Dynamical systems' predictability using machine learning

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1. Introduction

Many real-world problems can be recast within the framework of complex dynamical systems. Such systems can be modeled either as high-dimensional deterministic systems with chaotic, multiscale behavior [1, 2], or as stochastic systems that explicitly incorporate randomness [3, 4]. Regardless of the modeling paradigm used, complex dynamical systems, like the atmosphere, exhibit limited predictability horizons, causing forecast errors to grow over time [5, 6]. This statement holds true both when using traditional numerical methods to solve the equations governing these systems, as well as when using data-driven and artificial intelligence (AI) approaches. In addition, the challenge of predicting complex dynamical systems becomes even more pronounced when extreme events occur, given their short-lived and abrupt nature.

The evaluation of predictability of complex system traces back to the sensitivity analysis to the initial conditions in deterministic systems proposed by Lorenz [5], which was later formalized through the largest Lyapunov exponent [7], and its variants [8, 9, 10, 11, 12]. The framework of information theory was also proposed to study predictability [13, 14, 15, 16]. The above two classes of methods have intrinsic limitations. Lyapunov-based approaches tend to have restrictive assumption on the underlying data, while information-theory methods are impractical for high-dimensional systems due to their prohibitive computational costs.

Building on a different perspective, Lucarini et al. [17] proposed local dynamical indices based on extreme value theory and dynamical systems theory, which can be viewed as qualitative proxies of state-dependent predictability. However, they cannot directly provide a quantitative estimation of predictability. To address this limitation, stemming from the same framework of dynamical indices, time-lagged recurrence (TLR) [18] was recently proposed to analyze the state-dependent predictability of complex systems. This recent and promising approach was applied to several dynamical systems showing its ability to correctly capture known predictability, while also providing results for dynamical systems where Lyapunov exponents and information theory struggled.

In this work, we take yet another route, that is: we attempt to estimate predictability using machine learning, building upon some recent works [19, 20, 21].

2. Method

We combine machine learning with information theory to quantify the predictability limits of dynamical systems, focusing in particular on extreme events. Specifically, we utilize a diffusion-based machine learning model to obtain the distribution of predicted trajectories, and then define a variable based on information theory to quantify predictability limits of extreme events.

We employ the Autoregressive Conditional Diffusion Model (ACDM) [22] to ensure long-term stable predictions. ACDM extends Denoising Diffusion Probabilistic Models (DDPMs) [23] by introducing an autoregressive structure for sequential predictions, where the system's previous state conditions the predicted probability distribution at each time step (see Appendix, Fig. A1). Notably, this approach inherently provides a distribution of predicted system trajectories, allowing for better uncertainty and predictability assessment. The training process follows the standard diffusion model framework, where Gaussian noise is progressively added to the simulation states, transforming the original data into a noise distribution. This process helps the model learn the statistical dynamics of the system while incorporating variability.

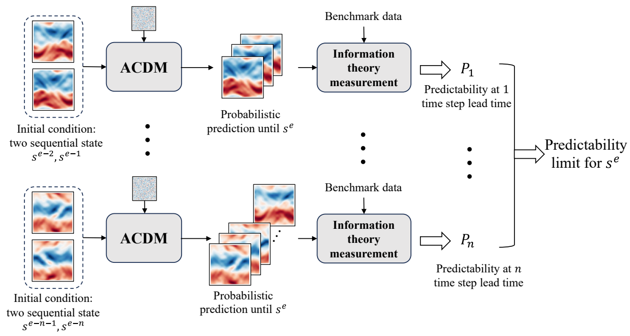

Fig. 1: Methodology to quantify the predictability of one extreme event that happens on the e^{th} time step. The variable s^e denotes the onset state of the extreme event, while P_n denotes the predictability of s^e from the n^{th} time step before the onset. In this figure, two sequential states before the onset of extreme events are used as initial conditions for probabilistic prediction.

The reverse process, which reconstructs the denoised data from the noise distribution, is learned using a U-Net (based on [24]) with various modern architectural improvements [25, 26, 27]. In the inference phase, noise is added to the conditions, and combined with a random distribution that represent current state. This random distribution is denoised stepwise to produce a predictive distribution for the current state. This approach maintains consistency and coherence in long simulations. Controlled noise perturbations help reduce error accumulation, enhancing stability and robustness. The trained ACDM is then used to predict the system's evolution, with initial conditions taken from various time steps before the onset of extreme events. To establish a benchmark, numerical methods are used to generate ground truth data, identifying the onset times of a large number of extreme events. A variable is introduced to evaluate the predictability of the distribution generated by the diffusion model, ultimately allowing us to determine the predictability limit for each extreme event. An illustration of how to find the predictability limit for one extreme event is shown in Fig. 1.

3. Preliminary Results

The proposed model is evaluated on a well-established dynamical system: namely the Kolmogorov flow, a two-dimensional incompressible flow driven by a sinusoidal body force with a specified wavenumber [28, 29]. At sufficiently high Reynolds numbers, this system exhibits extreme events characterized by sudden increase in instantaneous space-averaged enstrophy Ω [29], that is directly linked to the dissipation rate of the system. Indeed, in Kolmogorov flow with Reynolds number $Re = 100$, an extreme event is defined when the enstrophy is above 10.7, which represents the top 1% of the enstrophy distribution within the attractor. To generate ground truth data, we employ a pseudo-spectral method [30].

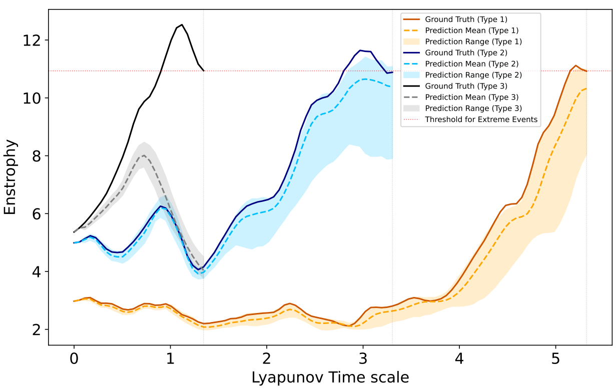

Fig. 2: Extreme events with different predictability limits in Kolmogorov flow.

Preliminary results indicate that extreme events in Kolmogorov flow can be classified into distinct groups based on their machine-learning-derived predictability, which is calculated based on information theory metrics. Some extreme events exhibit a relatively long predictability limit. One example is shown in Fig 2 in orange, labeled as Type 1. The probability predictions made by the machine learning model starting from 5 Lyapunov times (L_T) before the onset of extreme events are tightly concentrated around the ground truth, indicating that the system is still within the predictability limit. However, predictions starting from above 5 L_T before the event become widely dispersed across the attractor, suggesting that the model cannot accurately predict this extreme event. Some other extreme events shows a lower predictability limit at around 3 L_T. The successful prediction of one example, made from a lead time shorter than the predictability limit, is shown in Fig 2 in blue, labeled as Type 2. When predicting starting from above 3 L_T before the onset, the accuracy cannot be guaranteed. (The unsuccessful predictions that out of predictability limit for Type 1 and Type 2 are shown in Appendix, Fig. A2) Additionally, we observe that some extreme events are entirely unpredictable, with no clear indication of their occurrence even at shorter timescales. An example of this type of extreme events can be found in Fig 2 in gray, labeled as Type 3. Even starting the prediction from less than 1 L_T lead time before the occurrence of the extreme event, none of the trajectories reach the threshold of extreme events. This variability in predictability may stem from different underlying mechanisms driving extreme events, which warrants further investigation in future studies.

4. Conclusion

This work establishes a machine-learning-driven approach for quantifying the predictability of dynamical systems, with a focus on extreme events. The approach uses a diffusion-based model, and can pave the way to better understand the behaviour of real-world dynamical systems, especially for extreme events. Understanding why certain extreme events have longer or shorter predictability windows could reveal fundamental properties of chaotic systems and improve forecasting strategies.

Acknowledgments

GM acknowledges support from MOE Tier 2: Prediction-to-Mitigation with Digital Twins of the Earth's Weather, under grant number # T2EP50221-0017.

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Appendix A. Additional images

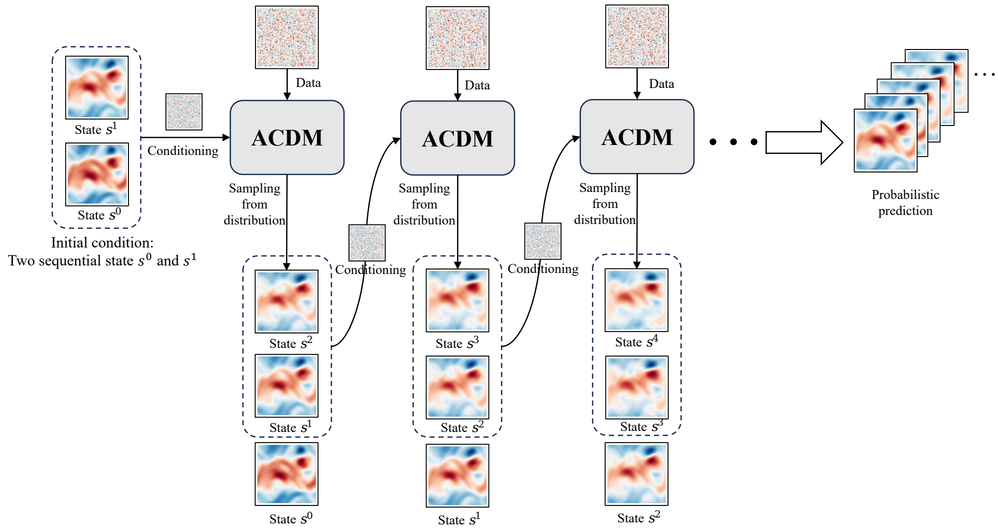

Fig. A1: The inference workflow of Autoregressive conditional diffusion model (ACDM) [22]. s^n denotes the state of the system at n^{th} time step. As an example, the input of ACDM is two sequential state for each time step prediction.

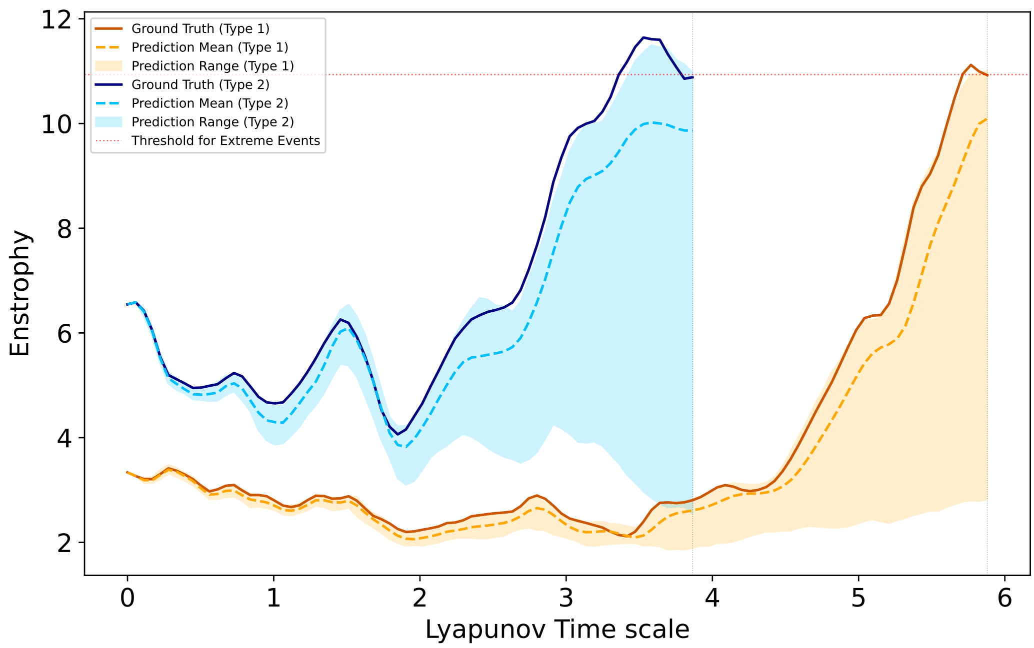

Fig. A2: Unsuccessful prediction of Type 1 and Type 2 extremes from initial conditions out of predictability limit.