On the relationship between Koopman operator approximations and neural ordinary differential equations for data-driven time-evolution predictions

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Abstract

This work explores the relationship between state space methods and Koopman operator-based methods for predicting the time-evolution of nonlinear dynamical systems. We demonstrate that extended dynamic mode decomposition with dictionary learning (EDMD-DL), when combined with a state space projection, is equivalent to a neural network representation of the nonlinear discretetime flow map on the state space. We highlight how this projection step introduces nonlinearity into the evolution equations, enabling significantly improved EDMD-DL predictions. With this projection, EDMD-DL leads to a nonlinear dynamical system on the state space, which can be represented in either discrete or continuous time. This system has a natural structure for neural networks, where the state is first expanded into a high dimensional feature space followed by a linear mapping which represents the discrete-time map or the vector field as a linear combination of these features. Inspired by these observations, we implement several variations of neural ordinary differential equations (ODEs) and EDMD-DL, developed by combining different aspects of their respective model structures and training procedures. We evaluate these methods using numerical experiments on chaotic dynamics in the Lorenz system and a nine-mode model of turbulent shear flow, showing comparable performance across methods in terms of short-time trajectory prediction, reconstruction of long-time statistics, and prediction of rare events. We also show that these methods provide comparable performance to a non-Markovian approach in terms of prediction of extreme events.

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Accurately predicting the behavior of complex dynamical systems is a critical challenge in many scientific and engineering fields, especially with the increasing availability of large datasets. Two promising approaches for developing predictive models from time-series data are neural ODEs, which construct continuoustime models directly on the space of the original data, and approaches based on Koopman operator theory, which lift the data to a high dimensional space where the dynamics can be represented linearly. Recent works have shown that the predictive performance of Koopman-based methods can be significantly improved by projecting the prediction back to the state space on each timestep. We show that this step converts the linear dynamics on the space of observables to a nonlinear system on the state space, rendering the method essentially equivalent to a neural ODE of a particular form. This insight helps to form new connections between these distinct approaches and inspires new methods that combine the strengths of each. We validate these findings through numerical experiments and performance comparisons on two chaotic systems arising in fluid dynamics, showing that methods arising from each approach exhibit excellent, and nearly equivalent predictive performance.

I. INTRODUCTION

Developing methods for forecasting the time-evolution of complex systems governed by ordinary differential equations (ODEs) using models derived directly from data is of great importance to many scientific and engineering applications, especially as data from many of these systems has become more readily available in recent years. This demand has driven the development of many neural network architectures tailored to time-series data. Some of the most popular and effective modeling techniques for time sequence data include neural networks with recurrent architectures, such as long short-term memory networks (LSTM) [1] or gated recurrent units (GRU) [2]; reservoir computing methods [3]; and transformerbased architectures [4] (see, for example, Refs. [5–8] for applications of these methods on dynamical systems). However, these approaches implicitly abandon the dynamical systems point of view by constructing models which predict future time evolution from long sequences of past states. That is, these models are non-Markovian and thus effectively operate on a space of much higher dimension than the original state space. Here, our focus is on developing models using data obtained from systems which are known to be governed by differential equations. Therefore, we restrict ourselves to Markovian models, in which future time evolution is uniquely determined from the present state. In this work we consider parallels between neural network-based methods for modeling dynamical systems which represent the dynamics directly on the state space and those which represent the dynamics in the space of observable functions using Koopman operator approximations, as illustrated in Fig. 1.

In recent years, data-driven modeling techniques derived from Koopman operator theory have gained significant research attention due to their potential to provide linear representations for complex, nonlinear dynamical systems [9–11]. In the Koopman formalism, time evolution is considered in the space of observable functions of the states, rather than in the state space of the system. Therefore, though the time evolution is determined by a linear operator, this operator typically acts on an infinite dimensional function space. Much of the work in this area has focused on constructing useful finite-dimensional approximations of the Koopman operator directly from data. Such approximations hold great promise for many application areas, as they enable the use of modal analysis to identify structure in nonlinear systems [10, 12], they can allow for model reduction when dealing with high-dimensional data [13], and they can potentially be paired with linear methods for forecasting, estimation, and control [14].

Many numerical techniques have been developed for constructing finite-dimensional approximations of the Koopman operator. One of the earliest and most common approaches is dynamic mode decomposition (DMD), originally proposed by Schmid [15], which determines a best-fit linear time-evolution operator (or its eigenvalues and eigenvectors) given time series data from the system (pairs of snapshots separated by one timestep). DMD is appealing to many practitioners due to its simplicity and its ability to extract physically meaningful features or modes directly from data without any a priori knowledge of the system or dynamics. The connection between DMD and the Koopman operator was made by Rowley et al. [16], which built upon the earlier works of Mezic that proposed a Koopman mode decomposition directly from data [12, 17].

As pointed out by Rowley, et al [16], the finite dimensional approximation obtained from DMD can only be rigorously connected to the Koopman operator if the observable functions



FIG. 1. Schematic illustrating how EDMD-DL with a projection to the state space directly leads to a neural network representation of the nonlinear dynamics on the state space.

used in the computation lie within an invariant subspace spanned by eigenfunctions of the Koopman operator. In practice, however, this is usually not the case, such as when the data is obtained directly from experimental observations. This lack of an invariant subspace then leads to closure issues with the numerically obtained matrix approximation of the operator, as the true operator propagates the selected observables forward in time into functions that cannot be represented as a linear combination of these observables. This leads to inaccurate approximations of Koopman modes and rapid error buildup when attempting to use the operator approximation for forecasting [18, 19]. These issues have led to numerous extensions of the original DMD algorithm [20], with many of them aiming to improve the function space on which the operator is approximated by a careful selection of observables. One of the most prominent variations is extended dynamic mode decomposition (EDMD) [21], which performs the DMD computation for the best-fit linear time evolution operator on measurement data that is "lifted" to a higher dimensional space by evaluating a pre-defined set of dictionary functions on the data. Williams et al. [21] showed that EDMD offers an improvement upon DMD, as it converges to the same results that would be obtained from a Galerkin method in the limit of a large data set. However, aside from some heuristic guidelines, the optimal choice of dictionary functions remained an open problem.

In light of this challenge, many works have proposed methods to learn or discover an appropriate choice of observables to be used in EDMD. Li et al. [22] proposed a method called EDMD with dictionary learning (EDMD-DL) which optimizes the dictionary used with EDMD by representing the dictionary as a neural network and optimizing its parameters by stochastic gradient descent to minimize a prediction loss. They showed that this method yielded great improvements over standard choices of dictionary, both in terms of approximating Koopman eigenfunctions and eigenvalues and in forecasting capabilities. Recently, this method was extended by Constante-Amores, et al. [23], who showed that the optimization of the dictionary and the operator can be combined into a streamlined training procedure by backpropagating through the EDMD pseudoinverse calculation. EDMD-DL typically allows for linear reconstruction of the state from the dictionary by explicitly including the state in the dictionary as non-trainable elements. Other works |24, 25| have proposed methods in which Koopman operators are approximated by learning linear dynamics on the latent space of an autoencoder, thus learning both a nonlinear encoding (lifting) transformation as well as a nonlinear decoding transformation to reconstruct the state. These works also typically optimize the matrix representation of the operator and a dictionary for lifting simultaneously by stochastic gradient descent without the need to perform a leastsquares or pseudoinverse calculation, as in standard EDMD. Relatedly, Constante-Amores, et al. [26, 27] applied EDMD-DL to learn a dynamic model for the latent state from an autoencoder-based reduced order model.

Despite these advances, Koopman-based methods with linear time-evolution still fail to provide accurate forecasts of complex systems (see, for example, Ref. [23, 28]). In many cases, this is likely due to the fact that certain systems are nonlinearizable [29]. That is, it is not possible to find a finite-dimensional linear representation of a nonlinear system with essentially nonlinear characteristics (such as multiple isolated attracting equilibria) because such systems cannot globally be smoothly conjugate to a finite-dimensional linear system. [18, 30–33]. This is due to the fact that any linear system can have at most one isolated, attracting equilibrium. Further discussions on the existence of smooth embeddings of nonlinear systems can be found in the recent works of Kvalheim and Arathoon [34, 35] and Liu et al [36, 37]. Another recent series of papers have indicated that, from an applied perspective, one mechanism that may be useful for constructing global linearizations is the introduction of discontinuous indicator functions which separate distinct regions of attraction [38–40], effectively giving a piecewise linear Koopman representation. It has also been shown that whether or not a system can be represented linearly in finite dimension is related to the spectrum of the Koopman operator [12, 41, 42], in that systems where the associated Koopman operator has a continuous spectrum do not admit a finite dimensional linear representation [42]. This is a substantial limitation of the predictive capability of Koopmanbased methods, as it indicates that it is not possible for these methods to fully capture the chaotic dynamics associated with the continuous spectrum.

Indeed, many Koopman-based methods for forecasting introduce a nonlinearity into the time-evolution formulation to improve performance, with some doing so explicitly and some subtly. Baddoo et al. [43] proposed learning a nonlinear forcing term jointly with a linear operator using a kernel-based learning strategy to identify a sparse dictionary for the nonlinear forcing. They show that by disambiguating the linear and nonlinear terms in this way, the identified linear operator is more robust, as it is not corrupted by noise effects from the nonlinear terms as in the standard DMD training procedure. Similarly, Eivazi et al. [44], introduced a modified version of Hankel-DMD [45, 46] (a Koopman-based model in time-delay coordinates) that explicitly includes a nonlinear term in the time evolution model, showing that their Koopman-based method provides models which achieve the same level of prediction accuracy as non-Markovian time-series models using recurrent neural networks (RNNs). Others have proposed that a way to avoid the issue of the impossibility of conjugacy to a linear system is to avoid including the full state explicitly in the Koopman observables and instead introducing a nonlinearity in decoding the full state from a latent state with linear time evolution. This is the idea behind many Koopman-based autoencoder frameworks [24, 25].

Of particular interest here is a more subtle nonlinearity that has been introduced in several Koopman-based prediction applications, where at each time step in the forward rollout of the observables by the Koopman operator, the observables are projected back to the state space and then "re-lifted" back to the observable space. This procedure was used in the implementation of EDMD-DL for prediction in the work of Li, et al. [22]. Jünker et al. [47] also pointed out the effectiveness of this method, showing that this strategy greatly improves the predictive capability of EDMD as compared to purely linear time evolution of the observables for damped pendulum and Duffing oscillator models. Recently, this procedure was further studied in the work of Constante-Amores et al. [23] in the context of EDMD-DL, where it was shown that this strategy also yields improved performance for several chaotic systems and a comparison was given in terms of the time between these correction steps. The method was also studied recently by van Goor et al. [48], who showed that by considering the lifting as a mapping to a manifold in a higher dimensional space, the re-lifting procedure can be thought of as a projection back to this manifold, which will not necessarily be invariant under the action of the matrix approximation of the operator. That is, the re-lifting corrects the EDMD prediction by projecting it back onto the manifold. This interpretation allows for a connection to be made between the projection method and the invariance of the function space spanned by the EDMD dictionary under the action of the Koopman operator. Nehma and Tiwari [49] also recently applied this method in their study of learning Koopman representations using Kolmogorov-Arnold networks, showing that this method can be used with a linear quadratic regulator control block.

While these Koopman-based approaches have shown great promise, other data-driven methods have sought to use neural networks to learn dynamics directly on the state space. When the vector field on the right hand side (RHS) of an ODE is represented as a neural network, the resulting model is known as a neural ODE. The neural ODE method was popularized in recent years by Chen et al. [50], who observed that gradients with respect to the network parameters can be computed by either backpropagating through the operations of a numerical ODE solver or by an adjoint sensitivity method. These gradients can then be used to optimize the network parameters by stochastic gradient descent. While neural ODEs have seen a resurgence in recent years, many of the underlying ideas can be found in papers dating back to the 1990s [51–54], such as the work of Rico-Martinez et al. [51], who used a neural ODE to develop a continuous-time model for a chemical reaction from experimental data and showed that the neural ODE model captured bifurcations observed in experiments.

Another popular approach to developing continuous time models directly on the state space is the sparse identification of nonlinear dynamics (SINDy)[55], which models a vector field on the state space as a sparse linear combination of a predefined dictionary of functions of the state (a.k.a. features). SINDy is often presented as more interpretable than neural network-based approaches, as the sparsity-promotion in the optimization attempts to eliminate all but the most significant contributors to the dynamics. However, determining an appropriate set of dictionary functions for a given system, is often challenging and may require expert domain knowledge. Additionally, SINDy requires access to data of the timederivatives of the states during training, whereas neural ODEs only require snapshot data during training. For these reasons, our focus here is on neural ODE models in comparison to EDMD-DL models, as both provide neural network-based modeling strategies to develop models directly from sequences of snapshots. We show here that EDMD-DL with a state space projection also represents the vector field as a linear combination of dictionary elements, where the dictionary is represented by a neural network. In this way, the method can be interpreted as being related to SINDy, without sparsity promotion but on an optimized feature space.

In this work, we elucidate the relationship between EDMD-DL with the projection correction step and neural ODEs. Specifically, we point out that by deviating from the typical, linear time evolution of observables in Koopman formulations, the projection step introduces a nonlinearity into the time evolution, which makes the method essentially equivalent to learning a neural network approximation of the flow map, as illustrated in Fig. 1. In this formulation, the flow map approximation has a natural neural network structure that expands out to a high dimensional set of nonlinear features (from EDMD-DL), followed by a linear mapping which selects from those features to represent the flow map. Moreover, EDMD-DL parameterizes the dictionary with neural networks, allowing us to draw parallels to neural ODEs, which represent the vector field of an ODE by a neural network. We show that converting the discrete time EDMD-DL model to a continuous time formulation directly yields a neural ODE, without the need for a separate training procedure. These parallels motivate several model variations developed by combining structures and training methods typically used in neural ODEs and EDMD-DL. In comparing the performance of these methods in numerical examples with chaotic dynamics, we further highlight that by including a projection back to the state space on each step of the EDMD-DL time evolution, the resulting model is essentially equivalent to a neural ODE.

The remainder of this paper is organized as follows. In Sec. II, we review the dynamical systems formalisms needed for developing models on the state space and based on the Koopman operator. In Sec. III, we review numerical methods for training neural network models for dynamical systems and discuss how these models are implemented for prediction tasks. In Sec. IV, we discuss how the parallels between EDMD-DL and neural ODE methods give rise to several variations of these models by combining aspects of each. We then

implement these model variations on two chaotic dynamical systems: the Lorenz system and a nine-mode model for a turbulent shear flow. With these implementations, we assess the performance of the models in terms of short-time prediction error, reconstruction of long-time statistics, and the prediction of rare events.

II. PRELIMINARIES

Consider an autonomous dynamical system in continuous time given by an ODE

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}).\tag{1}$$

where $\mathbf{x} \in \mathbb{R}^n$ is the state of the system and denote the associated discrete-time flow map for time interval τ by $\mathbf{F}_{\tau} : \mathbb{R}^n \to \mathbb{R}^n$ such that

$$\mathbf{x}(t+\tau) = \mathbf{F}_{\tau}(\mathbf{x}(t)). \tag{2}$$

We can also consider time evolution in a space \mathcal{O} of observable functions of the state, $g: \mathbb{R}^n \to \mathbb{R}$. Associated with this system is an operator, $\mathcal{K}_{\tau}: \mathcal{O} \to \mathcal{O}$ defined by

$$\mathcal{K}_{\tau}g(\mathbf{x}) = g \circ \mathbf{F}_{\tau}(\mathbf{x}) = g(\mathbf{F}_{\tau}(\mathbf{x})) \tag{3}$$

which propagates observable functions forward in time along trajectories of the system in Eq. 1. This operator \mathcal{K}_{τ} is known as the Koopman operator, or composition operator [56, 57]. The operator \mathcal{K}_{τ} is linear, as

$$\mathcal{K}_{\tau}(c_1g_1 + c_2g_2)(\mathbf{x}) = (c_1g_1 + c_2g_2)(\mathbf{F}_{\tau}(\mathbf{x}))$$
$$= c_1g_1(\mathbf{F}_{\tau}(\mathbf{x})) + c_2g_2(\mathbf{F}_{\tau}(\mathbf{x}))$$
$$= c_1\mathcal{K}_{\tau}g_1(\mathbf{x}) + c_2\mathcal{K}_{\tau}g_2(\mathbf{x})$$
(4)

for $c_1, c_2 \in \mathbb{R}$ and $g_1, g_2 \in \mathcal{O}$. The family of operators \mathcal{K}_{τ} parameterized by τ has a semigroup structure [57], and the infinitesimal generator of the Koopman semigroup can be used to express the continuous time form of the dynamics on \mathcal{O} . The infinitesimal generator, \mathcal{L} is defined by [57]

$$\mathcal{L}g = \lim_{t \to 0^+} \frac{g \circ \mathbf{F}_t - g}{t} = \lim_{t \to 0^+} \frac{\mathcal{K}_\tau g - g}{t} = \lim_{t \to 0^+} \frac{\mathcal{K}_\tau - \mathcal{I}}{t} g.$$
(5)

By this definition, the operator \mathcal{L} gives the time derivative of $g(\mathbf{F}_t(\mathbf{x}))$. Expanding this by chain rule gives the following explicit form.

$$\mathcal{L}g = \frac{d}{dt}g(\mathbf{F}_t(\mathbf{x})) = \frac{\partial g}{\partial \mathbf{x}} \cdot \frac{d\,\mathbf{F}_t(\mathbf{x})}{dt} = \frac{\partial g}{\partial \mathbf{x}} \cdot \mathbf{f}(\mathbf{x}) \tag{6}$$

The operator \mathcal{L} is commonly referred to as the Koopman generator or the Lie operator [11, 56], because $\mathcal{L}g$ is the Lie derivative of g along the vector field \mathbf{f} [58]. Further, by solving Eq. 6, the Koopman operator and Lie operator can be shown to be formally related by an exponential [59]

$$\mathcal{K}_{\tau} = e^{\tau \mathcal{L}} \,. \tag{7}$$

Also, we note that while the Lie operator given in Eq. 6 represents a linear partial differential equation, this equation is hyperbolic and can be solved by the method of characteristics, wherein each characteristic is determined by solving a nonlinear ODE. This conceptual point helps to provide some intuition as to how nonlinear dynamics can be represented by a linear operator.

III. NUMERICAL METHODS

Here we briefly review a set of numerical methods for constructing dynamic models from data based on the formalisms introduced in Sec. II. Specifically, we will be interested in learning models from a time series dataset, which we will typically organize as snapshot pairs

$$\{(\mathbf{x}_i, \mathbf{y}_i = \mathbf{F}_{\tau}(\mathbf{x}_i))\}_{i=1}^m \tag{8}$$

where $\mathbf{x}_i \equiv \mathbf{x}(t_i)$, $\tau = t_{i+1} - t_i$ is the sampling interval, and m is the number of data pairs. We note that for the continuous time formulations considered below, such as neural ODEs, it is not necessary to have a fixed time interval between datapoints in the dataset, but we will take it to be fixed here for consistency between methods. We will additionally be interested in fitting models using neural networks as function approximators, and those which preserve the Markovian structure assumed in the dynamical systems formulation above – that future time evolution is determined only from the present states. This requirement excludes several popular deep learning based time series modeling approaches, such as reservoir computing, LSTMs, and transformers.

A. Neural ODEs

Perhaps the most straightforward way to construct a dynamics model from data is to pose a functional form for the flow map in Eq. 2, as

$$\mathbf{x}_{i+1} = \mathbf{F}_{\tau}(\mathbf{x}_i; \theta_{\mathbf{F}}) \tag{9}$$

where the parameters $\theta_{\mathbf{F}}$ are chosen to minimize the prediction loss

$$J(\theta_{\mathbf{F}}) = \sum_{i=1}^{m} \|\mathbf{y}_i - \mathbf{F}_{\tau}(\mathbf{x}_i; \theta_{\mathbf{F}})\|_2^2.$$
(10)

For example, \mathbf{F}_{τ} can be represented as a simple feedforward neural network and the objective minimized by stochastic gradient descent. Alternatively, \mathbf{F}_{τ} could be assumed to be linear in a predefined set of features $\psi_j(\mathbf{x})$, such as monomials, radial basis functions, or a Fourier basis; and then the parameters can be optimized by solving a linear least squares problem.

In many cases, we would prefer a continuous time model, which requires an approximation of the ODE vector field $\mathbf{f}(\mathbf{x})$ in Eq. 1. When \mathbf{f} is approximated by a neural network $\mathbf{f}(\mathbf{x}; \theta_{\mathbf{f}})$, the resulting model is called a neural ODE [50]. The parameters of a neural ODE are optimized to minimize the objective

$$J(\theta_{\mathbf{f}}) = \sum_{i=1}^{m} \|\mathbf{y}_{i} - \hat{\mathbf{y}}_{i}\|_{2}^{2}, \qquad (11)$$

where $\hat{\mathbf{y}}_i$ is the prediction of \mathbf{y}_i found by integrating the ODE from t_i to $t_i + \tau$ from initial condition \mathbf{x}_i

$$\hat{\mathbf{y}}_i = \mathbf{x}_i + \int_{t_i}^{t_i + \tau} \mathbf{f}(\mathbf{x}(t); \theta_{\mathbf{f}}) dt \,.$$
(12)

The objective in Eq. 11 is typically optimized by stochastic gradient descent, where the gradients with respect to the parameters $\theta_{\mathbf{f}}$ are determined by either solving an adjoint equation backward in time from $t_i + \tau$ to t_i to obtain these sensitivities or by using modern automatic differentiation tools to backpropagate these gradients through the operations of a numerical ODE solver [50]. Once the neural ODE model is trained, it can be implemented to predict the time evolution of a system by simply integrating along the learned vector field using a numerical ODE solver from a given initial condition.

B. EDMD

Extended dynamic mode decomposition (EDMD) [21] is a method for constructing a matrix approximation of the Koopman operator from data by considering the operator acting on elements of a function subspace spanned by a predefined set of dictionary functions. Consider the dictionary

$$\mathbb{D} = \{\psi_j : \mathbb{R}^n \to \mathbb{R}\}_{j=1}^k \tag{13}$$

whose elements span a subspace $\mathcal{O}_{\mathbb{D}} \subset \mathcal{O}$. Any observable $g_{\mathbf{c}} \in \mathcal{O}_{\mathbb{D}}$ can be represented as a linear combination of the dictionary elements

$$g_{\mathbf{c}}(\mathbf{x}) = \sum_{j=1}^{k} \mathbf{c}_{j} \psi_{j}(\mathbf{x}) = \mathbf{c}^{\mathrm{T}} \Psi(\mathbf{x})$$
(14)

where $\Psi : \mathbb{R}^n \to \mathbb{R}^k$ is a vector-valued function containing the elements of \mathbb{D} , and $\mathbf{c} \in \mathbb{R}^k$ is a vector of projection coefficients. A time-evolved observable $\mathcal{K}_{\tau}g_{\mathbf{c}}$ can also be expressed in terms of the dictionary elements as

$$\mathcal{K}_{\tau} g_{\mathbf{c}}(\mathbf{x}) = \mathbf{c}^{\mathrm{T}} \mathbf{K}_{\tau}^{\mathrm{T}} \Psi(\mathbf{x}) + r_{\mathbf{c}}(\mathbf{x})$$
(15)

where $\mathbf{K}_{\tau} \in \mathbb{R}^{k \times k}$ is a matrix which approximates the action of the Koopman operator \mathcal{K}_{τ} by updating the projection coefficients \mathbf{c} and $r_{\mathbf{c}} \in \mathcal{O}$ is a residual, which we will seek to minimize by an appropriate choice of \mathbf{K}_{τ} . If $\mathcal{O}_{\mathbb{D}}$ is Koopman invariant, then the operator can be represented exactly as a matrix and the residual, $r_{\mathbf{c}}(\mathbf{x}) = 0$. Note that the time-evolved observable can also be represented, using Eq. 3, as

$$\mathcal{K}_{\tau} g_{\mathbf{c}}(\mathbf{x}) = g_{\mathbf{c}} \circ \mathbf{F}_{\tau}(\mathbf{x}) = \mathbf{c}^{\mathrm{T}} \Psi \circ \mathbf{F}_{\tau}(\mathbf{x}).$$
(16)

Equating Eq. 15 and Eq. 16, the residual $r_{\mathbf{c}}(\mathbf{x})$ can be written as

$$r_{\mathbf{c}}(\mathbf{x}) = \mathbf{c}^{\mathrm{T}} \left(\Psi(\mathbf{F}_{\tau}(\mathbf{x})) - \mathbf{K}_{\tau}^{\mathrm{T}} \Psi(\mathbf{x}) \right).$$
(17)

Since we would like to minimize the residual for arbitrary observables in $\mathcal{O}_{\mathbb{D}}$, we can drop the dependence on **c** and seek to minimize the objective

$$J(\mathbf{K}_{\tau}) = \sum_{i=1}^{m} \left\| \Psi(\mathbf{y}_{i}) - \mathbf{K}_{\tau}^{\mathrm{T}} \Psi(\mathbf{x}_{i}) \right\|_{2}^{2}$$
(18)

where $\mathbf{y}_i = \mathbf{x}_{i+1} = \mathbf{F}_{\tau}(\mathbf{x}_i)$. If the lifted measurement data is organized into the lifted data matrices $\Psi_X, \Psi_Y \in \mathbb{R}^{k \times m}$ as

$$\Psi_X = \left[\Psi(\mathbf{x}_1) \ , \ \cdots \ , \ \Psi(\mathbf{x}_m)\right] \qquad , \qquad \Psi_Y = \left[\Psi(\mathbf{y}_1) \ , \ \cdots \ , \ \Psi(\mathbf{y}_m)\right]$$

then $J(\mathbf{K}_{\tau})$ can be expressed succinctly as

$$J(\mathbf{K}_{\tau}) = \|\Psi_Y - \mathbf{K}_{\tau}^{\mathrm{T}}\Psi_X\|_F^2$$
(19)

where $\|\cdot\|_F$ denotes the Frobenius norm. The solution of this least-squares problem for **K** is given by

$$\mathbf{K}_{\tau}^{\mathrm{T}} = \Psi_{Y} \Psi_{X}^{\mathrm{T}} \left(\Psi_{X} \Psi_{X}^{\mathrm{T}} \right)^{\dagger} \tag{20}$$

where $(\cdot)^{\dagger}$ denotes the Moore-Penrose pseudoinverse [21]. We further detail how such a matrix approximation can be used for predicting the time evolution of the states below in Sec. III D.

C. EDMD with dictionary learning

A challenge of the EDMD approach is finding an appropriate dictionary \mathbb{D} on which to compute the operator \mathbf{K}_t , as the as the accuracy and convergence of the approximation depend heavily on this choice. Ideally, the subspace spanned by the dictionary should be Koopman invariant so that the residual can be driven to zero. To meet this requirement, it is necessary that the dictionary elements all lie in a space spanned by Koopman eigenfunctions [12, 16]. Additionally, we would like a dictionary from which the states can be recovered easily, and preferably linearly, for use in prediction applications. However, finding a dictionary that satisfies these properties is nontrivial, as the appropriate dictionary depends heavily on the underlying dynamical system and many common choices of dictionary do not scale well with the state dimension, making them challenging to apply to systems of dimension greater than 3 or 4.

An alternative approach proposed by Li et al. [22] is to allow the vector of dictionary elements Ψ to be represented by a neural network, parameterized by weights θ_{Ψ} ; that is, $\Psi(\mathbf{x}) = \Psi(\mathbf{x}; \theta_{\Psi})$. This allows the basis to be optimized jointly along with the matrix approximation of the Koopman operator, \mathbf{K}_{τ} , so that the objective in Eq. 18 becomes

$$J(\mathbf{K}_{\tau}, \theta_{\Psi}) = \sum_{i=1}^{m} \left\| \Psi(\mathbf{y}_{i}; \theta_{\Psi}) - \mathbf{K}_{\tau}^{\mathrm{T}} \Psi(\mathbf{x}_{i}; \theta_{\Psi}) \right\|_{2}^{2}$$
(21)

This approach is known as EDMD with dictionary learning (EDMD-DL). The original paper of Li et al [22] proposed an iterative procedure for solving Eq. 21 which alternates between two steps in which (1) the dictionary is fixed and the Koopman approximation \mathbf{K}_{τ} is optimized through the pseudoinverse calculation in Eq. 20 and then (2) the matrix \mathbf{K}_{τ} is fixed and the dictionary is optimized through stochastic gradient descent. Recently, Constante-Amores et al. showed that these steps can be combined by performing the least-squares calculation for \mathbf{K}_{τ} within the dictionary optimization step and backpropagating through this pseudoinverse-based solution of the least squares problem in optimizing the dictionary [23]. Other works have optimized the elements of \mathbf{K}_{τ} directly along with the dictionary by stochastic gradient descent, avoiding the least squares calculation entirely (e.g., [24, 25, 60]).

D. Forecasting with EDMD models

Here we discuss different variations of EDMD-DL for predicting the time-evolution of the states. First, we discuss the development of a projection operation which maps from the feature vector Ψ to the states. Then we discuss how such a projection may be implemented within time-series prediction. This can either be done as a post-processing step of a full trajectory predicted linearly in the space of observables or by projecting back to the state space on each timestep, thereby formulating a nonlinear map on the state space.

1. Recovering \mathbf{x} from Ψ

Once the dictionary Ψ and the matrix operator \mathbf{K}_{τ} are determined, the time evolution of an observable $g_{\mathbf{c}}$ in $\mathcal{O}_{\mathbb{D}}$ can be predicted by expressing it in terms of the dictionary \mathbb{D} as in Eq. 14 and then stepping the projection coefficients \mathbf{c} forward in time with \mathbf{K}_{τ} as in Eq. 15. However, we are often more interested in forecasting the evolution of \mathbf{x} along a single trajectory from an initial condition \mathbf{x}_0 at t = 0. This can be done by using \mathbf{K}_t to evolve the dictionary elements $\Psi(\mathbf{x})$ forward in time, as in the objective in Eq. 18,

$$\Psi(\mathbf{x}(\tau)) = \mathbf{K}_{\tau}^{\mathrm{T}} \Psi(\mathbf{x}_0).$$
(22)

Again, note that this will only be exact if the span of $\mathcal{O}_{\mathbb{D}}$ is Koopman invariant; otherwise, the residual can lead to significant error buildup in this prediction. While this method propagates the features Ψ linearly, it is still necessary to recover the states \mathbf{x} from the predictions of Ψ . That is, we need a mapping $\mathcal{P} : \mathbb{R}^n \to \mathbb{R}^d$, which effectively inverts the lifting Ψ , projecting the features back to the state space; i.e. $\mathbf{x} = \mathcal{P}\Psi(\mathbf{x})$. One common approach to this is to structure the dictionary so that the states \mathbf{x} are included explicitly [22, 23]; that is,

$$\Psi(\mathbf{x}) = \begin{bmatrix} \mathbf{x} \\ \tilde{\Psi}(\mathbf{x}) \end{bmatrix}$$
(23)

where $\tilde{\Psi}$ are dictionary elements which are nonlinear functions of \mathbf{x} . With this structure, the projection back to the state space takes the simple, linear form $\mathcal{P}\Psi(\mathbf{x}) = \mathbf{P}\Psi(\mathbf{x})$ with $\mathbf{P} = \begin{bmatrix} \mathbf{I}_{n \times n} & \mathbf{0}_{n \times (k-n)} \end{bmatrix}$. Alternatively, if the states are not explicitly included in the dictionary, the mapping \mathbf{P} can be learned as a linear mapping in a similar manner to \mathbf{K}_{τ} ; that is, by a least squares calculation for standard EDMD [61] or jointly by gradient descent for EDMD-DL. A more general approach is to assume that \mathcal{P} is a nonlinear mapping and represent it as a decoder neural network, as in many Koopman autoencoder formulations [24, 25]. Otto and Rowley [25] performed comparisons of nonlinear reconstruction versus linear reconstruction of the observables from the features, showing that for some examples performance actually degrades by allowing for nonlinear reconstruction. For this reason, in our implementations of EDMD-DL, we will include the state explicitly in the dictionary, as in Eq. 23. As noted by Li, et al [22], including the states \mathbf{x} as nontrainable dictionary elements also prevents the training procedure from learning the trivial solution, $\Psi(\mathbf{x}) = \mathbf{0}$, which is a minimizer of Eq. 21. As pointed out by Otto and Rowley [25], it is also useful to normalize the error in the state prediction and the dictionary prediction in the loss function

$$J(\mathbf{K}_{\tau};\theta_{\Psi}) = \sum_{i=1}^{m} \left[\frac{\|\mathbf{y}_{i} - \mathbf{P}\mathbf{K}_{\tau}^{\mathrm{T}}\Psi(\mathbf{x}_{i};\theta_{\Psi})\|_{2}}{\|\mathbf{y}_{i}\|_{2} + \epsilon} + \lambda \frac{\|\tilde{\Psi}(\mathbf{y}_{i};\theta_{\Psi}) - \tilde{\mathbf{P}}\mathbf{K}_{\tau}^{\mathrm{T}}\Psi(\mathbf{x}_{i};\theta_{\Psi})\|_{2}}{\|\tilde{\Psi}(\mathbf{y}_{i};\theta_{\Psi})\|_{2} + \epsilon} \right]$$
(24)

where $\tilde{\mathbf{P}} = \begin{bmatrix} \mathbf{0}_{(k-n) \times n} & \mathbf{I}_{(k-n) \times (k-n)} \end{bmatrix}$ is the matrix which extracts only the nonlinear functions $\tilde{\Psi}$ from the dictionary (but not the states \mathbf{x}), ϵ is a small parameter introduced to avoid divide-by-zero errors, and λ is an optional weighting parameter to adjust the relative effect of the two terms. The reasoning for this is that the objective in Eq. 21 can be reduced by simply choosing θ_{Ψ} to reduce the magnitude of $\Psi(\mathbf{x}; \theta_{\Psi})$, which may or may not improve the state prediction.

2. EDMD-DL with projection

The standard time-evolution strategy using an EDMD model, as described above, is to lift the initial state \mathbf{x}_0 to obtain the initial feature vector $\Psi_0 = \Psi(\mathbf{x}_0)$ and then propagate this lifted state forward linearly using the matrix approximation \mathbf{K}_{τ} as in Eq. 22,

$$\Psi_{i+1} = \mathbf{K}_{\tau}^{\mathrm{T}} \Psi_i \tag{25}$$

where the subscripts on Ψ refer to values at timesteps evenly spaced by time interval, τ . Iterating this for multiple timesteps allows us to obtain a trajectory in the feature space. Once this trajectory is obtained, the corresponding trajectory of the states, \mathbf{x} can be obtained by mapping back to the state space using the operator \mathcal{P} . A key characteristic of Koopmanbased approaches is that, as long as the operator \mathcal{P} is linear, these methods allow for state trajectories to be predicted from an initial condition using only linear operations (following the initial nonlinear mapping to the feature space). This is key, as preserving linearity is necessary in order to apply linear methods for control [61].

However, several recent works [23, 26, 47, 48] have shown that the predictive capabilities of EDMD models can be substantially improved by performing a projection during the forward rollout where after each step with the Koopman model, the prediction is projected from the lifted state $\Psi(\mathbf{x}_i)$ back to the original state space,

$$\mathbf{x}_{i+1} = \mathbf{P}\mathbf{K}_{\tau}^{\mathrm{T}}\Psi(\mathbf{x}_i) \,. \tag{26}$$

To understand why this subtle change offers such improved performance, we first note that Eq. 26 can be thought of as a nonlinear discrete-time model on the state space with a particular form, as depicted in Fig. 1. That is, the model in Eq. 26 is of the same form as Eq. 9 where

$$\mathbf{F}_{\tau}(\mathbf{x};\theta_{\Psi}) = \mathbf{P}\mathbf{K}_{\tau}^{\mathrm{T}}\Psi(\mathbf{x};\theta_{\Psi}).$$
(27)

So, in EDMD-DL, we learn a set of features Ψ which is typically of higher dimension than the original state representation, \mathbf{x} and whose time evolution is approximately linear. However, when we implement this model for state prediction with a reprojection on each step, we have essentially defined a nonlinear discrete time map on the state space of a form that first expands out to a high dimensional feature vector, followed by two linear mappings: the first, $\mathbf{K}_{\tau}^{\mathrm{T}}$, representing the time evolution and the second, \mathbf{P} , representing a projection back to

the original state space. Since it is common for the output layer of a neural network to be linear (with no activation function following it), this model is essentially a neural network representation of the flow map in a fairly standard form. This observation is the heart of the present work.

Van Goor, et al. [48] recently examined this method as well, showing that there is a geometric interpretation of this step as a projection onto a manifold. To see this, we can think of the nonlinear feature map Ψ as a coordinate mapping to a manifold in a higher dimensional space, $\Psi : \mathbb{R}^n \to \mathcal{M}_{\Psi} \subset \mathbb{R}^k$. That is, $\mathcal{M}_{\Psi} \subset \mathbb{R}^k$ is defined as the image of Ψ

$$\mathcal{M}_{\Psi} = \{ \Psi(\mathbf{x}) \mid \mathbf{x} \in \mathbb{R}^n \} \subset \mathbb{R}^k.$$
(28)

Then a trajectory in the state space, $\mathbf{x}(t)$, also defines a trajectory $\Psi(\mathbf{x}(t))$ on \mathcal{M}_{Ψ} . If the function space spanned by the elements of \mathbb{D} is Koopman invariant, then the dynamics on \mathcal{M}_{Ψ} can be represented exactly by a linear mapping

$$\Psi(\mathbf{F}_{\tau}(\mathbf{x})) = \mathbf{K}_{\tau}^{\mathrm{T}} \Psi(\mathbf{x}) \,. \tag{29}$$

However, if $\mathcal{O}_{\mathbb{D}}$ is not Koopman invariant, the true operator \mathcal{K}_t will map elements of $\mathcal{O}_{\mathbb{D}}$ out of this space, so a linear approximation of the dynamics on \mathcal{M}_{Ψ} will not be exact. That is, the EDMD approximation \mathbf{K}_{τ} will map elements of \mathcal{M}_{Ψ} off of this manifold even though \mathcal{M}_{Ψ} is invariant under the dynamics by definition (i.e., $\Psi(\mathbf{F}_{\tau}(\mathbf{x})) \in \mathcal{M}_{\Psi}$). Performing a projection step in the forward rollout can be viewed as a projection back onto the manifold \mathcal{M}_{Ψ} of the prediction using the EDMD approximation $\mathbf{K}_{\tau}^{\mathrm{T}}$ when the space $\mathcal{O}_{\mathbb{D}}$ is not Koopman invariant. By mapping back to the state space on each step and then re-lifting on the next step, it is ensured that the prediction remains on \mathcal{M}_{Ψ} . Specifically, $\Psi(\mathbf{PK}_{\tau}^{\mathrm{T}}\Psi(\mathbf{x})) \in \mathcal{M}_{\Psi}$ even when $\mathbf{K}_{\tau}^{\mathrm{T}}\Psi(\mathbf{x}) \notin \mathcal{M}_{\Psi}$.

E. Continuous-time models from EDMD

As noted in Sec. II, the Koopman formalism also gives rise to a continuous-time representation of the dynamics on the observable space, described by the infinitesimal generator, \mathcal{L} . Using this formulation, an analogous projection step can be performed, which directly yields a neural ODE representation of the state space dynamics, as illustrated in Fig. 2. Based on this, several previous works have shown that continuous-time representations can also be derived from EDMD or similar regression methods [62–66]. Similarly to standard EDMD, these methods produce a matrix representation \mathbf{L} of the Koopman generator, \mathcal{L} , which acts on observables $g_{\mathbf{c}} = \mathbf{c}^{\mathrm{T}} \Psi \in \mathcal{O}_{\mathbb{D}}$ by updating the projection coefficients:

$$\mathcal{L}g_{\mathbf{c}} = (\mathbf{L}\mathbf{c})^{\mathrm{T}}\Psi = \mathbf{c}^{\mathrm{T}}\mathbf{L}^{\mathrm{T}}\Psi + r_{\mathbf{c}}(\mathbf{x})$$
(30)

where, as before, the residual $r_{\mathbf{c}}(\mathbf{x})$ arises due to the space $\mathcal{O}_{\mathbb{D}}$ not being Koopman invariant. In many implementations, it is assumed that time derivative data of the states $\dot{\mathbf{x}}$ is available (or can be obtained by finite-differencing). If this velocity data is available, then using the generator definition in Eq. 6 we have

$$\mathcal{L}g_{\mathbf{c}} = \frac{\partial g_{\mathbf{c}}}{\partial \mathbf{x}} \cdot \dot{\mathbf{x}} = \mathbf{c} \cdot \frac{\partial \Psi(\mathbf{x})}{\partial \mathbf{x}} \cdot \dot{\mathbf{x}} \,. \tag{31}$$

Then equating Eqs. 30 and 31, we see that the residual can be written as

$$r_{\mathbf{c}}(\mathbf{x}) = \mathbf{c}^{\mathrm{T}} \left(\frac{\partial \Psi(\mathbf{x})}{\partial \mathbf{x}} \cdot \dot{\mathbf{x}} - \mathbf{L}^{\mathrm{T}} \Psi \right)$$
(32)

and so we can frame the EDMD regression for \mathbf{L} by minimizing the objective

$$J(\mathbf{L}) = \sum_{i=1}^{m} \left\| \dot{\Psi}(\mathbf{x}_i) - \mathbf{L}^{\mathrm{T}} \Psi(\mathbf{x}_i) \right\|_2^2$$
(33)

where $\dot{\Psi}(\mathbf{x}) = \frac{\partial \Psi}{\partial \mathbf{x}} \cdot \dot{\mathbf{x}}$. This is the approach taken in [64–66]. However, this is disadvantageous, as time derivative data can be difficult to acquire from experiments, and obtaining accurate finite-differencing approximations relies on measurements being closely spaced in time. Alternatively, one can obtain a matrix approximation of the generator from the EDMD approximation of the Koopman operator by applying the limit definition in Eq. 5 as

$$\mathbf{L} = \frac{\mathbf{K}_{\tau} - \mathbf{I}_{k \times k}}{\tau} \tag{34}$$

though this approach will only be accurate for sufficiently small time interval, τ . Similarly, we can make use of the exponential relationship between the Koopman operator and its generator in Eq. 7 and obtain the matrix approximation of \mathcal{L} using a matrix logarithm as

$$\mathbf{L} = \frac{1}{\tau} \log(\mathbf{K}_{\tau}) \,. \tag{35}$$

This is the approach taken by Mauroy and Goncalves [62, 63], where it was also shown that an ODE vector field can be computed directly from an EDMD approximation of the



FIG. 2. Schematic illustrating how the continuous-time EDMD-DL formulation with projection to the state space leads to a neural ODE representation of the state space dynamics.

Koopman operator by solving a linear least squares problem for systems linear in parameters. However, those works were limited to polynomial vector fields and vector fields composed of a linear combination of predefined dictionary functions, respectively.

Once the matrix representation of the generator is obtained, it can be used to predict the dynamics of the state, \mathbf{x} , as this matrix acts on the dictionary elements to return their time derivative. Specifically, given an initial state \mathbf{x}_0 , we can lift it to obtain an initial condition for the lifted state, $\Psi_0 = \Psi(\mathbf{x}_0)$, and then obtain a trajectory in this lifted state by integrating the equation

$$\frac{d\Psi}{dt} = \mathbf{L}^{\mathrm{T}}\Psi.$$
(36)

Integrating this yields a trajectory in the lifted state, Ψ , from which we can recover the state predictions by mapping back to the state space, $\mathbf{x} = \mathcal{P}\Psi$, as in Sec. III D. Note that Eq. 36 is a linear ODE in Ψ and is essentially a continuous time version of the linear time evolution using the Koopman operator (without projection) in Eqs. 22, 25.

Analogously the EDMD formulation, where we defined a nonlinear discrete-time evolution equation on the state space using the EDMD operator, \mathbf{K}_{τ} , by projecting back to the state space on each timestep (see Eq. 26), we can also define a nonlinear continuous time evolution equation on the state space using the generator obtained from EDMD by lifting the state $\Psi(\mathbf{x})$, computing the time derivative of the feature vector, and then projecting the time derivative back to the state space. This can be seen by simply taking the time derivative of the projection back to the state space $\mathbf{x} = \mathcal{P}\Psi(\mathbf{x})$ as

$$\frac{d\mathbf{x}}{dt} = \frac{\partial \mathcal{P}}{\partial \Psi} \frac{d\Psi}{dt} = \frac{\partial \mathcal{P}}{\partial \Psi} \mathbf{L}^{\mathrm{T}} \Psi(\mathbf{x}) \,. \tag{37}$$

This form is only necessary if the mapping \mathcal{P} back to the state space is nonlinear (such as

in Koopman autoencoder formulations). If \mathcal{P} is taken to be a linear mapping, $\mathcal{P}\Psi = \mathbf{P}\Psi$, such as when the state is explicitly included in the dictionary (see Sec. III D, Eq. 23), then $\frac{\partial \mathcal{P}}{\partial \Psi} = \mathbf{P}$ and Eq. 37 can be simplified to

$$\frac{d\mathbf{x}}{dt} = \mathbf{P}\mathbf{L}^{\mathrm{T}}\Psi(\mathbf{x})\,. \tag{38}$$

In the case of EDMD-DL, where the feature vector $\Psi(\mathbf{x})$ is parametrized by a neural network, $\Psi(\mathbf{x}; \theta_{\Psi})$ and optimized jointly with \mathbf{K}_{τ} , this implies that the EDMD-DL training procedure directly defines a neural ODE of a certain structure

$$\frac{d\mathbf{x}}{dt} = \mathbf{P}\mathbf{L}^{\mathrm{T}}\Psi(\mathbf{x};\theta_{\Psi}).$$
(39)

In particular, the structure of this neural ODE is such that the state is expanded out to a high dimensional set of features, $\Psi(\mathbf{x}; \theta_{\Psi})$ which have been chosen as important during EDMD-DL training, and then the linear mapping \mathbf{PL}^{T} selects a linear combination of these features to represent the vector field.

In summary, in both discrete time and continuous time, performing a projection back to the state space in the EDMD time evolution leads to a nonlinear dynamical system in the state space with a natural structure for neural networks. Specifically, the state is first expanded nonlinearly into a high dimensional feature space, followed by a linear mapping which represents the dynamics as a linear combination of these features. In the following section, we see how this observation motivates the development of several methods that combine different aspects of EDMD and neural ODE based models. We also see that the projection within EDMD-DL time evolution leads to greatly improved performance as compared to the linear time evolution strategy used in standard EDMD-DL. Additionally, the models using this projection achieve a level of accuracy in predicting extreme events comparable to the non-Markovian approach of Racca and Magri [67].

IV. PERFORMANCE COMPARISON

A. Model structures

The discussion in Sec. III of the parallels between data-driven state-space modeling techniques and the projected Koopman approach to predicting the state evolution motivates a comparison between the numerical methods arising from each. In particular, we will

Model	Time evolution	Training notes
Basic neural ODE	$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}; \theta_{\mathbf{f}})$	$\theta_{\mathbf{f}}$ optimized as neural ODE
	$\mathbf{x}(0) = \mathbf{x}_0$	(loss in Eq. 11)
EDMD structured neural ODE	$\dot{\mathbf{x}} = \mathbf{P} \mathbf{L}^{\mathrm{T}} \Psi(\mathbf{x}; \theta_{\Psi})$	θ_{Ψ} and matrix \mathbf{PL}^{T} optimized
	$\mathbf{x}(0) = \mathbf{x}_0$	as neural ODE (loss in Eq. 11)
EDMD-DL	$\Psi_{i+1} = \mathbf{K}^{\mathrm{T}} \Psi_i$	θ_{Ψ} and K optimized by EDMD-DL
	$\mathbf{x}_i = \mathbf{P} \Psi_i$	(loss in Eq. 24)
	$\Psi_0 = \Psi(\mathbf{x}_0; heta_\Psi)$	
EDMD-DL with projection	$\mathbf{x}_{i+1} = \mathbf{P}\mathbf{K}^{\mathrm{T}}\Psi(\mathbf{x}_i; \theta_{\Psi})$	θ_{Ψ} and K optimized by EDMD-DL
		(loss in Eq. 24)
EDMD basis neural ODE	$\dot{\mathbf{x}} = \mathbf{P} \mathbf{L}^{\mathrm{T}} \Psi(\mathbf{x}; \theta_{\Psi})$	θ_{Ψ} optimized by EDMD-DL (Eq. 24)
	$\mathbf{x}(0) = \mathbf{x}_0$	\mathbf{PL}^{T} optimized as neural ODE (Eq. 11)
EDMD direct neural ODE	$\dot{\mathbf{x}} = \mathbf{P} \mathbf{L}^{\mathrm{T}} \Psi(\mathbf{x}; \theta_{\Psi})$	$\theta_{\Psi}, \mathbf{K}$ optimized by EDMD-DL (Eq. 24)
	$\mathbf{x}(0) = \mathbf{x}_0$	$\mathbf{L} = rac{1}{ au} \log \mathbf{K}$

TABLE I. Summary of model structures based on neural ODEs and EDMD-DL

compare two neural ODE models arising directly from the state space view and four neural network models arising from EDMD approximations of the Koopman operator (with learned dictionaries). These model variations are described in the text below and summarized in Table I.

Neural ODE Models The first neural ODE model considered is a basic neural ODE, without any explicit structural constraints. This model approximates the right hand side of the ODE in Eq. 1 with a neural network, as described in Sec. III A and is trained to minimize the one-step state-prediction loss in Eq. 11. We also consider an *EDMD-structured neural ODE*, in which the output of the neural network is structured to represent the state space dynamics similarly to EDMD-based approaches. In this model, the neural network maps the state \mathbf{x} to a high-dimensional feature vector that explicitly contains the state (as in Eq. 23) before a final linear layer that selects a linear combination of these features to represent the vector field. This neural ODE therefore has the same structure as the model in Eq. 39, but is trained using the neural ODE training procedure, rather than any form of EDMD.

Discrete-time EDMD models The first EDMD approach that we consider is the standard EDMD-DL method, where a dictionary paremetrized by a neural network and the corresponding Koopman operator matrix representation are jointly learned by optimizing the objective in Eq. 24. Then to model the time-evolution, the initial state is lifted and propagated linearly in the lifted space using the Koopman matrix (see Eq. 25). We also consider the EDMD variation with reprojection, where the same dictionary and Koopman matrix are used, but where on each timestep, the state is lifted, evolved forward in time, and then reprojected (see. Eq. 26). In each EDMD-DL implementation, we constrain the dictionary to be of the form in Eq. 23, where the state is explicitly included as a nontrainable set of dictionary elements.

Continuous-time EDMD models We consider two variations of continuous-time models derived from EDMD. In the first, we use the dictionary obtained from EDMD-DL as the neural network in a neural ODE. That is, the dictionary is optimized, as in EDMD-DL, to minimize Eq. 24, and then the linear layer that maps to the output is optimized through the neural ODE training procedure. So the model has the structure of Eq. 39, where the dictionary $\Psi(\mathbf{x}; \theta_{\Psi})$ is determined by EDMD-DL and the linear mapping \mathbf{PL}^{T} is trained as with the neural ODE loss in Eq. 11. We refer to this variation as an *EDMD basis neural ODE*. Lastly, we consider a neural ODE model that is obtained directly from EDMD-DL, without a separate training procedure. That is, the matrix representation of the generator \mathbf{L} is obtained from the EDMD-DL Koopman matrix \mathbf{K}_{τ} by a matrix logarithm, as in Eq. 35. We refer to this variation as an *EDMD direct neural ODE*.

In the sections below, we provide a numerical comparison of the performance of these methods on two example systems: dynamics on the attractor of the Lorenz system and on a 9-mode model for a turbulent shear flow [68, 69]. In each implementation, we have made an effort to keep the neural network architectures, training procedures, and hyperparameters as consistent as possible between the different variations. In particular, all of the neural networks have 4 hidden layers with 200 nodes in each hidden layer and GELU activations between the layers. For the EDMD-DL models, the network output representing the nonlinear elements of the dictionary is of dimension 200, so that the total dictionary size is k = 200 + n, where n is the state dimension. The models are implemented in PyTorch and trained using the AdamW optimizer with weight decay of 10^{-6} and a OneCycle learning rate schedule which peaks at 10^{-3} after 30% of the total number of training iterations and then decays to 10^{-5} .



FIG. 3. Prediction results for the data-driven models on the Lorenz system for sampling interval $\tau = 0.02$. (a) Normalized ensemble-averaged error over time. (b) Representative trajectory timeseries of the states with predictions from each model.

B. Lorenz system

We consider the Lorenz system

$$\frac{dx}{dt} = \sigma(y - x) \tag{40a}$$

$$\frac{dy}{dt} = x(\rho - z) - y \tag{40b}$$

$$\frac{dz}{dt} = xy - \beta z \tag{40c}$$

with parameter values $\rho = 28$, $\sigma = 10$, and $\beta = 8/3$. For these parameter values, the Lyapunov timescale is $\tau_L \approx 1.1$ [70]. A training dataset is generated by integrating the system numerically using a Dormand-Prince (4)5 ODE solver and storing the solution with sampling time of 0.02. The first 1000 time units are neglected as transience so that the data lies on the attractor, and the next 50,000 time units are stored with an 80/20 train/test split. All models are trained for 100,000 training iterations with a batch size of 40. We also study the effects of the training timestep, τ , by training models with τ varying from 0.02 to 0.1.

Figure 3 demonstrates the short-time tracking error for each of the models on the Lorenz



FIG. 4. Normalized ensemble-averaged error of each model evaluated at t = 2 for varying training data sampling time, τ .

system, with $\tau = 0.02$. Fig. 3(a) shows an ensemble-averaged relative error,

$$\mathcal{E}(t) = \left\langle \frac{\|\hat{\mathbf{x}}(t) - \mathbf{x}(t)\|}{\|\mathbf{x}(t)\|} \right\rangle \tag{41}$$

where $\hat{\mathbf{x}}$ is the model prediction and $\langle \cdot \rangle$ denotes an ensemble average. We evaluate this error over time for each of the model by simulating the models from 1,000 randomly selected initial conditions from the test dataset. Fig. 3(b) shows an example trajectory timeseries, along with the predictions from each of the models. From these results, it is clear that the standard linear EDMD time evolution prediction diverges rapidly from the true trajectory, while the other models perform well, with less than 2% relative error at $t = \tau_L$. From the ensemble-averaged error, we also see that the EDMD with reprojection and the EDMDstructured neural ODE have a slightly slower error growth than the basic neural ODE, perhaps indicating that there are benefits to explicitly including the state in the dictionary.

We now compare the performance of the models when trained on data sampled at larger sampling times. For this, starting with the original training dataset we downsample it in time to effectively vary the sampling time interval, τ . We train new models on the downsampled datasets, while holding the total number of training iterations and other training parameters constant. We then compare the models in terms of the ensemble-averaged error, \mathcal{E} , evaluated at $t = 2\tau_L$. The results are shown in Fig. 4. We see that at large sampling times, the EDMD basis neural ODE and EDMD direct neural ODE begin to fail, while at small sampling times



FIG. 5. Long time predictions of each model from a common initial condition for 100 time units on the Lorenz system. Each of these models maintains the shape of the attractor for long times. These trajectories are generated by models trained with timestep $\tau = 0.02$.

(less than $\tau = 0.06$), all of the models perform well, with the relative error ranging from 1% to 5% at a prediction horizon of $2\tau_L$. The neural ODE models and EDMD-DL with projection maintain this level of accuracy even at larger sampling times up to $\tau = 0.1$.

Finally, while Figs. 3 and 4 analyzed the short-time performance of these models, we demonstrate the long-time performance of the models by simulating each model for 100 time units from a common initial condition. The resulting trajectory from each model is shown in Fig. 5. We see that each of the models considered (excluding the standard EDMD-DL approach) are able to capture the dynamics and reproduce the butterfly shape of the Lorenz attractor.

C. Low dimensional model of turbulent shear flow

Next we compare these methods on the nine-mode model for a sinusoidal shear flow between parallel plates developed by Moehlis, Faisst, and Eckhardt (MFE) in [68, 69]. This model provides a useful test case, as it displays complex dynamics with many characteristics associated with turbulent shear flows in the transition regime, such as long chaotic transient intervals with rare quasi-laminarization events, with all trajectories eventually collapsing to the laminar state. These complex dynamics allow us to assess not only a model's ability for short time predictions and reproduction of long time statistics in the turbulent region, but also the accuracy of the lifetime predictions and the model's ability to predict extreme events. For these reasons, this model has become a common test-case for data-driven time-series prediction methods, particularly in the fluid dynamics community [26, 28, 67, 71].

The domain is wall-bounded at $y = \pm 1$ and periodic in the streamwise and spanwise directions (x and z), with lengths $L_x = 4\pi$ and $L_z = 2\pi$, respectively; and we consider a channel Reynolds number of Re = 400, following Refs. [26, 28, 67, 71]. The Lyapunov timescale associated with these parameter values is $\tau_L \approx 61$ [67]. The nine mode model is constructed as a Galerkin projection of the Navier-Stokes equations onto nine Fourier modes, as described in [68]. That is, the fluid velocity field $\mathbf{u}(\mathbf{x}, t)$ is approximated as a superposition of the modes, $\mathbf{u}_i(\mathbf{x})$, with time-varying amplitudes $a_i(t)$

$$\mathbf{u}(\mathbf{x},t) = \sum_{i=1}^{9} a_i(t) \mathbf{u}_i(\mathbf{x}) \,. \tag{42}$$

Performing the Galerkin projection yields a set of nine ODEs for the amplitudes. These ODEs, as well as the Fourier modes for the model, are given explicitly in Ref. [68]. The first mode of the model, $\mathbf{u}_1(\mathbf{x})$, represents the base flow profile, so the laminar flow state is associated with the amplitudes $\mathbf{a} = [1, 0, 0, 0, 0, 0, 0, 0, 0]^{\mathrm{T}}$. The flow can be characterized using the energy $E(t) = \sum_{i=1}^{9} a_i^2(t)$. In the turbulent region of the state space, the system shows large bursts of energy, corresponding to quasi-laminarization events, while the laminar state corresponds to the steady value of E = 1. A typical time-series of the energy for this system is shown in Fig. 6

A training dataset is constructed by numerically integrating the system from 100 random initial conditions, $\mathbf{a}(0) \sim \mathcal{U}(-0.1, 0.1)$ for 30,000 time units or until laminarization occurs with data stored at time intervals of $\tau = 0.5$. The first 500 time units of each trajectory are



FIG. 6. Typical time series for the energy in the MFE model for a turbulent shear flow. The horizontal dashed line depicts the energy threshold used to define an extreme event.

discarded as transience. These trajectories have a mean lifetime of approximately 1.1×10^4 (or $180 \tau_L$) and the resulting dataset contains approximately 2.1×10^6 snapshots. A test dataset is generated using an identical procedure, using another set of randomly selected initial conditions. All models are trained for 10 epochs with batch size of 40 (5.25×10^5 iterations).

Figure 7 shows the short-time prediction results for the data-driven models on the MFE system. Fig. 7(a) shows the ensemble-averaged error over time for each model, computed (as before) by simulating the models from 1000 randomly selected initial conditions from the test dataset. Fig. 7(b) shows a representative trajectory from the test dataset, along with the model predictions for the first three mode amplitudes. As in the case of the Lorenz system, we see that the standard EDMD time evolution diverges rapidly from the true trajectory, while the other time evolution methods perform well. Here all of the models trained with the neural ODE training procedure outperform all of the EDMD-DL-based models in terms of ensemble-averaged relative error, with the EDMD-structured neural ODE performing slightly better than the basic neural ODE. Nevertheless, that all of these models perform quite well, with less than 3% relative error at $t = \tau_L$.

To assess the accuracy of the models in terms of reproducing the long-time statistics of the system, we simulate the models from the 100 initial conditions of the trajectories in the test dataset for 30,000 timesteps or until relaminarization is predicted. Shown in Fig. 8 are



FIG. 7. Prediction results for the data-driven models on the MFE model of a turbulent shear flow.(a) Normalized ensemble-averaged error. (b) Representative trajectory timeseries of the first three modes.

the joint probability density functions (PDFs) of the amplitudes a_1 and a_3 , from the test data set and as predicted by each of the models. The standard EDMD model is omitted here, since it tends to rapidly diverge from the true trajectory, as shown in Fig. 7. From Fig. 8, it is apparent that each of the other models reproduces the statistics qualitatively well. To quantify the accuracy of these long-time statistics, we compute a Wasserstein distance (a.k.a. earth mover's distance) to quantify the discrepancy between the predicted and true joint PDFs. This quantity measures the distance between distributions by solving an optimal tranport problem to determine the most efficient way to move mass between distributions. Given two discrete distributions, μ and ν (as obtained from a normalized histogram of the data using n_{μ} and n_{ν} bins, respectively), the Wasserstein-2 distance, $W_2(\mu, \nu)$ between the distributions is given by

$$\mathcal{W}_{2}(\mu,\nu) = \left(\min_{\gamma} \sum_{i,j} \gamma_{i,j} \|\mu^{(i)} - \nu^{(j)}\|_{2}^{2}\right)^{\frac{1}{2}}$$
s.t. $\gamma \mathbf{1} = \mu, \quad \gamma^{\mathrm{T}} \mathbf{1} = \nu, \quad \gamma \ge 0$

$$(43)$$

where $\gamma \in \mathbb{R}^{n_{\mu} \times n_{\nu}}$ is a transport plan (i.e., $\gamma_{i,j}$ assigns the amount of mass to move from bin $\mu^{(i)}$ to bin $\nu^{(j)}$). We compute the Wasserstein distances using the python library, Python Optimal Transport [72], and we report the distances normalized by the distance between the distributions of the test and training datasets. That is, we report the normalized Wasserstein



FIG. 8. Joint probability densities of amplitudes a_1 and a_3 for (a) the test data set, (b) the basic neural ODE model, (c) the EDMD-structured neural ODE model, (d) EDMD with reprojection (e) the EDMD basis neural ODE, and (f) the EDMD direct neural ODE. The inset values give normalized Wasserstein distance \overline{W}_2 between the distribution predicted by the model and the test data distribution. Note the logarithmic scale.

distance

$$\overline{\mathcal{W}}_2(\mu_{\text{pred}}, \mu_{\text{test}}) = \frac{\mathcal{W}_2(\mu_{\text{pred}}, \mu_{\text{test}})}{\mathcal{W}_2(\mu_{\text{train}}, \mu_{\text{test}})}.$$
(44)

for each model where μ_{pred} is the distribution of the dataset generated by a given model, and similarly μ_{test} and μ_{train} are the distributions of the test and training datasets respectively. So $\overline{W}_2 = 1$ indicates that the error between the predicted and test histograms is of the same magnitude as the error between the test and training datasets, which are generated by the same model with different initial conditions. The \overline{W}_2 values for each model are displayed as an inset in the joint PDF plots in Fig. 8. We see that each model has a \overline{W}_2 value of approximately 1 or less, with the exception of the EDMD basis neural ODE model, which appears to suffer from a large error near to the laminar state, indicating poor prediction of relaminarization, while otherwise appearing qualitatively accurate.

Using the same predicted and test datasets as used for quantifying the long-time statistics, we also evaluate the models in terms of their ability to predict the lifetime distribution for the system. The lifetime distribution describes the expected amount of time that trajectories spend in the turbulent region of the state space before laminarization. The lifetime distribution is quantified by the survival probability, S(t), which describes the probability that a trajectory will still be turbulent after time t [68]. For this, we say that the system has laminarized when it reaches a high-energy, near-laminar state $(E = \sum_{i=1}^{9} a_i^2 > 0.8)$ which remains steady for 5 time units (to within a tolerance of 10^{-6}). Fig. 9 shows the lifetime distribution of the test dataset along with the lifetime distribution predicted by each of the models. From the lifetime distribution of the test-dataset, it can be seen that trajectories tend to remain in the turbulent region for very long times, as the half-life of the survival function is over 100 Lyapunov times. Therefore, to produce accurate reconstructions of the long-time statistics, as in Fig. 8, the models are required to maintain accurate predictions over very long timescales. In Fig. 9, we see that each of the considered models, aside from the standard EDMD perform comparably, with each of them accurately approximating the lifetime distribution. The basic neural ODE and EDMD-structured neural ODE models appear to capture the distribution the best at shorter times $(t < 100\tau_L)$, while the EDMD-direct neural ODE performs better at larger times where the other models tend to overestimate the survival probability. The standard EDMD-DL model prediction tends to grow rapidly, and never collapses to the laminar state, which results in a survival probability of 1 by the definition above.

Finally, we assess the ability of the data-driven models to forecast rare quasi-laminarization events within a short time horizon by casting this task as a binary classification problem, following Racca and Magri [67]. That is, we evaluate whether extreme events predicted by the model within a specified time interval are true positives (TP) or false positives (FP). Similarly, when a model does not predict an extreme event in the interval, we evaluate whether this is a true negative (TN) or a false negative (FN). In this way, we can also evaluate how rapidly the quality of extreme event prediction degrades as the prediction horizon, h, before the interval of interest is increased. There are multiple ways to quantify the statistical accuracy of predictions in binary classification problems. Precision quantifies the fraction of true positive predictions out of all positive predictions, P = TP/(TP + FP),



FIG. 9. Lifetime distribution predictions for the models, given in terms of the survival function S(t).

while recall quantifies the ratio of true positive predictions to the total number of event occurrences, R = TP/(TP + FN). Here we report the *F*-score, which is given by the harmonic mean of precision and recall

$$F = \frac{2}{P^{-1} + R^{-1}} = \left(1 + \frac{FP + FN}{2TP}\right)^{-1}.$$
(45)

To compute the *F*-score for our models, we first select a set of starting points from the test dataset evenly spaced at 1 τ_L apart. From these starting points, we simulate the model forward for a time of $h + \tau_L$, and assess the model's extreme event prediction within the interval $[h, h + \tau_L]$. By processing the test dataset in this way, we construct a dataset containing 18,000 starting points (and intervals) with 947 quasi-laminarization events. We say that a quasi-laminarization event has occurred within a given interval if the energy is below the threshold value at the beginning of the interval and increases past the threshold within the interval. Some examples of these quasi-laminarization events are depicted in Fig. 6, along with the energy threshold considered here. We use an energy threshold of E = 0.2 and consider prediction horizons ranging from $0.5\tau_L$ to $4.5\tau_L$.

Figure 10 shows the *F*-score as a function of the prediction horizon normalized with Lyapunov time, h/τ_L , for each of the models. From these results, it is clear that the continuous time neural ODE models outperform the discrete time and EDMD-DL-based approaches, more accurately forecasting extreme events for every prediction horizon. Among the EDMD-



FIG. 10. F-score assessment of quasi-laminarization event prediction as a function of prediction horizon, h.

DL-based models, the EDMD-basis neural ODE outperforms EDMD-DL with reprojection and the EDMD direct neural ODE. The standard EDMD-DL prediction is poor for every prediction horizon, resulting in a much lower F-score than the other models. Also included for comparison in Fig. 10 are the *F*-score results from Racca and Magri [67], who developed a model using an echo state network, a type of recurrent neural network. Its predictions are based on long sequences of past states and are thus non-Markovian, while our model predictions are based only on the initial state. Nevertheless, their model only slightly outperforms the present models, especially for the case of the EDMD-structured neural ODE.

V. CONCLUSIONS

Developing and improving upon neural network-based methods for time evolution prediction of dynamical systems is a promising approach for the forecasting of complex dynamical systems. In this work, we have examined the parallels between neural ODE methods and methods based on finite-dimensional approximations of the Koopman operator using neural network-based dictionaries. While methods based on the Koopman operator lead to an approximation of linear dynamics on the space of observables, in practice they often provide poor predictions of the time-evolution of the states due to the difficulty associated with determining a dictionary which spans a Koopman invariant space for a given system. This is especially true for chaotic systems, such as the ones considered here. It has been seen that the state-predictions of these Koopman-based methods can be greatly improved by projecting back to the state space on each timestep. Here we have pointed out that by relifting to the observable space from the state space on each step, we introduce a nonlinearity into the time evolution formulation, resulting in a nonlinear discrete-time map on the state space. Therefore using an EDMD approximation of the operator in this way with a neural network dictionary can be seen as a discrete-time version of a neural ODE. Furthermore, we can also apply a similar projection strategy to the continuous time formulations of EDMD based on the Koopman generator to obtain a continuous time neural ODE directly from the EDMD-DL-optimized operator and dictionary without any further training. Additionally, the model structures arising from EDMD-DL with projection naturally possess a neural network structure that is commonly used in neural ODEs, in which the state is first expanded out to a high-dimensional feature vector (represented by a multi-layer neural network) followed by a linear mapping back to the state space to yield the vector field of the dynamics.

Inspired by these observations, we have implemented several variations of neural ODEs and EDMD-DL, developed by combining different aspects of their respective model structures and training procedures. We provide performance comparisons on two chaotic systems to demonstrate the equivalence of these methods and highlight the aspects of each model that lead to improved performance. Specifically, we show that the novel neural ODE architecture based on the dictionary structure typically used in EDMD-DL, where the state is explicitly separated from the nonlinear dictionary elements, leads to a small improvement in the short-time prediction performance of neural ODEs, as compared to the standard neural ODE architecture. In the context of neural ODEs, separating the linear and nonlinear parts of the vector field provides a nice structure, as the neural network only has to account for the nonlinear dynamics, with the linear terms represented separately. In the examples considered here, the EDMD-structured neural ODE architecture, trained with the usual neural ODE loss, performed best overall, suggesting that this should be the standard structure for neural ODEs.

We see that each of the neural ODE methods and EDMD-DL methods with projection tend to perform comparably on these systems in terms of short-time trajectory prediction, reconstruction of long-time statistics, and the prediction of extreme events; with all of them offering a significant improvement over the standard EDMD-DL linear time evolution on the space of observables. Furthermore, we emphasize that each of these models perform very well in terms of short-time prediction, with less than 3% relative error at $t = \tau_L$ for each of the chaotic systems considered here and rare event prediction capability comparable to the non-Markovian approach of Racca and Magri [67]. In addition to accurate short-time tracking, we have also demonstrated that the model predictions are statistically accurate for long times as well, as they yield accurate reconstructions of the long-time probability density functions on the state space and accurately predict the turbulent lifetime for the MFE model of a turbulent shear flow. These findings highlight the promise of neural ODEs and Koopman-based approaches for developing data-driven models capable of generating accurate time evolution predictions in complex and chaotic systems.

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