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Recurrent Neural Network based linear embeddings for time evolution of non-linear dynamics

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Abstract: In modern dynamical system modeling, finding coordinate transformation for representing highly non-linear dynamics in terms of approximate linear dynamics has been of crucial importance for enabling non-linear control, estimation, and prediction. Recently developed interest in Koopman operator theory has shown that its eigenfunctions can provide such coordinates that intrinsically linearize the global dynamics [11], [6], [2], [14]. But finding and representation of such eigenfunctions have been challenging. The present work leverages deep learning methods, specifically Recurrent Neural Networks (RNNs) [15] for discovering the Koopman eigenfunction representations and exploit RNNs ability to model temporal dependencies, to allow multi-step evolution of the dynamics, as long forecasting for such systems still remains a major challenge [16]. It has been shown by [11], that such embeddings can be found using deep neural networks. Current work is an incremental work on the network architecture, which is interpretable in terms of Koopman theory and parsimonious, allowing augmentation to the lacking interpretability to deep learning architectures, while capturing the fewest meaningful eigenfunctions. Some other challenges related to modeling such architectures are discussed in future work.

Keywords: Non-linear dynamics, time evolution, Koopman operator theory, Recurrent Neural Networks

1. Introduction

For any complex dynamical system, non-linearity brings out the most diverse features of the system evolution across disciplines of physics, chemistry, biology and applied sciences. Though such systems can be computationally evolved, there exists no general framework for their evolution given to non-linearity. Hence, the projection of such systems onto a linear frame is of particular interest, as well robust and powerful algorithms that have been developed for robust analysis and control. In this regard, Koopman operator [7] has shown much promise, emerging as a frontier in the data-driven analysis. The renewed interest in Koopman operators can be attributed to the advancements in theoretical [12], [8], algorithmic [17], [6] and the recent data-deluge. Work of [3], [11], [2], [13], have shown that eigenfunctions of Koopman operator provide intrinsic coordinates for linear evolution of non-linear dynamical system. Though the great confidence shown by Koopman embeddings, finding them has proven to be a major challenge, except for the simplest of case. Usually, such embeddings are identified using black-box optimizations which are often uninterpretable or intractably complex. The current work is an increment on the work by [11], which utilizes a deep neural network architecture for identifying the Koopman embeddings and the corresponding Koopman operator in a flexible and general manner, while keeping the architecture Koopman interpretable and parsimonious. The proposed architecture utilizes a Recurrent Neural Network on top of the present deep neural network, to better address the highly sensitive dependence of such dynamical systems on the initial condition and augment to the longer forecast of such systems.

Deep Learning methods have proved their excellence as the current state of the art methods for various tasks such as image classification, natural language process, among others. Inspired by the visual cortex of cats, neural networks, which form the underlying theoretical basis for most deep learning methods where hierarchically stacked neurons are employed to process the input signal. This hierarchical build of the features enables the efficient representation of complex functions. However, of concern to this approach is enabling interpretable, parsimonious and easily transferable models.

Evolution of non-linear dynamical systems can be thought of as *time-series forecasting* in the context of applying neural networks for their evolution as it satisfies the following basic criteria: 1) output data is dependent on temporal input data(s), 2) input data are endogenous, 3) requires multi-step prediction, 4) non-linear system is dynamic, meaning

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the model may receive new inputs for further evolution, 5) the input data may be discontinuous. In this aspect, Recurrent Neural Networks have shown great success in task pertaining to supervised learning of sequential data. Work done by [16] has shown the success of RNNs applied to effectively modeling aerial vehicles.

The focus of present research is while building upon the architecture by [11], which is interpretable and parsimonious in terms of Koopman eigenfunctions and eigenvalues, by integrating the network with a RNN type network for long-time system evolution, by limiting the error propagating through the evolution and all the while reducing the amount of data required for training the network.

2. Data-Driven non-linear systems

Before dwelling into the specifics of the present work for dynamical system evolution, a summary of challenges and highlights in data-driven modeling is presented. All formulation for this work assumes discrete-time dynamics of the form,

$$x_{t+1} = F(x_k)$$

where $x \in \mathbb{R}^n$ is the state space and F is the time map of the dynamics to future state. Discrete systems such as these are often used to define continuous systems, such that $x_k = F(k\Delta t)$, where Δt is the sampling time. Dynamics described by F are usually non-linear in nature, where x maybe a high-dimensional vector, but is usually assumed to unfold in a low-dimensional attractor dictated by persisting coherent structures. Though it must be noted that F is often not known and only measurements of the system are available.

Though representing the evolution of x in the state-space using differential equation allows for a compact and efficient representation of the system, but more often then not, such systems dynamics are arbitrarily complex in their construction and more, can be almost impossible to represent except for some particular cases. Here finding such coordinate transformations which can present the non-linear state-space embeddings as a linear embedding in a different space would be particular interest. For a linear system, where F would be a matrix that advances the system to future steps would be among the few systems through which a universal solution can be obtained in terms of the eigenfunctions and eigenvalues of the matrix F, popularly known as *spectral expansion*.

2.1 Koopman Operator Theory

In 1931, B. O. Koopman presented an alternate view of dynamical systems in terms of the evolution of the system on the *observable functions* in the Hilbert space. A mathematical framework relating the observables of the system to the state-space. Observables of the system can be thought of as all functions $y = g(x)$, on the infinite dimensional Hilbert space, where $x \in M$, M being the state-space. An example of this would free incompressible fluid flow in a box constituting a dynamical system, where the smooth velocity fields satisfying the incompressibility criteria can be thought of as the state-space of the system. For such a system, pressure, vorticity, velocity field at a discrete location or the total kinetic energy of the system can be thought of as the observables of the dynamical system [1]. Mathematically such dynamics can be represented as

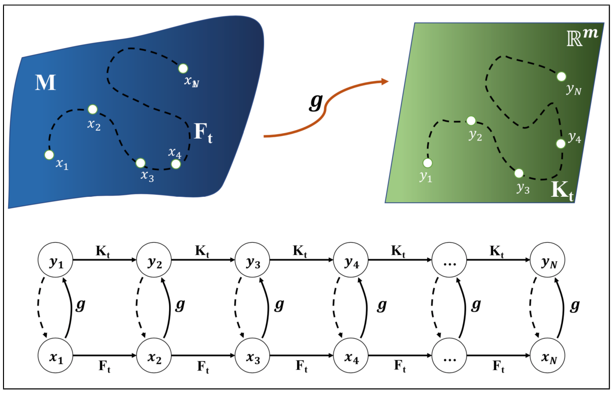

Fig. 1 Diagram representing the underlying principle of Koopman Operator theory.

$$\begin{aligned} &\frac{d}{dt}x = f(x), \\ &\Rightarrow F_t(x(t_0)) = x(t_0 + t) \\ &\qquad\qquad\quad = x(t_0) + \int_{t_0}^{t_0+t} f(x(\tau))d\tau \end{aligned}$$

For discrete-time update:

$$x_{k+1} = F_t(x_k)$$

where, x belongs the state-space of the system, $f(x)$ is a vector field on the state-space and F_t is the flow map operator, for advancing the state-space to future time-steps.

From the above discussion, given the knowledge of the observable of the system in the form of time series, what can be said about the evolution of the state? Let g be a real-valued observable of the dynamical system. Collection of all such observables form a linear vector space. The Koopman operator acts on the observable function as described by the following equation:

$$\begin{aligned} &K_t g = goF_t \\ &\Rightarrow K_t g(x_k) = g(F_t(x_k)) \\ &\qquad\qquad\quad = g(x_{k+1}) \end{aligned}$$

For discrete-time updates:

$$g(x_{k+1}) = K_t g(x_k)$$

Fig.1, diagrammatically represents the underpinnings of Koopman Operator theory.

Koopman analysis has garnered a lot of attention owing to the pioneering work of Mezic et al. [14], [13], [12], and to the data-deluge and incomplete understanding of system dynamics in various domains. Though the promise showed

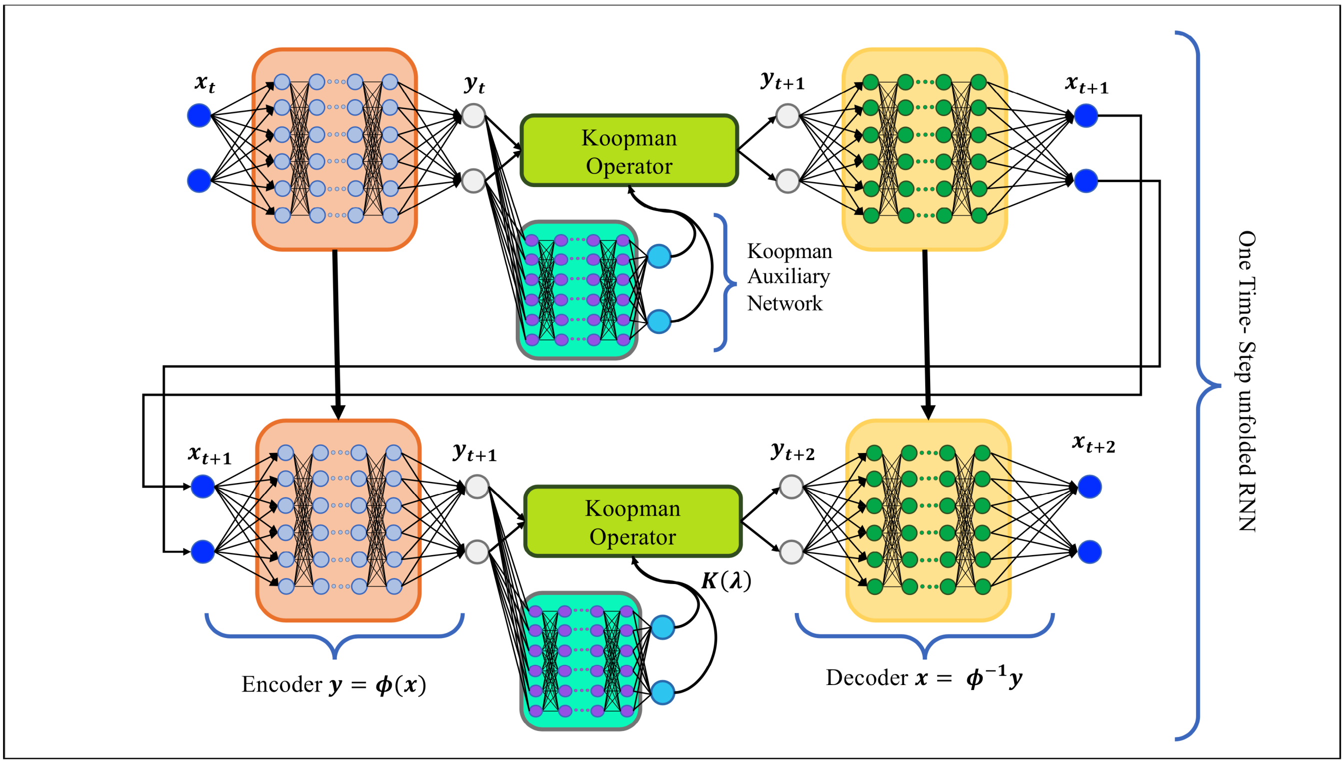

Fig. 2 Diagram of the current proposed architecture based on recurrent units. All the directional arrows represents the direction of data movement for the forward pass.

by Koopman theory leveraging on the extensive and robust advances made in linear theory, for control, estimation, and prediction, is commendable, however, finding the associated eigenfunctions and eigenvalues still remains a major challenge for practical application.

The various method, like Extended Dynamic Mode Decomposition and the related variational approach of conformation dynamics [9] do capture the non-linear features of the dynamics, but there is no guarantee that the measurements span the Koopman invariant sub-space, suffering from closure issues. Kernel methods likewise can be high dimensional and highly uninterpretable. Hence, many approaches try to directly represent the eigenfunctions associated with the Koopman operator. While finding these eigenfunctions, identifying continuous spectra, characterized by a continuous range of frequencies, is observed for a wide range of physical systems. This confounds trivial Koopman description as they cannot be approximated using a finite number of eigenfunctions.

The present architecture augments the accounting of the dependence of Koopman Operator $K(\lambda)$ on the varying eigenvalues λ, by first creating an auxiliary network to model the parametric dependence of the Koopman Operator on the frequency, creating a low-rank model of the intrinsic dynamics. If this explicit frequency dependence is left unaccounted for then deeper models are required to capture the effects of shifting frequency and eigenvalues.

3. Network Architecture

The primary goal of this work is to enable longer-time forecasting of complex dynamical systems while maintaining interpretability and the parsimony of the network. The present work builds upon the network architecture proposed by [11]. The architecture proposed is based on finding Koopman embeddings and evolving them using learned Koopman Operator. The architecture is so constructed as to be able to handle a ubiquitous class of non-linear systems characterized by continuous spectra, as interpretable and compact representation presents novel challenges This work in some sense, is constructing *local linear embeddings*, which also takes into account the previous state of the system. Rather than evolving the dynamics in globally linear embeddings, quasi-global linear embeddings are generated to propagate the dynamics.

The presented architecture employs a Recurrent Neural Network layers for the encoder and decoder part of the network as shown in Fig.2. The current objective of the network is to enable longer-time forecasting and reduce the number of training data needed to train the architecture while maintaining the interpretability and parsimony of the network architecture. In light of the latter objective, the network was modified such as to incorporate the following high-level requirements of the architecture:

(1) *Intrinsic coordinates assisting reconstruction.* Though the architecture is employed as an RNN, the architecture is still needed to satisfy encoding the observables $y = \phi x$, where ϕ is the encoder and $x = \phi^{-1} y$, where ϕ^{-1} is the decoder unit of the architecture. Fig.3 represents this diagrammatically. The loss for this autoencoder architecture is calculated as $||x - \phi^{-1}(\phi(x))||$

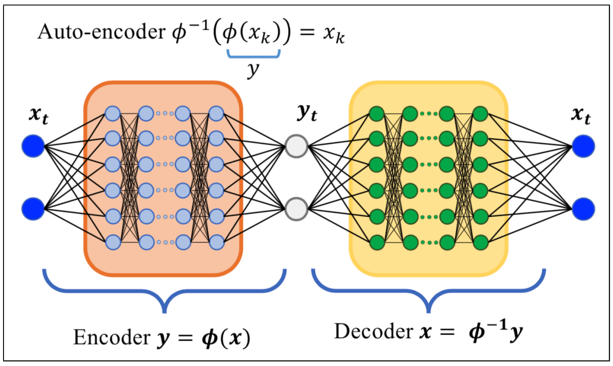

Fig. 3 Diagram representing the auto-encoder part of the network. This network is also implemented during the main network training, accounting for the reconstruction loss.

(2) *Linearity.* The Koopman Operator evolves the dynamics linearly on the identified eigenfunctions, parametrized by the eigenvalues, which are identified using the identified eigenfunctions. Linearization of the dynamics can be achieved by optimizing $||\phi(x_{k+1}) - K(\phi(x))||$ or in a more general way $||\phi(x_{k+m}) - K^m(\phi(x))||$. Fig.4 illustrates the linearity of the operator.

(3) *Dynamics evolution.* The overarching goal of the whole network is accurate future state prediction of the dynamics. Evolution loss can be defined as $||x_{k+1} - \phi^{-1}(K\phi(x_k))||$, which can be more generally specified as $||x_{k+m} - \phi^{-1}(K^m\phi(x_k))||$.

Over here $||\cdot||$ specifies the mean-squared error, average over all the dimensions for all time-steps for a given batch while training the network. All the kernels are l_2 regularized for avoiding over-fitting. One of the other enabling features of the current work is how all the previous described losses for the RNN architecture are computed.

The auxiliary network in the architecture address the continuous spectra, by parametrizing the eigenvalues of K by function $\lambda = \Lambda(y)$, allowing K to vary. The eigenvalues $\lambda_\pm = \mu \pm i\omega$, is used to form a parametrized $K(\mu, \omega)$ Jordan block of the form:

$$K(\mu, \omega) = exp(\mu\Delta t)\begin{bmatrix}\cos(\omega\Delta t) & -\sin(\omega t)\\ \sin(\omega t) & \cos(\omega\Delta t)\end{bmatrix}$$

The addition of the auxiliary network allows the eigenvalues to vary in the phase plan allowing a parsimonious representation of the continuous spectra.

4. Datasets

To demonstrate that the proposed architecture is capable of system dynamics evolution for multiple time steps, with requiring less training data for learning and at the same time maintaining the interpretability and parsimony of the architecture, several examples systems are considered. The considered systems are well-studied and incorporate both discrete and continuous spectra.

4.1 Model with Discrete spectrum

A simple model with a discrete spectrum presents a nice validation system for the proposed architecture, going past the complexities associated with a continuous spectrum. This model has been well studied in the literature [4], with a single fixed point and a discrete eigenvalue spectrum:

$$\dot{x_1} = \mu x_1$$
$$\dot{x_2} = \lambda(x_2 - x_1^2)$$

The model describes a slow manifold given by $x_2 = x_1^2$ for stable eigenvalues of $\lambda < \mu < 0$. Fig.5 represents the model for the $\mu = -0.05$ and $\lambda = -1$. For creating the data set, the earlier prescribed value of λ and μ are used.

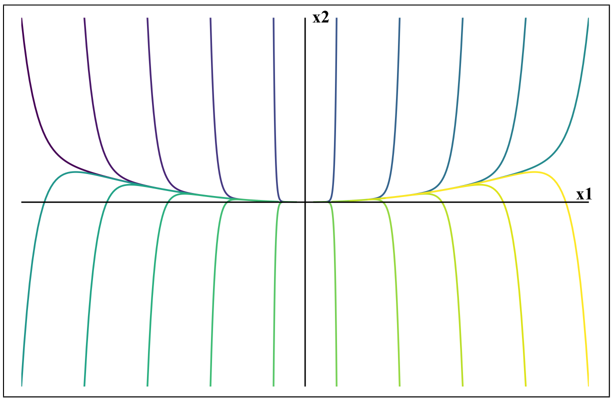

Fig. 5 Diagram representing the dynamics of the discrete case.

4.2 Non-linear Pendulum

One of the most studied models of chaotic systems, non-linear pendulum exhibits continuous eigenvalue spectrum, with increasing energy:

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

Parsimonious representation of non-linear pendulum has been challenging due to the continuous spectra, attributed to the increase in the Hamiltonian energy due to an elongation of the oscillation period. The initial points for the various trajectories for the training dataset were selected so as that the total potential energy of the system, described by $\frac{1}{2}x_2^2 - \cos x_1$ is less than 0.99.

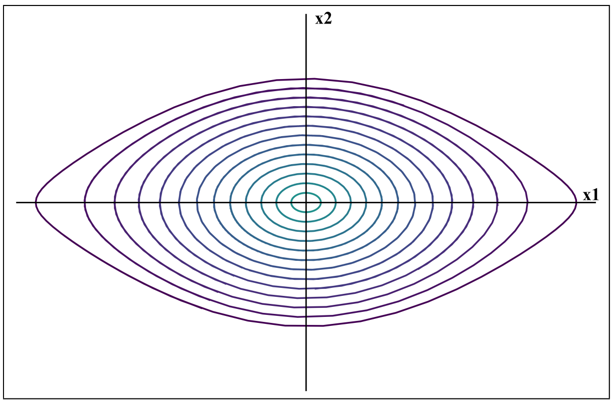

Fig. 6 Diagram representing dynamics of the nonlinear pendulum.

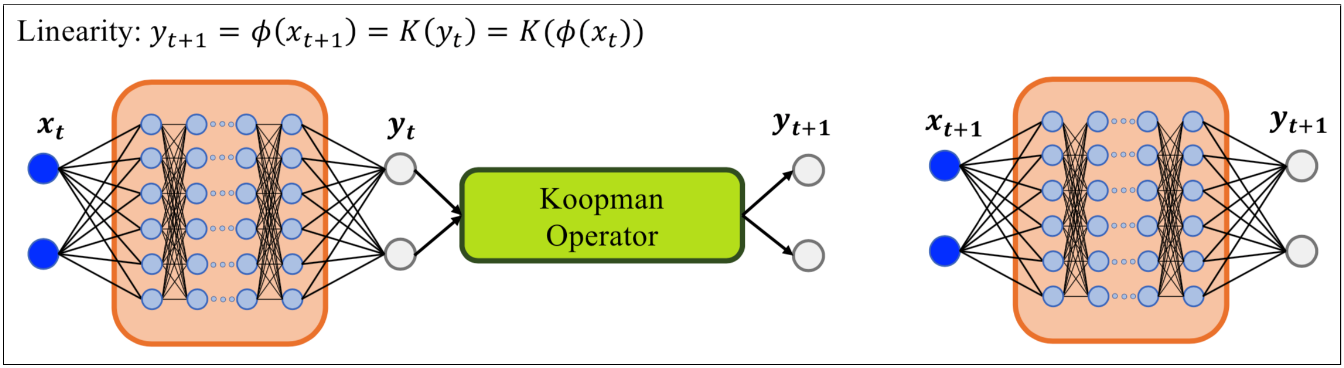

Fig. 4 Diagram representing the linearity reserving part of the network, accounting for the linearization loss in the represented in Fig. 8 a).

4.3 Lorenz System

A simplified model of atmospheric convection, first developed and studied by Edward Lorenz [10], is notable for having rich non-linearity embedded in a seemingly simple system, for certain parameter values and initial conditions. The model which is a system of three differential equation can be described as follows:

$$\begin{aligned}\dot{x_1} &= \sigma(x_2 - x_1),\\ \dot{x_2} &= x_1(\rho - x_3) - x_2,\\ \dot{x_3} &= x_1 x_2 - \beta x_3.\end{aligned}$$

The system describes a two-dimensional fluid flow, which is being uniformly heated from below and cooled from above. The parameters x_1 corresponds to the rate of convection and x_2 and x_3 corresponds to the horizontal and vertical temperature variations respectively. The constants σ, ρ and β corresponds to Prandtl's number, Rayleigh number and a constant related to the layer respectively. Such an equation arises in the modeling of various physical phenomena such as planetary atmospheres, models of lasers, dynamos, etc.

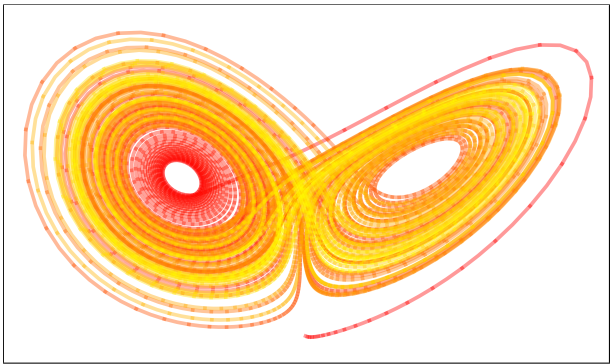

Fig. 7 Diagram representing the dynamics of Lorenz system.

5. Preliminary results

This work is still in its infancy, the current progress is limited. The progress until this point is the construction of the primary network architecture as depicted in Fig. 2, composed of stack of LSTM [5] and densely connected layers. Fig. 8 represents the various loss on training and validation set of the nonlinear pendulum dataset.

6. Future Work

As the current research is still in its infancy, a considerable amount of work needs to be done to see the desired results from the constructed pipeline for achieving longer forecasting of nonlinear system evolution while reducing the amount of data needed to train the model architecture. Future work for current research can be summarized as follows:

(1) Porting the network architecture created to supercomputers to experiment with various higher-parameters, as to obtain best parameter settings which gives the best train to validation loss ratio.

(2) Comparison of the proposed architecture for dynamics forecasting error with methods such as Extended Dynamic Model Decomposition and related variational approach of conformation dynamics (VAC), kernel methods, amongst others, while also considering the training data for each of them.

(3) One of the major addition to improving the forecasting ability of the network is to append a model for enhanced initial state initializer for the LSTM layers employed in the current architecture. Work by [16] has shown improved performance for their architecture by augmenting the initial state initialization.

Above mentioned is a list of work which is planned to be executed for the current research. As for further enhancing the prediction, control, and forecasting of such non-linear systems, the following directions are of particular interest for the community:

(1) *Bifurcation parameter estimation*. Being able to quantify the bifurcation parameters associated with the system is of crucial importance in control of a non-linear system, example fluid flows. The current architecture is defined for only a fixed set of bifurcation parameter and would give erroneous results if the parameters change during the system evolution.

(2) *Automatic detection of required eigenfunctions*. The current approach requires a trial and error based approach for identifying the number of eigenfunctions required to give the best possible fit to the system at hand. Making this process automatic is of crucial interest, to make it truly ubiquitous for dynamics evolution.

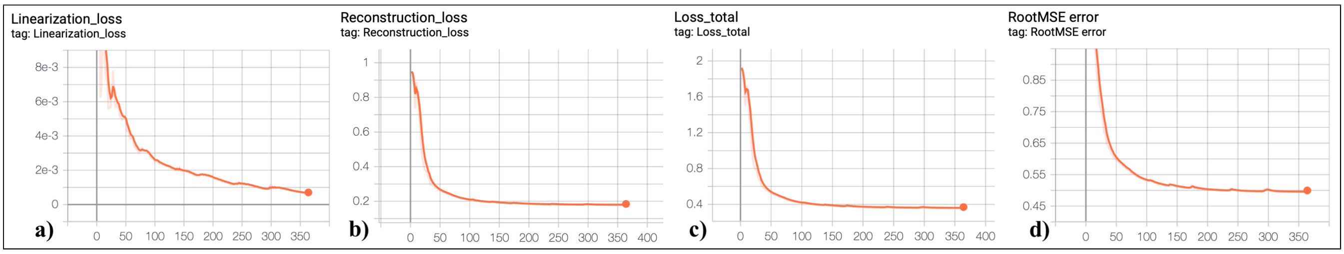

Fig. 8 Plot representing various loss during the training of dynamics of the non-linear pendulum. a) represents the linearization loss, b) represents the reconstruction loss, c) represents the total loss for the network and d) represents the trainig metric for the network.

(3) *Systems with higher complexity.* It is of crucial importance to apply these models to a system of high complexity such as turbulent flows, epidemiology, neurosciences, amongst others.

All of these future directions can be facilitated with more advanced network architecture, infusing the best of physics and applied mathematics.

References

[1] Arbabi, H.: Introduction to Koopman operator theory of dynamical systems, Technical report.
[2] Arbabi, H., Korda, M. and Mezic, I. M.: A data-driven Koopman model predictive control framework for nonlinear flows, Technical report (2018).
[3] Arbabi, H. and Mezic, I. M.: Ergodic theory, Dynamic Mode Decomposition and Computation of Spectral Properties of the Koopman operator, Technical report (2017).
[4] Brunton, S. L., Brunton, B. W., Proctor, J. L. and Kutz, J. N.: Koopman invariant subspaces and finite linear representations of nonlinear dynamical systems for control, *PloS one*, Vol. 11, No. 2, p. e0150171 (2016).
[5] Gers, F. A., Schmidhuber, J. and Cummins, F.: Learning to forget: Continual prediction with LSTM (1999).
[6] Kaiser, E., Kutz, J. N. and Brunton, S. L.: Data-driven discovery of Koopman eigenfunctions for control, Technical report (2018).
[7] Koopman, B. O.: Hamiltonian systems and transformation in Hilbert space, *Proceedings of the National Academy of Sciences of the United States of America*, Vol. 17, No. 5, p. 315 (1931).
[8] Korda, M. and Mezić, I.: Linear predictors for nonlinear dynamical systems: Koopman operator meets model predictive control, *Automatica*, Vol. 93, pp. 149–160 (2018).
[9] Korda, M. and Mezić, I.: On convergence of extended dynamic mode decomposition to the Koopman operator, *Journal of Nonlinear Science*, Vol. 28, No. 2, pp. 687–710 (2018).
[10] Lorenz, E. N.: Deterministic nonperiodic flow, *Journal of the atmospheric sciences*, Vol. 20, No. 2, pp. 130–141 (1963).
[11] Lusch, B., Nathan Kutz, J. and Brunton, S. L.: Deep learning for universal linear embeddings of nonlinear dynamics, Technical report.
[12] Mezić, I.: Spectral properties of dynamical systems, model reduction and decompositions, *Nonlinear Dynamics*, Vol. 41, No. 1-3, pp. 309–325 (2005).
[13] Mezic, I. M.: Analysis of Fluid Flows via Spectral Properties of the Koopman Operator, (online), DOI: 10.1146/annurev-fluid-011212-140652 (2012).
[14] Mezic, I. M.: Koopman Operator Spectrum and Data Analysis, Technical report (2017).
[15] Mikolov, T., Karafiát, M., Burget, L., Černockỳ, J. and Khudanpur, S.: Recurrent neural network based language model, *Eleventh annual conference of the international speech communication association* (2010).
[16] Mohajerin, N. and Waslander, S. L.: Multi-Step Prediction of Dynamic Systems with Recurrent Neural Networks, Technical report (2018).
[17] Schmid, P. J.: Dynamic mode decomposition of numerical and experimental data, *Journal of fluid mechanics*, Vol. 656, pp. 5–28 (2010).