Predicting Rare Events in Multiscale Dynamical Systems
Using Machine Learning

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We study the problem of rare event prediction for a class of slow-fast nonlinear dynamical systems. The state of the system of interest is described by a slow process, whereas a faster process drives its evolution. By taking advantage of recent advances in machine learning, we present a data-driven method to predict the future evolution of the state. We show that our method is capable of predicting a rare event at least several time steps in advance. We demonstrate our method using numerical experiments on two examples and discuss the mathematical and broader implications of our results.

Keywords: Rare event prediction, machine learning, deep echo state network, multiscale dynamical systems

I. INTRODUCTION

The dynamics of many systems in nature are nonlinear, multiscale and noisy, making both the theoretical and numerical modeling and prediction of their states challenging. Of particular interest are those dynamics that often lead to rare transition events. Namely, the system under study spends very long periods of time in various metastable states and only very rarely and at seemingly random times, it hops between states. Understanding the dynamics of such systems requires us to study the ensemble of transition paths between the different metastable states [19, 21, 32].

One mechanism that explains the hopping behavior is that it is induced by a fast signal influencing the state of the system. The usually noisy driving signal comes from an external source. It is often the case that there is a large separation of time scales on which the system state and the signal evolve. Without the driving signal, the system will remain in one state forever.

The above signal-induced phenomenon can be modeled by a class of non-autonomous dynamical systems, whose state $x(t) : [0, T] \rightarrow \mathbb{R}^n$, $T > 0$, is described by:

$$\dot{x}(t) = F(x(t), t) + f(t),$$

where $F(x(t), t)$ is a force field, providing a deterministic backbone, and $f(t)$ is a fast driving noisy signal, describing small perturbations imparted to the system. In principle, one does not have any a priori knowledge of the mathematical model for $f(t)$, but only has access to data for $x$ and, possibly, a mathematical model for $F(x(t), t)$ at their disposal. The unknown $f(t)$ is generally a random function, and it could be regular, chaotic or stochastic. It is challenging to infer an accurate model for $f(t)$ using only the data for $x$. In fact, in many cases one could construct several models that are capable of describing the data equally well, and often there are ambiguities in the choice of model. An example that illustrates this issue is the problem of distinguishing deterministic chaos from stochasticity [1, 15, 38]. Indeed, on one hand, when certain assumptions are satisfied, chaotic systems can be well approximated by a stochastic one [4, 17, 46]. On the other hand, many stochastic systems can be described by a chaotic model [27]. In the absence of a uniquely defined model for $f(t)$, one has to resort to a model-free, data-driven approach, which is currently an extremely active area in applied dynamical systems. We refer the reader to the book by Brunton and Kutz [11] for an excellent review of data-driven methods.

An important and practical question concerning the system (1) is the following – can we predict the future evolution of the system state using only its data [14, 34]? Moreover, can we achieve this for a sufficiently long time, and to a desired level of accuracy and certainty? Note that this is different from asking one to infer a mathematical model (which may have a very low predictive power, as in the case of a random walk model) from the data. Typically, the data is complex and multiscale in nature, thererby complicating analysis and prediction. The main goal of this work is to propose and test a machine
learning based solution to predict rare events in multiscale noisy nonlinear dynamical systems, making use of only the (slow) system state data and a partial knowledge of the physics of the generating system. Since the occurrence of rare events has significant deleterious or positive implications, it is important to quantify and predict them in advance to inform decision making [28] – this is the main motivation of this paper. It would appear that this is the first attempt to solve this problem using a machine learning method. Here we will focus on the case where the system of interest is one-dimensional (i.e., n = 1). While we focus on prediction of rare events, our method can be applied to predicting future states in general multiscale systems.

By exploiting recent advances in machine learning, we will construct an algorithm to solve the prediction problem. The field of machine learning itself is experiencing a major recent resurgence of interest, with wide ranging applications and significant implications in many areas of science and engineering [35, 47, 62]. We note in particular neural networks and deep learning, whose industry wide applications have been made possible due to availability of large amount of data and advances in computer hardware development [30]. For instance, by training on a sufficiently large set of data, one can classify handwritten digits to unprecedented accuracy [39], predict and analyze time series [24, 58, 67], infer the Hölder exponent of stochastic processes [65], characterize anomalous diffusion [10], learn how to construct linear embeddings of nonlinear dynamics [44], replicate chaotic attractors and calculate Lyapunov exponents [55], solve high-dimensional nonlinear PDEs [59], infer a person’s face from his/her voice [52], and others that are too numerous to list here. As powerful as it appears, we emphasize that it is by no means an easy task to apply the tools of machine learning to real world data sets and one needs to proceed with caution and avoid the pitfalls of machine learning[60]. Indeed, one of the main challenges in machine learning deals with the ability of the algorithm to be generalized to unseen data. Moreover, the methods in machine learning are based on a black-box empirical approach, guided only with useful practices that were mostly discovered by trial and error.

This paper is organized as follows. In Section II, we motivate and describe the class of dynamical systems of interest from which the data is generated. They are special cases of (1) with a specified model for f(t). We then introduce the problem of data-based rare event prediction. In Section III, we present a method to solve the prediction problem using a deep version of the echo state network. In Section IV, we apply and test the method to predict rare events in two different systems. We make concluding remarks in Section V.

II. MULTISCALE NOISY SYSTEMS AND THE PREDICTION PROBLEM

We consider scenarios where the available data is generated by the following family of continuous-time slow-fast systems (parametrized by ϵ > 0) [17, 57, 61]:

\[ \dot{x}(t) = F(x(t), t) + \frac{\sigma}{\epsilon} G(\xi(t)), \]  
\[ \dot{\xi}(t) = \frac{1}{\epsilon^2} H(\xi(t)), \]  

with the initial conditions x(0) = x₀ and \( \xi(0) = \xi_0 \), where \( x_0 \) and \( \xi_0 \) can be either fixed or random. In the case when both initial conditions are fixed, (2)-(3) describe a deterministic dynamical system; otherwise, it is a random dynamical system. In the above, x(t) : \( I \to \mathbb{R} \) is a slow process, \( \xi(t) : I \to \mathbb{R}^m \) is a fast process (noise), \( F(x, t) : \mathbb{R} \times I \to \mathbb{R} = \mathbb{R}^m \) is a deterministic force field, \( G(\xi) : \mathbb{R}^m \to \mathbb{R} \) is a functional (observable) of the fast process, \( H(\xi) : \mathbb{R}^m \to \mathbb{R}^m \) is a deterministic vector field describing the fast process, \( \sigma > 0 \) is a small constant controlling the strength of influence of the fast process on the slow one, and \( I \) is a time interval on which the system evolves. In many applications of interest, F, G and H may be highly nonlinear. The assumption that the data is modeled by the above systems is not too restrictive, for as is very often the case in the analysis of experimental data, there is not a unique single model for the system generating the data [3, 13].

Often one is interested in the dynamics of the slow process and the case where the driving signal, \( f(t) = \frac{\sigma}{\epsilon} G(\xi(t)) \), is a stochastic process such as Gaussian white noise. A crucial property of dynamical systems of the form (2)-(3) is that stochastic behavior emerges as \( \epsilon \) becomes smaller. Indeed, it can be rigorously shown that under appropriate assumptions on the initial conditions, F, G and H (usually a mixing assumption is imposed on the fast flow), x(t) converges in law to \( X(t) \) as \( \epsilon \to 0 \) for \( t \in I \), where \( X(t) \) is a diffusion process solving the SDE:

\[ dX(t) = F(X(t), t)dt + \sigma dW_t. \]
Here \( \sigma > 0 \) is a constant (involving the time integral of the correlation of the fast process) and \( W_t \) is a Wiener process \([17, 48]\). Therefore, the family of equations (2)-(3) can be viewed as approximations of a stochastic model. Such a perspective has been adopted to study a variety of noisy systems \([2, 8, 33, 49]\).

We refer to Section IV for two concrete examples. An important class of \( \xi(t) \) are those that exhibit deterministic chaos, which has been studied and observed \([27]\) in a class of physical systems. Note that \( G \) can be generalized to be dependent on \( x(t) \), in which case the limiting SDE will have a multiplicative noise, but we will not pursue this case here.

We now formulate the prediction problem introduced in Section I systematically. First, we lay out our assumptions. The only available data to us is that for \( x \), which is assumed to be generated by the systems (2)-(3), and we do not have access to the data for \( \xi \). Let \( \mathcal{I} = [0, t_{\text{obs}}] \cup [t_{\text{obs}}, t_f] \), where \( 0 < t_{\text{obs}} < t_f \). We have taken the initial time to be zero for simplicity. Here \( t_{\text{obs}} \) denotes observation time, beyond which we do not know the system state, and \( t_f \) denotes the final time at which the prediction will be made. Suppose that we are given a sufficiently long and high-frequency time series for \( x \) on \([0, t_{\text{obs}}]\).

Furthermore, we are blind to the actual mathematical model for the fast process. However, a partial knowledge of the physics of the system of interest is known. In particular, it is assumed that we know the exact expression describing the force field \( F \). This assumption is satisfied when one can reconstruct the force field from the data accurately, which may be possible in many practical situations \([26]\).

We are given a time series data for \( x \), a sequence \( (x_k)_{k=0,\ldots,N} = (x(t_0), x(t_1), x(t_2), \ldots, x(t_N)) \), where \( t_0 = 0, t_i = i\Delta t \ (i = 0, 1, \ldots, N) \) is the sampling time, \( \Delta t \) is the time step size, \( t_N = N\Delta t = t_{\text{obs}} \), and \( N \) is the number of available samples. Our time series does not record occurrence of a rare event and we assume that a rare event will occur shortly after time \( t_{\text{obs}} \). Any precursors for this rare event must then be hidden in the time series. We then attempt to answer the following questions.

- Can we predict if and when a rare event will occur in a given future time window? Can we infer the characteristics of the event?
- How far in advance can we predict the rare event?
- With what accuracy and certainty can we achieve these goals?
- Is it possible to answer all of these questions with a computationally inexpensive method and/or using a relatively short time series data for \( x \)?

Clearly these are challenging questions. The degree of difficulty depends on the characteristics of the dynamical systems generating the data for \( x \). For a given amount of data the difficulty increases as \( \epsilon \) becomes smaller, in which case the statistical behavior of the driving noise is closer to that of a white noise and so predictability is lost in the limit. Therefore, analysis of the data should be performed on a case by case basis.

III. A DEEP LEARNING BASED PREDICTION METHOD

A. The method

We first present a three-step procedure that will allow us to investigate the questions posed at the end of Section II. We then discuss a number of heuristic issues associated with our approach.

Algorithm III.1. Predicting rare events with deep learning.

Under the assumptions, setting and notation described in Section II:

(S1) **Feature extraction.** Extract the fast driving signal using the data for \( x \) and the known expression for \( F \):

\[
f(t_i) = \frac{x(t_{i+1}) - x(t_i)}{\Delta t} - F(x(t_i), t_i),
\]

for \( i = 0, 1, \ldots, N - 1 \), where \( \Delta t \) is a uniform time step.

(S2) **Deep learning.** Using \( (f(t_i))_{i=0,\ldots,N-1} \) as the training data, predict the values of \( f \) for \( M + 1 \) time steps into the future (i.e., beyond time \( t_{\text{obs}} - \Delta t \)) using a supervised machine learning algorithm (for instance, the Algorithm III.2 in Section IV) that is best fit for the task to infer \( (f(t_N), f(t_{N+1}), \ldots, f(t_{N+M})) \).
(S3) **Numerical integration.** Numerically evolve the system (2) up to time $t_{N+M}$, with $(f(t))_{t=t_0,...,t_{N+M}}$ in place of $\frac{\xi}{2}G(\xi(t))$ in (2), using the step size $\Delta t$. The predicted values for $x$ in the time window $[t_{\text{obs}} + \Delta t, t_f = (N + M)\Delta t]$ are then obtained from the resulting numerical solutions.

Algorithm III.1 is the method that we propose and use for predicting rare events. It allows the prediction of the system state $M$ time steps beyond the observation time $t_{\text{obs}}$, the result of which can be used to investigate the questions posed in Section II. To be able to answer these questions with a desired level of confidence, the predicted values should be as close as possible to the actual (target) values, i.e. the generalization error should be small.

Before we discuss the details of implementation for each of the three steps above, a few remarks are in order. A natural approach is to apply a suitable machine learning algorithm directly to the data for $x$ and attempt to predict the future states. While this seems like a sensible approach, it is unrealistic to expect an algorithm to learn the multiscale nature of the data accurately. In fact, it is not clear beforehand which algorithm is best and in many cases the rare event will not be detected successfully (see Section IV). Our method circumvents this challenge and provides an alternative route for handling multiscale data. Moreover, the simplicity of our method provides an additional advantage.

The quality and accuracy of the prediction results will rely heavily on how well each step in the algorithm is executed. Errors will accumulate as one progresses through the three steps. Indeed, (S1) involves a numerical approximation of the driving signal. In (S2), errors will arise from both the use of the training data (where the numerical errors from (S1) are hidden) as well as the machine learning algorithm itself. In (S3), an additional error due to numerical integration is inevitable. Provided that the accumulation of these errors is negligibly small and well controlled, one can learn and predict the system states with reasonably good accuracy, as demonstrated with the examples in Section IV. Rigorous error analysis will not be studied here.

Steps (S1) and (S3) are straightforward to implement, so we must discuss (S2), whose implementation is the most challenging part of the method. We will formulate this step as the problem of learning the training data $(f(t_i))_{i=0,...,N-1}$ with parametrized high-dimensional nonlinear dynamical systems.

### B. Deep echo state network (DESN)

There are many machine learning algorithms that one can use to implement step (S2). Algorithms from deep learning include convolutional neural networks, recurrent neural networks (RNNs), and encoder-decoder networks, each of which can be implemented using various architectures and training schemes [30]. As nonlinear state space models, RNNs have **dynamical memory**, which means that they are capable of preserving in their internal state a nonlinear transformation of the input history. They are, therefore, particularly well suited to deal with sequential data [18]. We will implement (S2) using a RNN known as the **echo state network** (ESN).

ESN belongs to the paradigm of reservoir computing and is computationally less costly to train than other variants of RNNs, which typically use a backpropagation through time algorithm for gradient descent based training [37, 43]. Similar to other RNNs, the ESN can, under fairly mild and general assumptions, be shown to be a universal approximator of arbitrary dynamical systems [31]. In contrast to standard design and training schemes for RNNs but conceptually similar to the kernel methods [9], the neural network (called the reservoir) in ESNs is generated randomly and only the readout from the reservoir is trained. The outputs are linear combinations of the internal states and the inputs. This reduces the training to solving a linear regression problem, minimizing the mean squared error between the outputs and the target values. For practical introductions and technical details on ESNs, we refer the reader to Refs. [36, 42].

Even though not all the weights of the network are trained, it has been shown that ESNs work surprisingly well and achieve excellent performance in many benchmark tasks. For example, the ESN has been shown to predict chaotic systems remarkably well [41, 54–56, 69]. They may outperform other machine learning algorithms in certain prediction tasks. For instance, it has been shown that ESN substantially outperforms deep feed-forward neural network and RNN with long short-term memory (LSTM) for predicting short-term evolution of a multiscale spatio-temporal Lorenz-96 system [16]. Moreover, ESNs do not suffer from the vanishing and exploding gradient problem typically encountered when training other RNNs [36]. For these reasons, we have chosen to use the ESN over other machine learning methods. We emphasize, however, that the ESN may not be the most optimal network for our prediction task and we remain mindful of its shortcomings.

To achieve our goals, we are going to use a deep version of the ESN (see also the discussion in Section IV(b)). Our deep echo state network (DESN) consists of organized hierarchically stacked ESNs, whose architecture and training algorithm will be described in the following subsections. Such deep ESNs
are more expressive than shallow ESNs, in the sense that they are able to develop in their internal states a multiple time-scale representation of the temporal information [22, 23]. We remark that in contrast to feed-forward neural networks, it is often not obvious how one should construct a deep RNN [53]. In particular, different variants of deep echo state networks can be constructed, depending on the task at hand [45, 66].

1. Architecture of the DESN

Similar to other RNNs, the DESN is a parametrized, high-dimensional, discrete-time, non-autonomous, nonlinear state-space model, describing a dynamical input-output relation:

\[ x(t_{n+1}) = f(x(t_n), u(t_{n+1}), y(t_n), \nu(t_n); \theta_f), \]
\[ y(t_{n+1}) = g(x(t_{n+1}), u(t_{n+1}), \nu(t_{n+1}); \theta_g), \]  

for \( n = 0, 1, \ldots, N - 1 \). Here \( u(t) \in \mathbb{R}^{n_u} \) is the input (bias) at time \( t \), \( x(t) \in \mathbb{R}^{n_x} \) is the internal/hidden state, \( y(t) \in \mathbb{R}^{n_y} \) is the output, \( \nu(t) \in \mathbb{R}^{n_\nu} \) is an external perturbation (noise/regularization), \( f \) and \( g \) are generally nonlinear functions, and \( \theta_f \) and \( \theta_g \) are model parameters. The network non-linearly embeds the input into a higher dimensional space where the original problem is more likely to be solved linearly. In the case of the DESN, the basis expansion is randomized, computed by a pool of randomized nonlinear filters.

Our DESN is a specific implementation of the above state-space model, putting constraints on a fully connected deep RNN. In the following, \( t_n = n\Delta t \), for \( n = 0, \ldots, N - 1 \), where \( \Delta t \) is a fixed time step size. If the number of layers, \( n_L := L + 1 \), is chosen to be one, i.e., a shallow ESN, then we have the following update for the states and outputs:

\[ x^{(0)}(t_{n+1}) = \tanh(W^{(0)}x^{(0)}(t_n) + W^{(0)}_{in}u(t_{n+1}) + W_{fb}y(t_n)) + \nu \xi^{(0)}, \]
\[ y(t_{n+1}) = W_{out}(x^{(0)}(t_{n+1}), u(t_{n+1})), \]

for \( n = 0, 1, \ldots, N - 1 \), with initial condition \( x(t_0) := x^{(0)}(t_0) = 0, y(t_0) = 0 \).

Otherwise, we employ the following deep version of ESN:

\[ x^{(0)}(t_{n+1}) = \tanh(W^{(0)}x^{(0)}(t_n) + W^{(0)}_{in}u(t_{n+1})) + \nu \xi^{(0)}, \]
\[ x^{(l)}(t_{n+1}) = \tanh(W^{(l)}x^{(l)}(t_n) + W^{(l)}_{in}x^{(l-1)}(t_{n+1}) + \nu \xi^{(l)}), \quad \text{for } l = 1, \ldots, L - 1, \]
\[ x^{(L)}(t_{n+1}) = \tanh(W^{(L)}x^{(L)}(t_n) + W^{(L)}_{in}x^{(L-1)}(t_{n+1}) + W_{fb}y(t_n) + \nu \xi^{(L)}), \]
\[ y(t_{n+1}) = W_{out}(x^{(0)}(t_{n+1}), \ldots, x^{(L)}(t_{n+1}), u(t_{n+1})), \]

for \( n = 0, 1, \ldots, N - 1 \), with initial condition \( x(t_0) := (x^{(0)}(t_0), \ldots, x^{(L)}(t_0)) = 0, y(t_0) = 0 \).

In (8)-(13), the training input \( u \) and output \( y \) come from a compact subset of \( \mathbb{R}^{n_u} \) and of \( \mathbb{R}^{n_y} \) respectively, the vector \( x^{(i)} \in \mathbb{R}^{n_x} \) (for \( i = 0, \ldots, L \)) is the \( i \)th hidden state, the vector \( y \in \mathbb{R}^{n_y} \) is the output, the matrices \( W^{(i)} \in \mathbb{R}^{n_x \times n_x} \) (for \( i = 0, \ldots, L \)), \( W^{(0)}_{in} \in \mathbb{R}^{n_x \times n_u} \), \( W^{(i)}_{in} \in \mathbb{R}^{n_x \times n_x(i)} \) (for \( i = 1, \ldots, L \)) and \( W_{fb} \in \mathbb{R}^{n_y \times n_x \times 1} \) are fixed internal connection weights whose values are set to random values, the matrix \( W_{out} \in \mathbb{R}^{n_y \times (n_x + n_x + \cdots + n_x + n_y)} \) is the readout weight matrix whose entries are to be learned. The vectors \( \xi^{(k)} \), \( k = 0, \ldots, L \), are random vectors describing added noise during the sampling at each layer and \( \nu \) is a noise (regularization) intensity parameter (we have taken the same noise level for each layer). The activation function in each layer is taken to be a (vectorized) hyperbolic tangent function. At each training step, the input is fed into the first layer, which is then connected to the next layer via the connection weights, and we have added an output-to-reservoir feedback connection in the last layer. The ansatz for the output at each update time is taken to be a linear combination of the elements of the hidden states and the input. For a schematic of a general DESN architecture, we refer to Figure 3 in [22].

2. Algorithm for training the DESN

The above implementation gives a randomly constructed RNN prior to training. It may generally develop oscillatory or chaotic behavior even in the absence of external excitation by the input, and therefore the subsequent network states, starting from an arbitrary state \( x(t_0) \), may not converge to the
zero state. To ensure that the DESN converges to the desired state, the internal connection weights are scaled such that the resulting (untrained) input-driven recurrent network (or the “dynamical reservoir”) is appropriately stabilized or “damped”, forcing it to have the so-called ”echo state property”. The echo state property says that the current network state is uniquely determined by the history of the input and the output provided that the RNN has been run for a sufficiently long time (see [36] for details, subtleties, and other equivalent conditions for the echo state property). Once this initialization is made, we can proceed to the training stage.

We now give a complete description of setting up and training the DESN. It is based closely on the techniques developed in [36].

**Algorithm III.2. Initializing and training the DESN.**

Given a training set consisting of the input-output sequence \((u(t_0), y(t_0)), \ldots, (u(t_{N-1}), y(t_{N-1}))\), find a trained DESN parametrized by \((W^{(i)}, W^{(j)}_\text{in}, W_{fb}, W_{out}, \nu)\) whose network output \((y(t_0), \ldots, y(t_{N-1}))\) approximates the actual output \((y_{ac}(t_0), \ldots, y_{ac}(t_{N-1}))\).

1. **Initialize the DESN to ensure the echo state property.**
   - Depending on the training data (length, difficulty of task, etc.), select appropriate dimensions/sizes (i.e., \(n_x, \ldots, n_{x_L}\)) for the connection weight matrices. These dimensions are hyperparameters that can be tuned. The matrix elements of these matrices are then selected randomly as follows:
     - \((W^{(i)}_\text{in})_{klt} \sim \text{Unif}(-1,1)\);
     - \((W^{(j)}_\text{in})_{klt} \sim \text{Unif}(-0.5,0.5)\), for \(j = 1, \ldots, L\);
     - \((W^{(i)}_{fb})_{klt} \sim \text{Unif}(-0.5,0.5)\), for \(i = 0, \ldots, L\);
     - \((W^{(i)}_{out})_{klt} \sim \text{Unif}(-1,1)\).

1b) **These matrices are rescaled as follows:**

\[
W^{(j)}_\text{in}, W^{(i)}_\text{in}, W_{fb} \mapsto \frac{W^{(j)}_\text{in}}{\|W^{(j)}_\text{in}\| + 0.001}, \quad \frac{W^{(i)}_\text{in}}{\|W^{(i)}_\text{in}\| + 0.001}, \quad \frac{W_{fb}}{\|W_{fb}\| + 0.001},
\]

where \(\| \cdot \|\) denotes the Frobenius norm.

1c) **Set a fraction of elements (connections) in the matrices** \(W^{(i)}\) **to zero** (the fraction, denoted \(r_i\), chosen is a hyperparameter for sparsity of the matrices used for each layer) and then rescale the resulting matrices \(\hat{W}^{(i)}\) **appropriately using their spectral radius** (to satisfy the necessary condition for the echo state property [36]), i.e.,

\[
\hat{W}^{(i)} \mapsto \hat{W}^{(i)} \rho_{des}^{(i)} = \rho^{(i)},
\]

where \(\rho^{(i)}\) is the spectral radius of \(\hat{W}^{(i)}\), \(\rho_{des}^{(i)}\) is the desired spectral radius, and \(i = 0, \ldots, L\). The spectral radius chosen is less than one to ensure contractivity and is another tunable hyperparameter. The sparsity hyperparameter is chosen to guarantee a rich variety of dynamics of different internal units/hidden states as well as to speed up computation.

1a)-(1c) should then give an untrained network (dynamical reservoir) that satisfies the required properties. We initialize the network state with \(x(t_0) = 0\).

2. **Train the readout by solving a linear least squares problem.**

2a) **Discard an initial transient** by disregarding the first \(i_{\text{transient}} = \min(\text{int}(N/10), 100)\) states, where \(\text{int}(x)\) is the integer part of \(x\) and \(\min(x,y)\) is the minimum of \(x\) and \(y\).

2b) **Run the network on the entire input sequence and collect the output sequence** (i.e. according to (8)-(9) for the shallow ESN and (10)-(13) for the DESN. During sampling we add a small amount of noise or regularization, whose intensity is determined by the hyperparameter \(\nu\), to stabilize the network and prevent overfitting [42]. We choose the elements of the noise vectors \(\xi^{(k)}, k = 0, \ldots, L\), to be \(\text{Unif}(-0.5,0.5)\).
A  Example 1: A bi-stable system, driven by a fast Lorenz-63 system

(2c) Solve the least squares problem:

\[
\text{arg min}_{W_{\text{out}}} \frac{1}{N-1-i_{\text{transient}}} \sum_{i=i_{\text{transient}}+1}^{N-1} \| W_{\text{out}} \hat{x}(t_i) - y_{\text{ac}}(t_i) \|_2^2,
\]

(20)

where \( \hat{x} = (x, u) \). We remind the reader that \( W_{\text{out}} \) is the only trainable matrix in the DESN. As the above problem admits a closed form solution, we obtain \( W_{\text{out}} \) directly by applying the Moore-Penrose pseudo-inversion, i.e.,

\[
W_{\text{out}} = y_{\text{ac}} \hat{x}^+ = y_{\text{ac}} \hat{x}^T (\hat{x} \hat{x}^T)^{-1},
\]

(21)

where + and T denote pseudo-inverse and transposition respectively.

(3) Apply the trained DESN to prediction task.

Using the solution to (2c), propagate the trained network forward in time and obtain the predicted values \((y(t_N), \ldots, y(t_{N+M}))\), where \( y(t_i) = W_{\text{out}} \hat{x}(t_i) \), for \( i = N, \ldots, N + M \). The smaller the generalization error \( \| W_{\text{out}} \hat{x} - y_{\text{ac}} \|_2^2 \) on the prediction time horizon, the more accurate is the prediction.

The quality of prediction achieved by our DESN depends on the selection of hyperparameters, which need to be chosen following an appropriate model selection procedure, adapting to the data set on hand. The important hyperparameters are \( n_i := L + 1 \) (number of layers in the DESN), \( n_{\text{ac}} \) (dimension of the connection weight matrices at layer \( i + 1 \)), the \( r_i \) (sparsity parameter), the \( \rho_{\text{des}}^{(i)} \) (the desired spectral radius of these matrices at layer \( i + 1 \)), and \( \nu \) (the noise intensity). We remark that the above algorithm gives a specific way to initialize and train the DESN. Other variants may also be considered [43]. In any case, due to a lack of theoretical understanding of ESNs, one can rely on only heuristics and experience to achieve good performance on many tasks. To implement (S2) in Algorithm III.1, we apply Algorithm III.2 to the training data \((f(t_i))_{i=0,...,N-1}\). Together with (S1) and (S3), this completes the description of our rare event prediction method.

IV. NUMERICAL EXPERIMENTS

We apply the method presented in Section III to study the questions posed in Section II for two data sets generated by dynamical systems of different complexity. We implement Algorithm III.1-III.2 in Python. The complete codes that reproduce all the results obtained in this section are available at the following website: https://github.com/shoelim/predicting_rare_events_multiscale_systems.

Throughout this section, all variables considered are real and one-dimensional.

A. Example 1: A bi-stable system, driven by a fast Lorenz-63 system

Data generation. The data for \( x \) is generated by the following slow-fast system [29]:

\[
\dot{x}(t) = x(t)[1 - x^2(t)] + \frac{\sigma}{\epsilon} y_2(t),
\]

(22)

\[
\dot{y}_1(t) = \frac{10}{\epsilon^2} [y_2(t) - y_1(t)],
\]

(23)

\[
\dot{y}_2(t) = \frac{1}{\epsilon^2} [28y_1(t) - y_2(t) - y_1(t)y_3(t)]
\]

(24)

\[
\dot{y}_3(t) = \frac{1}{\epsilon^2} [y_1(t)y_2(t) - \frac{8}{3}y_3(t)].
\]

(25)

In (22)-(25), \( x \) is the state of the system of interest and its evolution is driven by a fast chaotic signal \( y_2/\epsilon \), which is modeled as follows. The vector state \((y_1, y_2, y_3)\) is described by the Lorenz-63 model with parameter values that lead to a chaotic behavior [40]. At these parameter values, \( y_2(t) \) is ergodic with invariant measure supported on a set of zero volume. The equation for \( x \) is therefore an ODE driven by a fast chaotic signal with characteristic time \( \epsilon^2 \).

To generate the data, we use a uniform time step of \( \Delta t = 0.01 \) to integrate (22)-(25) with \( \sigma = 0.08 \), \( \epsilon = 0.5 \), \( x(0) = -1.5 \), and \( y_i(0) \sim \text{Unif}(-10,10) \) for \( i = 1,2,3 \), up to time \( t = 100 \). Note that the
Example 1: A bi-stable system, driven by a fast Lorenz-63 system

time step is chosen to be small enough so that we can sample the scale on which the fast driving signal takes place. The data generated is plotted in Figure 1. This data is split into a training and a testing set.

Figure 1: Time series data for $x$ in Example 1 up to time $t = 100$ (of which only a segment prior to $t = 37$ will be available for training) – Here, the x-axis is the number of time steps (i.e., 100$^t$).

Generating system: dynamics and applications. Applying the discussion in Section II, the family of systems (22)-(25) (parametrized by $\epsilon$) can be viewed as an approximation to the Markovian system:

$$dX(t) = X(t)[1 - X^2(t)]dt + \tilde{\sigma}dW(t),$$

where $\tilde{\sigma}$ is an effective diffusion constant and $W(t)$ is a Wiener process, in the sense that as $\epsilon$ becomes smaller $x(t)$ converges in law to the process $X(t)$ solving the SDE above. Recall that we have chosen $\epsilon = 0.5$ for data generation and therefore the data can be thought of coming from an approximately stochastic system.

In the absence of the driving signal, the equation for $x$ has two stable fixed points, at $x = -1$ and $x = 1$, and an unstable one at $x = 0$. Starting from an initial state, the system will eventually evolve towards a nearby stable state. The presence of noise alters this dynamics, causing an occasional transition of the system between stable states. In the case where the noise amplitude is small, such a transition is a rare event, occurring at a seemingly unpredictable time (see Figure 1). In our case, $x$ starts near the fixed point $x = -1$ and will eventually jump to that at $x = 1$, the prediction of which is of great interest.

From a statistical mechanical point of view, the system (22)-(25) describes an overdamped Brownian particle moving in a symmetric double-well potential. In this case, $x$ is the position of the particle and $y_2$ models the fluctuations due to its interaction with the environment. The above model for $x$ is also often used in climate physics, an example of which is to view $x$ as the sea-surface temperature anomaly and $\xi = \frac{\sigma}{\epsilon}y_2$ as the impact of small-scale atmospheric variability [8, 33, 49].

Training and prediction details. To obtain the results in Figures 2-10, we apply Algorithm III.1-III.2 using a shallow ESN (i.e., $n_L = 1$ and $L = 0$) with $n_y = 1$. The ESN is driven by a constant input sequence of ones for all simulations performed in this section. The values of hyperparameters used to generate the results in these figures are given in Table I. For Figure 6 and Figure 10(b), we refer to the caption in the figure for values of hyperparameters used there. The values of all these hyperparameters are not fully optimized, i.e., an exhaustive search over the hyperparameters has not been performed. For numerical integration in (S3), we use a Runge-Kutta method with a uniform step size of 0.01.

Table I: Values of hyperparameters used for obtaining the results for Example 1.

| Figure | Number of training data points | $n_{x_0}$ | $\rho^{(0)}$ | $\rho^{(0)}_{det}$ | $\nu$ |
|--------|-------------------------------|------------|--------------|-------------------|------|
| 2      | 3700                          | 720        |              |                   |      |
| 3      | 3690                          |            | 700          | 0.7               | 0.1  |
| 4      | 3680                          |            |              |                   | 0.001|
| 5      | 3670                          |            |              |                   |      |
| 7      | 3700                          | 720        |              |                   |      |
| 8      | 7080                          | 1000       | 0.8          |                   |      |
| 9      | 3080                          | 720        | 0.75         |                   |      |
| 10(a)  | 3700                          |            |              |                   | 0.7  |
We perform an ensemble-like prediction by running the trained network 10 times\cite{50} into the future, where each time ran with different random realizations (using different random seeds) for setting up the ESN. We are taking the averaged values as the predicted values. To evaluate the quality of the prediction, we study the statistics (the mean and standard deviation) of the difference between the predicted values and the actual (target) values. We remark that alternative measures for evaluating the predictive performance could also be considered. Our choice of measure here, in contrast to coarse-grained metrics such as the percentage of learned trajectories that display a jump at a time close to the actual one, reflects our focus on inferring the characteristics of the whole transition path.

Results and Discussions. The prediction results for different training scenarios using Algorithm III.1 are displayed in Figures 2-5. Each run of the algorithm is completed in a few minutes on a 5-core CPU.

Figure 2: Training using 3700 data points. (a) the actual trajectory for $x$ (in red), 10 predicted trajectories from 10 runs using different random realizations, and the averaged predicted trajectory (in blue) up to 600 time steps into the future; (b) a zoom-in view of the average (out of 10 runs) predicted values for $x$ (in blue) vs. the actual values for $x$ (in red) – the shaded light blue region represents the 90 percent confidence interval of the predicted values; (c) error of the predicted results and its mean value (in blue); (d) standard deviation of the errors from (c). The $x$-axis in (a)-(d) is the number of time steps (i.e., $100\tau$).

Figures 2-4 show that our method is capable of quite confidently predicting the rare event and its transition path at least 20 time steps in advance. In particular, the actual future trajectory lies almost entirely within the 90 percent confidence interval of the predicted trajectory. Given that a relatively short time series was used for training, it would appear that the accuracy of these predictions is remarkable. Note that the plots in Figure 3 and Figure 4 are very similar. This is because the numbers of data points used for training differ by only 10 and the same training setting is used to obtain the results in both figures. However, the standard deviation of the errors grows more rapidly near the beginning of prediction horizon in Figure 4(d) than that in Figure 3(d).

Figure 5 shows how the inability of the ESN to make accurate long-term predictions cripples the performance of the method, rendering prediction of the rare event from an earlier time more difficult. Indeed, the longer into the future the prediction is, the less confident the results are. This is shown by the growth of the standard deviation of the prediction errors, which seems to saturate about a maximum value that increases with fewer training data points.

Figure 7 confirms that our method is far better than the direct method of applying an ESN to the data for $x$, which we take as a baseline result for comparison. We emphasize that one can also apply other machine learning algorithms such as the gradient descent based deep RNN and the deep convolutional neural network to implement the direct method \cite{5}. However, after some experiments we found that the predictive performance is similar to the baseline result, i.e., they fail to predict the approaching rare event, rendering the prediction task almost impossible using the direct method. This comparison study enhances the veracity of our method, which exploits the crucial idea of appropriately taking into account the multiscale nature of the system generating the data. The success of our method in predicting the
Figure 3: *Training using 3690 data points.* (a) the actual trajectory for $x$ (in red), 10 predicted trajectories from 10 runs using different random realizations, and the averaged predicted trajectory (in blue) up to 610 time steps into the future; (b) a zoom-in view of the average (out of 10 runs) predicted values for $x$ (in blue) vs. the actual values for $x$ (in red) – the shaded light blue region represents the 90 percent confidence interval of the predicted values; (c) error of the predicted results and its mean value (in blue); (d) standard deviation of the errors from (c). The $x$-axis in (a)-(d) is the number of time steps (i.e., 100$t$).

Figure 4: *Training using 3680 data points.* (a) the actual trajectory for $x$ (in red), 10 predicted trajectories from 10 runs using different random realizations, and the averaged predicted trajectory (in blue) up to 620 time steps into the future; (b) a zoom-in view of the average (out of 10 runs) predicted values for $x$ (in blue) vs. the actual values for $x$ (in red) – the shaded light blue region represents the 90 percent confidence interval of the predicted values; (c) error of the predicted results and its mean value (in blue); (d) standard deviation of the errors from (c). The $x$-axis in (a)-(d) is the number of time steps (i.e., 100$t$).

A rare transition event lies in its ability to separate the slow and fast components of the data with the help of some physical knowledge about the generating system.

Figure 10(a) shows the result obtained if we run the trained network used to obtain Figure 2 much further into the future. In this case the predicted trajectory, not surprisingly, fails to capture the second transition that occurs around $t = 71$. However, we are able to predict the second transition confidently
Figure 5: Training using 3670 data points. (a) the actual trajectory for $x$ (in red), 10 predicted trajectories from 10 runs using different random realizations, and the averaged predicted trajectory (in blue) up to 630 time steps into the future; (b) a zoom-in view of the average (out of 10 runs) predicted values for $x$ (in blue) vs. the actual values for $x$ (in red) – the shaded light blue region represents the 90 percent confidence interval of the predicted values; (c) error of the predicted results and its mean value (in blue); (d) standard deviation of the errors from (c). The $x$-axis in (a)-(d) is the number of time steps (i.e., 100$t$).

Figure 6: Root mean squared error (RMSE) of predicted trajectories vs. number of training data points, at the same training setting as that in: (a) Figure 2; (b) Figure 3; (c) Figure 4; (d) Figure 5. The $x$-axis in (a)-(d) represents 100$t$ and std is the abbreviation for standard deviation.

if more data points are used for training. This result is illustrated in Figure 8, where 7080 data points are used for training.

All the results discussed so far are obtained by training on a trajectory that starts from the initial time ($t = 0$) and ends at a time before a rare event occurs. A natural question is whether one can achieve prediction results of comparable quality using a shorter trajectory that comes sufficiently close to the rare event but starts at a later time $t > 0$. Given the chaoticity of the generating system with a known predictability horizon determined by the Lyapunov exponent, one expects the answer to this question is affirmative. Indeed, this is demonstrated by the results in Figure 9, where a trajectory starting at
A Example 1: A bi-stable system, driven by a fast Lorenz-63 system

Figure 7: Training using 3700 data points with the naive direct method. (a) the actual trajectory for x (in red), 10 predicted trajectories from 10 runs using different random realizations, and the averaged predicted trajectory (in blue) up to 315 time steps into the future; (b) a zoom-in view of the average (out of 10 runs) predicted values for x (in blue) vs. the actual values for x (in red) – the shaded light blue region represents the 90 percent confidence interval of the predicted values; (c) error of the predicted results and its mean value (in blue); (d) standard deviation of the errors from (c). The x-axis in (a)-(d) is the number of time steps (i.e., 100t).

Figure 8: Training using 7080 data points. (a) the actual trajectory for x (in red), 10 predicted trajectories from 10 runs using different random realizations, and the averaged predicted trajectory (in blue) up to 935 time steps into the future; (b) a zoom-in view of the average (out of 10 runs) predicted values for x (in blue) vs. the actual values for x (in red) – the shaded light blue region represents the 90 percent confidence interval of the predicted values; (c) error of the predicted results and its mean value (in blue); (d) standard deviation of the errors from (c). The x-axis in (a)-(d) is the number of time steps (i.e., 100t).

t = 40 and consisting of only 3080 data points (i.e. a reduction of 4000 data points compared to that in the previous scenario) is used for training. However, the length of the trajectory has to be sufficiently long and there may be a lower bound on the length to achieve this goal. This argument is partially supported by the results in Figure 6 and Figure 10(b), which show how the root mean squared error of the predicted trajectories varies with the length of the trajectory (number of training data points) used.
B. Example 2: A tri-stable system, subject to periodic forcing and driven by a fast Ornstein-Uhlenbeck-like process

Data generation. The data for $x$ is generated by the following slow-fast system:

\[
\dot{x}(t) = x(t)[1 - x(t)][1 + x(t)][x(t) + 2][x(t) + 2] + A \cos(2\pi t) + \sigma_0 z(t), \tag{27}
\]

\[
\dot{z}(t) = -\alpha_1 z(t) + \frac{\sigma_1}{\epsilon} y_2(t), \tag{28}
\]

where $x$ describes the state of the system of interest whose evolution is driven by a fast Ornstein-Uhlenbeck like signal $z$, and $y_2$ is the second component of the Lorenz-63 system (23)-(25). For data generation, we use a uniform time step of $\Delta t = 0.01$ to integrate (27)-(28) with $x(0) = 0.1$, $z(0), y_i(0) \sim \text{Unif}(-10,10)$ (for $i = 1, 2, 3$), $A = 0.5$, $\epsilon = 0.5$, $\sigma_0 = 0.2$, $\alpha_1 = 1000$, and $\sigma_1 = 1000\epsilon$, up for training for a fixed training setting.

Figure 9: Training using 3080 data points. (a) the actual trajectory for $x$ (in red), 10 predicted trajectories from 10 runs using different random realizations, and the averaged predicted trajectory (in blue) up to 935 time steps into the future; (b) a zoom-in view of the average (out of 10 runs) predicted values for $x$ (in blue) vs. the actual values for $x$ (in red) – the shaded light blue region represents the 90 percent confidence interval of the predicted values; (c) error of the predicted results and its mean value (in blue); (d) standard deviation of the errors from (c). The $x$-axis in (a)-(d) is the number of time steps (i.e., $100t$).

Figure 10: (a) the actual trajectory for $x$ (in red), 10 predicted trajectories from 10 runs using different random realizations, and the averaged predicted trajectory (in blue) using 3700 data points for training; (b) RMSE of the predicted trajectories vs. number of training data points, at the same training setting as that in Figure 8. The $x$-axis in (a)-(b) represents $100t$ and std is the abbreviation for standard deviation.
B Example 2: A tri-stable system, subject to periodic forcing and driven by a fast Ornstein-Uhlenbeck-like process

to time $t = 100$. The time step is small enough to sample the scale on which the fast signal takes place. The data generated is plotted in Figure 11. This data is split into a training and a testing set.

Figure 11: Time series data for $x$ in Example 2 up to time $t = 100$ (of which only a segment prior to $t = 94$ will be available for training) – Here, the x-axis is the number of time steps (i.e., 100).

Generating system: dynamics and applications. The system (27)-(28), is more complex than that in Example 1, of which it is an extended version, in the sense that the force field is generalized to include a time-dependent external force and the driving signal is described by a higher dimensional system. One can view (27)-(28) as a family of systems (parametrized by $\epsilon$) approximating the following SDE system:

$$
\begin{align*}
 dX(t) &= X(t)[1 - X(t)][1 + X(t)][X(t) - 2][X(t) + 2]dt + A\cos(2\pi t)dt + \sigma_0 Z(t)dt, \\
 dZ(t) &= -\alpha_1 Z(t)dt + \tilde{\sigma}_1 dW(t),
\end{align*}
$$

where $\tilde{\sigma}_1$ is an effective diffusion constant and $W(t)$ is a Wiener process. As $\epsilon$ (chosen to be 0.5 for data generation here) becomes smaller, $(x(t), z(t))$ converges in law to $(X(t), Z(t))$ solving the non-autonomous SDE system (29)-(30).

In contrast to Example 1, in the absence of the driving signal $z(t)$, equation (27) for $x$ has three stable periodic orbits centered at $x = -2, 0, 2$ and two unstable ones centered at $x = -1, 1$. Here our system state starts in the middle potential well and will, due to influence of the driving signal as well as the periodic forcing, transits to one of the left or right nearby stable orbits at a random time (see Figure 11). It is thus natural to ask which potential well will the system transit to and at what time will the transition occur?

The addition of the periodic forcing $A\cos(2\pi t)$ introduces another time scale into the system. When this time scale is of the same order of the mean exit time from the potential (the Kramers time), a resonance-like mechanism where the noise can lead to the amplification of the periodic signal takes place. This resonance is induced by a chaotic signal, and is closely related to stochastic resonance, a noise-induced phenomenon first introduced in the context of climate modeling [6, 7], which has been found to occur in many physical and biological systems [25].

One example of such systems describes the dynamics of an overdamped self-propelled active particle, which converts energy absorbed from the environment into a directed motion, rendering the system out of equilibrium. The position of the particle can be described by $X$ in (29) and the active force or self-propulsion is modeled by $Z$ in (30), in which case the particle is trapped in a triple-well potential and subject to periodic forcing. This is a variant of the model of an active Ornstein-Uhlenbeck process widely used to study active matter [12, 63].

Training and prediction details. To obtain the results in Figures 12-16, we apply Algorithm III.1-III.2 using a three-layered ESN (i.e., $n_L = 3, L = 2$) with $n_y = 1$. The DESN is driven by a constant input sequences of ones. The values of hyperparameters used to generate the results in these figures are given in Table II. For Figure 15, we refer to the caption for value of hyperparameters used there. The values of all these hyperparameters are not fully optimized. For numerical integration in (S3), we use a Runge-Kutta method with a uniform step size of 0.01.

We again perform an ensemble-like prediction by running the trained network 10 times into the future, each time run with different random realizations. We take the averaged values as the predicted values. To evaluate the quality of the predictions, we study the statistics (the mean and standard deviation) of the error between the predicted values and the actual values.

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Example 2: A tri-stable system, subject to periodic forcing and driven by a fast Ornstein-Uhlenbeck-like process

Table II: Values of hyperparameters used for obtaining the results for Example 2.

| Figure | Number of training data points | $n_{x_0} = n_{x_1} = n_{x_2}$ | $P_{des}^{(0)}$ | $P_{des}^{(1)}$ | $P_{des}^{(2)}$ | $r_0 = r_1 = r_2$ | $\nu$ |
|--------|-------------------------------|--------------------------------|----------------|----------------|----------------|------------------|-----|
| 12     | 9400                          | 200                           | 0.6            | 0.7            | 0.8            | 0.05             | 0.003 |
| 13     | 9390                          |                                |                |                |                |                  |      |
| 14     | 9380                          | 150                           | 0.55           | 0.65           | 0.75           | 0.08             | 0.002 |
| 16     | 9400                          | 200                           | 0.6            | 0.7            | 0.8            | 0.05             | 0.003 |

are displayed in Figures 12-14. Despite using a DESN with more than one layer, each run of the algorithm takes only a few minutes to complete on a 5-core CPU.

Figure 12: Training using 9400 data points. (a) the actual trajectory for $x$ (in red), 10 predicted trajectories from 10 runs using different random realizations, and the averaged predicted trajectory (in blue) up to 600 time steps into the future; (b) a zoom-in view of the average (out of 10 runs) predicted values for $x$ (in blue) vs. the actual values for $x$ (in red) – the shaded light blue region represents the 90 percent confidence interval of the predicted values; (c) error of the predicted results and its mean value (in blue); (d) standard deviation of the errors from (c). The $x$-axis in (a)-(d) is the number of time steps (i.e., 100$\ell$).

Figures 12-13 show that our method is capable of very confidently predicting the rare event and its transition path at least 10 time steps in advance. Note that the plots in Figure 12 and Figure 13 are very similar. This is because the numbers of data points used for training differ by only 10 and the same training setting is used to obtain the results in both figures, as discussed earlier in a similar case in Example 1. There is, however, a small quantitative difference between the results for these two cases, as demonstrated by the plots for standard deviation of the errors (see Figure 12(d) and Figure 13(d)).

However, Figure 14 shows how the inability of the DESN to make accurate long-term predictions again cripples the performance of the prediction method, making prediction of the rare event from an earlier time a very challenging task. We emphasize that these results are used primarily to demonstrate our method. It may be possible to improve these results by using a different training setting (with a higher number of layers and optimized values of hyperparameters), enabling successful longer-term prediction and therefore prediction of a rare event from an earlier time.

There is one notable difference from the results obtained for Example 1. The standard deviation for the errors of prediction grows initially but then peaks at a maximum value before decreasing, giving a bell-shaped curve (see Figures 12(d), 13(d)). This maximum value of standard deviation is about half of the saturated value of those in Example 1. A plausible explanation for this difference is as follows. Note that the orbit around one stable minimum of the potential in Example 2 is much more stable than the orbit around a stable minimum of the potential in Example 1. In fact, the Lyapunov exponent in Example 1 can be estimated to be about $-6$, whereas in Example 2 the exponent is about $-2$. Therefore, in Example 2 we expect that when we try to reconstruct the shape of the system path near the jump using many different (realizations of) trajectories provided by a trained DESN, they will differ significantly.
Example 2: A tri-stable system, subject to periodic forcing and driven by a fast Ornstein-Uhlenbeck-like process.

Figure 13: Training using 9390 data points. (a) the actual trajectory for \( x \) (in red), 10 predicted trajectories from 10 runs using different random realizations, and the averaged predicted trajectory (in blue) up to 610 time steps into the future; (b) a zoom-in view of the average (out of 10 runs) predicted values for \( x \) (in blue) vs. the actual values for \( x \) (in red) – the shaded light blue region represents the 90 percent confidence interval of the predicted values; (c) error of the predicted results and its mean value (in blue); (d) standard deviation of the errors from (c). The \( x \)-axis in (a)-(d) is the number of time steps (i.e., 100\( t \)).

Figure 14: Training using 9380 data points. (a) the actual trajectory for \( x \) (in red), 10 predicted trajectories from 10 runs using different random realizations, and the averaged predicted trajectory (in blue) up to 620 time steps into the future; (b) a zoom-in view of the average (out of 10 runs) predicted values for \( x \) (in blue) vs. the actual values for \( x \) (in red) – the shaded light blue region represents the 90 percent confidence interval of the predicted values; (c) error of the predicted results and its mean value (in blue); (d) standard deviation of the errors from (c). The \( x \)-axis in (a)-(d) is the number of time steps (i.e., 100\( t \)).

because here we are training the machine with the signal \( z(t) \) instead of the signal generated by the Lorenz-63 system. However, due to the high stability of that orbit, each of these trajectories will rapidly fall into it thereby rapidly decreasing the variance.

This heuristic argument can be extended to any shape of the attractive potential inside which the evolution of the system takes place. Two different conflicting tendencies can be found in the predicted...
Example 2: A tri-stable system, subject to periodic forcing and driven by a fast Ornstein-Uhlenbeck-like process.

Figure 15: Root mean squared error (RMSE) of predicted trajectories vs. number of training data points, at the same training setting as that in: (a) Figure 12; (b) Figure 13; (c) Figure 14. The $x$-axis in (a)-(c) represents 100$t$ and std is the abbreviation for standard deviation.

Figure 16: Training using 9400 data points with the naive direct method. (a) the actual trajectory for $x$ (in red), 10 predicted trajectories from 10 runs using different random realizations, and the averaged predicted trajectory (in blue) up to 600 time steps into the future; (b) a zoom-in view of the average (out of 10 runs) predicted values for $x$ (in blue) vs. the actual values for $x$ (in red) – the shaded light blue region represents the 90 percent confidence interval of the predicted values; (c) error of the predicted results and its mean value (in blue); (d) standard deviation of the errors from (c).

The machine learning algorithm is only able to reconstruct the immediate future of the system state and the quality of the predictions degrades for longer-term predictions. The second is the strength of the attraction of the potential that drives the system towards a stable orbit, which is characterized by the Lyapunov exponent. The first depends on the learning algorithm and the second depends on the physical model generating the data, and one of these tendencies will dominate the other.

We find that it is very difficult to obtain a comparable quality of prediction if we work with a shallow ESN, instead of the three-layered variant that we have used here. A closer look at the model for the driving signal $z(t)$ reveals that there are actually two widely separated time scales in the system.
generating it, instead of only one time scale as in the case of Example 1. This difference in the multiscale behavior of the system generating the driving signal explains why a shallow ESN works well for Example 1 but not for Example 2. A deep version of the ESN is needed to handle the multiscale nature of the data for $z$ in Example 2. This supports the intuition that increasing the depth of the ESN can lead to a better multiple time scale representation of the temporal information. This motivates our use of a deep version of the ESN for our method in Section III.

Figure 16 confirms that our method is far superior to the baseline method of applying a DESN to the data for $x$. Indeed, the ability of our method to predict, at least 10 time steps (0.1 period) in advance, has significant importance for many systems exhibiting stochastic resonance. The results in Figure 15 suggest the possibility of achieving prediction results of comparable quality using a shorter but sufficiently long trajectory starting at a later time $t > 0$ and coming sufficiently close to the rare event (see the relevant discussion on this in Subsection IV A).

V. CONCLUSIONS AND FINAL REMARKS

In this paper, we have presented a data-driven method for tackling the challenging task of predicting rare events in a large class of multiscale nonlinear dynamical systems. The method is demonstrated on two examples of different complexity, each providing a model for many important physical and biological systems. For both examples, we obtain excellent predictive performance, which would not be possible by using a direct method that does not take into account the multiscale nature of the problem. In particular, our method predicts a rare transition event up to several time steps in advance. The method incurs relatively low computational cost, thanks to the use of a reservoir computing based training technique, rather than a gradient descent based one. These results demonstrate the promise of our machine learning based method in predicting rare events occurring in a wide range of dynamical systems, a problem that is of substantial interest in science and engineering. We expect the accuracy of these results to improve by carefully optimizing the hyperparameters and using a more sophisticated machine learning algorithm.

We now discuss a few potential future directions. So far we have applied the method to two toy examples, where there are two widely separated time scales. In many systems of interest there may be more than two widely separated time scales and the competition between them may be crucial in triggering a rare event. The driving noise may also be multiplicative in nature. Therefore, it is important to extend the present work to these systems. In many realistic situations, the available time series data may be multivariate, rather than univariate, and moreover there may be missing and/or uneven data. It would then be important to extend our method to cover these situations.

It is also of practical interest to apply the method presented here to study more non-trivial yet physically relevant data sets, such as that generated by a chaotic version of the model in [20] and real world data from climate science [62, 64]. On the other hand, because the method is based on the use of a deep version of echo state network, a firm theoretical understanding of the underpinnings behind such a network, in particular its initialization and the generalization error, will shed light on the nature of the prediction results. Therefore, it is important to carry out a systematic theoretical study of how and why the network works.

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One could of course run the network a different number of times, but we choose to work with 10 runs here.

It is a partial argument because the relationship between the RMSE and number of data points used for training does vary with the training setting as well as the length of the prediction horizon. Moreover, one usually adapts the training setting (tuning the hyperparameters) according to the number of data points available for training to minimize the RMSE.

One could of course run the network a different number of times, but we choose to work with 10 runs here.

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