Villani. <i>Optimal transport – Old and new</i> , volume 338, pp. xxii+973. 01 2008. doi: 10.1007/978-3-540-71050-9.
654 655 656	James Vuckovic, Aristide Baratin, and Rémi Tachet des Combes. A mathematical theory of attention. <i>ArXiv</i> , abs/2007.02876, 2020. URL https://api.semanticscholar.org/CorpusID: 220363994.
657 658 659	E Weinan and Ting Yu. The deep ritz method: A deep learning-based numerical algorithm for solving variational problems. <i>Communications in Mathematics and Statistics</i> , 6:1–12, 2017.
660 661	Dmitry Yarotsky. Optimal approximation of continuous functions by very deep relu networks. In <i>Conference on learning theory</i> , pp. 639–649. PMLR, 2018.
662 663 664 665 666	Chulhee Yun, Srinadh Bhojanapalli, Ankit Singh Rawat, Sashank Reddi, and Sanjiv Kumar. Are transformers universal approximators of sequence-to-sequence functions? In <i>International Conference on Learning Representations</i> , 2020. URL https://openreview.net/forum?id=ByxRMONtvr.
667 668 669	Yinhao Zhu and Nicholas Zabaras. Bayesian deep convolutional encoder–decoder networks for surrogate modeling and uncertainty quantification. <i>Journal of Computational Physics</i> , 366:415–447, 2018.
670 671 672	
673 674	
675 676 677	
678 679	
680 681 682	
683 684	
685 686	
688 689	
690 691	
692 693 694	
695 696	
697 698 699	
700 701	

A PROOF OF THEOREM 3

Theorem 3 (Universal Approximation). Let $\varepsilon > 0$. Let $\Omega \subset \mathbb{R}^d$ be a compact set containing 0. Let $\mathcal{F} : \Omega \times \mathcal{P}(\Omega) \to \mathbb{R}^d$ satisfy Assumption 1a) for a given p. Suppose that there exists a transformer network $T : \Omega^{n+1} \to \mathbb{R}^{(n+1) \times d}$ such that

$$\sup_{z_1,\dots,z_{n+1}\in\Omega} \|T(z_1,\dots,z_{n+1}) - F_{n+1}(z_1,\dots,z_{n+1})\|_{\infty} \le \varepsilon.$$
(16)

Then, for any q > p there exists a constant C(p, q, d), depending only on p, q, and d, such that for all $n \ge 1$, the corresponding continuum version $\mathcal{T}_n : \Omega \times \mathcal{P}(\Omega) \to \mathbb{R}^d$ (equation 7) satisfies

$$\|\mathcal{T}_n - \mathcal{F}\| \le \varepsilon + C\mathscr{L}diam(\Omega)^p \left(\frac{1}{n^{\frac{q-p}{q}}} + \begin{cases} n^{-1/2} & p > d/2, \ q \ne 2p \\ n^{-1/2}\log(n+1) & p = d/2, \ q \ne 2p \\ n^{-p/d} & p < d/2, \ q \ne d/(d-p) \end{cases}\right).$$

Proof.

702

703 704

705

706

707 708

709 710

749

750 751

$$\begin{split} \|\mathcal{F} - \mathcal{T}_{n}\| &= \sup_{\mu} \sup_{x} \left\| \mathcal{F}(x,\mu) - \int_{\Omega^{n}} (T(x,\mathbf{z}))_{1} d\mu^{\otimes n}(\mathbf{z}) \right\|_{\infty} \\ &\leq \sup_{\mu} \sup_{x} \int_{\Omega^{n}} \|\mathcal{F}(x,\mu) - (T(x,\mathbf{z}))_{1}\|_{\infty} d\mu^{\otimes n}(\mathbf{z}) \\ &= \sup_{\mu} \sup_{x} \int_{\Omega^{n}} \|\mathcal{F}(x,\mu) - \mathcal{F}(x,\nu_{\mathbf{z}}^{n}) + \mathcal{F}(x,\nu_{\mathbf{z}}^{n}) - (T(x,\mathbf{z}))_{1}\|_{\infty} d\mu^{\otimes n}(\mathbf{z}) \\ &\leq \sup_{\mu} \sup_{x} \int_{\Omega^{n}} \|\mathcal{F}(x,\mu) - \mathcal{F}(x,\nu_{\mathbf{z}}^{n})\|_{\infty} d\mu^{\otimes n}(\mathbf{z}) \\ &+ \sup_{\mu} \sup_{x} \int_{\Omega^{n}} \|\mathcal{F}(x,\nu_{\mathbf{z}}^{n}) - (T(x,\mathbf{z}))_{1}\|_{\infty} d\mu^{\otimes n}(\mathbf{z}) \quad (*) \end{split}$$

The second inequality follows from the standard triangle inequality. The first integral on the RHS can be bounded from above as,

$$\begin{aligned} \sup_{\mu} \sup_{x} \int_{\Omega^{n}} \|\mathcal{F}(x,\mu) - \mathcal{F}(x,\nu_{\mathbf{z}}^{n})\|_{\infty} d\mu^{\otimes n}(\mathbf{z}) \\ & \leq \sup_{\mu} \int_{\Omega^{n}} \sup_{x} \|\mathcal{F}(x,\mu) - \mathcal{F}(x,\nu_{\mathbf{z}}^{n})\|_{\infty} d\mu^{\otimes n}(\mathbf{z}) \\ & \leq \sup_{\mu} \int_{\Omega^{n}} \mathcal{L} \|\mu - \nu_{\mathbf{z}}^{n}\|_{\mathcal{W}_{p}} d\mu^{\otimes n}(\mathbf{z}) \\ & = \mathcal{L} \sup_{\mu} \mathbb{E}_{\mathbf{z} \sim \mu^{\otimes n}} [\mathcal{W}_{p}(\mu,\nu_{\mathbf{z}}^{n})] \quad (**) \end{aligned}$$

743 We let $M_q(\mu)$ be the q-moment of μ i.e. $M_q(\mu) := \int_{\Omega} |x|^q d\mu(x)$ and 744

$$G(n) = \begin{cases} n^{-1/2} & p > d/2, \ q \neq 2p \\ n^{-1/2} \log(n+1) & p = d/2, \ q \neq 2p \\ n^{-p/d} & p < d/2, \ q \neq d/(d-p) \end{cases}.$$

Then as per Theorem 1 of Fournier & Guillin (2015), there exists a constant C(p, q, d) (a function of p, q, d) such that, $\mathbb{E}_{\mathbf{z} \sim \mu^{\otimes n}}$ from (**) can be bounded from above by $CM_q^{p/q}(\mu)G(n)$. We obtain:

752
753
754
755

$$\sup_{\mu} \sup_{x} \int_{\Omega^{n}} \|\mathcal{F}(x,\mu) - \mathcal{F}(x,\nu_{\mathbf{z}}^{n})\|_{\infty} d\mu^{\otimes n}(\mathbf{z}) \leq \mathscr{L} \sup_{\mu} CM_{q}^{p/q}(\mu)G(n)$$

$$\leq \mathscr{L}C \operatorname{diam}(\Omega)^{p}G(n), \quad (22)$$

where we have used the fact that μ is a probability measure on Ω .

Next, we obtain an upper bound for the second integral in (*).

758
759
$$\sup_{\mu} \sup_{x} \int_{\Omega^{n}} \|\mathcal{F}(x,\nu_{\mathbf{z}}^{n}) - (T(x,\mathbf{z}))_{1}\|_{\infty} d\mu^{\otimes n}(\mathbf{z})$$

760
761
$$\leq \sup \int_{\Omega^n} \sup \|\mathcal{F}(x,\nu_{\mathbf{z}}^n) - (F_{n+1}(x,z_1,\ldots,z_n))_1\|_{\infty} d\mu^{\otimes n}(\mathbf{z})$$

762
763
764

$$\mu J_{\Omega^n} x$$

 $+ \sup_{\mu} \int_{\Omega^n} \sup_{x} \|(F_{n+1}(x, z_1, \dots, z_n))_1 - (T(x, \mathbf{z}))_1\|_{\infty} d\mu^{\otimes n}(\mathbf{z})$

765 Consider the first term in the expression above

$$\begin{aligned}
& \sup_{\mu} \int_{\Omega^{n}} \sup_{x} \|\mathcal{F}(x,\nu_{\mathbf{z}}^{n}) - (F_{n+1}(x,z_{1},\ldots,z_{n}))_{1}\|_{\infty} d\mu^{\otimes n}(\mathbf{z}) \\
& = \sup_{\mu} \int_{\Omega^{n}} \sup_{x} \|\mathcal{F}(x,\nu_{\mathbf{z}}^{n}) - \mathcal{F}\left(x,\nu_{(x,\mathbf{z})}^{n+1}\right)\|_{\infty} d\mu^{\otimes n}(\mathbf{z}) \\
& = \sup_{\mu} \int_{\Omega^{n}} \mathscr{L} \|\nu_{\mathbf{z}}^{n} - \nu_{(x,\mathbf{z})}^{n+1}\|_{W_{p}} d\mu^{\otimes n}(\mathbf{z}) \\
& \leq \sup_{\mu} \int_{\Omega^{n}} \mathscr{L} \frac{2}{n+1} d\mu^{\otimes n}(\mathbf{z}) \\
& = \mathscr{L} \frac{2}{n+1}
\end{aligned}$$
(23)

Since we have assumed 16, we have

$$\sup_{\mu} \int_{\Omega^n} \sup_{x} \left\| (F_{n+1}(x, z_1, \dots, z_n))_1 - (T(x, \mathbf{z}))_1 \right\|_{\infty} d\mu^{\otimes n}(\mathbf{z}) \le \varepsilon$$
(24)

Putting together 22, 23, and 24, we get that

$$\|\mathcal{T}_n - \mathcal{F}\| \leq \mathscr{L}C \operatorname{diam}(\Omega)^p G(n) + \mathscr{L}\frac{2}{n+1} + \varepsilon.$$

B PROOF OF THEOREM 4

Proposition 1. Suppose there exists a Lagrangian solution $\mu \in C([0, \tau]; \mathcal{P}(\mathbb{R}^d))$ of equation 2. Additionally, suppose that \mathcal{F} satisfies Assumption 1. Then the solution satisfies,

$$\operatorname{supp} \mu(t) \subseteq B_{C_t}(0) \tag{25}$$

for all $t \in [0, \tau]$, where $C_t = (R + 2\mathcal{M}t)e^{3\mathcal{M}t}$.

Proof. By definition of the Lagrangian solution,

$$\|X(t,x)\|_{L_1} \le \|x\|_{L_1} + \int_0^t \|\mathcal{F}(X(s,x),\mu(s))\|_{L_1} ds$$
(26)

$$\leq \|x\|_{L_1} + \int_0^t \mathscr{M}(1 + \|X(s, x)\|_{L_1} + M_1(\mu(s)))ds$$
(27)

Integrating both sides of 27 with respect to μ_0 we get,

$$M_1(\mu(t)) \le M_1(\mu_0) + \mathscr{M} \int_0^t (1 + 2M_1(\mu(s))) ds$$

Combining this with 27 itself we get,

$$\|X(t,x)\|_{L_1} + M_1(\mu(t)) \le M_1(\mu_0) + \mathscr{M} \int_0^t (2 + \|X(s,x)\|_{L_1} + 3M_1(\mu(s))) ds$$

Using Gronwall's lemma, this implies

 $||X(t,x)||_{L_1} + M_1(\mu(t)) \le (M_1(\mu_0) + 2\mathscr{M}t))e^{3\mathscr{M}t}$ $\leq (R+2\mathscr{M}t)e^{3\mathscr{M}t}$

Theorem 4 (Mean Field Dynamics Approximation Using Transformers). Let $\delta > 0$ and n > 1. Suppose \mathcal{F} satisfies Assumption 1 for some p and Assumption 2 for $\mu_0 \in \mathcal{P}_c(\mathbb{R}^d)$. If $\operatorname{supp} \mu_0 \subseteq B_R(0)$ for some R > 0, and $K \in \mathbb{R}$ is such that $K > (R + 2\mathcal{M}\tau e^{3(\mathcal{M}\tau)})$. \mathcal{T}_n satisfies for all $z \in \bar{B}_K(0)$ and $\mu \in \mathcal{P}(\bar{B}_K(0))$ $\|\mathcal{T}_n(x,\mu) - \mathcal{F}(z,\mu)\|_{L_{\infty}} < \delta$

Then we have that

$$W_p(\mu^{\mathcal{F}}(t), \mu^{\mathcal{T}_n}(t)) < \delta \cdot 2^p t \exp(2^p \mathscr{L} t)$$
(19)

where $\mu^{\mathcal{F}}$ and $\mu^{\mathcal{T}_n}$ are the solutions to equation 2 and equation 10, respectively, and the constants are independent of $\mu_0 \in \mathcal{P}(B_R(0))$.

Proof. Let X, Y be the flow maps associated with with respect the vector fields \mathcal{F} and \mathcal{T}_n , respectively. From the definition of Lagrangian solutions we know that,

$$X(t,x) = x + \int_0^t \mathcal{F}(X(s,x),\mu^{\mathcal{F}}(s))ds$$
$$Y(t,x) = x + \int_0^t \mathcal{T}_n(Y(s,x)),\mu^{\mathcal{T}_n}(s))ds$$

for all $t \in [0, \tau]$. From this we get

$$\begin{aligned} \|Y(t,x) - X(t,x)\|_{p}^{p} &= \left\|\int_{0}^{t} \mathcal{T}_{n}(Y(s,x),\mu^{\mathcal{T}_{n}}(s))ds - \int_{0}^{t} \mathcal{F}(X(s,x),\mu^{\mathcal{F}}(s))ds\right\|_{p}^{p} \\ &\leq 2^{p-1} \left\|\int_{0}^{t} \mathcal{T}_{n}(Y(s,x),\mu^{\mathcal{T}_{n}}(s))ds - \int_{0}^{t} \mathcal{F}(Y(s,x),\mu^{\mathcal{F}}(s))ds\right\|_{p}^{p} \\ &+ 2^{p-1} \left\|\int_{0}^{t} \mathcal{F}(Y(s,x),\mu^{\mathcal{F}}(s))ds - \int_{0}^{t} \mathcal{F}(X(s,x),\mu^{\mathcal{F}}(s))ds\right\|_{p}^{p} \end{aligned}$$

843
844
845
$$\leq 2^{p-1} \left\| \int_0^t \mathcal{T}_n(Y(s,x),\mu^{\mathcal{T}_n}(s)) ds - \int_0^t \mathcal{F}(Y(s,x),\mu^{\mathcal{T}_n}(s)) ds \right\|$$

$$+2^{p-1} \left\| \int_0^t \mathcal{F}(Y(s,x),\mu^{\mathcal{T}_n}(s)) ds - \int_0^t \mathcal{F}(Y(s,x),\mu^{\mathcal{F}}(s)) ds \right\|_p^p$$

$$+ 2^{p-1} \left\| \int_0^t \mathcal{F}(Y(s,x),\mu^{\mathcal{F}}(s)) ds - \int_0^t \mathcal{F}(X(s,x),\mu^{\mathcal{F}}(s)) ds \right\|_p^p$$

The first inequality follows from Young's inequality. Since, $K > (R + 2\mathcal{M}\tau e^{3(\mathcal{M}\tau)})$, for $\varepsilon > 0$ small enough, and n large enough we can conclude that, $K > (R + 2(\mathcal{M} + \varepsilon + \varepsilon))$ $\delta(n,K)$) $\tau e^{3((\mathcal{M}+\varepsilon+\delta(n,K))\tau)})$. We can approximate \mathcal{F} using \mathcal{T}_n on $B_K(0)$. Using the uniform norm approximation, we can conclude that

$$\|\mathcal{T}_n(x,\mu)\|_{L_1} \le (\mathscr{M} + \varepsilon + \delta(n,K))(1 + \|x\|_{L_1} + M_1(\mu))$$

for all $x \in \mathbb{R}^d$ and $\mu \in \mathcal{P}(B_K(0))$. From this we get,

$$\operatorname{supp} \mu^{\mathcal{T}_n(s)} \subseteq B_K(0)$$

by Proposition 1.

$$2^{1-p} \|Y(t,x) - X(t,x)\|_{p}^{p} \leq \int_{0}^{t} \varepsilon + \delta(n,K) ds + \int_{0}^{t} \mathscr{L} W_{p}^{p}(\mu^{\mathcal{F}}(s),\mu^{\mathcal{T}_{n}}(s)) ds + \int_{0}^{t} \mathscr{L} \|Y(s,x) - X(s,x)\|_{L_{1}} ds.$$

Taking expectation with respect to the initial condition we obtain,

$$2^{1-p} \int_{\mathbb{R}^d} \||Y(t,x) - X(t,x)\|_p^p d\mu_0(x) \le (\varepsilon + \delta(n,K))t + \int_0^t \mathscr{L}\mathcal{W}_1(\mu^{\mathcal{F}}(s),\mu^{\mathcal{T}_n}(s))ds + \int_{\mathbb{R}^d} \int_0^t \mathscr{L}\|Y(s,x) - X(s,x)\|_p ds \ d\mu_0(x)$$

Using the fact that

$$\begin{aligned} \mathcal{W}_p(\mu^{\mathcal{F}}(t), \mu^{\mathcal{T}_n}(t)) &\leq \int_{\mathbb{R}^d} \|x - X(t, Y^{-1}(t, x))\|_p^p d(Y(t, \cdot)_{\#} \mu_0)(x) \\ &= \int_{\mathbb{R}^d} \|Y(t, x) - X(t, x)\|_p^p d\mu_0(x), \end{aligned}$$

we can conclude that

$$2^{-p} \int_{\mathbb{R}^d} \|Y(t,x) - X(t,x)\|_p^p d\mu_0(x) + 2^{-p} \mathcal{W}_p^p(\mu^{\mathcal{F}}(t),\mu^{\mathcal{T}_n}(t)) \le (\varepsilon + \delta(n,K))t$$
$$+ \int_0^t \mathscr{L} \mathcal{W}_p^p(\mu^{\mathcal{F}}(s),\mu^{\mathcal{T}_n}(s)) ds + \int_{\mathbb{R}^d} \int_0^t \mathscr{L} |Y(s,x) - X(s,x)| ds \ d\mu_0(x).$$

This implies that

$$2^{-p} \int_{\mathbb{R}^d} \|Y(t,x) - X(t,x)\|_p^p d\mu_0(x) + 2^{-p} \mathcal{W}_p^p(\mu^{\mathcal{F}}(t),\mu^{\mathcal{T}_n}(t)) \le (\varepsilon + \delta(n,K))t$$
$$+ \mathscr{L} \int_0^t \mathcal{W}_p^p(\mu^{\mathcal{F}}(s),\mu^{\mathcal{T}_n}(s)) ds + \mathscr{L} \int_{\mathbb{R}^d} \int_0^t |Y(s,x) - X(s,x)| ds \ d\mu_0(x)$$

Now, applying Gronwall's inequality, we get,

$$\int_{\mathbb{R}^d} \|Y(t,x) - X(t,x)\|_p^p d\mu_0(x) + \mathcal{W}_p^p(\mu^{\mathcal{F}}(t),\mu^{\mathcal{T}_n}(t)) \le 2^p(\varepsilon + \delta(n,K))t\exp(2\mathscr{L}t)$$

This implies that

$$\mathcal{W}_p^p(\mu^{\mathcal{F}}(t), \mu^{\mathcal{T}_n}(t)) \le 2^p(\varepsilon + \delta(n, K))t\exp(2\mathscr{L}t)$$