SAND2022-14099C

State Space Reconstruction from Embeddings of Partial Observables in Structural Dynamic Systems for Structure-Preserving Data-Driven Methods

David A. Najera-Flores[1,2] and Michael D. Todd[1]

[1]Department of Structural Engineering
University of California San Diego, La Jolla, CA USA 92093

[2]ATA Engineering, Inc., San Diego, CA USA 92128

ABSTRACT
Data-driven machine learning models are useful for modeling complex structures based on empirical observations, bypassing the need to generate a physical model in cases where the physics is not well known or easily modeled. One disadvantage of purely data-driven approaches is that they tend to perform poorly in regions outside the original training domain. To mitigate this limitation, physical knowledge about the structure can be embedded in the model architecture via the model topology or numerical constraints in the formulation. We propose a neural network framework based on Hamiltonian mechanics to enforce a physics-informed structure to the model. The Hamiltonian framework allows us to relate the energy of the system to the measured quantities (e.g., accelerations) through the Euler-Lagrange equations of motion. A challenge with this hybrid data-driven, physics-constrained approach is the problem of limited observability, or not being able to measure structural response in a complete coordinate system that is compatible with the physical constraints being enforced. To overcome this issue, we propose combining a neural network autoencoder architecture with knowledge from embedding theory to enrich the limited observable data with time-delay embeddings. From Taken's theorem, we know that a sufficient time-delay embedding is diffeomorphically equivalent to the underlying state space of the system. We use this information to find time-delays of the original data and build the diffeomorphic mapping with a neural network encoder. The approach is demonstrated on computational examples.

Keywords: embedding theory, structure-preserving machine learning, nonlinear dynamics, structural health monitoring, digital twin

INTRODUCTION

Data-driven machine learning models of structural systems are appealing because they capture the state of the as-built as-deployed structure. Furthermore, they enable bypassing the process of physical model generation, which may be expensive and time-consuming. One disadvantage of purely data-driven approaches is that they tend to perform poorly in regions outside the original training domain. To mitigate this limitation, physical knowledge about the structure can be embedded in the model architecture via the model topology or numerical constraints in the formulation. Najera and Todd [1] previously developed a framework based on Hamiltonian mechanics structure-preservation to address the challenge associated with purely data-driven approaches. However, one challenge associated with this Hamiltonian-constrained approach is the problem of limited observability, or not being able to measure structural response in a complete coordinate system that is compatible with the physical constraints being enforced. To overcome this issue, we propose combining a neural network autoencoder architecture with knowledge from embedding theory to enrich the limited observable data with time-delay embeddings.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

BACKGROUND

As described in [1], an autoencoder is used to transform a set of arbitrary coordinates to generalized coordinates. As described in the introduction, a challenge arises when there is only partial observability of the dynamic response, which is a typical problem in practical applications where only a limited number of sensors can be used. To address this challenge, we rely on Taken's theorem [2] which states that a dynamical system can be reconstructed from a sequence of observations and a set of corresponding time-delayed copies. Combining the time-delayed copies we form a time-delay embedding which, according to Taken's theorem, should be greater than twice the state-space dimension. However, the dimensionality of the state space is often not known a priori.

This problem of attractor reconstruction via embeddings has been widely studied in the literature. One of the biggest questions researchers have posed is that of determining the embedding dimension and time-delay size for practical applications. This question was addressed by Pecora et al. [3] by approaching the problem from the perspective of obtaining an accurate reconstruction. To this end, Pecora et al. defined a continuity statistic to test for general, nonlinear functional dependence between observed coordinates and time-delayed copies. Kraemer et al. [4] built upon the initial work by Pecora and combined it with the work by Uzal et al. [5] to establish a unified and automated approach to attractor reconstruction called PECUZAL.

In this work, we employ the PECUZAL algorithm to determine the optimal embedding dimension and the size of the time delays of the observed signals. The state space is reconstructed by finding the diffeomorphic mapping between the time-delay embedding and the generalized coordinate system that satisfies the Hamiltonian constraints imposed on the neural network. The dimensionality of the state space is defined by the size of the latent space, which is determined iteratively by trying to maximize reconstruction accuracy. The coordinate transformation operation is performed as

$$\mathbf{q} = \mathscr{E}_{nn}(\mathbf{r}), \quad \mathbf{r} = \mathscr{D}_{nn}(\mathbf{q}), \tag{1}$$

where $\mathbf{r}$ is the time-delay embedding vector obtained from the PECUZAL algorithm, $\mathbf{q}$ is the vector of generalized coordinates, and $\mathscr{E}$ and $\mathscr{D}$ are the encoder and decoder neural networks, respectively. The generalized velocity and acceleration vectors can be obtained via autodifferentiation as

$$\dot{q}_i = \sum_{j=1}^{n} \frac{\partial q_i}{\partial r_j} \cdot \dot{r}_j, \quad \ddot{q}_i = \sum_{j=1}^{n} \frac{\partial q_i}{\partial r_j} \cdot \ddot{r}_j + \sum_{j=1}^{n} \frac{\partial \dot{q}_i}{\partial r_j} \cdot \dot{r}_j. \tag{2}$$

In the latent space, the neural network is constrained to preserve the physical structure of Hamiltonian mechanics. The details of these constraints are described in [1]. The network training is performed by supervising the accuracy of the reconstruction of the observable coordinates in physical space, while time integration occurs in the latent space where physics are enforced.

ANALYSIS

To demonstrate the proposed approach, we considered an eight degree-of-freedom (DOF) mass-spring damped oscillator with cubic nonlinearities. It is assumed that only four DOFs are observed. The parameters of the problem are as follow: $k = 1.0$, $m = 1.0$, $c = 0.008$, and $k_{nl} = 5.0$. The cubic spring is only present between every other mass with a total of four cubic springs. The training data is generated by prescribing random initial conditions. The four observed DOFs correspond to masses 2,4,5, and 8. The PECUZAL algorithm determined that the optimal time-delay embedding dimension was 6 and was composed as $\mathbf{r} = [x_0^{(2)}, x_{300}^{(4)}, x_0^{(6)}, x_{392}^{(6)}, x_0^{(8)}, x_{352}^{(8)}]$, where the superscript represents the mass number and the subscript represents the time delay.

The latent dimension is assumed to be 6 as well. Once trained, the model is a neural differential operator that is solved using the RK45 solver implemented in the Python package Scipy [6]. Once the network has been trained with a single response realization example, the trained model can be used to predict the response for new initial conditions or external forcing. An example of the prediction for different initial conditions is illustrated in Figure 1 (left).

Lastly, a number of manifold learning techniques were applied to the original 16-dimensional state space (8 displacements and 8 velocities) to compare its topology to the learned 12-dimensional latent space. The result from applying a spectral embedding method is shown in Figure **??**. The color represents the time index going from bright to dark. As illustrated, the learned two-dimensional manifold is the same between the original state space and the reconstructed lower dimensional one found by

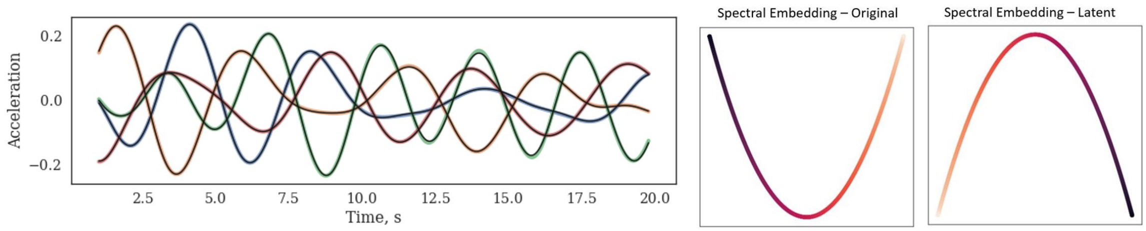

Figure 1: Time history response in the physical domain (left); analytical response shown in color and network prediction shown in black. Spectral embedding of original (center) and learned (right) state space.

the network. This result suggests that the state space was reconstructed accurately by the network. This conclusion is further reinforced by the accuracy of the results presented in Figure 1 where it is shown that the learned dynamic system is able to represent the actual dynamics even after changing the initial conditions.

CONCLUSION

This work demonstrated an approach that combines embedding theory with Hamiltonian-constrained neural networks to reconstruct the state space of a dynamic system based on partial observables. The results presented here demonstrate a viable path forward to enable practical physics-constrained, data-driven modeling for as-built as-deployed structures for digital twin applications, including structural health monitoring.

ACKNOWLEDGEMENTS

This work was funded by Sandia National Laboratories, Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. The University of California San Diego acknowledges Sub-Contract Agreement 2169310 from Sandia National Laboratories for its participation in this work.

REFERENCES

[1] David A. Najera-Flores and Michael D. Todd. "Ensemble of numerics-informed neural networks with embedded hamiltonian constraints for modeling nonlinear structural dynamics". In Matthew R.W. Brake, Ludovic Renson, Robert J. Kuether, and Paolo Tiso, editors, *Nonlinear Structures & Systems, Volume 1*, pages 27–30, Cham, 2023. Springer International Publishing.

[2] Floris Takens. "Detecting strange attractors in turbulence". In David Rand and Lai-Sang Young, editors, *Dynamical Systems and Turbulence, Warwick 1980*, pages 366–381, Berlin, Heidelberg, 1981. Springer Berlin Heidelberg.

[3] Louis M. Pecora, Linda Moniz, Jonathan Nichols, and Thomas L. Carroll. "A unified approach to attractor reconstruction". *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 17(1):013110, 2007.

[4] K H Kraemer, G Datseris, J Kurths, I Z Kiss, J L Ocampo-Espindola, and N Marwan. "A unified and automated approach to attractor reconstruction". *New Journal of Physics*, 23(3):033017, mar 2021.

[5] L. C. Uzal, G. L. Grinblat, and P. F. Verdes. "Optimal reconstruction of dynamical systems: A noise amplification approach". *Phys. Rev. E*, 84:016223, Jul 2011.

[6] Pauli Virtanen, Ralf Gommers, Travis E. Oliphant, Matt Haberland, Tyler Reddy, David Cournapeau, Evgeni Burovski, Pearu Peterson, Warren Weckesser, Jonathan Bright, Stéfan J. van der Walt, Matthew Brett, Joshua Wilson, K. Jarrod Millman, Nikolay Mayorov, Andrew R. J. Nelson, Eric Jones, Robert Kern, Eric Larson, C J Carey, İlhan Polat, Yu Feng, Eric W. Moore, Jake VanderPlas, Denis Laxalde, Josef Perktold, Robert Cimrman, Ian Henriksen, E. A. Quintero, Charles R. Harris, Anne M. Archibald, Antônio H. Ribeiro, Fabian Pedregosa, Paul van Mulbregt, and SciPy 1.0 Contributors. "SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python". *Nature Methods*, 17:261–272, 2020.