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AUTOMATIC DISCOVERY OF LOW-DIMENSIONAL DYNAMICS UNDERPINNING TIME-DEPENDENT PDES BY MEANS OF LATENT DYNAMICS NETWORKS

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We present a novel Machine Learning technique able to learn differential equations that surrogate the solution of space-time-dependent problems. Our method exploits a finite number of latent variables, providing a compact representation of the system state, automatically discovered during training. It allows building, in a fully non-intrusive manner, surrogate models accounting for the dependence on parameters and time-dependent inputs. This work pushes forward a novel technology towards the construction of data-driven digital twins in various application fields.

Keywords: *data-driven modeling, scientific machine learning, surrogate modeling, latent dynamics networks*

1. Introduction

Predicting the evolution of systems that exhibit spatio-temporal dynamics in response to external stimuli is a key enabling technology fostering scientific innovation. Traditional equations-based approaches leverage first principles to yield predictions through the numerical approximation of high-dimensional systems of differential equations, thus calling for large-scale parallel computing platforms and requiring large computational costs. Data-driven approaches, instead, enable the description of systems evolution in low-dimensional latent spaces, by leveraging dimensionality reduction and deep learning algorithms [1, 2, 3, 4, 5, 6]. Through the data-driven modeling approach, our work provides a solid methodological foundation for creating digital twins, enabling predictive simulation in a fast and accurate manner [7].

2. Methods

We propose a novel architecture, named Latent Dynamics Network (LDNet), which is able to discover low-dimensional intrinsic dynamics of possibly non-Markovian dynamical systems, thus predicting the time evolution of space-dependent fields in response to external inputs [8]. Unlike popular approaches, in which the latent representation of the solution manifold is learned by means of auto-encoders that map a high-dimensional discretization of the system state into itself, LDNets automatically discover a low-dimensional manifold while learning the latent dynamics, without ever operating in the high-dimensional space. Furthermore, LDNets are meshless algorithms that do not reconstruct the output on a predetermined grid of points, but rather at any point of the domain, thus enabling weight-sharing across query-points. These features make LDNets lightweight and easy-to-train, with excellent accuracy and generalization properties, even in time-extrapolation regimes.

3. Results

We demonstrate the effectiveness of LDNets through several test cases. First, we consider a linear PDE model to analyze the ability of LDNets to extract a compact latent representation of models that are progressively less amenable to reduction. Then, we consider the time-dependent version of a benchmark problem in fluid dynamics. Finally, we compare LDNets with state-of-the-art methods in a challenging task, that is, learning the dynamics of the Aliev-Panfilov model [9], a highly non-linear excitation-propagation PDE model used in the field of cardiac electrophysiology modeling. In the latter test case (see Fig. 1) we show that LDNets outperform state-of-the-art methods in terms of accuracy (normalized error 5 times smaller), by employing a dramatically smaller number of trainable parameters (more than 10 times fewer).

We focus on synthetically generated data obtained by numerical approximation of differential models, thus allowing us to test LDNet predictions against ground-truth results. We evaluate the prediction accuracy of the trained models using two metrics: the normalized root-mean-square error (NRMSE) and the Pearson dissimilarity, $1 - \rho$, where ρ is the Pearson correlation coefficient. To tune hyperparameters, we employ a Bayesian approach, namely the Tree-structured Parzen Estimator algorithm [10], combined with Asynchronous Successive Halving scheduler to early terminate bad hyperparameters configurations [11].

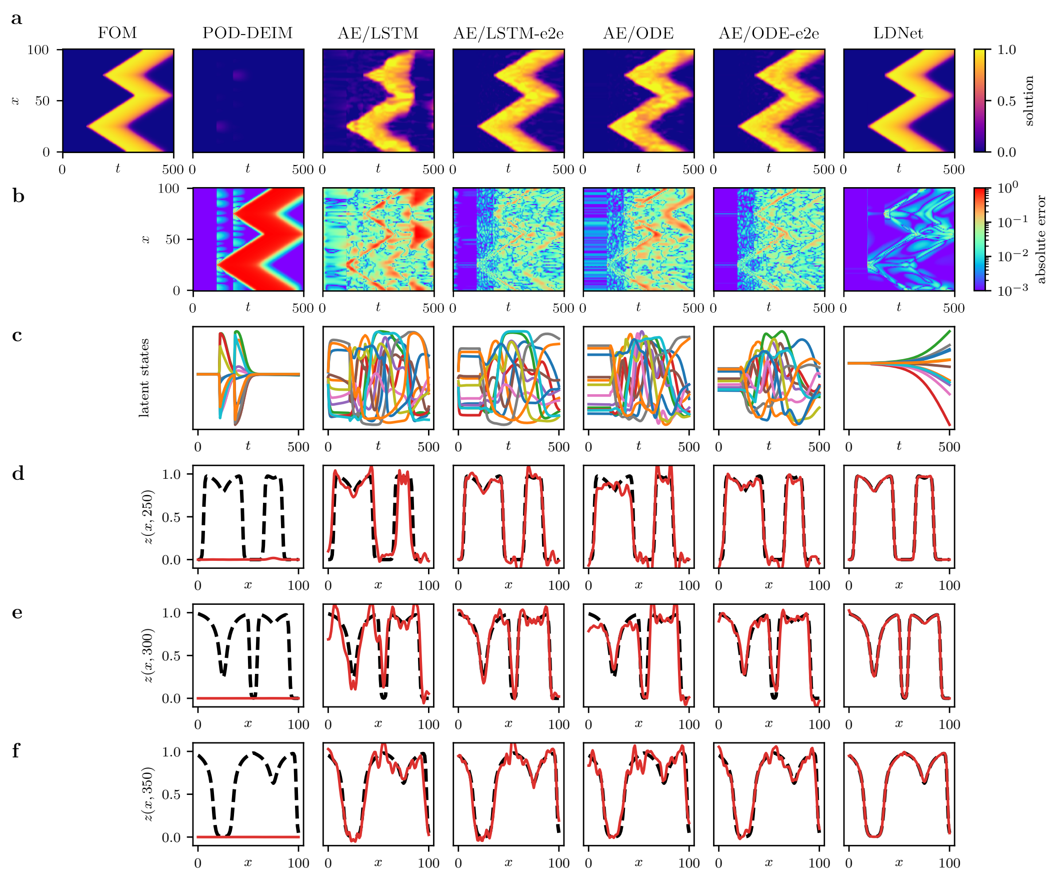

Figure 1: Results of the Aliev-Panfilov test case. We compare the results obtained different methods (reported in the captions) for a sample belonging to the test dataset. The left-most column reports the FOM solution of the AP model (the abscissa denotes time, the ordinate denotes space). For each method we report: **(a)** the space-time solution; **(b)** the space-time error with respect to the FOM solution; **(c)** the time-evolution of the 12 latent variables; **(d)**-**(e)**-**(f)** three snapshots of the space-dependent output field at $t = 250$, 300 and 350, in which we compare the predicted solution (red solid line) with the FOM solution (black dashed line).

4. Conclusions

LDNets represent, as proved by the results of this work, an innovative tool capable of learning spatio-temporal dynamics with great accuracy and by using a remarkably small number of trainable parameters. They are able to discover, simultaneously with the system dynamics, compact representations of the system state, as shown in Test Case 1 where the Fourier transform of a sinusoidal signal is automatically discovered. Once trained, LDNets provide predictions for unseen inputs with negligible computational effort (order of milliseconds for the considered Test Cases). LDNets provide a new flexible and powerful tool for data-driven digital twins that is open to a wide range of variations in the definition of the loss function (like, e.g., including physics-informed terms), in the training strategies, and, finally, in the NN architectures. The comparison with state-of-the-art methods on a challenging problem, such as predicting the excitation-propagation pattern of a biological tissue in response to external stimuli, highlights the full potential of LDNets, which outperform the accuracy of existing methods while still using a significantly lighter architecture.

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