gLaSDI: Parametric physics-informed greedy latent space dynamics identification

6th Annual Sandia MLDL Workshop

July 25th, 2022



Youngsoo Choi

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

LLNL-PRES-836951



Awesome reduced order model team and collaborators



Dylan Copeland











Tarek Zohdi Jessie Lauzon Jon Belof

Quincy Huhn

re manufact

Michael Juhasz





Kevin Carlberg



Brown

Sean

Bob Anderson

McBane



Rob Karen Rieben Willcox



Saad

Debojyoti Ghosh







Springer

Dan White

Trenton Kirchdoerfer Oxberry





Teeratorn Xiaolong He William Fries Karen Wang Kadeethum





Nikolaos Bouklas



David

Widemann

Yeonjong Shin



Khairallah



Bedros Afevan Jean Ragusa





Geoff



Charles Fredrick Jekel





Lawrence Livermore National Laboratory LLNL-PRES-836951



Physical simulations play an important role in modern science







How can you accelerate existing physical simulations with data?

1. Generate Simulation data



2. Get the relation between input and output, e.g., training a neural network



Conditional Generative Adversarial Neural Network

Blackbox approach

*Kadeethum, O'Malley, Fuhg, Choi, Lee, Viswanathan, Bouklas. "A framework for data-driven solution and parameter estimation of PDEs using conditional generative adversarial networks." *Nature Computational Science*, 2021.

Blackbox

How can we get an interpretability? LaSDI

Radial advection:
$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{u} = \in \Omega = [-1, 1] \times [-1, 1], \quad t \in [0, 3], \qquad \mathbf{v} = \frac{\pi}{2} d[x_2, -x_1]^T, \quad d = (1 - x_1^2)^2 (1 - x_2^2)^2 \\ u(\mathbf{x}, t; \boldsymbol{\mu}) = \mathbf{0} \quad \text{on} \quad \partial \Omega, \end{aligned}$$
Parameterized initial condition: $u(\mathbf{x}, 0; \boldsymbol{\mu}) = \sin(w_1 x_1) \sin(w_2 x_2) \end{aligned}$





Interpretable

Parameterized latent space dynamics identification (LaSDI)



Fries, He, Choi, "Lasdi: Parametric latent space dynamics identification." arXiv:2203.02076, 2022.



Performance of LaSDI to radial advection problem

Radial advection:
$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{u} = \in \Omega = [-1, 1] \times [-1, 1], \quad t \in [0, 3], \qquad \mathbf{v} = \frac{\pi}{2} d[x_2, -x_1]^T, \quad d = (1 - x_1^2)^2 (1 - x_2^2)^2$$
$$u(\mathbf{x}, t; \boldsymbol{\mu}) = \mathbf{0} \quad \text{on} \quad \partial \Omega, \qquad \text{Parameterized initial condition:} \quad u(\mathbf{x}, 0; \boldsymbol{\mu}) = \sin(w_1 x_1) \sin(w_2 x_2)$$

Maximum relative error: High dimensional simulation data 5.4% with 25 uniformly sampled training points **Speed-up** of 200x 2.4 2.5 2.3 1.9 1.4 3.3 2.8 2.2 2.3 1.4 3.7 3.0 2.2 2.9 1.5 4.2 3.3 2.3 2.1 1.4 2.1 2.3 1.8 1.1 1.6 2.9 2.6 2.1 1.2 1.8 3.1 2.8 2.2 1.2 1.8 3.2 2.9 2.3 1.1 2.0 3.3 1.8 1.5 1.7 1.7 2.3 3.0 1.7 1.9 1.9 2.6 3.2 1.9 2.1 2.0 2.8 3.2 1.9 2.1 2.0 1.9 1.3 1.7 1.6 2.1 2.5 1.5 2.0 1.9 2.3 2.7 1.7 2.1 2.0 2.5 2.9 1.7 2.2 2.0 1.56 2.4 2.2 2.1 1.3 1.3 2.4 2.5 2.4 1.5 1.2 2.6 2.8 2.5 1.6 1.1 2.8 3.1 2.7 1.6 1.1 3.9 Latent space dynamics identification 9 3.0 1.5 1.6 1.5 3.3 3.4 1.8 1.9 1.5 3.6 3.7 2.4 2.5 1.6 1.57 1.59 2 1.7 2.8 2.4 2.2 1.4 2.0 3.0 2.5 2.4 1.5 2.4 3.4 2.7 with a dimension of 3 .6 1.8 1.7 2.2 2.7 1.6 1.9 1.9 2.3 3.0 1.8 2.0 2.0 2.5 3.3 1.9 2.2 2.2 t = 0 sect = 0.7 sec 1.6 1.8 1.7 2.2 2.8 1.6 1.9 1.8 2.4 3.0 1.8 2.0 1.9 2.5 3.2 1.9 2.2 2.1 2.8 5.4 2.8 2.4 2.0 1.3 1.2 2.7 2.6 2.1 1.4 1.3 2.9 2.9 2.2 1.8 1.2 3.2 3.2 2.5 2.2 10 Encoder 8 2.9 1.3 1.4 1.5 3.0 3.1 1.7 1.8 1.5 3.3 3.4 2.3 2.4 1.6 3.7 3.9 3.2 5 1.65 --- DI 21 14 17 29 21 22 14 20 32 22 24 15 25 37 23 26 8 24 33 18 19 18 25 35 19 19 19 27 1.6 3.1 2.7 2.0 1.3 1.6 3.4 3.0 2.0 1.6 1.6 3.0 1.4 1.5 1.6 3.2 3.3 2.1 2.2 1.7 3.3 1.8 2.1 1.6 1.7 3.0 1.9 2.3 1.6 2.0 3.4 2.0 2.4 1.6 2.6 3.9 2.1 2.6 1.7 20 14 17 17 18 29 15 18 17 19 33 16 18 17 19 38 20 19 19 21 36 1.5 1.7 1.7 1.6 2.3 3.3 1.8 1.7 1.7 2.4 3.5 1.8 1.8 1.7 2.5 3.6 2.0 1.9 1.8 -102.4 2.4 1.6 1.4 1.6 3.2 2.6 1.7 1.5 1.6 3.4 2.8 1.7 1.9 1.6 1.79 t = 1.7 sect = 3.0 sec1.80 1.4 1.9 3.0 3.6 2.0 1.3 2.4 3.1 4.1 2.5 1.4 2.6 3.4 4.8 3.2 2.25 0.753.00 0.001.50

National Nuclear Security Administration 7

Interpretable

Lawrence Livermore National Laboratory

Is uniform sampling enough? No, so we need physics-informed greedy sampling!

Uniform sampling



5.4% with 25 uniformly sampled training points

Physics-informed greedy sampling



2.0% with 25 greedy sampling points

*He, Choi, Fries, Belof, Chen. "gLaSDI: Parametric Physics-informed Greedy Latent Space Dynamics Identification." arXiv:2204.12005. 2022.



gLaSDI: physics-informed greedy latent space dynamics identification*



*He, Choi, Fries, Belof, Chen. "gLaSDI: Parametric Physics-informed Greedy Latent Space Dynamics Identification." arXiv:2204.12005. 2022



Curious about the physics-informed greedy procedure?

• Watch this YouTube video (less than 10minutes) : https://youtu.be/A5JIIXRHxrl





Does linear compression always work? No Benefit of nonlinear compression





Linear subspace

Nonlinear compression outperforms!



2D Burgers

advection-dominated

Nonlinear manifold



*Fries, He, Choi, "LaSDI: Parametric latent space dynamics identification." arXiv:2203.02076, 2022.

*He, Choi, Fries, Belof, Chen. "gLaSDI: Parametric Physics-informed Greedy Latent Space Dynamics Identification." arXiv:2204.12005. 2022



Questions? Email choi15@llnl.gov















Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.