Major Project-II Report

On

# Predicting Non-Linear Systems Through Koopman Based Autoencoder

**Submitted by**

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## Abstract

Conventional approaches to modeling nonlinear dynamical systems face significant challenges in achieving accurate prediction and efficient representation due to inherent complexity and absence of linear structure. Because of their inherent complexity and lack of linear structure, conventional approaches to modeling nonlinear dynamical systems have a difficult time producing accurate predictions and effective representation. The scalability, interpretability, and long-term forecasting capabilities of models applied to dynamical systems in the real world are all significantly impacted by these limitations. By creating a novel Koopman-based autoencoder architecture that effectively blends Koopman operator theory and deep learning techniques, this study tackles these issues. Without requiring explicit knowledge of the governing equations, the suggested framework learns a latent space where the dynamics of nonlinear systems evolve linearly, allowing for both reliable long-term prediction and effective reconstruction.

Our approach uses Transformer architectures and autoencoders to find observable functions that make it easier to apply Koopman operator theory, successfully linearizing intricate nonlinear dynamics while maintaining system properties. This data-driven approach allows for generalization across unknown conditions while improving model interpretability, stability, and forecasting performance. Proton Exchange Membrane Fuel Cell (PEMFC) data and synthetic datasets are used to thoroughly assess our framework's performance on a variety of benchmark systems, such as the Pendulum, Lorenz, Rossler, and Chen systems. With potential applications in a variety of fields, such as fluid dynamics, climate modeling, and renewable energy systems, this work makes a substantial contribution to the field of nonlinear system identification and prediction.

## Declaration

We hereby *declare* that the Major Project-II Report entitled **"Predicting Non-Linear Systems Through Koopman Based Autoencoder"**, which is being submitted to the ***National Institute of Technology Karnataka, Surathkal*** in partial fulfillment of the requirements for the award of the Bachelor of Technology (B.Tech) degree in ***Electrical and Electronics Engineering*** is a *bonafide report of the research work carried out by us.* The material contained in this report has not been submitted to any University or Institution for the award of any degree.

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## Certificate

This is to *certify* that the Major Project-II Report entitled **"Predicting Non-Linear Systems Through Koopman Based Autoencoder "**, submitted by **Gaurangee Parashar** (Register Number: 2110510) and **Rajashri Varadaraj** (Register Number: 2110165) as the record of the project work carried out by them, is *accepted* as the *Major Project-II Report* in partial fulfillment of the requirements for the award of degree of ***Bachelor of Technology(B.Tech)***.

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# Contents

## 1 Introduction

Dynamical systems pervade our natural and engineered world, from weather patterns and fluid flows to chemical reactions and economic cycles. Our natural and artificial environments are replete with dynamic systems, ranging from fluid flows and weather patterns to chemical reactions and economic cycles. States that change over time in accordance with governing equations or rules define these systems. The majority of real-world phenomena display nonlinear dynamics, despite the fact that linear dynamical systems—those whose future states depend linearly on their current states—are comparatively easy to study and forecast. Complex behaviors that are not captured by linear models, such as chaos, bifurcations, limit cycles, and strange attractors, are exhibited by nonlinear systems. Because of these features, studying non-linear systems is both challenging and fascinating.

The mathematical description of a nonlinear dynamical system typically takes the form:

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(\mathbf{x})$$

where $\mathbf{x} \in R^n$ represents the system state, and $\mathbf{F} : R^n \to R^n$ is a nonlinear vector field. Unlike linear systems where $\mathbf{F}(\mathbf{x}) = \mathbf{A}\mathbf{x}$ with $\mathbf{A}$ being a constant matrix, nonlinear functions cannot be represented as simple matrix operations.

This essential distinction leads to a number of difficulties:
(i) **Analytical Intractability:** Nonlinear systems rarely have closed-form solutions, so numerical approximations are required;
(ii) **Computational Cost:** Large amounts of computing power and precise time discretization are frequently needed for numerical simulations;
(iii) **Sensitivity to Initial Conditions:** The hallmark of chaotic systems is prediction, which is made more difficult by the fact that minor perturbations can result in drastically different trajectories;
(iv) **Limited Generalizability:** It is uncommon for solutions or approximations created for one nonlinear system to be transferred to another; and
(v) **Difficulties in Model Identification:** Compared to linear systems, it is much more challenging to infer the governing equations from data.

Linearization around equilibrium points, numerical integration schemes, and approximation techniques like perturbation theory are examples of traditional methods for dealing with nonlinear systems. For high-dimensional systems, these approaches, however, frequently fall short in capturing global dynamics or become unaffordable. The need for increasingly complex frameworks becomes evident as systems become more complex.

Bernard O. Koopman presented a ground-breaking viewpoint for dynamical system analysis in 1931. Koopman suggested looking at the evolution of observable functions, which are scalar functions that translate the state space to real numbers, rather than the evolution of state variables directly. The evolution of these observables over time is described by the Koopman operator, $\mathcal{K}$.

The Koopman framework offers several compelling advantages:

- **Linear Representation:** The linear nature of the Koopman operator enables the application of powerful linear analysis tools.
- **Global Perspective:** Unlike linearization around equilibrium points, the Koopman approach captures global dynamics.

- **Spectral Analysis:** The eigenvalues and eigenfunctions of the Koopman operator provide deep insights into system behavior.
- **Data-Driven Applicability:** Koopman methods can be applied directly to data, without explicit knowledge of governing equations.

Despite these advantages, practical implementation of Koopman theory faces a fundamental challenge: how to identify a suitable finite set of observable functions that effectively capture the system's dynamics? This question has motivated extensive research in recent decades, with approaches ranging from Extended Dynamic Mode Decomposition (EDMD) to various machine learning techniques.

The remainder of this report is organized as follows. Section 1 introduces several classical nonlinear dynamical systems, including the Pendulum, Lorenz, Rossler, and Chen systems, as well as real-world systems that exhibit nonlinear behavior. Section 2 presents the theoretical foundations of Koopman operator theory and explains how it enables linear analysis of nonlinear systems through a transformation of observables. Section 3 surveys the relevant literature, including methods such as Dynamic Mode Decomposition (DMD), Extended DMD (EDMD), and deep learning approaches like Deep Koopman models. Section 4 describes the architecture of our proposed model, which combines autoencoders, a Koopman matrix for linear latent dynamics, and Transformer-based attention mechanisms to enhance representational power. Section 5 outlines the methodology used to generate data, train the network, and define loss functions that enforce reconstruction, forecasting accuracy, and Koopman consistency. Section 6 discusses the results obtained from experiments, evaluates the relevance and limitations of the model, and highlights its generalization capabilities. Section 7 concludes the report with a summary of contributions, and Section 8 outlines potential directions for future research and model improvements.

## 2 Nonlinear Dynamical Systems

Differential equations with state variable evolutions that depend nonlinearly on their current values are known as nonlinear dynamical systems. Nonlinear systems can display rich dynamical phenomena such as multiple equilibria, limit cycles, bifurcations, and chaotic behavior, in contrast to linear systems, which behave relatively simply and adhere to the superposition principle. A nonlinear continuous-time dynamical system's general form is as follows:

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

where $\mathbf{x} \in R^n$ is the state vector and $\mathbf{F} : R^n \rightarrow R^n$ is a nonlinear vector field. One of the distinguishing features of many nonlinear systems is their sensitivity to initial conditions, which frequently takes the form of the "butterfly effect" in chaotic systems where even the smallest perturbations can result in radically different long-term behaviors. This characteristic makes precise forecasting extremely difficult, especially when considering long time horizons.

In this work, we focus on several canonical nonlinear systems that have been extensively studied in the literature and serve as benchmarks for evaluating new methodologies. Each system exhibits unique dynamical properties that challenge traditional modeling approaches and make them ideal candidates for testing our Koopman-based autoencoder framework.

### 2.1 Pendulum System

The nonlinear pendulum represents one of the simplest yet profoundly important nonlinear systems in classical mechanics. It consists of a mass attached to a rigid rod or string, swinging under the influence of gravity. While small oscillations can be approximated by linear models, the full dynamics require nonlinear treatment. The system is governed by:

$$\frac{d^2\theta}{dt^2} + \frac{g}{l}\sin(\theta) + \gamma\frac{d\theta}{dt} = 0 \tag{2}$$

where $\theta$ represents the angular displacement from the vertical position, $g$ is the acceleration due to gravity, $l$ is the length of the pendulum, and $\gamma$ is an optional damping coefficient accounting for friction. For modeling purposes, this second-order differential equation can be reformulated as a system of first-order equations by defining $\omega = \frac{d\theta}{dt}$ as the angular velocity:

$$\frac{d\theta}{dt} = \omega \tag{3}$$

$$\frac{d\omega}{dt} = -\frac{g}{l}\sin(\theta) - \gamma\omega \tag{4}$$

The pendulum system is particularly relevant to our analysis for several reasons:

1. **Variable Nonlinearity**: By adding a nonlinearity whose magnitude changes with displacement, the sine term enables us to test our model in various behavioral regimes.

2. **Space Phase:** A rich phase space structure is produced by the pendulum's unique dynamical regimes, which are oscillatory for low energy and rotational for high energy, and are divided by a homoclinic orbit.

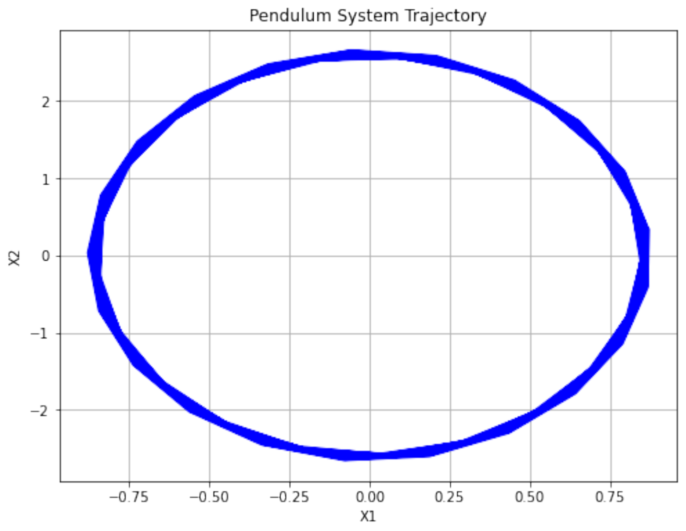


Figure 1: Pendulum system dynamics illustration.

3. **Applicable Relevance:** Pendulum dynamics are used as simplified models for more intricate mechanical systems in a wide range of applications, from robotics to clocks.
4. **"**Analytical Tractability:" The pendulum provides ground truth for confirming numerical methods because, in spite of its nonlinearity, it admits unique analytical solutions in terms of elliptic functions.

To test the model's generalization across different dynamical behaviors, we create training data in our experiments by numerically integrating the pendulum equations across a range of initial conditions, including both oscillatory and rotational regimes.

## 2.2 Lorenz System

Introduced by Edward Lorenz in 1963 while researching atmospheric convection, the Lorenz system has come to represent deterministic chaos. This three-dimensional system is controlled by:

$$\frac{dx}{dt} = \sigma(y - x) \tag{5}$$

$$\frac{dy}{dt} = x(\rho - z) - y \tag{6}$$

$$\frac{dz}{dt} = xy - \beta z \tag{7}$$

where the standard parameter values are $\sigma = 10$ (the Prandtl number), $\rho = 28$ (the Rayleigh number), and $\beta = \frac{8}{3}$ (a geometric factor). With these parameters, the system exhibits chaotic behavior as shown below.

Several characteristics of chaotic dynamical systems are present in the Lorenz system:

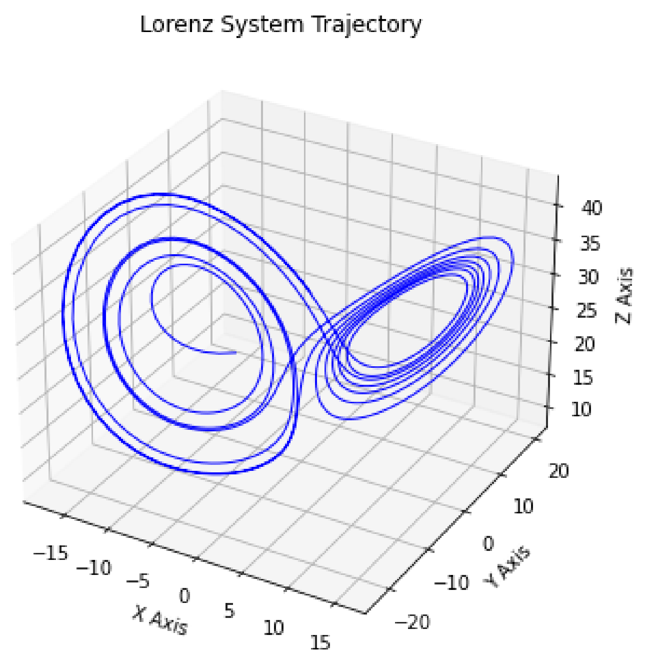


Figure 2: Lorentz system dynamics illustration.

1. **Strange Attractor:** The well-known ”butterfly” or ”figure-eight” pattern in phase space is the result of trajectories convergent to a fractal set with non-integer dimension.

2. **Sensitive Reliance on Starting Conditions:** With a positive Lyapunov exponent of roughly 0.9, nearby trajectories diverge exponentially quickly.

3. **Bounded but Aperiodic Motion:** Trajectories are still limited to a bounded area of phase space in spite of the chaotic behavior.

4. **Deterministic Unpredictability:** Long-term prediction is essentially constrained by the amplification of initial uncertainties, even though it is completely deterministic.

The Lorenz system serves as an excellent test case for our Koopman-based methodology due to the following reasons:

1. **Challenging Prediction Problem:** Accurate long-term forecasting is particularly challenging for conventional methods due to the chaotic nature.

2. **Low-Dimensional Complexity:** It offers a manageable but difficult problem for algorithm development and testing because it only has three dimensions.

3. **Well-Studied Dynamics:** Our approach can be evaluated using benchmarks and insights from extensive prior research.

4. **Continuous Spectrum:** The Koopman operator for the Lorenz system has a continuous spectrum component, testing the approximation capabilities of our finite-dimensional representation.

By successfully modeling the Lorenz system, we demonstrate our approach's ability to capture complex chaotic dynamics in a manner that enables improved prediction compared to conventional techniques.

## 2.3 Rössler System

The Rössler system, proposed by Otto Rössler in 1976, represents another paradigmatic chaotic system, but with simpler mathematical structure than the Lorenz system. It is described by:

$$\frac{dx}{dt} = -y - z \tag{8}$$

$$\frac{dy}{dt} = x + ay \tag{9}$$

$$\frac{dz}{dt} = b + z(x - c) \tag{10}$$

Standard parameter values are $a = 0.2$, $b = 0.2$, and $c = 5.7$, which produce chaotic behavior. Unlike the Lorenz system, which has a more intricate strange attractor, the Rössler system generates a simpler attractor that predominantly lies in a plane with a folded structure in one region.

Key characteristics of the Rössler system include:

1. **Single-Scroll Structure:** The attractor forms a single scroll or funnel in phase space, compared to the double-scroll of the Lorenz attractor.
2. **Simpler Nonlinearity:** The system contains only one nonlinear term ($xz$), making it structurally simpler than the Lorenz system.
3. **Chaotic Behavior:** Despite its relative simplicity, it exhibits chaotic dynamics with sensitivity to initial conditions.
4. **Variable Dimensionality:** By adjusting parameters, the attractor's dimension can be varied, allowing for testing across different complexity levels.

The Rössler system is valuable for our analysis because:

1. **Intermediate Complexity:** It bridges the complexity gap between the pendulum and Lorenz systems.
2. **Different Attractor Topology:** The model's ability to generalize across topologically distinct strange attractors is tested by its different structure.
3. **Sparse Nonlinearity:** The isolated nonlinearity term assesses how well our approach handles particular types of nonlinearity instead of pervasive nonlinearity.
4. **Multiscale Dynamics:** The system exhibits slow drift along with fast oscillations, testing the model's capacity to capture multiscale temporal behavior.

We make sure that our methodology is tested against a variety of chaotic system types with varying structural properties by incorporating the Rössler system into our benchmark suite.

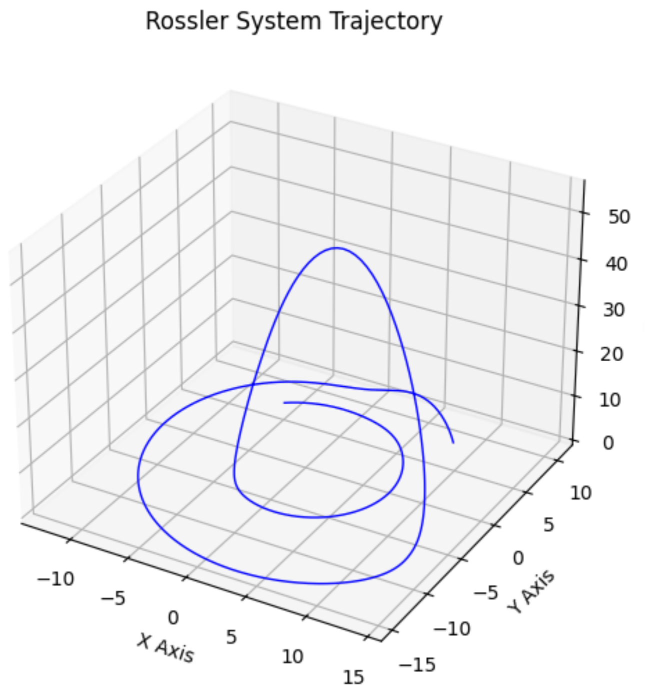


Figure 3: Rossler system dynamics illustration.

## 2.4 Chen System

The Chen system, introduced in 1999, represents a family of chaotic systems that share some structural similarities with the Lorenz system but exhibit distinct dynamical behaviors. The system is defined by:

$$\frac{dx}{dt} = a(y - x) \tag{11}$$
$$\frac{dy}{dt} = (c - a)x - xz + cy \tag{12}$$
$$\frac{dz}{dt} = xy - bz \tag{13}$$

Typical parameter values are $a = 35$, $b = 3$, and $c = 28$, which generate chaotic dynamics. The Chen system is notable for being the first example of a dual system to the Lorenz system, meaning it has similar structure but fundamentally different dynamics.

Distinguishing features of the Chen system include:

1. **Higher Complexity:** Compared to the Lorenz system, it typically displays more complex dynamical behavior; stronger chaos is indicated by higher Lyapunov exponents.
2. **Different Bifurcation Structure:** The routes to chaos differ from those in the Lorenz system.

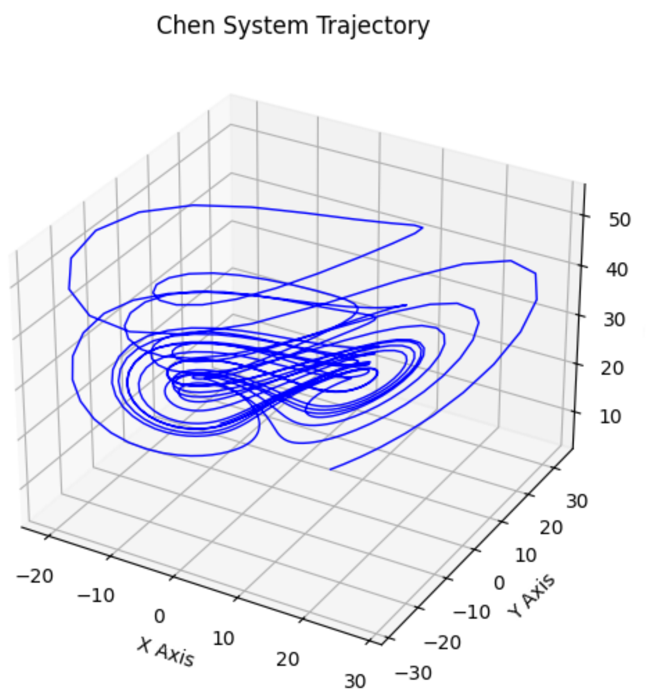


Figure 4: Chen system dynamics illustration.

3. **Anti-Control Properties:** The system has been studied for its properties in anti-control of chaos, where chaos is deliberately enhanced rather than suppressed.

4. **Parameter Sensitivity:** Robustness can be tested by observing how minor adjustments to parameters can result in notable behavioral changes.

The Chen system contributes to our analysis by:

1. **Testing Generalization:** Its structural similarity but dynamical difference from the Lorenz system tests the model's ability to distinguish between superficially similar systems.

2. **Stronger Chaos:** The more pronounced chaotic behavior challenges prediction capabilities more severely.

3. **Different Spectral Properties:** dditional test cases for our method are provided by the different spectral characteristics of the Koopman operator for the Chen system.

4. **Practical Applications:** The Chen system has found applications in secure communication and encryption, connecting our theoretical work to practical applications.

Including the Chen system guarantees that our approach is assessed across a wide range of chaotic behaviors, from the more intense chaos of the Chen system to the milder chaos of the Rössler system.

## 2.5 Synthetically Generated Fuel Cell Data

In order to bridge the gap between theoretical benchmark systems and practical applications, we also take into consideration synthetically generated data that simulates the behavior of PEMFCs. This synthetic dataset incorporates realistic complexities encountered in practical fuel cell operation while representing a controlled environment with known ground truth.

The synthetic PEMFC model incorporates several key factors that are integral to the behavior of a real Proton Exchange Membrane Fuel Cell (PEMFC). These include electrochemical kinetics, where the Butler–Volmer equations describe the relationship between current density and overpotential. Mass transport limitations are also considered, where concentration gradients and diffusion restrictions affect the availability of reactants. Ohmic losses are taken into account, which represent the resistance to electron and ion flow through the components of the system. Temperature effects are included, with variations in temperature impacting reaction rates and transport properties. Additionally, degradation mechanisms are modeled, reflecting the time-dependent performance decay due to catalyst dissolution, membrane thinning, and other related factors.

Coupled nonlinear differential equations are used to represent these processes, and the parameters are calibrated to match typical PEMFC behavior. The synthetic data generation includes multiple components to simulate realistic operation: degradation trajectories, which simulate the long-term performance evolution according to established degradation models; transient responses, where step changes in load capture the dynamic behavior of the system; sensor noise is added to the data to simulate real-world measurement inaccuracies; and several operating conditions.

This synthetic dataset serves several important purposes in our analysis:

1. **Controlled Complexity:** It allows us to test our methodology on a system of intermediate complexity between benchmark systems and fully real-world data.
2. **Ground Truth Availability:** Unlike real-world data, we have access to all state variables and exact system equations for validation.
3. **Domain Relevance:** The dataset connects our theoretical approach to practical energy applications.
4. **Scalability Testing:** The higher dimensionality tests the scalability of our methods to larger systems.

The synthetic dataset for the fuel cell stack voltage was generated by simulating the voltage behavior of a Proton Exchange Membrane Fuel Cell (PEMFC) over time.

The voltage decay was modeled with an exponential decay function, where the initial voltage was set to 50V and the decay rate was 0.02. Random noise with amplitude 0.5 was added to simulate the natural fluctuations that occur in real-world voltage measurements.

$$V(t) = V_0 \cdot e^{-\lambda t} + \eta(t) \tag{14}$$

Where:

- $V(t)$: Voltage at time $t$
- $V_0 = 50$: Nominal (initial) stack voltage

- $\lambda = 0.02$: Exponential decay rate
- $\eta(t) \sim N(0, \sigma^2)$: Additive Gaussian noise with standard deviation $\sigma = 0.5$
- $t$: Time (from 0 to 200 seconds)

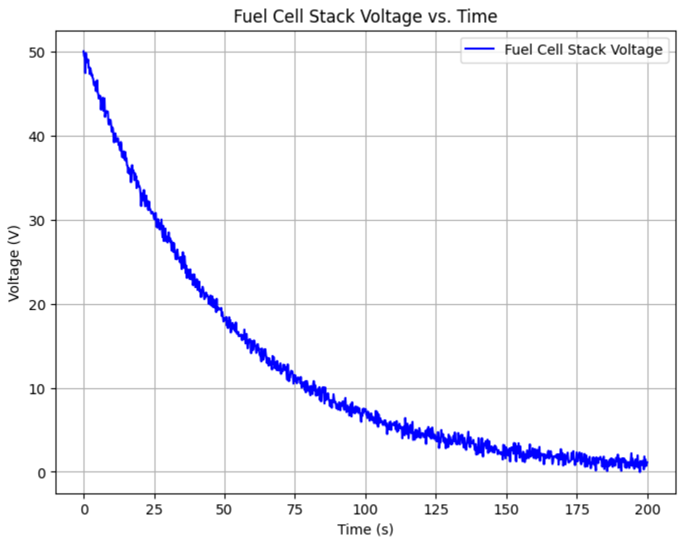


Figure 5: Evolution of Generated Fuel Cell Stack Voltage with time.

By successfully modeling this synthetic PEMFC data, we demonstrate the potential of our approach for real-world engineering applications while maintaining the ability to rigorously validate results against known ground truth.

## 2.6 Real-World Systems: IEEE 2014 Challenge Data

The ultimate objective of our research is to develop methods applicable to real-world systems where governing equations may be unknown or incompletely specified, even though theoretical benchmark systems offer useful test cases with known properties. To this end, we evaluate our approach on the IEEE PHM 2014 Data Challenge dataset, which contains operational data from real Proton Exchange Membrane Fuel Cells (PEMFCs).

### 2.6.1 Dataset Description

The IEEE PHM 2014 Data Challenge dataset consists of time series measurements from a Proton Exchange Membrane Fuel Cell (PEMFC) stack, which was operated under various conditions designed to accelerate degradation. This dataset includes a variety of key variables: the stack voltage, which represents the overall voltage output from the fuel cell stack; individual cell voltages, which capture the voltage measurements from each cell within the stack and reveal cell-to-cell variations; current load, which is the applied electrical load varying according to predefined profiles; temperature measurements, collected from multiple temperature sensors placed at different locations;

coolant flow rate, which measures the operation of the cooling system; pressure readings, which reflect gas pressure at various points in the system; and humidity levels, which are relative humidity measurements for inlet gases. The data was collected from a commercial PEMFC stack over approximately 1,000 hours of operation, with measurements recorded at 1-second intervals during normal operation and at higher frequencies during specific transient events.

#### 2.6.2 Challenges and Relevance

With dozens of measured variables, the IEEE 2014 Challenge Data has a high dimensionality compared to the benchmark systems previously discussed, which is a major challenge that makes it a great test case for our Koopman-based autoencoder approach. Additionally, the dataset captures both fast electrochemical processes, occurring on sub-second timescales, and slow degradation processes that unfold over hundreds of hours, making it a multi-scale dynamic system. Another challenge is partial observability, as not all relevant state variables are directly measured, requiring the inference of hidden states. The real sensor measurements also introduce noise, calibration errors, and other uncertainties, further complicating analysis. Moreover, while general principles of fuel cell operation are well understood, precise governing equations for this specific system are not available, adding to the complexity. Finally, the system exhibits hybrid dynamics, with both continuous evolution and discrete mode changes occurring when operating conditions are altered.

These qualities perfectly complement our Koopman-based approach's advantages. Without the use of explicit governing equations, our data-driven approach enables us to infer system dynamics straight from the data. While the linear Koopman representation allows for stable long-term prediction despite the complexity of the system, the nonlinear encoder can find the right transformations to capture the intricate fuel cell dynamics. Furthermore, effective dimensionality reduction is made possible by the autoencoder architecture's inherent handling of high-dimensional data through effective latent representations.

#### 2.6.3 Application Significance

There are important applications for accurately simulating PEMFC behavior. Optimizing operating conditions through improved predictive models can result in the highest possible energy efficiency. Furthermore, precise prediction of degradation trajectories aids in lifespan estimation and maintenance scheduling, extending the fuel cells' useful life. Another important advantage is early fault detection, which enables preventative measures to be taken before catastrophic failure occurs by identifying emerging faults through deviations from expected behavior. Better models also make it possible to create sophisticated control schemes that optimize fuel cell performance, improving the overall efficiency and dependability of the system.

By applying our methodology to this real-world dataset, we demonstrate its potential for practical impact in energy systems and beyond. The IEEE 2014 Challenge Data provides a stringent test of our approach's ability to handle the complexities encountered in actual engineering systems, effectively bridging the gap between theoretical advances and practical applications.

## 2.7 Synergistic Analysis Across Systems

The diverse collection of systems described above—ranging from the classic pendulum to complex real-world fuel cells—allows us to evaluate our Koopman-based autoencoder approach across a spectrum of complexity and application domains. This comprehensive benchmarking strategy enables several important analyses. First, the scalability of our method is assessed by testing on systems with increasing dimensionality, helping us understand how the method performs as system complexity grows. Additionally, success across diverse systems with different underlying physics demonstrates the generalizability of our approach. Performance across both synthetic and real data with varying noise levels also tests the robustness of the method to uncertainty in real-world measurements.

Furthermore, comparing the learned representations across systems may reveal fundamental structural similarities not immediately apparent from the governing equations, offering insights into the underlying dynamics. Finally, the relationship between system characteristics and achievable prediction horizons is explored through a range of systems with varying degrees of chaotic behavior, providing valuable insights into the limits of prediction in nonlinear dynamical systems.

By means of this methodical assessment, we hope to demonstrate not only how well our method works on particular benchmark problems but also how broadly applicable it is as a general framework for modeling and predicting nonlinear dynamical systems.

## 3 Koopman Operator Theory

Koopman operator theory offers a powerful framework for analyzing nonlinear dynamical systems using linear techniques. The central idea is to shift focus from the evolution of the system state to the evolution of observables — functions that map the system state to scalar or vector quantities. This perspective allows nonlinear dynamics to be studied through the action of a linear, though typically infinite-dimensional, operator.

Consider a discrete-time deterministic dynamical system:

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

where $x_k \in R^n$ represents the state of the system at time $k$, and $f : R^n \to R^n$ is a potentially nonlinear function governing the system dynamics.

Instead of working directly with $x_k$, Koopman theory examines observables $g : R^n \to C$, which are scalar- or vector-valued functions defined on the state space. The Koopman operator $\mathcal{K}$ is defined to act on these observables as:

$$\mathcal{K}g(x) = g(f(x))$$

This means that the Koopman operator advances the observable by composing it with the dynamics. Notably, $\mathcal{K}$ is linear:

$$\mathcal{K}(ag_1 + bg_2) = a\mathcal{K}g_1 + b\mathcal{K}g_2$$

for any scalars $a, b$ and observables $g_1, g_2$, even if $f$ is nonlinear. The cost of this linearity is that $\mathcal{K}$ operates on an infinite-dimensional function space.

A central focus in Koopman theory is on the eigenfunctions of $\mathcal{K}$. Suppose $\phi$ is an eigenfunction of $\mathcal{K}$ with eigenvalue $\lambda$, then:

$$\mathcal{K}\phi(x) = \phi(f(x)) = \lambda\phi(x)$$

This implies that as the system evolves, the eigenfunction evolves linearly:

$$\phi(x_k) = \lambda^k \phi(x_0)$$

The complete dynamics of the system can be expressed in terms of linear evolution in a transformed coordinate space if the observables of the system can be represented as linear combinations of Koopman eigenfunctions, where each eigenfunction has a Koopman mode that maps the eigenfunction space back to the initial state variables.

In practice, since working with the infinite-dimensional Koopman operator is intractable, finite-dimensional approximations are used. This involves selecting a finite set of observables or basis functions $\{g_1, g_2, \ldots, g_d\}$, and approximating the action of $\mathcal{K}$ using a matrix $\mathbf{K} \in C^{d\times d}$. Techniques such as Dynamic Mode Decomposition (DMD), Extended DMD (EDMD), and deep learning approaches like Koopman Autoencoders are commonly employed to compute this finite approximation from data.

The Koopman framework offers several advantages:

- It provides a global linear representation of nonlinear dynamics.
- It is compatible with data-driven methods and modern machine learning.
- Once learned, the linear model can be used for prediction, control, and system identification.

But there are still difficulties. The selection of observables has a significant impact on the approximation's quality. Inadequate observables may lead to non-closure under the Koopman operator, introducing errors. Additionally, computational cost increases with system dimensionality and the complexity of observables.

Neural networks and Koopman theory are combined in recent advances to automatically learn the proper coordinate transformations. A neural encoder in Koopman Autoencoders maps states $x$ to a latent space $z$, where a learned linear operator $\mathbf{K}$ evolves $z$ forward in time. Using the latent variables, a decoder recreates the initial state. End-to-end training efficiently learns an approximate Koopman-invariant subspace by minimizing reconstruction and prediction loss.

In conclusion, by taking into account the evolution of observables, Koopman operator theory makes it possible to apply linear analysis techniques to nonlinear dynamical systems. Despite being theoretically infinite-dimensional, real-world approximations made possible by data and learning offer a potent tool for control, prediction, and modeling. The theoretical and applied aspects of Koopman operator theory have been greatly advanced by scholars like Steven L. Brunton, whose work is based on the foundational insights of Koopman.

## 4 Literature Survey

Through the evolution of observable functions of the state, Koopman operator theory offers a linear (albeit infinite-dimensional) representation of nonlinear dynamical systems. From time-series data, data-driven techniques like Extended DMD (EDMD) and Dynamic Mode Decomposition (DMD) look for finite-dimensional approximations of this operator. Accuracy and interpretability may be limited by the manual selection of observables used in traditional DMD. Recent deep learning techniques, on the other hand, teach neural networks to automatically learn the observables (or coordinate transforms). Yeung *et al.* (2019), for instance, demonstrated that deep neural networks are capable of producing rich dictionaries and higher-fidelity Koopman models for long-term prediction[17]. The Koopman embedding can be found end-to-end by using neural nets, which eliminates the need for manually created features.

Koopman-based learning typically involves three key components: an *encoder* (or embedding) network that maps states $x$ into a latent space $y = \varphi(x)$, a linear operator $K$ governing $y_{k+1} = Ky_k$ in this space, and optionally a *decoder* mapping $y$ back to the original state. Deep models impose losses that enforce linear evolution in the latent space (e.g., regression or spectral losses) and that reconstruct the original states from the latent variables [9, 8]. For instance, Lusch *et al.* (2018) used a modified autoencoder to learn Koopman eigenfunctions: the encoder finds intrinsic coordinates that "globally linearize" the dynamics, and a linear model is fit in that space [8]. Table **??** summarizes representative deep Koopman methodologies.

A major approach is to use *autoencoder*-style networks to learn the Koopman embedding. In this scheme, an encoder neural network $\varphi(x)$ maps the state (or a delay-embedded state) into a latent space, and a decoder $h(y)$ reconstructs the original state. The training losses combine a linear-dynamics error in latent space with a reconstruction error. For example, Lusch *et al.* employed a deep autoencoder that simultaneously learns the Koopman eigenfunctions and a global linear model [8]. Their loss enforces $\varphi(x_{k+1}) \approx K\varphi(x_k)$ while penalizing reconstruction error $x \approx h(\varphi(x))$. The result is a parsimonious latent representation where the nonlinear pendulum and fluid flow dynamics evolve linearly. Similarly, Azencot *et al.* proposed "Koopman Autoencoder" architectures with consistency losses to enforce accurate multi-step forecasting [23].

**Deep Koopman Autoencoders:** Networks that enforce $y_{k+1} = Ky_k$ and learn $\varphi$ and optionally $h$ through backpropagation. For instance, Nayak *et al.* (2024) significantly improves generalization under noisy data [19] by introducing a temporally-consistent KAE (tcKAE) with a regularizer enforcing coherent predictions across time. Choi *et al.* (2024) improve long-term stability [**?**] by augmenting the KAE with an SVD-based eigenvalue loss to maintain the learned Koopman matrix eigenvalues on the unit circle. Some techniques use deep networks to learn a dictionary of observables. For example, LKIS (Learning Koopman Invariant Subspaces), as proposed by Takeishi *et al.* (2017), minimizes the linear regression residual in latent space. They implement the observables $g(x)$ and (if needed) a reconstructor $h(y)$ as neural networks, learning them by minimizing a least-squares loss (RSS) [9]. This yields a set of features spanning a Koopman-invariant subspace, without requiring manual dictionary selection.

**DeepDMD and Variational Embedding:** Deep nets are viewed as general nonlinear dictionaries in other works (e.g., Lusch *et al.* and Yeung *et al.*). Yeung *et al.* (2019) show that deep dictionaries perform significantly better than fixed EDMD bases by explicitly training deep networks to output lifted observables for DMD[17]. To capture complex embeddings, the networks can employ a variety of activations and architectures (ReLU, residual layers, etc.)[8].

Neural DMD frameworks integrate neural nets with the modal (spectral) viewpoint of Koopman theory. In particular, Iwata and Kawahara (2020) propose a *Neural Dynamic Mode Decomposition* (NDMD) that trains an end-to-end network to minimize multi-step prediction error under a spectral model[10]. Their architecture lifts the state via a neural network, performs an eigendecomposition to obtain a linear operator $K$, and then reconstructs and forecasts the state. The key idea is that the network weights are adjusted by backpropagating the forecasting error through the spectral decomposition of $K$[10]. They also extend NDMD to controlled systems by adding an auxiliary network to model nonlinear control inputs, effectively learning a Koopman representation of both dynamics and input terms[10]. This allows the learned model to be used in linear control designs (e.g., LQR) despite original nonlinearity.

Integrating Koopman models with control is the subject of several recent studies. An end-to-end *Deep Koopman Operator with Control* framework is proposed by Shi and Meng (2022). They introduce an auxiliary network to encode state-dependent control inputs and jointly train a neural Koopman embedding and operator using a multi-step (K-step) prediction loss[14]. The output of the control network maintains the latent dynamics linear by acting as a new effective control variable. A learned linear model in latent space that is appropriate for LQR design is the end result. Similar to this, techniques such as DKRCI (Deep Koopman for images) map raw sensory data to a latent space using convolutional encoders. From there, they identify a linear Koopman model from latent state and actions, allowing for control from high-dimensional observations.

Inspired by the success of attention models, recent works have proposed transformer architectures for Koopman embedding. Rana *et al.* (2024) develop a *Transformer-based Koopman Autoencoder* for spatiotemporal PDEs (e.g., the Fisher reaction-diffusion equation)[11]. Their model uses a transformer encoder-decoder to learn global latent coordinates that linearize the dynamics. Extensive experiments show the transformer-KAE can accurately predict multiple PDEs (Fisher, Kuramoto–Sivashinsky, Burgers, etc.) from data alone, outperforming other architectures. This highlights the potential of self-attention to capture complex spatiotemporal patterns within the Koopman framework.

Several works explore alternative network types for improved Koopman learning. For example, Nehma and Tiwari (2024) introduce *Kolmogorov–Arnold Networks* (KANs) as an alternative to standard MLPs for learning Koopman embeddings. They demonstrate on two-body and pendulum problems that KANs train much faster, use far fewer parameters, and achieve slightly better accuracy than MLPs in a deep Koopman framework[12]. These results suggest that certain architectures (e.g., networks inspired by Kolmogorov–Arnold representation) may be especially well-suited for approximating complex observables in Koopman learning.

Deep Koopman methods have been validated on classic benchmark systems. For example, the Lorenz and R"ossler chaotic oscillators are standard testbeds. The LKIS-DMD model of Takeishi *et al.* was explicitly tested on Lorenz-$x$ and R"ossler-$x$ time-series: it produced more accurate multi-step forecasts than standard Hankel DMD or LSTM baselines (Fig.$\tilde{6}$ in their paper)[9]. Lusch *et al.* and others have used the nonlinear pendulum as an example of a system with a continuous spectrum; their deep autoencoder identifies latent coordinates that linearize the pendulum dynamics[8]. Indeed, Nayak *et al.* (2024) report superior long-horizon forecasts on a simple pendulum and on fluid flow data using their tcKAE model[19].

Engineering systems have also been subjected to Deep Koopman methods. Proton-exchange-membrane fuel cells (PEMFCs) are a prominent example. For a 5kilowatt open-cathode PEMFC stack, Huo and Hall (2023–2024) created Koopman-based models. They derived a linear, time-invariant model of the thermal dynamics of the stack [13] using data-driven Koopman identification. By combining this Koopman model with a LQR controller, they demonstrated better thermal management: the Koopman-LQR outperforms a baseline PI controller in terms of output efficiency and temperature variation reduction [13]. The Koopman approach, according to the authors, "smoothly integrates with linear optimal control algorithms, effectively minimizing temperature variations" in the stack [13]. This example demonstrates how data-driven Koopman embeddings can generate precise, low-order linear models appropriate for complex electrochemical systems' real-time control.

Other domains employing Koopman-based models include robotics (e.g., learning linear embeddings of the cart-pole or robotic manipulators via deep Koopman networks[14]), power systems, fluid flows, and even neuroscience. In all cases, the goal is similar: discover latent coordinates in which predictions and control are simplified.

Recent years have seen a proliferation of deep Koopman architectures. Neural-network-based embeddings allow learning Koopman eigenfunctions directly from data, often outperforming classical basis expansions in predictive accuracy and scalability. Key advantages include: automatic feature discovery, compatibility with end-to-end training, and the ability to encode physical constraints (e.g., stability, known symmetries) via specialized losses[17, 8]. Challenges remain: ensuring interpretability of latent coordinates, handling high-dimensional state spaces, and dealing with process noise or unmodeled dynamics. Some works address these by adding noise-robust losses or Bayesian formulations.

In this field, transformer-based and other contemporary architectures are just starting to appear. They can effectively learn global spatiotemporal patterns, according to preliminary evidence (e.g., the Fisher equation study[11]). In the future, attention mechanisms and sequence models (like Koopman-augmented RNNs or GRUs) for time-series forecasting are likely to be more integrated. Additionally promising are hybrid methods that incorporate Koopman embeddings with physics knowledge (such as conservation laws). Last but not least, reliable identification and real-time Koopman model updating as data is gathered are necessary for practical deployment (such as in fuel cells or robotics).

Along with the fundamental advancements in Koopman operator theory, Brunton [1] offers thorough and easily readable lecture notes that serve as a useful starting point for both theorists and practitioners. Building on these theoretical insights, Gadia et al. [2] presented a Koopman-inspired neural network (KoNN) for battery State-of-Charge (SoC) estimation. This network uses an autoencoder architecture customized with a custom loss to predict future SoC across a range of temperatures with remarkable accuracy. In order to predict voltage degradation in PEMFCs, Liu et al. [3] presented a deep learning framework that combines residual CNNs, LSTMs, and random attention mechanisms. In terms of short- and medium-term prediction accuracy, this data-driven model performs noticeably better than conventional prognostics. Moreover, a Transformer-based Koopman autoencoder created especially for linearizing Fisher's reaction-diffusion equation was presented by Rana and Kumari [4]. Their model highlights the increasing convergence of Koopman theory and attention-based deep learning models by showcasing the scalability of Koopman-based approaches to spatiotemporal PDE systems.

In conclusion, deep learning-driven Koopman techniques provide a unified framework for linearizing and managing nonlinear systems. Their applicability has been greatly increased by recent developments in spectral training, deep autoencoders, and attention models. Their potential is demonstrated by case studies such as PEMFCs and benchmarks on chaotic oscillators. We anticipate that these techniques will become more prevalent in the modeling and control of dynamical systems as they develop further.

## 5 Model Architecture

### 5.1 Autoencoders: Nonlinear Representation Learning

Autoencoders are a class of unsupervised neural networks designed to learn efficient, compressed representations of high-dimensional data through self-reconstruction. The core architecture consists of two components: an **encoder** and a **decoder**.

The encoder is responsible for mapping input data from its original, often high-dimensional space, into a lower-dimensional latent space that captures the essential features of the data. The decoder then takes this latent representation and attempts to reconstruct the original input, effectively learning to reverse the compression process.

In the context of dynamical systems such as the Rössler attractor, autoencoders provide a powerful means of uncovering latent dynamics embedded in noisy or nonlinear measurements. Given an input $\mathbf{x}_t \in R^n$ (in our case, $n = 3$ corresponding to the $(x, y, z)$ state of the Rössler system at time $t$), the encoder network $E_\theta$ with parameters $\theta$ transforms it into a latent vector $\mathbf{v}_t \in R^d$:

$$\mathbf{v}_t = E_\theta(\mathbf{x}_t)$$

The decoder $D_\phi$, parameterized by $\phi$, then reconstructs the original signal:

$$\hat{\mathbf{x}}_t = D_\phi(\mathbf{v}_t)$$

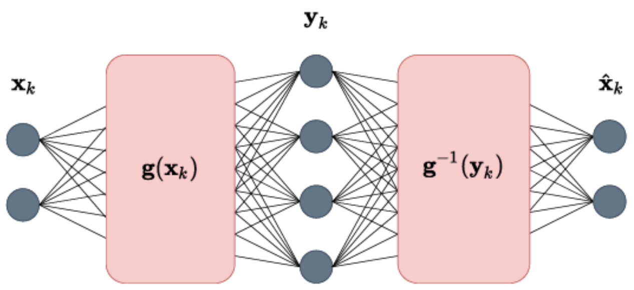


Figure 6: Schematic of an autoencoder

The goal during training is to minimize the difference between the original input $\mathbf{x}_t$ and its reconstruction $\hat{\mathbf{x}}_t$, typically using a loss function such as mean squared error.

In our model, both the encoder and decoder consist of two to three fully connected neural layers, often referred to as dense layers, where each neuron in one layer is connected to every neuron in the next. The encoder uses a ReLU (Rectified Linear Unit) activation in the first layer to introduce nonlinearity and enable the model to learn complex, non-linear transformations of the input. This is followed by a tanh activation in the next layer which serves to constrain the latent representations to a bounded range. Layer normalization is applied to stabilize the output distribution and improve convergence. Additionally, dropout regularization is used to mitigate overfitting by randomly disabling a fraction of the network's neurons in each iteration, thus promoting generalization. The decoder mirrors this structure in reverse, producing a reconstruction $\hat{\mathbf{x}}_t$ from the latent vector $\mathbf{v}_t$.

## 5.2 Koopman Matrix: Linear Dynamics in Latent Space

The Koopman operator provides a linear surrogate model for nonlinear dynamical systems by lifting the system into a latent space where evolution becomes linear. In our Koopman Autoencoder framework, we assume that the latent state $\mathbf{v}_t \in R^d$ evolves according to a learned Koopman matrix $\mathbf{K} \in R^{d\times d}$:

$$\mathbf{v}_{t+1} = \mathbf{K}\mathbf{v}_t$$

This linear relation enables time propagation using repeated matrix multiplication:

$$\mathbf{v}_{t+s} = \mathbf{K}^s\mathbf{v}_t$$

This is a powerful property: rather than requiring a complex recurrent or convolutional model to learn temporal dependencies, we can rely on a fixed, learned linear operator to evolve latent dynamics forward in time.

**Koopman Layer Operation:** During training, the Koopman layer operates on an encoded sequence of latent vectors $\{\mathbf{v}_0, \mathbf{v}_1, \ldots, \mathbf{v}_S\}$ produced by the encoder. It performs the following steps:

1. Take the initial latent state $\mathbf{v}_0 = E_\theta(\mathbf{x}_0)$.
2. Iteratively apply the Koopman matrix to propagate forward:
$$\tilde{\mathbf{v}}_1 = \mathbf{K}\mathbf{v}_0, \quad \tilde{\mathbf{v}}_2 = \mathbf{K}^2\mathbf{v}_0, \quad \ldots, \quad \tilde{\mathbf{v}}_S = \mathbf{K}^S\mathbf{v}_0$$
3. Decode the propagated latent states to obtain predicted future states:
$$\tilde{\mathbf{x}}_t = D_\phi(\tilde{\mathbf{v}}_t)$$

The true shifted latent states $\mathbf{v}_1, \mathbf{v}_2, \ldots$ serve as targets for training the Koopman operator. This enforces the latent space structure to not only reconstruct the original data but also conform to a linear dynamical evolution.

**Koopman Matrix Dimension:** The dimensionality of the Koopman matrix is $d \times d$, where $d$ is the latent dimension. In our implementation for the Rössler system, we typically choose $d = 8$, resulting in a Koopman matrix $\mathbf{K} \in R^{8\times 8}$. This dimension is sufficient to capture the essential nonlinear modes of the Rössler attractor while maintaining computational tractability.

**Experiment on Known Dynamic Systems:** In this section, we present experiments conducted on nonlinear dynamic systems for which the Koopman matrix is known in closed form. Specifically, these are cases where nonlinear systems can be effectively represented linearly in a higher-dimensional space, as outlined by Koopman operator theory. Leveraging this theoretical framework, we designed experiments to validate the performance of the Koopman-inspired neural network architecture in capturing and forecasting system dynamics. These experiments demonstrate the model's ability to approximate the Koopman operator and accurately model system behavior over time.

- Dynamic System 1

  The first system is defined by the following set of differential equations:

$$\dot{x}_1 = \mu x_1 \tag{15}$$
$$\dot{x}_2 = \lambda(x_2 - x_1^2) \tag{16}$$

This system can be linearized in a higher-dimensional space using the following coordinate transformations:

$$y_1 = x_1 \tag{17}$$
$$y_2 = x_2 \tag{18}$$
$$y_3 = x_1^2 \tag{19}$$

Under these transformations, the Koopman operator $\mathbf{K}$ takes the form:

$$\mathbf{K} = \begin{bmatrix} \mu & 0 & 0 \\ 0 & \lambda & -\lambda \\ 0 & 0 & 2\mu \end{bmatrix} \tag{20}$$

- Dynamic System 2

  The second system involves a more complex set of nonlinear dynamics given by:

$$\dot{x}_1 = \mu x_1 \tag{21}$$
$$\dot{x}_2 = \lambda(x_2 - x_1^4 + 2x_1^2) \tag{22}$$

  In this case, the dynamics are linear in a latent space of four dimensions. The corresponding Koopman operator $\mathbf{K}$ is given by:

$$\mathbf{K} = \begin{bmatrix} \mu & 0 & 0 & 0 \\ 0 & \lambda & 0 & 0 \\ 0 & 0 & 2\mu & 0 \\ 0 & 0 & 0 & 4\mu \end{bmatrix} \tag{23}$$

## 5.3 Koopman-based Autoencoder

Here, we describe the architecture and functionality of a Koopman-based Autoencoder, which leverages the Koopman operator for dynamic system prediction and state reconstruction. The model consists of three main components: the encoder network, the Koopman operator, and the decoder network.

- Encoder Network:

  The encoder network is responsible for transforming the original state, denoted as $\mathbf{x}_n$, into an embedding of observables, denoted as $\mathbf{y}_n = g(\mathbf{x}_n)$. This transformation maps the high-dimensional input state into a lower-dimensional latent space, where key dynamical features are captured and represented as observables. The encoder learns this mapping in such a way that it preserves the critical information required for both reconstruction and prediction tasks.

- Prediction with the Koopman Operator:

  Once the state has been encoded into the latent space, prediction is performed using the approximated Koopman operator $\mathbf{K}$. The Koopman operator provides a linear evolution of the system's dynamics in the latent space. Specifically, a linear transformation of the augmented state $\mathbf{y}_n$ is applied to predict the next state $\mathbf{y}_{n+1}$, as follows:

$$\mathbf{y}_{n+1} = \mathbf{K}\mathbf{y}_n$$

  This allows the system to model the temporal evolution of the underlying nonlinear system by capturing its behavior in a linearized form within the latent space, facilitating long-term forecasting and dynamic evolution prediction.

- Decoder Network:

  After the prediction step, the **decoder network** is tasked with reconstructing the original state $\mathbf{x}_n$ from the latent embedding $\mathbf{y}_n$. The decoder learns the inverse transformation $g^{-1}$, which maps the latent state $\mathbf{y}_n$ back to the original high-dimensional space. The reconstructed state $\mathbf{x}'$ is given by:

$$\mathbf{x}' = g^{-1}(\mathbf{y}_n)$$

  The decoder aims to minimize the reconstruction error, ensuring that the model can accurately recreate the system's original state from the latent representation. This process completes the cycle of encoding, predicting, and reconstructing the system's dynamics.

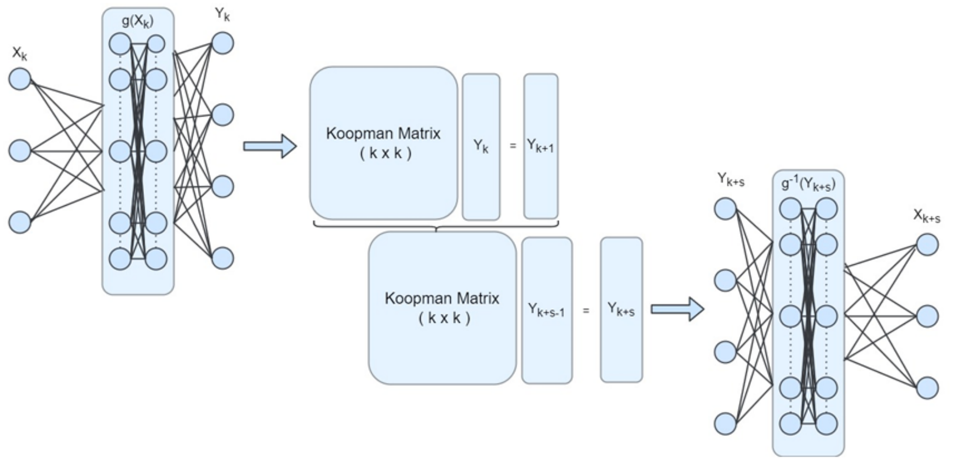


Figure 7: Schematic of a Koopman-based Autoencoder

**Loss Function and Training Objective:** The model is trained by minimizing a composite loss function comprising three components:

1. **Reconstruction Loss:** This term measures the accuracy with which the autoencoder can reconstruct the original input state $\mathbf{x}_t$ from its latent representation. It is defined as the mean squared error (MSE) between the true state and the reconstructed state $\hat{\mathbf{x}}_t$:

$$\mathcal{L}_{\text{rec}} = \|\mathbf{x}_t - \hat{\mathbf{x}}_t\|_{MSE}$$

   Minimizing this loss ensures that the encoder-decoder pair can effectively compress and reconstruct the data, preserving the essential features of the input signal.

2. **Linear Loss:** To promote long-term predictive accuracy, the model is trained to minimize prediction error not just for the next time step but over a sequence of $S$ steps into the future. In the lifted (latent) space, the true future latent states $g(\mathbf{x}_{k+s})$ are compared against the Koopman-propagated predictions $\mathbf{K}^{[s]}g(\mathbf{x}_k)$. This loss is defined as:

$$\mathcal{L}_{\text{lin}} = \frac{1}{S}\sum_{s=1}^{S} \left\| g(\mathbf{x}_{k+s}) - \mathbf{K}^{[s]}g(\mathbf{x}_k) \right\|_{MSE}$$

   This term ensures that the learned Koopman operator captures the linear evolution of the system across multiple future steps in the latent space.

3. **Prediction Loss:** In addition to the latent space, prediction performance is evaluated in the original state space. After applying the Koopman operator in latent space, the predicted state is mapped back to the original space using the decoder. The predicted future state $\tilde{\mathbf{x}}_{k+s}$ is compared to the true state $\mathbf{x}_{k+s}$, and the loss is averaged across all $S$ steps:

$$\mathcal{L}_{\text{pred}} = \frac{1}{S}\sum_{s=1}^{S} \left\| \mathbf{x}_{k+s} - g^{-1}(\mathbf{K}^{[s]}g(\mathbf{x}_k)) \right\|_{MSE}$$

   This component ensures that the model performs accurate long-horizon prediction in the original state space, which is essential for real-world forecasting tasks.

4. **Regularization Loss:** This term penalizes large values in the weight matrix $\mathbf{W}$ to ensure stability and prevent overfitting. Without such a constraint, the model may learn overly complex or unstable transformations. The regularization loss is given by the squared Frobenius norm (or $\ell_2$-norm) of the Koopman matrix:

$$\mathcal{L}_{\text{reg}} = \|\mathbf{W}\|^2$$

   This encourages smoother and more interpretable linear dynamics in the latent space.

These losses are combined into a single loss function, weighted by the hyperparameters $\alpha_1, \alpha_2, \alpha_3, \alpha_4$, as shown below:

$$\mathcal{L}_{\text{total}} = \alpha_1\mathcal{L}_{\text{rec}} + \alpha_2\mathcal{L}_{\text{lin}} + \alpha_3\mathcal{L}_{\text{pred}} + \alpha_4\mathcal{L}_{\text{reg}}$$

Empirical values used in our experiments are:

$$\alpha_1 = 1.0, \quad \alpha_2 = 50.0, \quad \alpha_3 = 10.0, \quad \alpha_4 = 10^{-6}$$

**Visualization and Interpretation:** After training, the model's accuracy is evaluated by plotting the original, reconstructed, and predicted trajectories in 3D. Close alignment of these curves indicates successful modeling of the system's attractor and its dynamics. This visual agreement—especially over multiple future steps—demonstrates both the representational power of the encoder and the predictive capacity of the Koopman operator.

Overall, this architecture combines nonlinear representation learning with linear dynamical modeling to yield a powerful hybrid system capable of reconstructing and forecasting complex chaotic dynamics from time-series data.

## 5.4 Transformers and Attention

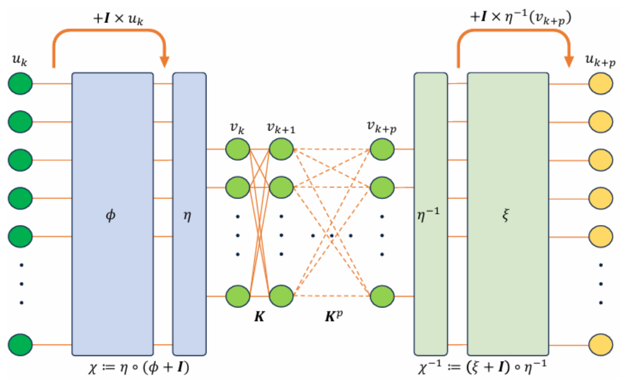
Transformers are a type of deep learning architecture originally introduced for sequence modeling tasks, such as natural language processing. They rely on a mechanism called attention, which allows the model to weigh the importance of different parts of the input sequence when making predictions. Unlike traditional recurrent models, transformers process the entire sequence in parallel, enabling faster training and better handling of long-range dependencies. The self-attention mechanism at the core of transformers helps capture complex relationships within the data by dynamically adjusting how much attention each input element pays to others.

By integrating transformers into the encoder or decoder, the model gains the ability to learn richer and more structured latent representations that better capture the underlying dynamics of the system. This enhanced representation leads to a more accurate approximation of the Koopman operator, which is crucial for modeling linear dynamics in the transformed space. As a result, the model becomes more reliable in making long-term predictions. This integration effectively combines the strengths of both approaches—transformers for capturing complex sequence patterns, and Koopman theory for simplifying nonlinear systems into linear ones in the latent space.

The entire architecture is illustrated in the figure given below. It is composed of three main components: an encoder denoted by $\chi$, a linear dynamics module represented by the Koopman operator $K$, and a decoder $\chi^{-1}$. Both the encoder and decoder consist of two segments.

The encoder comprises an *inner encoder* $\eta$ and an *outer encoder* $\phi + I$, where $I$ is the identity matrix. The inner encoder $\eta$ performs dimensionality reduction and facilitates diagonalization of the system, while the outer encoder applies a coordinate transformation to map the input into a space where linear dynamics apply. Correspondingly, the decoder consists of the inverses of these two components: the *inner decoder* $\eta^{-1}$ and the *outer decoder* $\xi + I$. Residual connections are utilized in both the outer encoder and outer decoder to enhance training stability and information flow.

The function $\phi$, detailed in given figure, includes a Transformer block. This block features a multi-head self-attention mechanism, followed by layer normalization and feedforward neural networks. The transformer processes the input data $u_k$, enabling the model to capture complex temporal dependencies and patterns. Residual connections within the transformer block further support the efficient propagation of information.



$+\boldsymbol{I} \times u_k$
$+\boldsymbol{I} \times \eta^{-1}(v_{k+p})$
$u_k$
$u_{k+p}$
$\phi$
$\eta$
$v_k$
$v_{k+1}$
$v_{k+p}$
$\boldsymbol{K}$
$\boldsymbol{K}^p$
$\eta^{-1}$
$\xi$
$\chi \coloneqq \eta \circ (\phi + \boldsymbol{I})$
$\chi^{-1} \coloneqq (\xi + \boldsymbol{I}) \circ \eta^{-1}$

Figure 8: Schematic of a Koopman-based Autoencoder having an outer encoder/decoder,an inner encoder/decoder and a matrix K

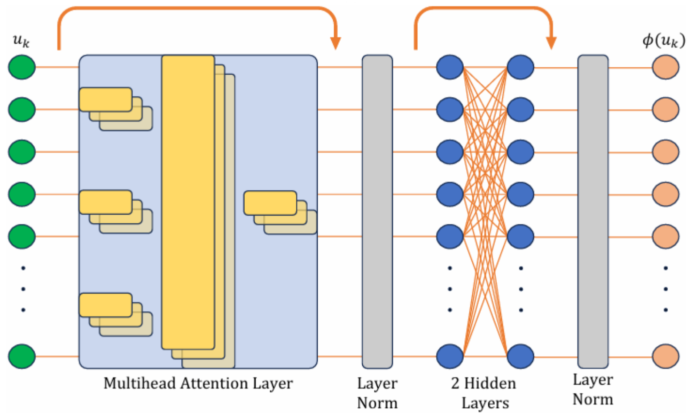


Figure 9: Schematic of a Transformer block that identifies the set of intrinsic coordinates of a linearized dynamical system

**Loss Function and Training Objective:**

Training the network involves a composite loss function composed of five terms, each designed to enforce specific structural and dynamical constraints:

- **Loss 1:** $\|u_k - \chi^{-1}(\chi(u_k))\|$
  Enforces the autoencoder property, ensuring reversibility between the state space and the intrinsic (latent) coordinates.
- **Loss 2:** $\|u_{k+p} - \chi^{-1}(K^p \chi(u_k))\|$
  Promotes accurate multi-step forecasting in the original space by applying the Koopman operator $K$ iteratively.
- **Loss 3:** $\|\chi(u_{k+p}) - K^p \chi(u_k)\|$
  Encourages linear evolution of states in the lifted (latent) space.
- **Loss 4:** $\|u_k - (\xi + I)((\phi + I)(u_k))\|$
  Ensures that the outer encoder-decoder pair adheres to the autoencoder principle, preserving the coordinate transformation and its inverse.
- **Loss 5:** $\|(\phi + I)(u_k) - \eta^{-1}(\eta((\phi + I)(u_k)))\|$
  Focuses on the inner encoder-decoder pair, reinforcing the autoencoding of the lower-dimensional, diagonalized representation.

The total loss $\mathcal{L}_{\text{total}}$ is computed by summing all five losses with equal weight.

## 6 Methodology

The datasets used in this study are derived from various dynamical systems and real-world applications, each designed to test the Koopman Autoencoder model's ability to capture system evolution and predict future states.

### 6.1 Pendulum System

A dataset of 800 training samples, 200 validation samples, and 100 testing samples was generated using the Runge-Kutta method, a widely used numerical integration technique that approximates solutions to ordinary differential equations. Each sample consists of 100 time steps of the pendulum system's evolution. The system's state consists of two dimensions: the angle and angular velocity. The initial conditions for the pendulum were uniformly sampled within the range $[-2.0, 2.0]$ for both the angle and angular velocity. This ensures a diverse set of initial conditions for training, validation, and testing, allowing the model to generalize to a wide range of scenarios.

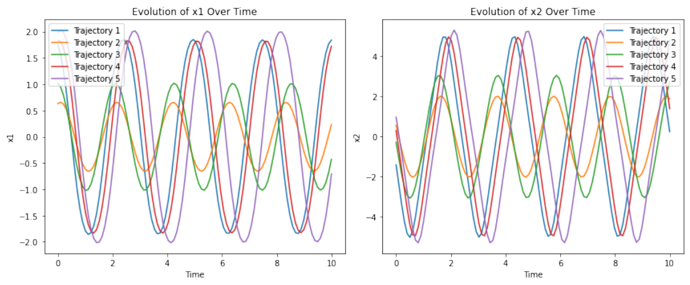


Figure 10: Evolution of state variables x1 and x2 of a pendulum with time

For the koopman based autoencoder, the encoder architecture for this system consists of two hidden layers. The first hidden layer contains 30 neurons, and the second hidden layer also contains 30 neurons, with ReLU (Rectified Linear Unit) activation functions applied to both layers. The output layer of the encoder contains 3 neurons, representing the latent space dimension, which maps the input state of the pendulum into a compressed representation in the latent space. The Koopman matrix used in this model has a size of $3 \times 3$, corresponding to the three latent variables used to represent the system's dynamics.

The decoder architecture mirrors the encoder's structure, with two hidden layers of 30 neurons each, again with ReLU activations, and an output layer containing 2 neurons that represent the reconstructed state of the pendulum (angle and angular velocity). This architecture allows the model to learn both the dynamics of the system and the inverse mapping from the latent space back to the system's state space.

For the transformer-based neural network, the encoder begins with a dense projection layer that maps the 2-dimensional input state of the pendulum to a higher-dimensional embedding space of size 30. This projection is followed by a custom transformer encoder layer, which includes multi-head self-attention with 6 heads and a feedforward network of 30 units. The transformer encoder incorporates layer normalization and dropout for improved training stability and generalization. After processing through the transformer, the output is passed through a linear dense layer with

3 output units, which represents the latent space. This latent space serves as the lifted representation of the input, suitable for linear evolution under the Koopman operator. Thus, the encoder compresses the input trajectory into a 3-dimensional latent space.

The Koopman operator layer is defined as a trainable matrix of size $3 \times 3$, corresponding to the latent space dimension. Given the latent trajectory $Z$, the layer computes a sequence of future latent states by iteratively applying the Koopman matrix. The first element of the trajectory is used as the initial state, and future predictions are obtained by repeated application of the Koopman matrix. The model also keeps track of the true shifted latent states, enabling multi-step loss computation for training.

The decoder architecture mirrors the encoder's structure. It also begins with a dense projection from the 3-dimensional latent space to a 30-dimensional embedding. This is followed by a transformer encoder block identical to the one used in the encoder. After passing through the transformer, the data is mapped back to the original 2-dimensional space (representing the angle and angular velocity of the pendulum) using a final dense layer. This structure allows the decoder to reconstruct both the original and predicted system states from their respective latent representations.

The training process for both these model was conducted over 20 epochs. During each epoch, the model was exposed to the training data, with the objective of minimizing the reconstruction error between the predicted and actual states of the pendulum. After training, the model was evaluated on its ability to predict the pendulum's state 30 time steps into the future.

## 6.2 Lorenz System

For the Lorenz system, a dataset of 800 training samples, 200 validation samples, and 200 testing samples was generated, again using the Runge-Kutta method for numerical integration. Each sample in these datasets consists of 256 time steps, representing the evolution of the system over a sufficiently long period to capture its chaotic behavior. The initial conditions for the systems were sampled uniformly within specific ranges for each system:

- The $x$ and $y$ initial conditions were uniformly sampled from the range $[-20, 20]$,
- The $z$ initial condition was uniformly sampled from the range $[10, 40]$.

These ranges were chosen to ensure that the system's dynamics span a wide region of phase space, capturing both regular and chaotic behaviors.

For the koopman based autoencoder, the encoder architecture for this system consists of two layers. The first layer contains 500 neurons with ReLU activation, and the second layer consists of 32 neurons. The large number of neurons in the first layer allows the encoder to capture the complex relationships in the data, while the smaller second layer helps compress the information into a more manageable latent representation. The Koopman matrix in this case has a size of $32 \times 32$, reflecting the dimensionality of the latent space representation.

The decoder for this model also has two layers: the first layer has 500 neurons with ReLU activation, and the output layer contains 3 neurons, corresponding to the three state variables $x$, $y$, and $z$. This decoder is designed to reconstruct the original state of the system from the latent space representation.

The encoder architecture of the transformer-based autoencoder begins with a dense layer that projects the input into a higher-dimensional space with 500 neurons, using a ReLU activation function to introduce nonlinearity and enable the network to learn complex representations. This is followed by a second dense layer with 32 neurons, which serves to compress the high-dimensional embedding into a compact 32-dimensional latent representation. Additionally, the encoder incorporates a multi-head attention mechanism with a 4 attention heads and 32 key dimensions to model long-range dependencies across time steps in the trajectory data. The attention output is processed with a residual connection and passed through a layer normalization step to stabilize training. Finally, a feedforward MLP network refines the latent features, again followed by a residual connection. This results in a temporally encoded latent representation suitable for linear propagation via the Koopman operator.

The Koopman layer serves as the core component that enables linear evolution of dynamics in the latent space. This layer introduces a trainable Koopman matrix of size $32 \times 32$, consistent with the dimension of the latent space. Given a latent trajectory $Z$, the Koopman operator is applied iteratively to generate future latent states. The first latent state is used as the base input, and subsequent states are predicted via repeated multiplication with the Koopman matrix. The output of this layer includes the original latent sequence, the Koopman-predicted latent sequence $Z_{\text{tilde}}$, and the ground truth latent sequence shifted forward in time, all of which are used for computing multi-step prediction losses during training.

The decoder architecture mirrors the structure of the encoder in reverse, aiming to reconstruct the original state of the system from its Koopman-evolved latent representation. It begins with a dense layer that expands the 32-dimensional latent input into a higher-dimensional representation of 500 neurons with ReLU activation. This allows the decoder to reintroduce the complexity of the original system dynamics. Following this, a final dense layer with 3 output units is used to map the high-dimensional intermediate representation back to the original system's state space, which in this case includes the three state variables $x$, $y$, and $z$. This design enables the full autoencoder pipeline to learn a nonlinear lifting and projection to a space where dynamics can be approximated linearly, and then accurately reconstruct the trajectory back in the original state space.

The training process was conducted over 20 epochs, similar to the pendulum system. The model was trained to minimize the reconstruction error and evaluated on its ability to predict 256 steps into the future, ensuring that the model could generalize to longer-term predictions.

## 6.3 Synthetic Generated Fuel Cell Data

The synthetic dataset for the fuel cell stack voltage was generated by simulating the voltage behavior of a Proton Exchange Membrane Fuel Cell (PEMFC) over time. The voltage decay was modeled with an exponential decay function, where the initial voltage was set to 50V and the decay rate was 0.02. Random noise with amplitude 0.5 was added to simulate the natural fluctuations that occur in real-world voltage measurements.

The time array $t$ was defined from 0 to 200 seconds, with 1000 evenly spaced time points. The voltage values were then normalized to the range $[0, 1]$ for compatibility with machine learning models. This normalization ensures that the voltage data is scaled appropriately for input to the model, allowing the network to focus on learning the temporal patterns without being affected by large variations in the raw voltage values.

The dataset was split into 80% training, 10% validation, and 10% testing. The training, validation, and test data were then reshaped and processed to be compatible with TensorFlow models. The voltage data, originally a 1D sequence, was reshaped into 3D data by repeating the voltage values across three dimensions, simulating a multivariate time-series input. This reshaping ensures that the data is compatible with models trained on multiple features, even though the data is univariate.

The voltage data was then further preprocessed by splitting it into sequences of 256 time steps. These sequences were used to train the model to predict future voltage values based on past observations. The data was normalized by scaling it between the minimum and maximum values from the training set, ensuring consistent scaling across all datasets.

## 6.4 IEEE 2014 Data Challenge Data

The IEEE 2014 Data Challenge dataset focuses on estimating the remaining useful life (RUL) of a Proton Exchange Membrane Fuel Cell (PEMFC). This dataset includes temporal and frequential data from fuel cell stacks under both normal and accelerated aging conditions. The main goal of the dataset is to predict the state of health (SoH) of the fuel cells and estimate their remaining useful life.

The dataset includes multiple variables, with the stack voltage being the primary variable used in this study. The voltage data was first cleaned using the Local Outlier Factor (LOF) method to remove any extreme outliers that could skew the training process. The cleaned voltage data was then normalized using the StandardScaler from scikit-learn, which standardizes the data to have zero mean and unit variance. This preprocessing step ensures that the voltage data is appropriately scaled for machine learning models.

To simulate real-time conditions, the voltage data was downsampled by selecting every 300th data point. This downsampling reduces the size of the dataset, making it more manageable while preserving the overall trends and patterns in the data. The downsampled voltage data was then reshaped into sequences of 256 time steps, ensuring that the model could be trained to predict future states of the system based on past observations.

The sequences were padded to a 3D format by repeating the voltage values across three dimensions, ensuring compatibility with the Koopman Autoencoder model. The dataset was split into 80% training, 10% validation, and 10% testing, and each sequence was reshaped to ensure consistency with the expected input format of the model.

The dataset was then converted into TensorFlow datasets for efficient training. Each batch contains sequences of voltage data, and the model was trained to predict future voltage values based on past observations. The validation dataset was used to evaluate the model's performance during training, ensuring that it could generalize to unseen data.

## 7 Results and discussion

To evaluate the efficacy of the proposed Koopman-based autoencoder models, both qualitative and quantitative methods are employed. Visualization is conducted using **reconstruction plots** and **prediction plots**, which provide insight into the model's ability to reproduce and forecast system dynamics. The **reconstruction plots** illustrate how accurately the decoder can recover the original system states from the latent representation. In contrast, the **prediction plots** demonstrate the model's ability to perform forward forecasting by evolving the latent state using the Koopman operator and decoding it back to the original space.

Quantitative evaluation is carried out by computing three primary metrics: the **reconstruction loss**, which measures the error between the original and reconstructed states; the **prediction loss**, which evaluates the discrepancy between the true future states and the predicted ones; and the **average test loss**, which aggregates performance across the test dataset. Together, these assessments provide a comprehensive understanding of the model's capability to learn, generalize, and forecast the underlying dynamics.

### 7.1 Lorenz System

In all the plots given below, the blue solid lines represent the actual ground truth trajectories, whereas the red solid lines correspond to the outputs generated by the model—either through reconstruction or prediction.

The **koopman based autoencoder** achieved an **average test loss** of **0.4452**, with a **reconstruction loss** of **0.0024** and a **prediction loss** of **0.0443**.

The **transformer based koopman autoencoder** achieved an **average test loss** of **0.513**, with a **reconstruction loss** of **0.0044** and a **prediction loss** of **0.0625**.

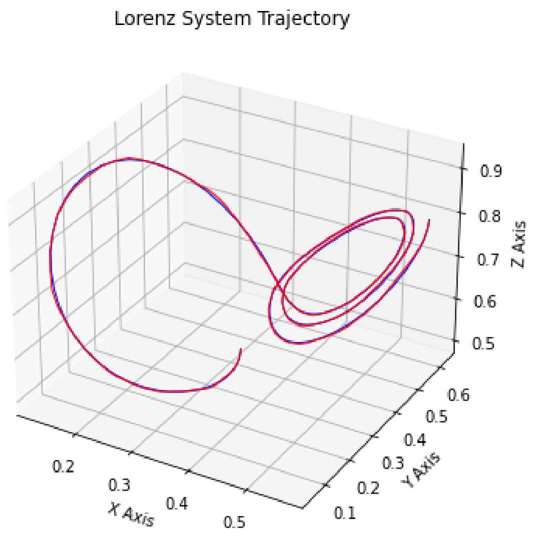


Figure 11: Reconstruction plot for koopman based autoencoder

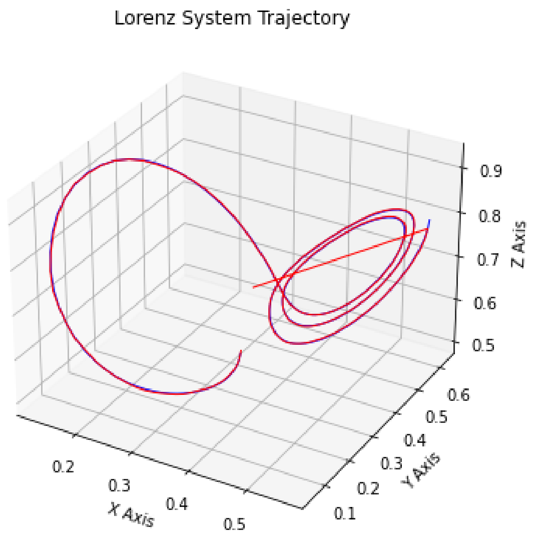


Figure 12: Prediction plot for koopman based autoencoder

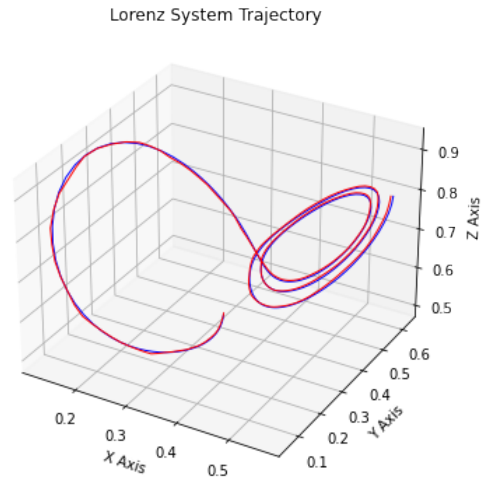


Figure 13: Reconstruction plot for transformer based koopman autoencoder

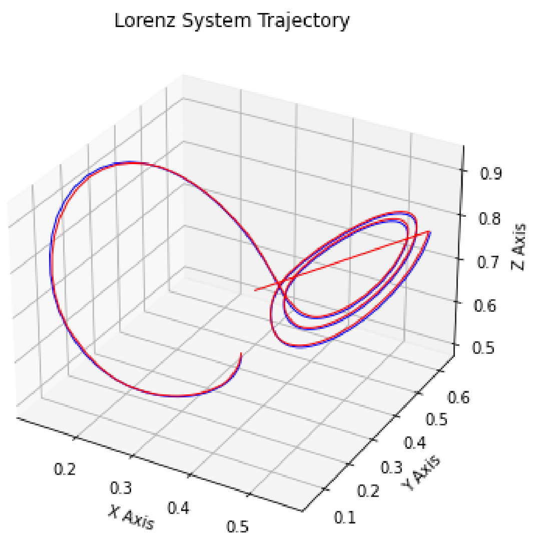


Figure 14: Prediction plot for transformer based koopman autoencoder

## 7.2 Pendulum System

In all the plots given below, the solid lines represent the actual ground truth trajectories, whereas the dotted lines correspond to the outputs generated by the model—either through reconstruction or prediction. Specifically, the green lines denote the first state variable, x1, and the red lines represent the second state variable, x2.

In the context of the **Koopman-based autoencoder**, two plots are presented to illustrate the model's performance. The first plot showcases the reconstruction of the input time-series data over a span of 50 time steps, while the second plot demonstrates the model's prediction capability over a horizon of 30 future time steps.

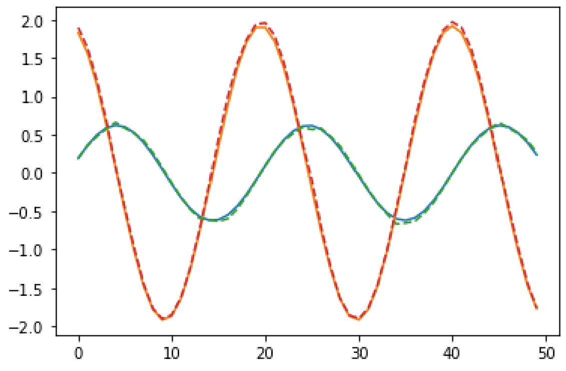


Figure 15: Reconstruction plot

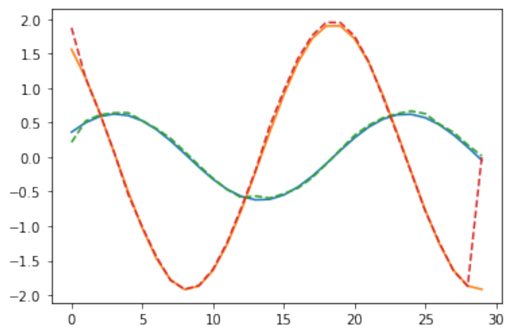


Figure 16: Prediction plot

The two plots shown below pertain to **transformer based koopman autoencoders**. The reconstruction plot shows data for 50 time steps and prediction plot for 30 time steps.

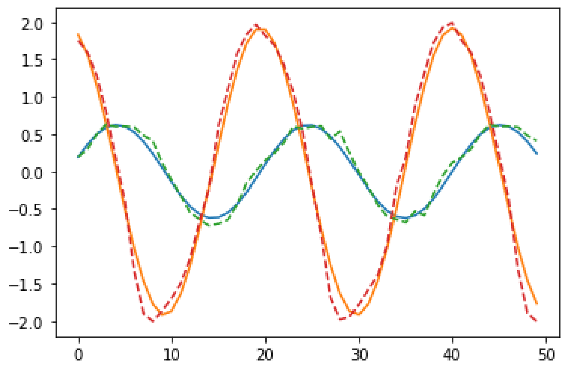


Figure 17: Reconstruction plot

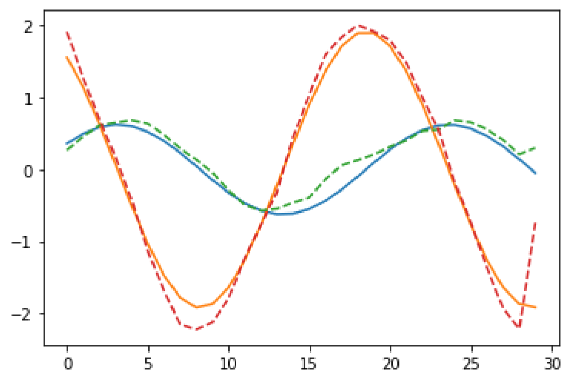


Figure 18: Prediction plot

## 7.3 Chen System

In all the plots given below, the blue solid lines represent the actual ground truth trajectories, whereas the red solid lines correspond to the outputs generated by the model—either through reconstruction or prediction.

The model achieved an **average test loss** of **0.2186**, with a **reconstruction loss** of **0.0008** and a **prediction loss** of **0.02178**.

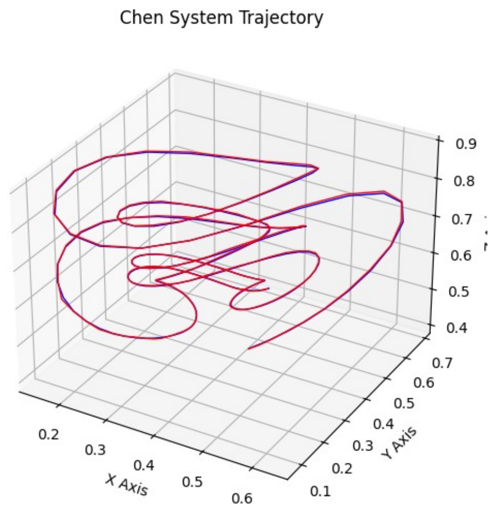


Figure 19: Reconstruction plot

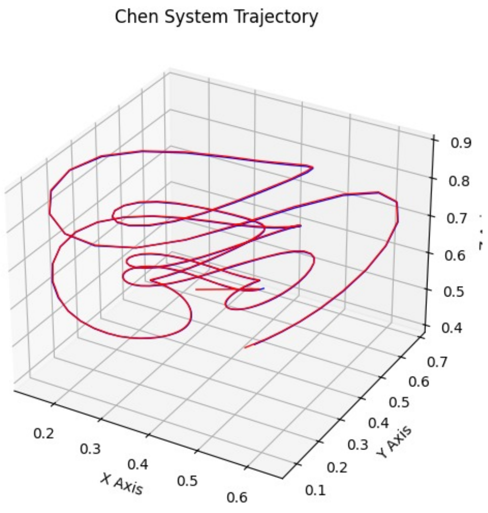


Figure 20: Prediction plot

## 7.4 Rossler System

In all the plots given below, the blue solid lines represent the actual ground truth trajectories, whereas the red solid lines correspond to the outputs generated by the model—either through reconstruction or prediction.

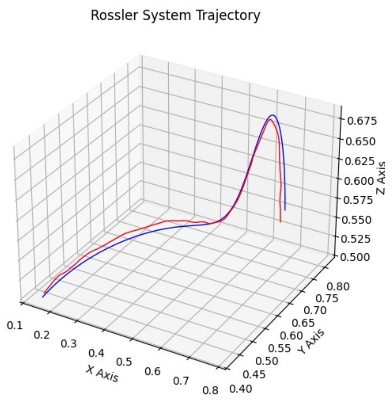


Figure 21: Reconstruction plot

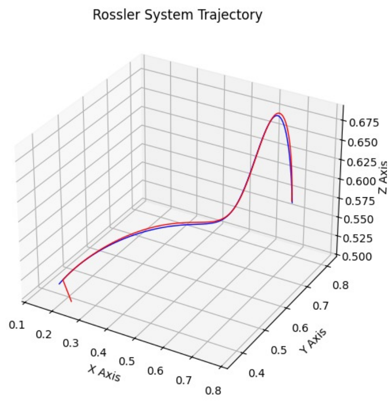


Figure 22: Prediction plot

## 7.5 Synthetic Generated Fuel Cell Data

The model achieved an **average test loss** of **0.5572**, with a **reconstruction loss** of **0.0041** and a **prediction loss** of **0.0553**.

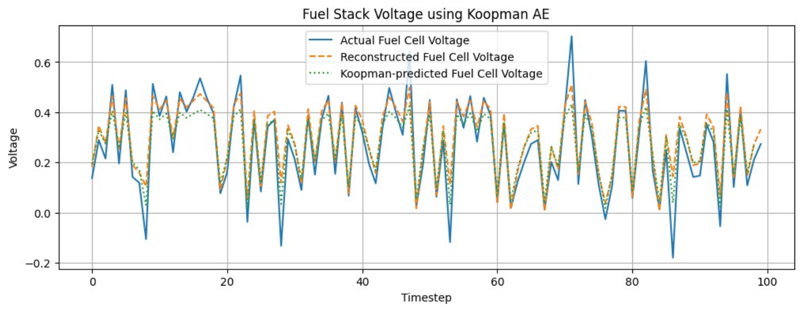


Figure 23: Reconstruction and Prediction plot

## 7.6 IEEE 2014 Data Challenge Data

The model achieved an **average test loss** of **0.2353**, with a **reconstruction loss** of **0.00035** and a **prediction loss** of **0.0235**.

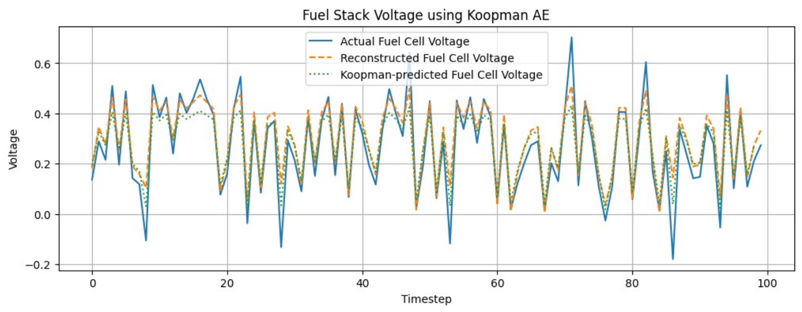


Figure 24: Reconstruction and Prediction plot

## 7.7 Relevance of the results

The Koopman-based autoencoder demonstrates accurate predictions across all the nonlinear systems tested and shows strong generalization to unseen initial conditions. Its ability to capture the underlying dynamics with a simple linear evolution in the latent space makes it both efficient and interpretable. Furthermore, the low reconstruction and prediction errors indicate that the model effectively learns meaningful latent representations that preserve the essential behavior of the original system, even in complex and chaotic regimes.

In contrast, the transformer-based Koopman autoencoder performs noticeably worse for both the pendulum and Lorenz systems. A likely reason for this decline in performance is that the transformer introduces unnecessary model complexity, which can interfere with the Koopman framework's fundamental assumption of linear evolution in the latent space. Although transformers excel at capturing complex temporal dependencies, they do not inherently promote the smooth, linear dynamics that Koopman-based models rely on. As a result, the transformer may learn overly flexible or nonlinear latent representations, making it challenging for the Koopman operator to accurately capture the system's time evolution. This mismatch often leads to less reliable reconstructions and degraded prediction accuracy, especially over extended time horizons.

## 7.8 Limitations of this Project

- **High Data Requirement:** The current model relies heavily on large volumes of training data to learn accurate Koopman embeddings and capture the underlying system dynamics effectively. This can pose a challenge in scenarios where labeled or high-quality time-series data is limited.
- **Interpretability of Koopman Embeddings:** While the Koopman framework aims to linearize nonlinear dynamics in a latent space, the resulting embeddings can be difficult to interpret, especially when combined with deep neural networks. This lack of interpretability limits the model's transparency and hampers insights into the learned dynamics.

- **Computational Overhead:** The use of transformer architectures, known for their self-attention mechanisms and depth, introduces significant computational complexity. This leads to longer training times and higher memory consumption, making it less practical for deployment on resource-constrained devices or large-scale systems.

Future improvements could involve training the model on real-world datasets to assess its robustness and practical utility. Additionally, the incorporation of attention-based refinement blocks may enhance the model's ability to focus on critical temporal features, potentially improving prediction accuracy and stability in challenging dynamical environments.

## 8 Conclusion and Future Scope

In this work, we presented a powerful data-driven framework for modeling nonlinear dynamical systems by integrating Koopman operator theory with deep neural architectures, specifically incorporating Transformer mechanisms into an autoencoder structure. The proposed Koopman-based autoencoder learns a latent representation in which the nonlinear dynamics evolve linearly. Transformer layers improve the model's ability to represent hierarchical structure and long-range temporal dependencies in the data, which is particularly useful for chaotic or multi-scale systems. Our findings on standard dynamical systems, such as the pendulum, Lorenz, Rössler, and Chen attractors, show that the model can generalize across qualitatively distinct regimes while retaining stability and interpretability. Custom loss formulations enforce Koopman consistency in the latent space, allowing the model to learn physically meaningful and computationally efficient dynamics.

The Transformer-based variant did not consistently outperform traditional autoencoder formulations in terms of forecasting loss or generalization, which was contrary to initial expectations. Although attention mechanisms are theoretically advantageous for capturing long-range dependencies, their applicability in this situation seems to vary depending on the system and be influenced by factors such as data scale, model capacity, and training dynamics. This result highlights how difficult it is to learn linear representations for nonlinear systems and implies that, despite their strength, attention-based architectures might not always provide better results when predicting chaotic dynamics. Nonetheless, this experiment provided valuable insights into the interplay between model architecture and dynamical behavior, and it highlights the need for careful architectural tuning and potentially hybridizing attention with other inductive biases. Despite these limitations, the broader contribution of this research remains intact: it demonstrates a principled integration of Koopman operator theory with deep learning, yielding interpretable, physics-informed models for nonlinear systems.

The ability of this research to combine the flexibility of deep learning with traditional dynamical systems theory results in a hybrid approach that is based on physics but scalable through data, which is one of its main contributions. In addition to synthetic systems, we also highlighted real-world applications, such as the thermal management of proton exchange membrane fuel cells (PEMFCs), where Koopman embeddings allow integration with optimal control frameworks like LQR and show improvements over classical controllers in terms of system efficiency and stability.

Looking ahead, this framework can be extended in several impactful directions. Future work should further reduce forecasting loss by refining the architecture and loss design. Other complicated real-world systems, like electric vehicle battery state-of-charge (SoC) estimation, which faces difficulties like sensor noise, temperature fluctuations, and long-term deterioration, can be modeled. Under these less-than-ideal circumstances, the Koopman-based method provides a way to make SoC predictions that are more precise, comprehensible, and controllable. Furthermore, spectral regularization techniques may guarantee long-term stability by constraining Koopman eigenvalues, while real-time adaptation via online learning could improve performance in non-stationary environments. Finally, this work lays the groundwork for future advancements in interpretable, generalizable, and physically consistent models for complex dynamical systems and provides opportunities to apply linear control strategies to otherwise nonlinear domains.

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