Discovering Dynamical Parameters by Interpreting Echo State Networks

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Abstract

Reservoir computing architectures known as echo state networks (ESNs) have been shown to have exceptional predictive capabilities when trained on chaotic systems. However, ESN models are often seen as black-box predictors that lack interpretability. We show that the parameters governing the dynamics of a complex nonlinear system can be encoded in the learned readout layer of an ESN. We can extract these dynamical parameters by examining the geometry of the readout layer weights through principal component analysis. We demonstrate this approach by extracting the values of three dynamical parameters (σ, ρ, β) from a dataset of Lorenz systems where all three parameters are varying among different trajectories. Our proposed method not only demonstrates the interpretability of the ESN readout layer but also provides a computationally inexpensive, unsupervised data-driven approach for identifying uncontrolled variables affecting real-world data from nonlinear dynamical systems.

1 Introduction

The analysis and modeling of complex nonlinear dynamics is a key problem across a broad range of disciplines in science and engineering [1]. While supervised deep learning approaches can provide excellent predictive performance on dynamical systems [2–4], difficulties with interpretability limit their usefulness in some scientific applications. For example, consider the problem of identifying uncontrolled dynamical parameters causing variations in the dynamics of a set of observed trajectories. Directly learning a black-box predictor for each trajectory does not provide any insight into how the dynamics are changing between trajectories. Potential approaches for solving this problem include methods that attempt to directly recover the symbolic governing equations [5–9], which often require a large library of possible terms along with assumptions about the sparsity of the equations, and Koopman operator-based methods [10–13] that map the nonlinear dynamics to an interpretable linear system but struggle with chaotic dynamics. Unsupervised learning approaches that use deep autoencoder architectures to provide interpretability have also been investigated [14, 15].

We propose an alternative approach for discovering varying dynamical parameters that is based on echo state networks (ESNs), a type of reservoir computing architecture [16, 17]. ESNs provide a fast and easy way to build predictive models for dynamical systems [18–20] and have been shown to perform remarkably well when trained to forecast complex nonlinear dynamics exhibiting high-dimensional chaos [4, 19, 21]. While superficially similar to recurrent architectures in deep learning, ESNs are inexpensive to train and do not suffer from exploding or vanishing gradients due to their use of a large sparse reservoir with fixed weights [4, 18]. Correctly constructed ESNs also exhibit the echo state property [16, 22], which provides many nice theoretical guarantees and allows for the ESN to be effectively trained by only fitting the output weights of the final readout layer via linear regression.

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However, ESNs are generally considered black-box predictors that have the same issues with interpretability as deep learning approaches. Our work demonstrates that this is not the case. By sharing the fixed weights across a series of separately trained ESNs, we can interpret the learned output weights from the readout layer as a representation of the system dynamics and use manifold learning to extracted the varying dynamical parameters affecting the data. Using the chaotic Lorenz system [23] as an example, we show that this approach is able to quickly and accurately learn high-quality predictive models and then extract an embedding which encodes three distinct varying parameters that affect the dynamics of the system.

2 Methods

To produce a set of interpretable representations of the system dynamics, we train a series of echo state networks (ESNs) that share the same reservoir and input weights. Each ESN is trained on a distinct trajectory in the dataset and, after training, produces a linear readout layer which we use as our representation of the dynamics. We then analyze the geometry of the readout layer weights using a manifold learning method—in our case, principal component analysis (PCA)—and extract parameters that account for the varying dynamics among the trajectories in the dataset.

2.1 ESN training and prediction

ESNs are reservoir computing architectures that consist of a large, fixed sparse reservoir $\mathbf{A} \in \mathbb{R}^{n \times n}$ with hidden size n, a fixed set of input weights $\mathbf{W}_{\text{in}} \in \mathbb{R}^{n \times d}$, and a trained set of output or readout weights $\mathbf{W}_{\text{out}} \in \mathbb{R}^{d \times n}$. A standard discrete time ESN can model a d-dimensional dynamical system

$$\frac{\mathrm{d}\mathbf{u}(t)}{\mathrm{d}t} = \mathbf{F}_\theta(\mathbf{u}(t)) \tag{1}$$

with dynamical parameters θ and states $\mathbf{u}(t) \in \mathbb{R}^d$ discretized as a time series $\{\mathbf{u}_{t_0}, \mathbf{u}_{t_0+\Delta t}, \ldots\}$ with a fixed time step Δt.

Training—To train the output weights $\mathbf{W}_{\text{out}}$, we first feed a training trajectory $\{\mathbf{u}_t\}_{t=t_0}^{T_{\text{train}}}$ into the ESN in a recurrent fashion

$$\mathbf{r}_{t+\Delta t} = \tanh(\mathbf{A}\mathbf{r}_t + \mathbf{W}_{\text{in}}\mathbf{u}_t), \tag{2}$$

producing a series of hidden reservoir states $\{\mathbf{r}_{t_0}, \mathbf{r}_{t_0+\Delta t}, \ldots\}$ where each $\mathbf{r}_t \in \mathbb{R}^n$ and $\mathbf{r}_{t_0} = \mathbf{0}$ is initialized as the zero vector. The output weights $\mathbf{W}_{\text{out}}$ are then fitted using a (regularized) linear regression to map the hidden states $\mathbf{r}_t$ back to the physical states $\mathbf{u}_t$ such that $\mathbf{u}_t \approx \mathbf{W}_{\text{out}}\mathbf{r}_t$, corresponding to the final readout layer of the ESN. Because the training only involves passing the inputs through the ESN once and then fitting the final readout layer using linear regression, this process is both fast and computationally inexpensive.

Prediction—To predict the future states of a test trajectory $\{\mathbf{u}_t\}_{t=t_0}^{T_{\text{test}}}$, the new trajectory is fed recurrently into the ESN as during training (2), and then future physical states $\hat{\mathbf{u}}_t = \mathbf{W}_{\text{out}}\mathbf{r}_t$ for $t > T_{\text{test}}$ are computed using the output weights from the readout layer. The predicted states $\hat{\mathbf{u}}_t$ are then fed back into the recurrent architecture to obtain subsequent hidden states

$$\mathbf{r}_{t+\Delta t} = \tanh(\mathbf{A}\mathbf{r}_t + \mathbf{W}_{\text{in}}\hat{\mathbf{u}}_t). \tag{3}$$

2.2 Training ESNs with unique and comparable readout layers

Because our approach treats the trained output weights $\mathbf{W}_{\text{out}}$ from the readout layer as a representation of the system dynamics, we require $\mathbf{W}_{\text{out}}$ to be comparable across ESNs trained on distinct trajectories with varying dynamics. To ensure this, we use the same fixed reservoir and input weights for all our ESNs and impose L_2 regularization on the linear regression (i.e. ridge regression) when fitting $\mathbf{W}_{\text{out}}$. Along with proper initialization of the ESN to ensure the echo state property (ESP) is fulfilled [16, 22], these conditions also maintain uniqueness among the learned readout layers corresponding to different dynamics. The ESP guarantees that each input sequence $\{\mathbf{u}_t\}_{t=-\infty}^{T-1}$ corresponds to a unique reservoir state $\mathbf{r}_T$. Then, because the dynamical system is Markovian (1), each set of dynamical parameters θ and physical state $\mathbf{u}_T$ have a unique input sequence history and so correspond to a unique $\mathbf{r}_T$. Therefore, the mapping $\mathbf{r}_T \to \mathbf{u}_T$, which is approximated by the readout layer, is also unique for each θ. Finally, by using ridge regression to fit the readout layer—a common practice for training ESNs—we obtain a unique set of output weights $\mathbf{W}_{\text{out}}$ for each θ.

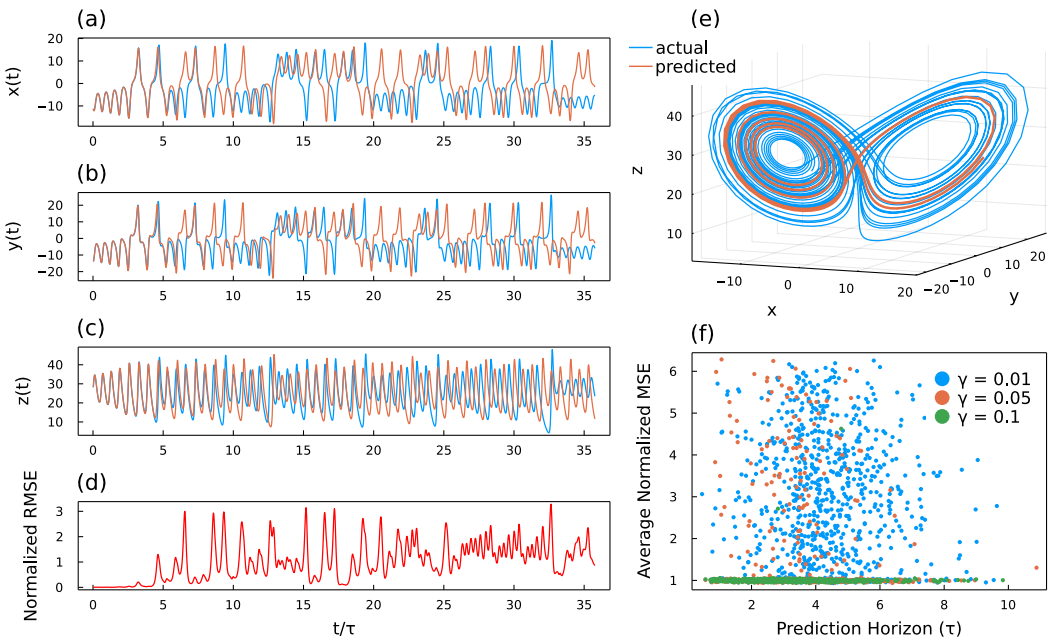

Figure 1: Prediction example for a test trajectory with dynamical parameters $\sigma = 10.3$, $\rho = 29.2$, $\beta = 2.58$. (a)–(c) The plots of the individual states x, y, z of the Lorenz system show the predicted dynamics (orange) compared with the actual ground truth dynamics (blue). Times are given in units of τ, the Lyapunov time of the dynamics. (d) The root mean squared error (RMSE) between the predicted and actual dynamics (normalized by the standard deviation over the entire trajectory) is used to define the prediction horizon, which corresponds to the first time at which the normalized RMSE rises above 1. The prediction horizon for this example is 4.56τ. (e) The phase space plot consists of the full trajectory of the actual dynamics (blue) alongside a partial trajectory of the predicted dynamics (orange), showing the predicted trajectory up to the prediction horizon where the two trajectories diverge. (f) For three sets of ESNs trained with ridge regression parameters $\gamma = 0.01$, 0.05, 0.1, the average mean squared error (MSE) over the entire test trajectory (normalized by twice the variance) is plotted versus the prediction horizon for each example in the test set. We ultimately chose to use $\gamma = 0.1$, which results in good long-term prediction stability as indicated by an average normalized MSE that is consistently low and close to 1.

2.3 Extracting dynamical parameters using manifold learning

Once we have the dynamics encoded in the output weights $\mathbf{W}_{\text{out}}$, we can analyze the geometry of this representation by performing manifold learning. In our experiments, we found that applying PCA to the flattened output weights was enough to extract a reasonable low-dimensional embedding that encodes the dynamical parameters θ.

3 Lorenz System Experiment

The Lorenz system [23] is a three-dimensional chaotic dynamical system governed by

$$\begin{aligned} \frac{\mathrm{d}x}{\mathrm{d}t} &= \sigma(y - x) \\ \frac{\mathrm{d}y}{\mathrm{d}t} &= x(\rho - z) - y \\ \frac{\mathrm{d}z}{\mathrm{d}t} &= xy - \beta z \end{aligned} \tag{4}$$

with the parameters σ, ρ, β traditionally chosen to be 10, 28, $8/3$, respectively. For our dataset, we generate 1000 trajectories each with 300,000 time steps ($\Delta t = 0.02$) for training and a subsequent 50,000 time steps for testing. For each trajectory, we independently sample the three dynamical

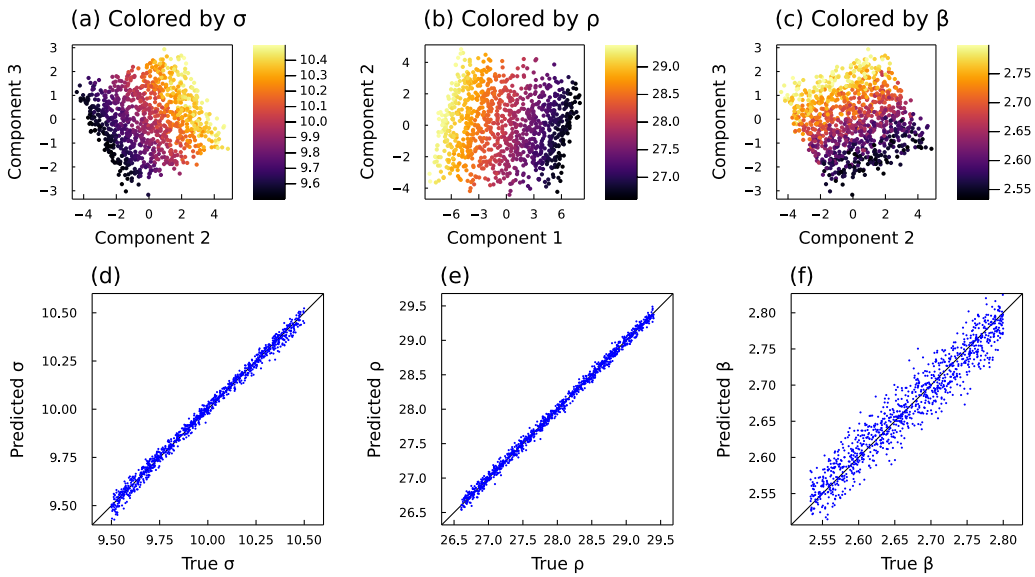

Figure 2: Three-dimensional embedding of the varying dynamical parameters σ, ρ, β of the Lorenz system extracted from the trained output weights $\mathbf{W}_{\text{out}}$ using PCA. (a)–(c) The scatter plots show cross-sections of the extracted embedding colored by the ground truth parameters σ, ρ, β. ρ is primarily aligned with component 1, while σ and β are embedded in components 2 and 3. (d)–(f) The predicted dynamical parameters, based on a linear fit from the extracted embedding, are plotted versus the ground truth parameters. The parameters σ and ρ are very well represented with $R^2 = 0.993$ and 0.996, respectively, while the embedding of β is slight noisier with $R^2 = 0.925$.

parameters σ, ρ, β from uniform distributions that cover $\pm 5\%$ of their standard values to mimic uncontrolled variations in the dynamics. Using ESN initialization hyperparameters suggested by Haluszczynski and Räth [20] and ridge regression regularization parameter $\gamma = 0.1$, we achieve long-term stability and good prediction performance (Fig. 1) with a mean prediction horizon of 3.2τ. Here, $\tau = \Lambda_{\max}^{-1}$ refers to the Lyapunov time, i.e. the inverse of the maximum Lyapunov exponent $\Lambda_{\max}$, of the chaotic system which characterizes how quickly two similar trajectories diverge.

Applying PCA to the trained output weights $\mathbf{W}_{\text{out}}$, we are able to extract a three-dimensional embedding that directly corresponds to the varying dynamical parameters σ, ρ, β of the Lorenz system (Fig. 2(a)–(c)). We also obtain high-quality linear fits for the parameters σ, ρ, β from the extracted three-dimensional embedding (Fig. 2(d)–(f)) with R^2 correlation coefficients of 0.993, 0.996, 0.925, respectively.

4 Conclusion

We have empirically confirmed that parameters governing the dynamics of a nonlinear system are encoded in the readout layer of a trained ESN and have demonstrated a method for extracting an embedding of the varying dynamical parameters using PCA. Our proposed method for analyzing data from dynamical systems, including chaotic systems, provides a fast and computationally inexpensive approach for both predicting future states and understanding the uncontrolled variables causing variations in the dynamics. Given the extracted embedding of the dynamical parameters, it should also be feasible to approximately reconstruct ESN output weights as a function of the identified dynamical parameters, effectively creating a tunable model for the dynamics learned from the data. This would aid in directly interpreting unknown dynamical parameters extracted using our method, so we hope to explore this direction in the near future. Also, because our approach builds on top of standard ESN training methods, it would be straightforward to adapt for any applications where ESNs are currently being used purely for prediction. These applications include modeling EEG signals [24], making atmospheric climate predictions [25], and scaling up ESNs to model arbitrarily high-dimensional chaotic attractors [21]. As such, we plan to test our method on a wider variety of examples, including systems exhibiting spatiotemporal chaos.

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