Deep learning for universal linear embeddings of nonlinear dynamics

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Abstract

Identifying coordinate transformations that make strongly nonlinear dynamics approximately linear is a central challenge in modern dynamical systems. These transformations have the potential to enable prediction, estimation, and control of nonlinear systems using standard linear theory. The Koopman operator has emerged as a leading data-driven embedding, as eigenfunctions of this operator provide intrinsic coordinates that globally linearize the dynamics. However, identifying and representing these eigenfunctions has proven to be mathematically and computationally challenging. This work leverages the power of deep learning to discover representations of Koopman eigenfunctions from trajectory data of dynamical systems. Our network is parsimonious and interpretable by constructing, embedding the dynamics on a low-dimensional manifold that is of the intrinsic rank of the dynamics and parameterized by the Koopman eigenfunctions. In particular, we identify nonlinear coordinates on which the dynamics are globally linear using a modified auto-encoder. We also generalize Koopman representations to include a ubiquitous class of systems that exhibit continuous spectra, ranging from the simple pendulum to nonlinear optics and broadband turbulence. Our framework parametrizes the continuous frequency using an auxiliary network, enabling a compact and efficient embedding at the intrinsic rank, while connecting our models to half a century of asymptotics. In this way, we benefit from the power and generality of deep learning, while retaining the physical interpretability of Koopman embeddings.

Keywords— Dynamical systems, Koopman theory, machine learning, deep learning.

1 Introduction

Nonlinearity is a hallmark feature of complex systems, giving rise to a rich diversity of observed dynamical behaviors across the physical, biological, and engineering sciences \cite{58, 57}. Although computationally tractable, there exists no general mathematical framework for solving nonlinear dynamical systems. Thus representing nonlinear dynamics in a linear framework is particularly appealing because of powerful and comprehensive techniques for the analysis and control of linear systems \cite{1}, which do not readily generalize to nonlinear systems. Koopman operator theory, developed in 1931 \cite{54, 55}, has recently emerged as a leading candidate for the systematic linear representation of nonlinear systems \cite{17, 18}. This renewed interest in Koopman analysis has been driven by a combination of theoretical advances \cite{17, 18, 19, 20}, improved numerical methods such as dynamic mode decomposition (DMD) \cite{46, 47, 48}, and an increasing abundance of data. Eigenfunctions of the Koopman operator are now widely sought, as they provide intrinsic coordinates that globally linearize nonlinear dynamics. Despite the immense promise of Koopman embeddings, obtaining representations has proven difficult in all but the simplest systems, and representations are often intractably complex or are the output of uninterpretable black-box optimizations. In this work, we utilize the power of deep learning for flexible and general representations of the Koopman operator, while enforcing a network structure that promotes parsimony and interpretability of the resulting models.

Neural networks (NNs), which form the theoretical architecture of deep learning, were inspired by the primary visual cortex of cats where neurons are organized in hierarchical layers of cells to process visual stimulus \cite{64}. The first mathematical model of such NNs was the neocognitron \cite{65} which has many of the features of modern deep neural networks (DNNs), including a multi-layer structure, convolution, max pooling and nonlinear dynamical nodes. Importantly, the universal approximation theorem \cite{66, 67, 68} guarantees that a NN with sufficiently many hidden units and a linear output layer is capable of representing any arbitrary function, including our desired Koopman eigenfunctions. Although NNs have a four-decade history, the analysis of the ImageNet data set \cite{69}, containing over 15 million labeled images in 22,000 categories, provided a watershed moment \cite{70}. Indeed, powered by the rise of big data and increased computational power, deep learning is resulting in transformative progress in many data-driven classification and identification tasks \cite{70, 71, 72}. A strength of deep learning is that features of the data are built in a hierarchical, or layered, way, which enables the representation of com-
Figure 1: Diagram of our deep learning schema to identify Koopman eigenfunctions $\varphi(x)$. (a) Our network is based on a deep auto-encoder, which is able to identify intrinsic coordinates $y = \varphi(x)$ and decode these coordinates to recover $x = \varphi^{-1}(y)$. (b,c) We add an additional loss function to identify a linear Koopman model $K$ that advances the variables $y$ forward in time. In practice, we enforce agreement with the trajectory data for several iterations through the dynamics, i.e. $K^m$. In (b), the loss function is evaluated on the state variable $x$ and in (c) it is evaluated on $y$.

The focus of this work is on developing DNN representations of Koopman eigenfunctions that remain interpretable and parsimonious, even for high-dimensional and strongly nonlinear systems. Our approach (See Fig. 1) differs from previous studies, as we are focused specifically on obtaining models that match the intrinsic low-rank dynamics while avoiding overfitting, thus merging the best of DNN architectures and Koopman theory. In particular, many dynamical systems exhibit a continuous eigenvalue spectrum, which confounds low-dimensional representation using existing DNN or Koopman representations. This work develops a generalized framework and enforces new constraints specifically designed to extract the fewest meaningful eigenfunctions in an interpretable manner. For systems with continuous spectra, we utilize an augmented network to parameterize the linear dynamics on the intrinsic coordinates, avoiding an infinite asymptotic expansion in harmonic eigenfunctions. Thus, the resulting networks remain parsimonious, and the few key eigenfunctions are interpretable. We demonstrate our deep learning approach to Koopman on several examples designed to illustrate the strength of the method, while remaining intuitive in terms of classic dynamical systems.
2 Background on data-driven dynamical systems

To give context to our deep learning approach to identify Koopman eigenfunctions, we first summarize highlights and challenges in the data-driven discovery of dynamics. Throughout this work, we will consider discrete-time dynamical systems,

\[ x_{k+1} = F(x_k), \tag{1} \]

where \( x \in \mathbb{R}^n \) is the state of the system and \( F \) represents the dynamics that map the state of the system forward in time. Discrete-time dynamics often describe a continuous-time system that is sampled discretely in time, so that \( x_k = x(k \Delta t) \) with sampling time \( \Delta t \). The dynamics in \( F \) are generally nonlinear, and the state \( x \) may be high dimensional, although we typically assume that the dynamics evolve on a low-dimensional attractor governed by persistent coherent structures in the state space \( \mathcal{F} \). Note that \( F \) if often unknown and only measurements of the dynamics are available.

The dominant geometric perspective of dynamical systems, in the tradition of Poincaré, concerns the organization of trajectories of \( \mathcal{F} \), including fixed points, periodic orbits, and attractors. Formulating the dynamics as a system of differential equations in \( x \) often admits compact and efficient representations for many natural systems \( \mathcal{F} \); for example, Newton’s second law is naturally expressed by \( \mathcal{F} \). However, the solution to these dynamics may be arbitrarily complicated, and possibly even irrepresentable, except for special classes of systems. Linear dynamics, where the map \( F \) is a matrix that advances the state \( x \), are among the few systems that admit a universal solution, in terms of eigenvalues and eigenvectors of \( F \), also known as the spectral expansion.

Koopman operator theory

In 1931, B. O. Koopman provided an alternative description of dynamical systems in terms of the evolution of functions in the Hilbert space of possible measurements \( y = g(x) \) of the state \( x \). The so-called Koopman operator, \( \mathcal{K} \), that advances measurement functions is an infinite-dimensional linear operator:

\[ \mathcal{K}g \triangleq g \circ F \implies \mathcal{K}g(x_k) = g(x_{k+1}). \tag{2} \]

Koopman analysis has gained significant attention recently with the pioneering work of Mezic et al. \( \mathcal{K} \), and in response to the growing wealth of measurement data and the lack of known equations for many systems \( \mathcal{F} \). Representing nonlinear dynamics in a linear framework, via the Koopman operator, has the potential to enable advanced nonlinear prediction, estimation, and control using the comprehensive theory developed for linear systems. However, obtaining finite-dimensional approximations of the infinite-dimensional Koopman operator has proven challenging in practical applications.

Finite-dimensional representations of the Koopman operator are often approximated using the dynamic mode decomposition (DMD) \( \mathcal{K} \), introduced by Schmid \( \mathcal{K} \). By construction, DMD identifies spatio-temporal coherent structures from a high-dimensional dynamical system, although it does not generally capture nonlinear transients since it is based on linear measurements, \( g(x) = x \), of the system. Extended DMD (eDMD) and the related variational approach of conformation dynamics (VAC) \( \mathcal{K} \), enriched the model with nonlinear measurements \( \mathcal{K} \), for more details, see SI Appendix. Identifying regression models based on nonlinear measurements will generally result in closure issues, as there is no guarantee that these measurements form a Koopman invariant subspace \( \mathcal{F} \). In addition, the resulting models are of exceedingly high dimension, and when kernel methods are employed \( \mathcal{F} \), the models may become uninterpretable. Instead, many approaches seek to identify eigenfunctions of the Koopman operator directly, satisfying:

\[ \varphi(x_{k+1}) = \mathcal{K}\varphi(x_k) = \lambda \varphi(x_k). \tag{3} \]

Eigenfunctions are guaranteed to span an invariant subspace, and the Koopman operator will yield a matrix when restricted to this subspace \( \mathcal{F} \). In practice, Koopman eigenfunctions may be more difficult to obtain than the solution of \( \mathcal{F} \); however, this is a one-time up-front cost that yields a compact linear description. The challenge of identifying and representing Koopman eigenfunctions provides strong motivation for the use of emerging deep learning methods \( \mathcal{F} \).

Koopman for systems with continuous spectra

The Koopman operator provides a global linearization of the dynamics. The concept of linearizing dynamics is not new, and locally linear representations are commonly obtained by linearizing around fixed points and periodic orbits \( \mathcal{F} \). Indeed, asymptotic and perturbation methods have been widely used since the time of Newton to approximate solutions of nonlinear problems by starting from the exact solution of a related, typically linear problem. The classic pendulum, for instance, satisfies the differential equation \( \ddot{x} = -\sin(wx) \) and has eluded an analytic solution since its mathematical inception. The linear problem associated with the pendulum involves the small angle approximation whereby \( \sin(wx) = wx - (wx)^3/3! \) and only the first term is retained in order to yield exact sinusoidal solutions. The next correction involving the cubic term gives the Duffing equation which is one of the most commonly studied nonlinear oscillators in all of physics \( \mathcal{F} \). Importantly, the cubic contribution is known to shift the linear oscillation frequency of the pendulum, \( \omega \) to \( \omega + \Delta \omega \) as well as generate harmonics such as \( \exp(\pm3i\omega) \). An exact representation of the solution can be derived in terms of Jacobi elliptic functions which have a Taylor series representation in terms of an infinite sum of sinusoids with frequencies \( (2n-1)\omega \) where \( n = 1, 2, \ldots, \infty \). Thus, the simple pendulum oscillates at the linear natural frequency \( \omega \) for small deflections,
and as the pendulum energy is increased, the frequency decreases continuously, resulting in a so-called continuous spectrum.

The importance of accounting for the continuous spectrum in Koopman theory was realized shortly after the original 1931 paper in an extension by Koopman and von Neumann [25]. A continuous spectrum, as described for the simple pendulum, is characterized by a continuous range of observed frequencies, as opposed to the discrete spectrum consisting of isolated, fixed frequencies. This phenomena is observed in a wide range of physical systems that exhibit broadband frequency content, such as in turbulence and nonlinear optics. The continuous spectrum thus confounds simple Koopman descriptions, as there is no a straightforward finite approximation in terms of a small number of eigenfunctions [32]. Indeed, away from the linear regime, an infinite Fourier sum is required to approximate the shift in frequency and eigenfunctions. In fact, in some cases, eigenfunctions may not exist at all.

Recently, there have been several algorithmic advances to approximate systems with continuous spectra, including nonlinear Laplacian spectral analysis [13] and the use of delay coordinates [3,2]. A critically enabling innovation of this work is explicitly accounting for the parametric dependence of the Koopman operator $K(\omega)$ on the continuously varying frequency $\omega$, which is directly related to the classic perturbation results above. By constructing an auxiliary network (See Fig. 2) to first determine the parametric dependence of the Koopman operator on the frequency $\omega$, an interpretable low-rank model of the intrinsic dynamics can then be constructed. If this explicit frequency dependence is unaccounted for, then a high-dimensional network is necessary to account for the shifting frequency and eigenvalues, i.e. a Taylor series expansion is required for an accurate model. We conjecture that previous Koopman models using high-dimensional DNNs actually approximate the harmonic series expansion required to approximate the continuous spectrum for systems such as the Duffing oscillator.

3 Deep learning to identify Koopman eigenfunctions

The overarching goal of this work is to leverage the power of deep learning to discover and represent eigenfunctions of the Koopman operator at its intrinsic rank. Our perspective is driven by the need for parsimonious representations that are efficient, avoid overfitting, and provide minimal descriptions of the dynamics on interpretable intrinsic coordinates. Unlike previous deep learning approaches to Koopman [46,31,44,49], our network architecture is designed specifically to handle a ubiquitous class of nonlinear systems characterized by a continuous frequency spectrum generated by the nonlinearity. A continuous spectrum presents unique challenges for compact and interpretable representation, and our approach is inspired by the classical asymptotic and perturbation approaches in dynamical systems.

Our core network architecture is shown in Fig. 1 and it is modified in Fig. 2 to handle the continuous spectrum. Our network identifies the intrinsic coordinates $y = \varphi(x)$ spanned by a set of Koopman eigenfunctions $\varphi: \mathbb{R}^n \rightarrow \mathbb{R}^p$, along with a dynamical system $y_{k+1} = Ky_k$. There are three high-level requirements for the network, corresponding to three types of loss functions used in training:

1. **Intrinsic coordinates that are useful for reconstruction.** We seek to identify a few intrinsic coordinates $y = \varphi(x)$ where the dynamics evolve, along with an inverse $x = \varphi^{-1}(y)$ so that the state $x$ may be recovered. This is achieved using an auto-encoder (See Figure 1a.), where $\varphi$ is the encoder and $\varphi^{-1}$ is the decoder. The dimension $p$ of the auto-encoder subspace is a hyperparameter of the network, and this choice may be guided by knowledge of the system. Reconstruction accuracy of the auto-encoder is achieved using the following loss: $\|x - \varphi^{-1}(\varphi(x))\|_2$.

2. **Linear dynamics.** To discover Koopman eigenfunctions, we learn the linear dynamics $K$ on the intrinsic coordinates, i.e., $y_{k+1} = Ky_k$. Linear dynamics are achieved using the following loss: $\|\varphi(x_{k+1}) - K\varphi(x_k)\|_2$. More generally, we enforce linear prediction over $m$ time steps with the loss: $\|\varphi(x_{k+m}) - K^m\varphi(x_k)\|_2$. (See Figure 1c.)

3. **Future state prediction.** Finally, the intrinsic coordinates must enable future state prediction. Specifically, we identify via linear dynamics in the matrix $K$. This corresponds to the loss $\|x_{k+1} - \varphi^{-1}(K\varphi(x_k))\|_2$, and more generally $\|x_{k+m} - \varphi^{-1}(K^m\varphi(x_k))\|_2$. (See Figure 1b.)

To account for the continuous spectrum, we parametrize the matrix $K$ by the frequency $\omega$. As shown in Fig. 2 an auxiliary network learns the frequency $\omega$ as...
a function of the input $x$. The output $\omega$ is then used to parametrize $K(\omega)$:

$$K(\omega) = \begin{bmatrix} \cos(\omega t) & -\sin(\omega t) \\ \sin(\omega t) & \cos(\omega t) \end{bmatrix}.$$ 

This network structure allows the eigenvalues to vary across phase space, facilitating a small number of eigenfunctions. The prediction loss becomes $\|x_{k+m} - \varphi^{-1}(K(\omega)^m \varphi(x_k))\|$, and the linearity loss becomes $\|\varphi(x_{k+m}) - K(\omega)^m \varphi(x_k)\|$.

To train our network, we generate trajectories from random initial conditions, which are split into training, validation, and testing sets. Models are trained on the training set and compared on the validation set, which is also used for early stopping to prevent overfitting. We report accuracy on the testing set.

4 Results

We demonstrate our deep learning approach to identify Koopman eigenfunctions on example systems, including a simple model with a discrete spectrum and the nonlinear pendulum, which exhibits a continuous spectrum.

Simple model with discrete spectrum

Before analyzing systems with the additional challenges of a continuous spectrum and high-dimensionality, we consider a simple nonlinear system with a single fixed point and a discrete eigenvalue spectrum:

$$\begin{align*}
\dot{x}_1 &= \mu x_1 \\
\dot{x}_2 &= \lambda (x_2 - x_1^2).
\end{align*}$$

This dynamical system has been well-studied in the literature [45–6], and for stable eigenvalues $\lambda < \mu < 0$, the system exhibits a slow manifold given by $x_2 = x_1^2$; we use $\mu = -0.05$ and $\lambda = -1$. As shown in Fig. 3, the Koopman embedding identifies nonlinear coordinates that flatten this inertial manifold, providing a globally linear representation of the dynamics; moreover, the correct Koopman eigenvalues are identified. Specific details about the network and training procedure are provided in the SI Appendix.

Nonlinear pendulum with continuous spectrum

As a second example, we consider the nonlinear pendulum, which exhibits a continuous eigenvalue spectrum with increasing energy:

$$\ddot{x} = -\sin(x) \quad \Rightarrow \quad \begin{cases} 
\dot{x}_1 = x_2 \\
\dot{x}_2 = -\sin(x_1).
\end{cases}$$

Although this is a simple mechanical system, it has proven extremely challenging to obtain compact global representations of the solution, and this system has eluded parsimonious representation in the Koopman framework. The deep Koopman embedding is shown in Fig. 4, where it is clear that the dynamics are linear in the eigenfunction coordinates, given by $y = \varphi(x)$. Even as the Hamiltonian energy of the system increases, corresponding to an elongation of the oscillation period, the parameterized Koopman network is able to account for this continuous frequency shift and provide a compact representation in terms of two eigenfunctions. Alternative network architectures that are not specifically designed to account for continuous spectra with an auxiliary network would be forced to approximate this frequency shift with the classical asymptotic expansion in terms of harmonics. The resulting network would be overly bulky and would limit interpretability.

Recall that we have three types of losses on the network: reconstruction, prediction, and linearity. Figure 4.I.A shows that the network is able to function as an auto-encoder, accurately reconstructing the ten example trajectories. Next, we show that the network is able to predict the evolution of the system. Figure 4.I.B shows the prediction horizon for ten initial conditions that are simulated forward with the network, stopping the prediction when the relative error reaches 10%. As expected, the prediction horizon deteriorates as the energy of the initial condition increases, although the prediction is still quite accurate. Finally, we demonstrate that the dynamics in the intrinsic coordinates $y$ are truly linear, as shown by the nearly concentric circles in Fig. 4.II.C. The eigenfunctions $\varphi_1(x)$ and $\varphi_2(x)$ are shown in Fig. 4.III.

5 Discussion

In summary, we have employed powerful deep learning approaches to identify and represent coordinate transformations that recast strongly nonlinear dynamics into a globally linear framework. Our approach is designed to discover eigenfunctions of the Koopman operator, which provide an intrinsic coordinate system to linearize nonlinear systems, and have been notoriously difficult to identify and represent using alternative methods. Building on a deep auto-encoder framework, we enforce additional constraints and loss functions to identify Koopman eigenfunctions where the dynamics evolve linearly. Moreover, we generalize this framework to include a broad class of nonlinear systems.
that exhibit a continuous spectrum, where a continuous range of frequencies is observed. Continuous-spectrum systems are notoriously difficult to analyze, especially with Koopman theory, and naive learning approaches require asymptotic expansions in terms of higher order harmonics of the fundamental frequency, leading to bloated and unwieldy models. In contrast, we utilize an auxiliary network to parametrize and identify the continuous frequency, which then parameterizes a compact Koopman model on the auto-encoder coordinates. Thus, our deep neural network models remain both parsimonious and interpretable, merging the best of neural network representations and Koopman embeddings.

The use of deep learning in physics and engineering is increasing rapidly, and this trend is only expected to accelerate. Nearly every field of science is revisiting challenging problems of central importance from the perspective of big data and deep learning. With this growing interest, it is imperative that we as a community seek machine learning models that favor interpretability and promote physical insight and intuition. In this challenge, there is a tremendous opportunity to gain new understanding and insight by applying increasingly powerful techniques to data. For example, discovering Koopman eigenfunctions will result in new symmetries and conservation laws, as conserved eigenfunctions are related to conservation laws via a generalized Noether’s theorem. It will also be important to apply these techniques to increasingly challenging problems, such as turbulence, epidemiology, and neuroscience, where data is abundant and models are needed. Finally, the use of deep learning to discover Koopman eigenfunctions may enable transformative advances in the nonlinear control of complex systems. All of these future directions will be facilitated by more powerful network representations.

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Supporting Information (SI)

Code

We used the Python API for the TensorFlow framework \[1\] and the Adam optimizer \[22\] for training. More in-depth information about the deep learning model is available in the SI. All of our code is available online at [github.com/BethanyL/DeepKoopman](https://github.com/BethanyL/DeepKoopman).

Creating the Datasets

For each dynamical system, we chose 4200 initial conditions for the test set, 8400 for the validation set, and 2,940,000 for the training set. For each initial condition, we solved the differential equations for \( t = 0, 0.02, \ldots, 1 \) (51 time points).

The discrete spectrum dataset consists of random initial conditions \( x \) where \( x_1, x_2 \in [-0.5, 0.5] \). The pendulum dataset consists of random initial conditions \( x \) where \( x_1 \in [-3.1, 3.1], x_2 \in [-2, 2] \), and the potential function is under 0.99. The potential function for the pendulum is \( \frac{1}{2} x_2^2 - \cos(x_1) \).

Network Architecture

Each hidden layer had the form of \( Wx + b \) followed by an activation with the rectified linear unit (ReLU): \( f(x) = \max\{0, x\} \). There were four hidden layers in the encoder, four in the decoder, and four in the frequency network. See Table 1 for the width of each hidden layer. The output layers of the encoder, decoder, and frequency network were linear (simply \( Wx + b \)).

Training

We initialized each weight matrix \( W \) randomly from a uniform distribution in the range \([-s, s]\) for \( s = \sqrt{a} \), where \( a \) is the dimension of the input of the layer. This distribution was suggested in [15]. Each bias vector \( b \) was initialized to 0.1. The model for the discrete spectrum example was trained for four hours on an NVIDIA K80 GPU, and the pendulum model was trained for six hours. The prediction loss was averaged over three steps: predicting \( x_{k+1}, x_{k+2}, \) and \( x_{k+3} \). The linearity loss was averaged over fifty steps: \( y_{k+1}, y_{k+2}, \ldots, y_{k+50} \). The learning rate for the Adam optimizer was 0.001. For the pendulum only, the prediction and reconstruction losses were weighted by 0.001. For each dynamical system, we trained multiple models in a random search of parameter space and chose the one with the lowest validation error. Each model was initialized with different random weights. We also used early stopping; for each model, at the end of training, we resumed the step with the lowest validation error. See Table 1 for the rest of the training hyperparameters.

Connection between eDMD and VAC

It has recently been shown that eDMD is equivalent to the variational approach of conformation dynamics (VAC) \[37, 39\], first derived by Noé and Nüske in 2013 to simulate molecular dynamics with a broad separation of timescales. Further connections between eDMD and VAC and between DMD and the time lagged independent component analysis (TICA) are explored in a recent review \[23\]. A key contribution of VAC is a variational score enabling the objective assessment of Koopman models via cross-validation. Recently, eDMD has been demonstrated to improve model predictive control performance in nonlinear systems \[28\].

| Layer width | Discrete spectrum | Pendulum |
|-------------|------------------|----------|
| Batch size  | 491              | 339      |
| \( \ell_2 \) | \( 1.44 \times 10^{-14} \) | \( 3.18 \times 10^{-16} \) |
| \( \ell_1 \) | \( 7.27 \times 10^{-17} \) | \( 6.53 \times 10^{-16} \) |
| \( \ell_\infty \) | \( 10^{-6} \) | \( 6.95 \times 10^{-9} \) |