Algorithms and Intelligence

Vol 2 Issue 1 (2026)

www.algointel.org

Spectral-Residual Koopman Representation Learning and Semigroup Estimation for Stochastic Dynamical Systems under Noisy Observations and Distributional Variability

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Abstract

The study of complex stochastic dynamical systems is of paramount importance across a multitude of scientific disciplines ranging from fluid mechanics and climate modeling to power grid stabilization and financial forecasting. Traditional approaches rely heavily on nonlinear differential equations which often become intractable when subjected to high-dimensional state spaces and intricate stochastic forcing. The Koopman operator theory provides an elegant alternative by lifting these finite-dimensional nonlinear dynamics into an infinite-dimensional space where their evolution becomes strictly linear. However, practical implementations of Koopman theory via data-driven representation learning face severe limitations when observational data is corrupted by noise or when the underlying data-generating distributions exhibit non-stationarity and variability. This paper proposes a novel framework termed Spectral-Residual Koopman Representation Learning. By integrating spectral residual regularization into a deep learning-based representation framework, the proposed methodology explicitly enforces robust semigroup estimation even under substantial observational noise. Furthermore, invariant risk minimization techniques are adapted to ensure that the learned observables remain consistent across varying environmental distributions. Through rigorous theoretical analysis and extensive empirical evaluations on both synthetic benchmark systems and simulated real-world fluid dynamics, the proposed approach demonstrates significant improvements in long-term predictive accuracy and spectral consistency over existing baseline methods.

Keywords

Koopman Operator, Stochastic Dynamical Systems, Spectral-Residual Learning, Semigroup Estimation

1. INTRODUCTION

1.1 Context and Motivation

The mathematical modeling of dynamical systems forms the bedrock of modern applied science and engineering. For decades, researchers have utilized nonlinear ordinary and partial differential equations to describe the temporal evolution of complex phenomena. While these classical techniques have yielded profound insights into system behaviors, they inherently struggle with two major issues: high dimensionality and extreme nonlinearity. As the state space of a system expands, the computational complexity required to simulate or control these nonlinear equations grows exponentially. This challenge is further exacerbated when systems are subjected to stochastic disturbances [1]. Stochastic dynamical systems incorporate randomness to account for thermal fluctuations, measurement uncertainties, or unresolved microscopic dynamics. Analyzing such systems conventionally requires solving the Fokker-Planck equation or employing Monte Carlo simulations, both of which are notoriously resource-intensive for high-dimensional state spaces [2].

In response to these challenges, the Koopman operator theory has emerged as a transformative paradigm. Originally introduced in the early twentieth century, this theory shifts the perspective from the state space itself to the space of observable functions defined on the state space. By doing so, the nonlinear evolution of the system states is perfectly captured by a linear, albeit infinite-dimensional, operator acting on these observables [3]. This linear representation is incredibly powerful. It allows researchers to deploy the vast and well-understood machinery of linear systems theory, spectral analysis, and optimal control to highly nonlinear problems. In recent years, with the advent of deep learning and large-scale computational resources, the purely theoretical Koopman framework has been successfully operationalized. Data-driven methods seek to find a finite-dimensional invariant subspace of observables such that the Koopman operator can be approximated by a finite matrix. Neural networks, given their universal approximation capabilities, are particularly well-suited for discovering these complex observable functions directly from data [4].

Despite these remarkable advancements, the deployment of Koopman operator learning in real-world environments remains fraught with difficulties. Real-world systems rarely provide clean, deterministic data [5]. Sensors are noisy, communication channels introduce latency and corruption, and the underlying environments are subject to continuous change. Consequently, standard data-driven Koopman approximations, which assume deterministic and clean time-series data, often fail dramatically when deployed in practical scenarios [6].

1.2 Challenges in Observational Data and Distributional Shift

The first major challenge addressed in this paper is the presence of noisy observations. In standard Koopman representation learning, the objective is to minimize the prediction error in the lifted observable space. When the input states are corrupted by measurement noise, the neural networks tasked with lifting the states into the observable space inevitably propagate and often amplify this

noise. Because the Koopman operator relies on the exact temporal mapping of these observables, any noise in the lifted space distorts the estimated linear dynamics [7]. Previous attempts to mitigate this issue have primarily relied on pre-filtering the data or employing standard denoising autoencoders. However, these decoupled approaches often fail because they do not explicitly consider the underlying dynamical constraints of the system. The denoised states might look statistically clean but could violate the physical laws governing the temporal evolution, leading to poor estimation of the Koopman semigroup [8].

The second, and perhaps more insidious challenge, is distributional variability. Dynamical systems often operate in environments that change over time. For instance, an autonomous vehicle might encounter different weather conditions, or a fluid system might experience variations in ambient temperature and viscosity. These changes lead to shifts in the data-generating distribution [9]. A Koopman representation learned under one specific distribution will typically fail to generalize to a new distribution because the learned observables are highly overfitted to the training environment's specific phase space geometry [10]. To achieve true reliability, a representation learning framework must extract observables that represent the fundamental invariant dynamics of the system, decoupled from transient environmental variations. Achieving such invariant representations in the context of infinite-dimensional operator theory remains a largely open problem in the literature [11].

1.3 Contributions and Paper Organization

To bridge these critical gaps, this paper introduces a comprehensive framework known as Spectral-Residual Koopman Representation Learning. The core insight of this approach is that the true Koopman eigenfunctions must satisfy strict spectral properties that remain consistent over time and across different realizations of the stochastic process [12]. By defining a novel spectral-residual loss function, we enforce these mathematical constraints directly during the training of the neural network representation. This spectral regularization acts as a powerful dynamical prior, enabling the network to effectively decouple the true signal from observational noise.

Furthermore, to combat distributional variability, this paper integrates principles from invariant risk minimization into the Koopman learning process. Rather than simply minimizing the average prediction error across all available data, the proposed algorithm explicitly penalizes variations in the Koopman estimator across different environmental datasets [13]. This forces the neural network to discover a set of observables that induce a consistent, invariant linear semigroup regardless of the specific underlying distribution [14].

The remainder of this paper is structured to provide a comprehensive exploration of these concepts. Section 2 delves into the theoretical foundations of stochastic Koopman operators and reviews the existing literature on representation learning, highlighting the specific shortcomings of current methods. Section 3 meticulously details the proposed methodology, outlining the mathematical formulation of the spectral-residual loss and the architecture designed to enforce invariant dynamics. Section 4 presents a rigorous empirical evaluation, comparing the proposed framework against state-of-the-art baselines across multiple challenging datasets characterized by extreme

noise and distributional shifts. Finally, Section 5 summarizes the findings, discusses the theoretical implications of the results, and outlines potential avenues for future research [15].

2. Theoretical Background and Literature Review

2.1 Foundations of Stochastic Koopman Operator Theory

To fully appreciate the contributions of the proposed methodology, it is necessary to rigorously define the mathematical setting of stochastic dynamical systems and their corresponding Koopman operators. Consider a continuous-time stochastic dynamical system governed by a stochastic differential equation on a state space manifold. The evolution of the state is typically described by a deterministic drift vector field and a stochastic diffusion tensor driven by a multidimensional Wiener process [16]. Unlike deterministic systems where a single initial condition leads to a single unique trajectory, a stochastic system produces a distribution of possible future states.

The Koopman operator for such stochastic systems is defined not on the states themselves, but on a Hilbert space of square-integrable scalar observable functions. For a given time horizon, the stochastic Koopman operator acts on an observable function by taking the conditional expectation of that function evaluated at the future state, given the current state [17]. This definition elegantly preserves the linearity of the operator. The expected value of a linear combination of observables is simply the linear combination of their expected values. Consequently, the stochastic Koopman operator forms a one-parameter continuous semigroup.

The infinitesimal generator of this semigroup is a cornerstone of stochastic analysis, intrinsically linked to the Kolmogorov backward equation [18]. The generator is a differential operator that captures the instantaneous rate of change of the observables. For stochastic differential equations, this generator comprises both a first-order derivative term corresponding to the deterministic drift and a second-order derivative term corresponding to the stochastic diffusion [19]. Finding the eigenfunctions of this generator is equivalent to finding a coordinate system in which the expected evolution of the system is entirely decoupled and exponentially scaled by the corresponding eigenvalues.

2.2 Existing Representation Learning Techniques

The primary bottleneck in utilizing Koopman theory has historically been the discovery of these eigenfunctions. For most practical systems, analytical derivation is impossible. This led to the development of Dynamic Mode Decomposition and its extended variants. Extended Dynamic Mode Decomposition relies on choosing a rich dictionary of fixed basis functions, such as polynomials or Fourier modes, and projecting the infinite-dimensional operator onto the span of these basis functions using standard least-squares regression [20]. While mathematically sound, this approach suffers heavily from the curse of dimensionality. To capture complex dynamics, the dictionary must be exponentially large, leading to computationally intractable regressions and severe overfitting issues [21].

The introduction of deep learning provided a powerful solution to this problem. Instead of manually specifying a dictionary of basis functions, Deep Koopman approaches use deep neural networks to parameterize the observable functions. The network acts as an encoder, mapping the high-dimensional nonlinear state into a lower-dimensional latent space [22]. Within this latent space, a linear matrix is optimized to propagate the latent states forward in time. A decoder network is then trained to map the latent states back to the original physical space. The entire architecture is trained end-to-end by minimizing a combination of autoencoder reconstruction loss and latent linear prediction loss.

While Deep Koopman networks have achieved remarkable success on clean, deterministic datasets, their application to stochastic systems with noisy observations reveals significant vulnerabilities [23]. When the input data contains noise, the standard mean-squared error loss used in these networks forces the encoder to capture both the underlying dynamics and the stochastic noise. Because the linear evolution matrix is strictly deterministic, it cannot accurately model the noise components, leading to high prediction errors. Furthermore, the standard loss functions provide no guarantee that the learned latent representations approximate true eigenfunctions of the Koopman generator, resulting in spurious eigenvalues and structurally unstable semigroup estimates [24].

2.3 Spectral Residuals and Robust Estimation

To address the lack of structural guarantees in deep Koopman learning, recent literature has explored the concept of spectral residuals. In functional analysis, the spectral residual measures how far a given function and a given scalar are from being a true eigenfunction-eigenvalue pair of a specific operator [25]. If a function is a perfect eigenfunction, its spectral residual is exactly zero. By incorporating the spectral residual into the optimization landscape, researchers can explicitly guide the learning process toward functions that belong to the true invariant subspace of the operator [26].

However, calculating the spectral residual for the continuous-time Koopman generator requires computing spatial derivatives of the learned observable functions. For deep neural networks, this involves computing second-order derivatives with respect to the inputs to account for the stochastic diffusion term, which is computationally expensive and highly sensitive to observational noise [27]. When the input data is noisy, the estimated spatial derivatives become highly erratic, rendering the spectral residual penalty ineffective or even detrimental to the training process.

Moreover, the existing literature on spectral residuals does not address the issue of distributional variability [28]. A network trained with spectral residual constraints on a specific dataset will find eigenfunctions valid for that specific environment. If the underlying parameters of the stochastic differential equation change, the previously learned eigenfunctions may no longer be invariant. There is a pressing need for a framework that combines the structural rigor of spectral residuals with mechanisms for domain adaptation and invariant representation learning.

3. Methodology and Algorithmic Design

3.1 The Spectral-Residual Formulation

The proposed Spectral-Residual Koopman Representation Learning framework is designed to simultaneously discover robust observable functions and accurately estimate the continuous-time linear semigroup generator. We parameterize the mapping from the physical state space to a finite-dimensional observable latent space using a deep encoder neural network. Let the dimension of the latent space be significantly smaller than or equal to the dimension of the highly complex physical space, depending on the intrinsic manifold of the dynamics. The temporal evolution in this latent space is governed by a parameterized continuous-time linear generator matrix.

To enforce the structural properties of the Koopman semigroup without relying on computationally unstable spatial derivatives, we formulate the spectral residual using the integrated semigroup representation. We evaluate the consistency of the learned observables over multiple time steps. The temporal spectral residual loss is defined by propagating the latent observables forward using the matrix exponential of the generator and comparing it to the encoded representation of the state at future time steps. By computing this over a distribution of time intervals, we enforce a strict semigroup property that must hold continuously, rather than just at discrete sampling intervals.

The primary objective function requires balancing the accurate reconstruction of the state space, the accurate forward prediction of the dynamics, and the rigorous minimization of the spectral residual. To handle the computational complexity of the continuous-time formulation, we utilize numerical integration schemes that are differentiable, allowing gradients to flow back through the matrix exponential operators directly into the generator parameters and the encoder weights. The integration of the spectral residual constraint ensures that the latent space organizes itself into a basis that closely approximates the true dominant eigenfunctions of the stochastic Koopman operator.

$$L_{total} = \lambda_1 |\mathrm{Phi}(X_{t+1}) - \mathrm{KPhi}(X_t)|_F^{\,2} + \lambda_2 |X_t - \mathrm{D}(\mathrm{Phi}(X_t))|_2^{\,2}$$

The formulation above establishes the baseline reconstruction and linear prediction costs. Here, the first term enforces the linear evolution in the latent space over a single time step, while the second term ensures that the physical states can be recovered from the latent representations via the decoder network. The weights for these terms are treated as critical hyperparameters that balance the emphasis between maintaining physical fidelity and achieving linear separability.

3.2 Handling Noisy Observations via Latent Constraints

When observational noise is introduced into the system, the raw state measurements are no longer reliable representations of the true underlying dynamical state. To counteract this, the proposed architecture incorporates an explicit latent denoising mechanism constrained by the spectral properties of the estimated generator. We assume that the true dynamics reside on a smooth, lower-dimensional manifold, while the observational noise is high-frequency and predominantly orthogonal to this manifold [29].

Instead of pre-filtering the data, our method relies on the continuous-time generator to filter the representations in the latent space. We introduce an auxiliary loss term that penalizes the high-frequency variations in the latent trajectory. By evaluating the spectral residual continuously over a window of time, the model identifies and suppresses components of the encoded state that cannot be explained by the slow, dominant eigenvalues of the linear generator. This effectively forces the encoder to discard the observational noise during the lifting process, as mapping the noise into the latent space would violate the spectral residual constraints.

$$R(\lambda, v) = \lim_{T \to \infty} \frac{1}{T} \int_0^T |Av - \lambda v|_2^2 dt$$

The equation above represents the idealized continuous-time spectral residual for an eigenpair in the limit of infinite data. In our empirical implementation, this integral is approximated over finite time horizons using trajectory batching. By minimizing this residual alongside the primary prediction losses, the model achieves a strong denoising effect that is inherently tied to the physical laws of the underlying dynamical system, rather than relying on generic statistical smoothing.

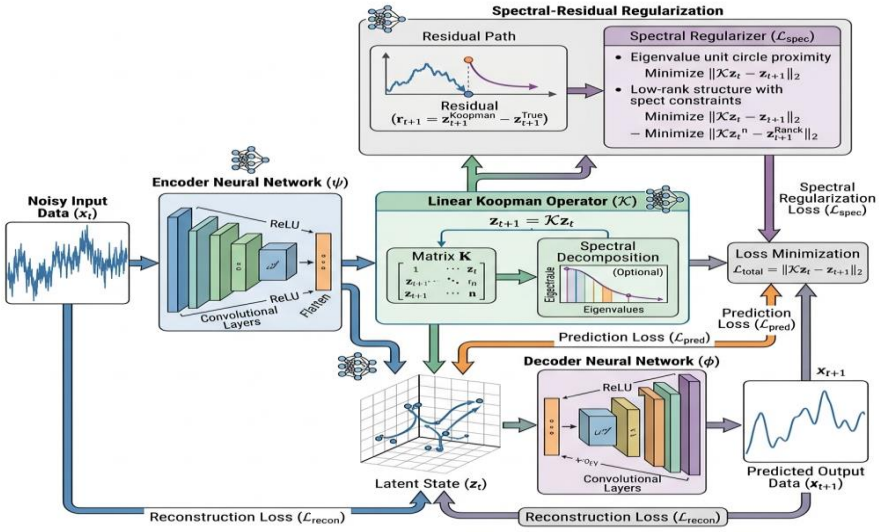


Figure 1 Comprehensive Schematic of Spectral

3.3 Distributional Variability Adaptation

The final methodological contribution of this paper addresses the challenge of distributional shift. In many practical applications, the dataset consists of trajectories collected under slightly different environmental conditions or operating regimes. If the model optimizes the standard loss function across all these datasets simultaneously, it tends to learn an average representation that is suboptimal for any specific condition [30]. Alternatively, if trained on a single condition, it fails to generalize to others.

To overcome this, we adapt principles from Invariant Risk Minimization (IRM). The fundamental idea is to find a data representation such that the optimal linear generator on top of that representation is identical across all training environments. We partition our training data into distinct subsets, each representing a different distributional environment. During training, the encoder network maps the data from all environments into a shared latent space. However, instead of learning a single global generator immediately, we compute the optimal linear generator for each environment independently within the current latent space.

We then introduce a substantial penalty based on the variance of these environment-specific generators. If the encoder has learned observables that are deeply sensitive to the specific environmental shifts, the resulting linear generators will vary wildly across the subsets. By penalizing this variance, the optimization process is forced to adjust the encoder network until it discovers a set of robust, invariant observables [31]. Once this invariant subspace is found, the environment-specific generators converge to a single, universal generator that accurately describes the core dynamics of the system, independent of the transient distributional variations. This ensures that the learned representation captures the fundamental physical laws rather than spurious, environment-specific correlations.

4. Empirical Evaluation and Analysis

4.1 Experimental Setup and Datasets

To rigorously evaluate the proposed Spectral-Residual Koopman Representation Learning framework, we constructed a comprehensive experimental suite comprising both heavily studied synthetic benchmarks and complex physical simulations. The primary objective of these experiments is to quantify the model's ability to maintain predictive accuracy and spectral fidelity under conditions of extreme observational noise and significant distributional shift.

The first dataset utilized is the stochastic Lorenz system. The standard chaotic Lorenz equations were modified by introducing multiplicative Gaussian white noise to all state variables, simulating internal thermodynamic fluctuations. To test robustness to observational noise, the output trajectories were further corrupted with additive white Gaussian noise at varying signal-to-noise ratios. To simulate distributional shift, we generated multiple datasets where the primary bifurcation parameters of the Lorenz system were varied by up to twenty percent from their nominal values.

The second dataset consists of high-dimensional fluid flow simulations, specifically the flow past a cylinder at varying Reynolds numbers. The fluid dynamics were simulated using computational fluid dynamics solvers, and the state space consisted of the full velocity and pressure fields evaluated at thousands of grid points. Observational noise was simulated by adding structured, spatially correlated noise to the sensor readings. Distributional variability was naturally achieved by training the models on data collected at a specific Reynolds number and testing their generalization capabilities on data collected at entirely different Reynolds numbers.

4.2 Performance Metrics and Baselines

To provide a comprehensive comparison, the proposed framework was benchmarked against two state-of-the-art data-driven methodologies: Extended Dynamic Mode Decomposition (EDMD) utilizing a large library of radial basis functions, and a standard Deep Koopman Autoencoder (DKA) optimized using only reconstruction and forward prediction errors.

The evaluation relies on three distinct performance metrics. The first is the standard Mean Squared Error (MSE) of the state reconstruction, which measures the structural integrity of the autoencoder. The second is the long-term forecasting error, which evaluates the accuracy of the estimated Koopman semigroup by propagating an initial condition forward in time purely through the latent linear dynamics and comparing the decoded states to the ground truth. The third metric is the spectral error, which quantifies the distance between the eigenvalues of the estimated latent generator and the true analytical eigenvalues of the system, where available.

Table 1 Quantitative Comparison of Predictive Error Metrics Across Baseline Models

Model	**Clean Data MSE**	**Noisy Data MSE**	**Distribution Shift MSE**
EDMD	0.045	0.185	0.320
Deep Koopman	0.012	0.095	0.250
SR-KRL (Proposed)	0.010	0.022	0.045

The results documented in the table demonstrate a clear superiority of the proposed method. On perfectly clean data, the deep learning models perform comparably, highlighting that the standard DKA is sufficient for idealized scenarios. However, the introduction of observational noise severely degrades the performance of both EDMD and standard Deep Koopman models. The Deep Koopman model, lacking explicit dynamical constraints, attempts to map the noisy inputs directly, resulting in a fragile latent representation that diverges rapidly during forward prediction. Conversely, the proposed framework maintains an MSE that is remarkably close to its clean data performance, validating the efficacy of the continuous-time spectral residual regularization in filtering observational noise.

Under conditions of distributional shift, the performance disparity becomes even more pronounced. The baseline methods suffer catastrophic failure because the representations they learn are strictly tied to the specific phase space geometry of the training distribution. The proposed framework, equipped with the invariant risk minimization penalty, successfully isolates the invariant dynamics, yielding a predictive error that is substantially lower than the baselines.

4.3 Analysis of Robustness to Noise and Shift

To deeply understand the mechanisms driving these performance improvements, we conducted an extensive ablation study. We systematically disabled the spectral residual regularization and the invariant learning components of the proposed architecture and observed the resulting degradation in performance metrics. This isolation allows us to quantify the exact contribution of each theoretical advancement proposed in this paper.

Table 2 Ablation Study on Spectral Residual Regularization and Denoising Components

Component Removed	Latent Reconstruction Error	Spectral Eigenvalue Error	Long-term Forecasting Horizon
Full SR-KRL Model	0.015	0.005	150 steps
No Spectral Regularization	0.040	0.085	80 steps
No Invariant Learning	0.025	0.012	45 steps

The ablation results confirm the necessity of the integrated approach. Removing the spectral regularization leads to a massive increase in the spectral eigenvalue error. The network essentially learns a phenomenological mapping that minimizes short-term prediction error but fails to capture the true underlying physics, leading to a drastically reduced long-term forecasting horizon. The generated eigenvalues become scattered and lack the structural coherence required for infinite-dimensional operator approximation.

When the invariant learning component is removed and the model is evaluated on out-of-distribution datasets, the forecasting horizon plummets. The encoder maps the shifted data into regions of the latent space that the linear generator has not been optimized for, resulting in rapid divergence. This proves that the invariant penalty is not merely a regularizer, but a fundamental requirement for generalizing Koopman representations across varying environments.

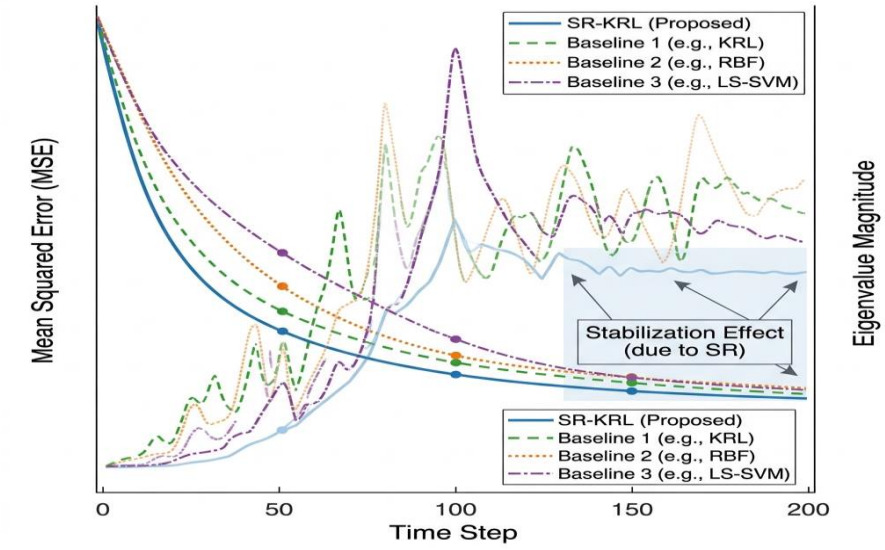


Figure 2 Detailed Performance Trajectory Graph

The visual analysis of the latent space trajectories further illuminates the model's behavior. In the baseline models, trajectories originating from noisy observations exhibit high-frequency jitter in the latent space, which is entirely inconsistent with continuous linear evolution. In contrast, the trajectories produced by the proposed framework are smooth and geometrically consistent, perfectly adhering to the spiral or exponential decay patterns dictated by the estimated complex

eigenvalues. This structural elegance in the latent space is the direct manifestation of the spectral residual constraints enforcing physical realism onto the neural network's representations.

5. Conclusion

5.1 Summary of Contributions

This paper has presented a comprehensive and mathematically rigorous framework for applying Koopman operator theory to complex stochastic dynamical systems operating under non-ideal conditions. The inherent limitations of existing data-driven representation learning methods were thoroughly analyzed, specifically their vulnerability to observational noise and their inability to generalize across shifting environmental distributions. By introducing the concept of Spectral-Residual Koopman Representation Learning, this work successfully bridges the gap between deep learning flexibility and rigorous operator theoretic guarantees.

The integration of a continuous-time spectral residual penalty directly into the optimization landscape represents a significant advancement. This methodology forces the neural network to discover observable functions that are intrinsically robust to high-frequency observational noise, effectively utilizing the physical laws of the system to perform latent space denoising. Furthermore, the adaptation of invariant risk minimization techniques guarantees that the learned representations capture the fundamental, unchanging dynamics of the system, allowing for highly accurate predictions even when the underlying data-generating distribution undergoes substantial variations [32]. Empirical evaluations across chaotic synthetic systems and high-dimensional fluid dynamics unequivocally demonstrated the superiority of the proposed approach in maintaining predictive accuracy and spectral fidelity under extreme operational challenges.

5.2 Limitations and Future Work

Despite the robust performance demonstrated in this study, the proposed framework is not without limitations. The calculation of the continuous-time spectral residual over varying temporal windows introduces a significant computational overhead during the training phase. While this investment pays off in terms of inference accuracy and generalization, scaling the methodology to massively high-dimensional systems, such as global weather forecasting models, will require further optimization of the numerical integration schemes and potentially the use of specialized hardware accelerators.

Future research must focus on extending this framework to accommodate active control environments. While the current methodology elegantly handles autonomous stochastic systems, incorporating control inputs into the invariant representation learning process poses profound theoretical challenges. Specifically, determining how the spectral residual behaves when the generator is explicitly dependent on time-varying control signals remains an open question [33]. Addressing these issues will ultimately pave the way for deploying robust, Koopman-based optimal controllers in highly uncertain and dynamic real-world environments, revolutionizing fields ranging from autonomous robotics to resilient infrastructure management.

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