Auto-Encoded Reservoir Computing for Turbulence Learning

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Abstract. We present an Auto-Encoded Reservoir-Computing (AE-RC) approach to learn the dynamics of a 2D turbulent flow. The AE-RC consists of a Convolutional Autoencoder, which discovers an efficient manifold representation of the flow state, and an Echo State Network, which learns the time evolution of the flow in the manifold. The AE-RC is able to both learn the time-accurate dynamics of the turbulent flow and predict its first-order statistical moments. The AE-RC approach opens up new possibilities for the spatio-temporal prediction of turbulent flows with machine learning.

Keywords: Echo State Network · Autoencoder · Turbulence.

1 Introduction

The spatio-temporal prediction of turbulence is challenging because of the flow’s extreme sensitivity to perturbations, the nonlinear interactions between turbulent structures of different scales, and the unpredictable nature of energy/dissipation bursts. Despite these complex characteristics of turbulence, many advances have been achieved in its understanding with, for example, the energy cascade concept that provides a statistical description of the energy transfer between different scales in turbulent flows [5]. Additionally, the existence of coherent structures, such as vortices, that evolve in a deterministic way, provides us with basic building blocks that can serve as basis for our understanding and prediction of turbulence [11]. These findings indicate that, within the apparent chaotic nature of turbulence, there exist identifiable patterns that can help us predict the evolution of turbulent flows. To discover such features, recent works have relied on machine learning techniques [1]. In particular, the dynamics of models of turbulent flows has been learned by recurrent neural networks (RNNs) such as the Long Short-Term Memory units [9,10] or a physics-informed reservoir computing (RC) approach, based on Echo State Networks (ESN) [2]. Despite

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their success, because RNNs are generally limited to low-dimensional datasets due to the complexity in training, past studies have been limited to fairly low-dimensional systems. To deal with high dimensional fluid mechanical systems, recent approaches based on convolutional neural networks (CNNs), and in particular Autoencoders (AE), have shown great potential in discovering coherent structures in turbulent flows and reducing the dimensionality of flows [1,7].

In this paper, we propose the Auto-Encoded Reservoir Computing framework (AE-RC). This combines an ESN and an AE with the objective of learning the spatio-temporal dynamics of a two-dimensional turbulent flow governed by the Navier-Stokes equations (the Kolmogorov flow). The flow is discussed in Section 2. The AE-RC framework is presented in Section 3. The predictions of the AE-RC framework are presented in Section 4. The final section summarizes the results and outlines avenues for future work.

2 Turbulent flow

We investigate two-dimensional turbulence governed by the incompressible Navier-Stokes equations

\[
\nabla \cdot \mathbf{u} = 0
\]

\[
\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \Delta \mathbf{u} + \mathbf{f}
\]

where \(\mathbf{u} = (u, v)\) is the velocity field, \(p\) is the pressure, \(Re\) is the Reynolds number, and \(\mathbf{f}\) is a harmonic volume force defined as \(\mathbf{f} = (\sin(k_f y), 0)\) in Cartesian coordinates. The Navier-Stokes equations are solved on a domain \(\Omega \equiv [0, 2\pi] \times [0, 2\pi]\) with periodic boundary conditions. (The solution of this problem is also known as the 2D Kolmogorov flow.) The flow has a laminar solution \(u = Re k_f^{-2} \sin(k_f y), v = 0\), which is unstable for sufficiently large Reynolds numbers and wave numbers \(k_f\) [8]. Here, we take \(k_f = 4\) and \(Re = 30\) to guarantee the development of a turbulent solution [10]. The set of Eqs. (1) and (2) is solved on a uniform \(N \times N\) grid, with \(N = 24\), using a pseudo-spectral code with explicit Euler time-stepping similar to the one in [10] with a timestep, \(\Delta t = 0.01\), to ensure numerical stability. Snapshots of the velocity and vorticity, \(\omega\), fields are shown in Fig. 1, in which the complexity and chaotic pattern of the turbulent flow can be observed. Figures 3b and 3c show the time evolution of the kinetic energy, \(k\), and dissipation, \(D\), which are calculated as \(k(\mathbf{u}) = (2\pi)^{-2} \int_\Omega \frac{1}{2} |\mathbf{u}|^2 d\Omega\) and \(D(\mathbf{u}) = Re^{-1} (2\pi)^{-2} \int_\Omega |\nabla \mathbf{u}|^2 d\Omega\), respectively. The solution is turbulent.

3 Auto-Encoded Reservoir Computing

The proposed Auto-Encoded Reservoir Computing (AE-RC) framework is shown in Fig. 3a. The AE-RC is composed of two parts: (i) an autoencoder (AE), which is composed of an encoder and a decoder; and (ii) an echo state network, which is a form of reservoir computing [6]. The role of the AE is to discover an efficient
Fig. 1. Isocontours of (a) $u$, (b) $v$ and (c) vorticity for the 2D turbulent flow at Re = 30 at time $t = 0$. (d) Time evolution of kinetic energy, $k$, and (e) dissipation, $D$, of the 2D turbulent flow.

reduced-order representation of the original data, $u \in \mathbb{R}^{N \times N \times 2} = N_u$. On the one hand, the encoder reduces the dimension of the data to a code, $c \in \mathbb{R}^{N_c}$, where $N_c < N_u$. On the other hand, the decoder reconstructs the data from the code, $c$, by minimizing the error between the reconstructed solution, $\hat{u}$, and the data. Here, the AE consists of a series of CNNs, which identify patterns within images through kernel operations \[3\]. The details of the AE are shown in Fig. 2b. On the downsampling side, the encoder is composed of multiple blocks of successive 2D CNNs, max pooling and dropout layers. Dropout layers, with a dropout rate of 0.001, avoid overfitting, while max pooling layers decrease the dimension of the input data. The value of the dropout rate was chosen during the training of the AE, which is described below, to ensure a similar level of accuracy on the training and validation datasets. At the last layer of the encoder, a dense feedforward neural network is used to fully combine the information from the previous layer to compress the data into the final code of dimension 192, compared to the original data of dimension $24 \times 24 \times 2 = 1152$. On the upsampling side, the decoder has an architecture that mirrors that of the encoder, but the dimension of the code is progressively increased using bilinear upsampling layers to recover the original information \[7\].

To learn the temporal dynamics of the reduced representation obtained with the AE, an Echo State Network (ESN) similar to that introduced in \[6\], given their accuracy in learning the dynamics of chaotic systems \[2\] \[6\]. The ESN receives the code as an input at a time $n$, $c(n)$, and approximates the code at the subsequent time step, $c(n + 1)$, as an output. An ESN is composed of three parts: (i) a randomized high dimensional dynamical system, called the reservoir, whose states of neurons (or units) states at time $n$ are represented by a vector, $x(n) \in \mathbb{R}^{N_x}$; (ii) an input matrix, $W_{in} \in \mathbb{R}^{N_x \times N_c}$, and (iii) an output matrix, $W_{out} \in \mathbb{R}^{N_y \times N_x}$ where $N_y$ is the dimension of the output of the ESN. The output of the ESN, $\hat{y}$, is a linear combination of the reservoir states, $\hat{y}(n) = W_{out}x(n)$. 
The evolution of the neurons’ states is given by the discrete nonlinear law

$$x(n) = \tanh (W_{in} c(n) + W x(n - 1))$$

(3)

Because the aim is to predict the dynamics of the reduced order representation, the output of the ESN is the predicted subsequent state of the reduced order representation, i.e., $\hat{y}(n) \approx c(n + 1)$. In the ESN approach, $W_{in}$ and $W$ are randomly initialized once and are not trained. Only $W_{out}$ is trained. The sparse matrices $W_{in}$ and $W$ are constructed to satisfy the Echo State Property. Following [2], $W_{in}$ is generated such that each row of the matrix has only one randomly chosen nonzero element, which is independently taken from a uniform distribution in the interval $[-\sigma_{in}, \sigma_{in}]$. Matrix $W$ is constructed with an average connectivity $\langle d \rangle$, and the non-zero elements are taken from a uniform distribution over the interval $[-1, 1]$. All the coefficients of $W$ are then multiplied by a constant coefficient for the largest absolute eigenvalue of $W$, i.e. the spectral radius, to be equal to a value $\lambda$, which is typically smaller than (or equal to) unity. The exact parameters of the ESN used here are provided in Fig. 2b. The training procedure to train the AE-RC is provided in the grey box below.

**AE-RC TRAINING PROCEDURE**

1. **Pre-train the AE** with the 2D velocity field as input/output. The reconstruction error, $E = \frac{1}{N_t} \sum_{n=1}^{N_t} ||u(n) - \hat{u}(n)||^2$ where $N_t$ is the number of samples, is minimized. The AE learns an appropriate reduced order representation, $c$, of $u$. 

Fig. 2. (a) Schematic and (b) details of the AE-RC. Number in boxes indicate the number of filters (for CNN) or neurons (for Dense layer). [:] : dimension of the signal. tanh activation is used for all layers except the last layer in which a linear activation is used to reconstruct the velocity in the full range of real numbers. All MaxPool and upsampling layers have a window of $(2, 2)$. All CNNs layers have a kernel of $(3, 3)$.
2. **Construct the reduced representation** of the original dataset with the pre-trained AE. Using the encoder part of the AE, the time-series \( c(n) \) is computed from \( u(n) \).

3. **Pre-train the ESN** using the dataset \( c(n) \) and ridge regression, 
   \[
   W_{out} = Y X^T \left( X X^T + \gamma I \right)^{-1},
   \]
   where \( Y \) and \( X \) are the horizontal concatenation of the target data, \( c(n) \), and the associated ESN states \( x(n) \), respectively. \( \gamma \) is the Tikhonov regularization factor [6].

4. **Train the combined AE-RC** for further fine-tuning. The AE-RC receives \( u(n) \) as an input and predicts \( \hat{u}(n+1) \). The training minimizes 
   \[
   L = \frac{1}{N_t} \sum_{n=1}^{N_t} ||u(n+1) - \hat{u}(n+1)||^2,
   \]
   where \( \hat{u}(n+1) \) is the prediction of the AE-RC at the next timestep, given an input \( u(n) \).

Steps 1 to 3 are used to obtain an initial AE-RC that is the initial guess for the training of the entire AE-RC in Step 4. This accelerates the overall training of the AE-RC by taking advantage of the fast training of the ESN with ridge regression compared to a random initialization of the AE-RC. The ADAM optimizer [4] is used for Steps 1 and 4 with a learning rate of 0.0001.

4 **Results**

The AE-RC framework presented in Sec. 3 is applied for learning the dynamics of the two-dimensional turbulent flow described above (Kolmogorov flow). The training dataset corresponds to the first 70% of the time-evolution shown in Fig. 1 and the subsequent 10% are used for validation. The AE-RC receives the 2D velocity field at a given timestep, as the input, and predicts the velocity field at the next timestep, as the output. The predictions of the kinetic energy, \( k \), and dissipation, \( D \), during training are shown in Fig. 3. The AE-RC accurately reproduces the evolution in the training data. To assess the extrapolation capability, the output of the AE-RC is looped back as an input so that the AE-RC can evolve autonomously. The learned extrapolated time-series of \( k \) and \( D \) are shown in Fig. 4 (the insets of the vorticity fields are shown for different time instants). The AE-RC reproduces the spatio-temporal evolution of \( k \) and \( D \), which is in agreement with the physical evolution of the turbulent flow. The instantaneous differences between the physical solution and the machine-learned solution stem from the spatio-temporally chaotic nature of the flow, in which small errors in the initial conditions propagate exponentially until nonlinear saturation (the “butterfly effect”). Thus, in chaotic systems, the statistics of the velocity field are typically compared to assess the accuracy of a solution. Figure 5 shows the time-averaged velocity profiles respectively, computed over the duration shown in Fig. 4. Because the error is small (less than 6% and 4% of error on average for \( u \) and \( v \) respectively), it is concluded that the AE-RC has learned the dynamics of the Kolmogorov flow also in a statistical sense (for the first moment). The standard deviations of the velocity profile were also computed and found to be of similar accuracy as those of time-averaged velocity (not shown here).
Fig. 3. Time evolution of (a) $k$ and (b) $D$ for the 2D turbulent flow during the training stage. The AE-RC is “teacher-forced” (the input is provided by the training data). Blue lines: actual evolution. Dashed red lines: AE-RC.

Fig. 4. Time evolution of (a) $k$ and (b) $D$ for the 2D turbulent flow. Vertical dotted lines indicates the time-instants for the snapshots (i) to (iii) of vorticity. For each snippets: (left) actual evolution, (right) AE-RC prediction.

Fig. 5. Prediction of time-averaged $u$ (top row) and $v$ (bottom row) profile. Right column: absolute error between AE-RC prediction and actual profile.
5 Conclusions and future directions

We propose the Auto-Encoded Reservoir-Computing framework (AE-RC) to learn the dynamics of high-dimensional turbulent flows, which are both spatially and temporally chaotic. This framework is composed of an Autoencoder, which learns an efficient reduced order representation of the flow state, and an Echo State Network, which learns the dynamics of the reduced order representation. With these two components, the AE-RC is able to learn both the instantaneous and average dynamics of the two-dimensional turbulent flow governed by the incompressible Navier-Stokes equations (the Kolmogorov flow). In future work, this framework is being assessed on flow conditions that also exhibit bursts of kinetic energy.

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