

- **What?** → Approximation of real-valued functions in any dimension with Tensor Networks (TNs), approximation rates for smoothness classes, properties of TN-approximable functions
- **Who?** → Mazen Ali (joint work with Anthony Nouy) from Centrale Nantes, France
- **When?** → December 16, 2020, 7-10 PM ET
- **Where?** → Online at <https://ec-nantes.zoom.us/j/93836109808>
- **Contact?** → mazen.ali@ec-nantes.fr, <https://ali-mazen.com>

Variational Autoencoders for Learning Nonlinear Dynamics of Physical Systems

R. Lopez, P. J. Atzberger, UC Santa Barbara

Summary:

Data-driven learning of dynamics \rightarrow non-linear state space representations.

Probabilistic Autoencoders (PAE) for regularized learning.

Geometric and topological priors for general manifold latent spaces.

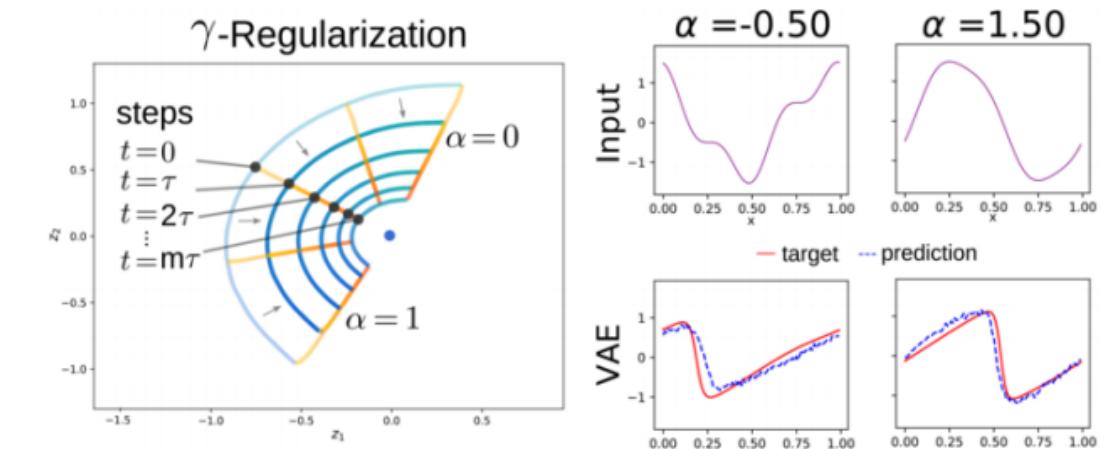
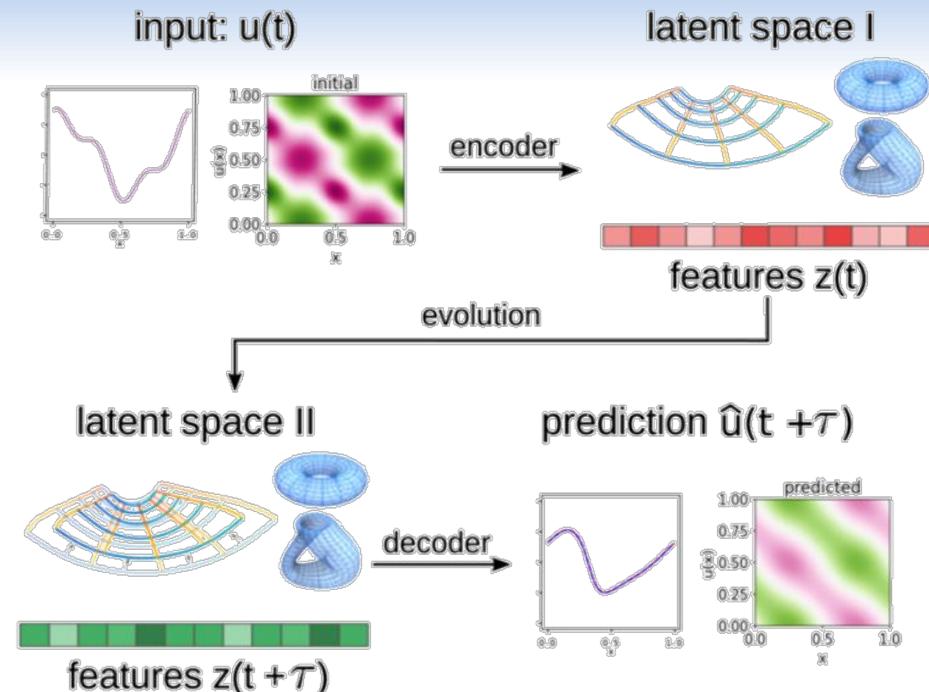
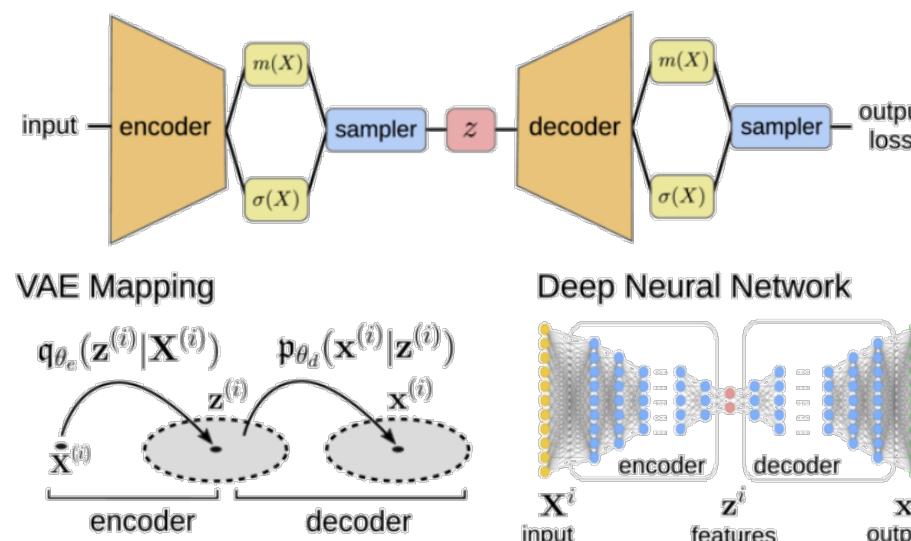
Results:

Nonlinear PDEs \rightarrow learned non-linear features \rightarrow reduced order models.
Constrained Mechanics \rightarrow learning on manifolds \rightarrow constrained motions.

Poster Session:

Zoom link: <https://ucsb.zoom.us/j/89003755986>
Paper: <http://arxiv.org/abs/2012.03448>

Variational Autoencoders



Training Sparse Neural Networks using Compressed Sensing

Jianhong Chen

Department of Mathematics, The Pennsylvania State University

Poster highlights

1. Our method trains sparser, more accurate networks than existing state-of-the-art methods. For example, we can use **less than 1%** of the parameters of VGG-19 to get 94.18% test accuracy.
2. It can also be used effectively to obtain **structured sparsity**.
3. It can be used to train sparse networks from **scratch**, i.e. from a random initialization, as opposed to initializing with a well-trained model.
4. It acts as an **effective regularizer**, improving generalization accuracy.

Zoom link: <https://psu.zoom.us/j/9431692739>

Joint work with Jonathan W. Siegel and Jinchao Xu

pSVGD: Projected Stein Variational Gradient Descent

A fast and scalable **Bayesian inference** method in **high dimensions**

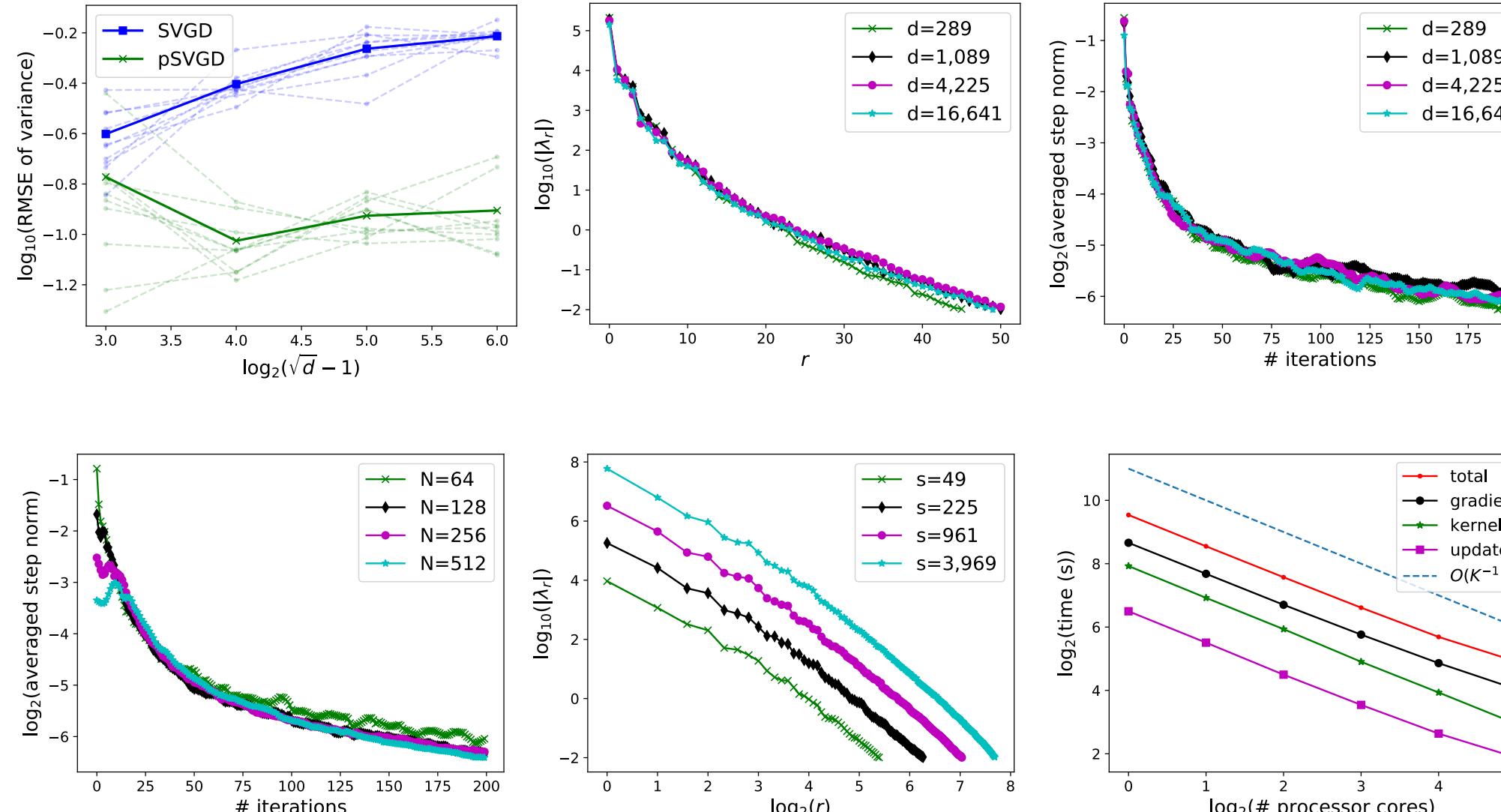
Peng Chen and Omar Ghattas {peng, omar}@oden.utexas.edu

1. Break the curse of dimensionality

2. Scalable with respect to
 - a. # parameters
 - b. # samples
 - c. # data points
 - d. # processor cores

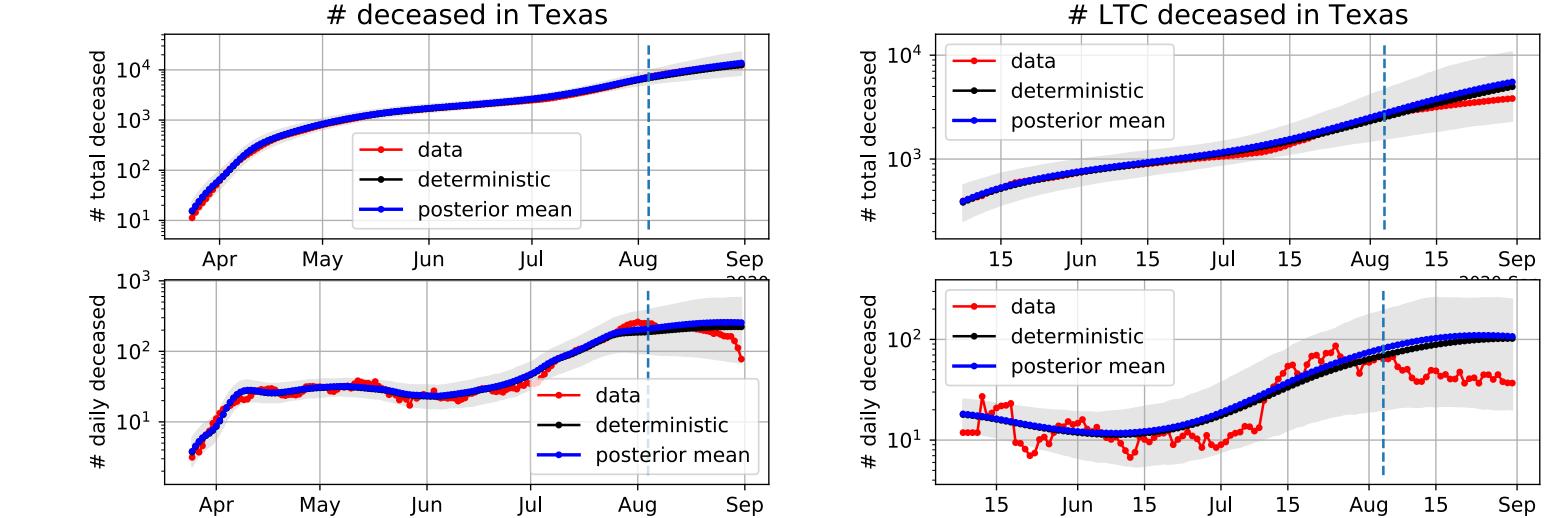
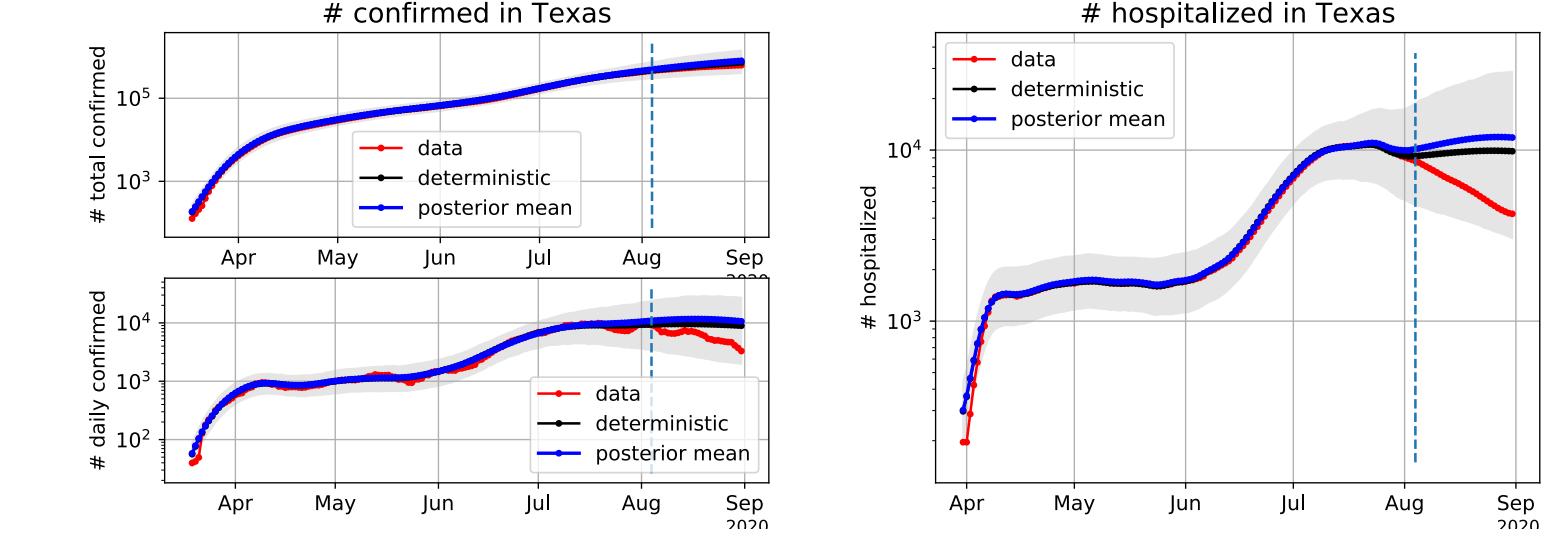
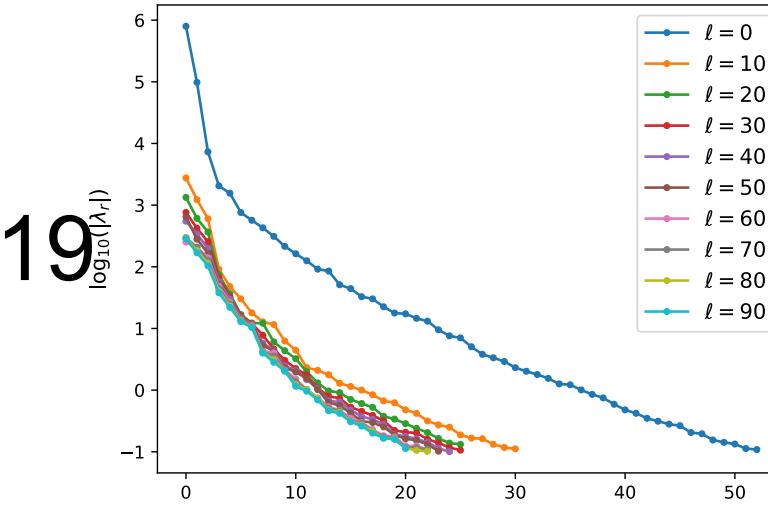
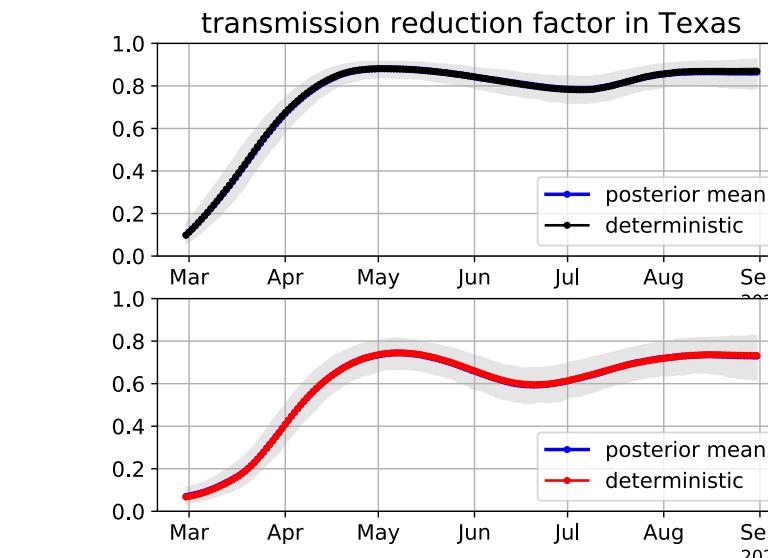
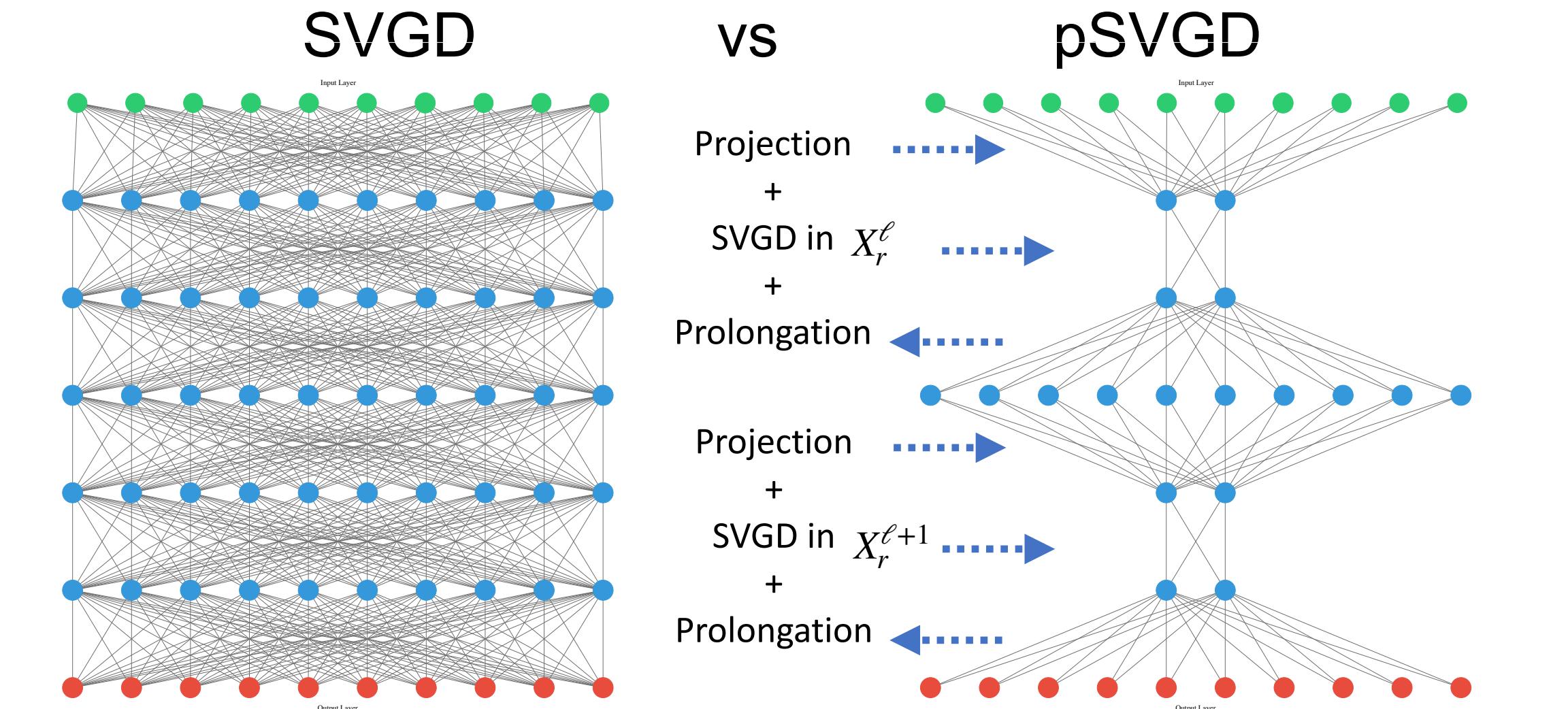
3. Applications to PDEs and COVID-19

Please click to join in Zoom: <https://utexas.zoom.us/j/4636973549>



PDEs

COVID-19



Poster Title

Deep Learning of Parameterized Equations with Applications to Uncertainty Quantification

Authors

Tong Qin¹, Zhen Chen^{2,*}, John D. Jakeman³, & Dongbin Xiu²

¹University of Michigan, ²The Ohio State University, ³Sandia National Laboratories.

*Presenting Author

Abstract

We propose a learning algorithm for discovering unknown parameterized dynamical systems by using observational data of the state variables. Our method is built upon and extends the recent work of discovering unknown dynamical systems, in particular those using deep neural network (DNN). We propose a DNN structure, largely based upon the residual network (ResNet), to not only learn the unknown form of the governing equation but also take into account the random effect embedded in the system, which is generated by the random parameters. Once the DNN model is successfully constructed, it is able to produce system prediction over longer term and for arbitrary parameter values. For uncertainty quantification, it allows us to conduct uncertainty analysis by evaluating solution statistics over the parameter space.

Key Words: Deep neural network, residual network, uncertainty quantification.

Presenter Brief Bio

Zhen Chen is a fifth year PhD student in Mathematics at the Ohio State University (OSU). His thesis advisor is Prof. Dongbin Xiu. His research interest is in scientific machine learning, uncertainty quantification and data assimilation. He is expected to graduate from OSU in Spring 2021.

Sparse Harmonic Transforms: Best s-Term Approximation Guarantees for Bounded Orthonormal Product Bases in Sublinear-Time

Bosu Choi^a, Mark Iwen^b, Toni Volkmer^c

Contact: bosuchoi@gmail.com | Website: <https://sites.google.com/view/bosuchoi/>

a) (former) Oden Institute for Computational Engineering and Sciences, UT Austin

(b) Department of Mathematics and Department of Computational Mathematics, Science and Engineering,
Michigan State University

(c) Department of Mathematics, Chemnitz University of Technology, Germany

In this poster, we will present the development of a sublinear-time compressive sensing algorithm learning multivariate functions which are well approximated by the expansion of a few Bounded Orthonormal Product Basis (BOPB). Such functions appear in many applications including, e.g., various Uncertainty Quantification (UQ) problems where the quantity of interest regarding the solution of parametric PDEs is approximately sparse in such basis functions. In detail, we will discuss a new variant of CoSaMP algorithm with a sublinear-time support identification using a dimension incremental method. As well as the theoretical guarantees, numerical experiment results will be shown for exactly and approximately sparse test functions. The sublinear-time CoSaMP can deal with the approximation of the functions in the spans of fairly general sets of as many as 10^{230} orthonormal basis functions.

Come and join in my poster session here:

Bosu Choi is inviting you to a scheduled Zoom meeting.

Join Zoom Meeting

<https://us02web.zoom.us/j/73568828874?pwd=cUQ1cWo5UUZZZmVKYUpVZFBWXZ4Zz09>

Meeting ID: 735 6882 8874

Passcode: 0000

One tap mobile

+13462487799,,73568828874#,,,,,0#,,0000# US (Houston)

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Dial by your location

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+1 253 215 8782 US (Tacoma)

+1 669 900 6833 US (San Jose)

+1 301 715 8592 US (Washington D.C.)

+1 312 626 6799 US (Chicago)

+1 929 205 6099 US (New York)

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Passcode: 0000

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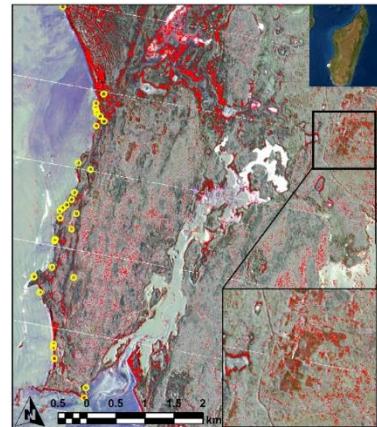
“Quantifying Ancient Landscape Modifications using Machine Learning and Evolutionary Theory: A Case Study from Madagascar”

Dylan Davis, M.A.

PhD Candidate, Department of Anthropology, Penn State University



planet.



Dylan is a PhD candidate in the Anthropology Department at Penn State. His research focuses on human-environmental dynamics and how machine learning methods can be applied to archaeological investigations. Dylan's poster focuses on the use of a random forest probability algorithm to quantify landscape changes caused by ancient foraging communities on Madagascar.

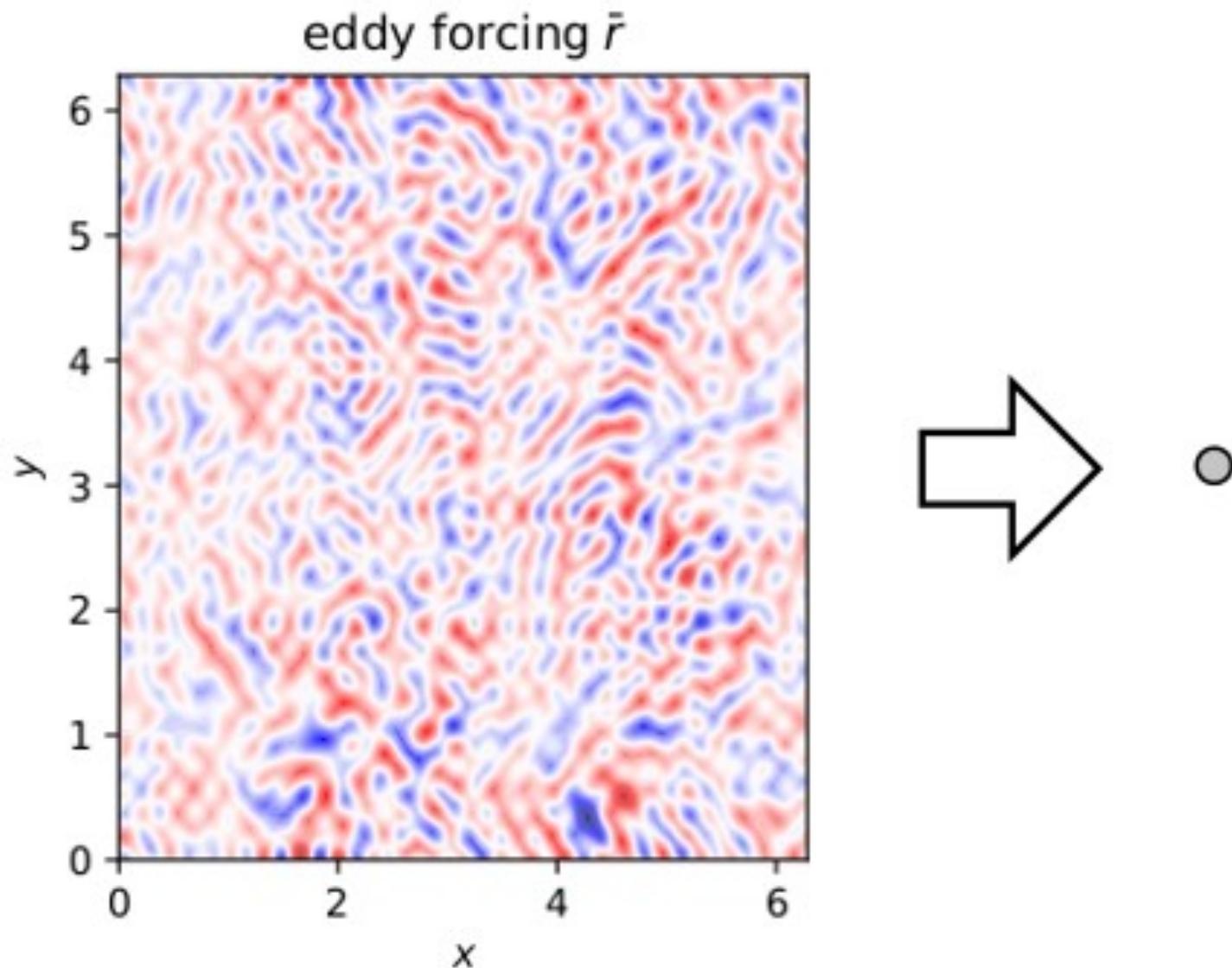
ABSTRACT: Madagascar is the subject of intense debate among archaeologists and holds important information pertaining to human-environmental interactions, particularly related to coping with extreme climate change. The archaeological record can elucidate these important dynamics, but archaeological deposits in this area generally bear ephemeral traces of past human activity and lack intensive landscape modifications that archaeologists typically look for as evidence of human impact or niche construction (e.g., agricultural development, monumental architecture, etc.). To remedy this issue, I use high-resolution satellite imagery and machine learning to reveal a history of human-induced landscape changes by comparing geophysical characteristics of archaeological sites to locations with no documented archaeological materials. Using a random forest probability algorithm, I quantify the extent of ancient human activity and contextualize modern-day landscape impacts in this region. The results of this analysis inform on the question of how we can develop successful machine learning models to understand dynamic systems. This study thus expands the spatial- and temporal-scale at which we can evaluate human-environment dynamics, including during early periods of human history for which the archaeological record is comprised of very subtle traces that are otherwise difficult to detect.

Zoom Link For Presentation:

<https://psu.zoom.us/j/94315489741?pwd=NWt0d0RZd0laL3VGRDd1bC95d1hEQT09> (Zoom Password: 119593)

Reduced training data

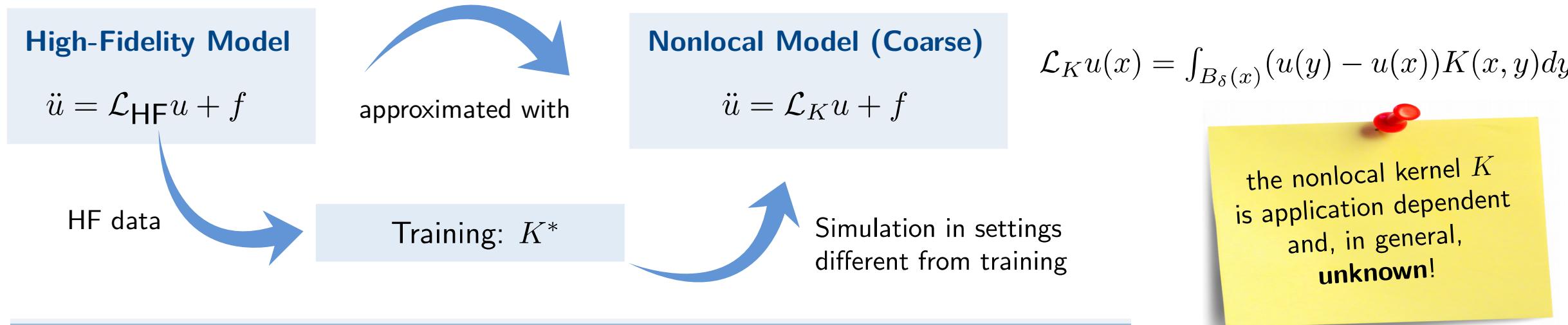
Wouter Edeling, CWI Amsterdam



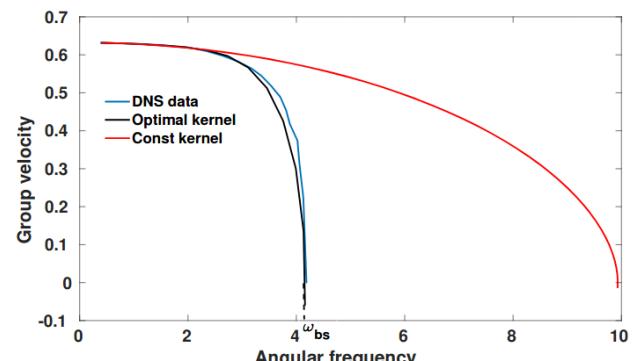
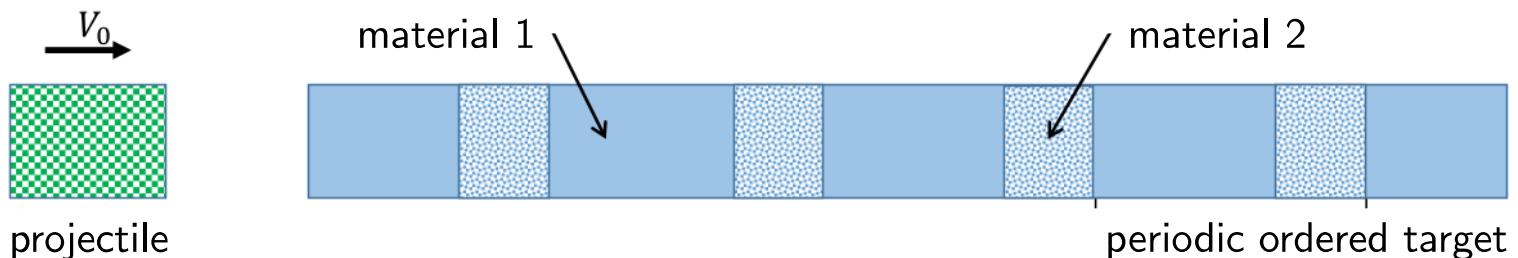
Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws



Marta D'Elia, Stewart Silling (Sandia National Laboratories) Huaiqian You, Yue Yu (Lehigh University)



Application to **wave propagation in a bar with heterogeneous microstructure**



Fast prediction of riverine flow velocity using deep learning

Mojtaba Forghani¹, Yizhou Qian², Jonghyun H. Lee³, Matthew Farthing⁴, Tyler Hesser⁴, Peter K. Kitanidis⁵, Eric F. Darve^{1,2}

¹ Department of Mechanical Engineering, Stanford University, CA

² Institute for Computational and Mathematical Engineering, Stanford University, CA

³ Department of Civil and Environmental Engineering and Water Resources Research Center, University of Hawaii at Manoa, Honolulu, HI

⁴ US Army Engineer Research and Development Center, Vicksburg, MS

⁵ Department of Civil and Environmental Engineering, Stanford University, CA

Abstract

Fast and reliable prediction of river flow velocities is important in many applications, including flood risk management. The shallow water equations (SWEs) are commonly used for this purpose. However, traditional numerical solvers of the SWEs are computationally expensive and require high-resolution riverbed profile measurement (bathymetry). In this presentation, we propose a two-stage process in which, first, using the principal component geostatistical approach (PCGA) we estimate the probability density function of the bathymetry from flow velocity measurements, and then use machine learning (ML) algorithms to obtain a fast solver for the SWEs. The fast solver uses realizations from the posterior bathymetry distribution and takes as input the prescribed range of BCs. The first stage allows us to predict flow velocities without any direct measurement of the bathymetry. Furthermore, we augment the bathymetry posterior distribution to a more general class of distributions before providing them as inputs to ML algorithm in the second stage. This allows the solver to incorporate future direct bathymetry measurements into the flow velocity prediction for improved accuracy, even if the bathymetry changes over time compared to its original indirect estimation. We propose and benchmark three different solvers, referred to as PCA-DNN (principal component analysis-deep neural network), SE (supervised encoder), and SVE (supervised variational encoder), and validate them on the Savannah river near Augusta, GA. Our results show that the fast solvers are capable of predicting flow velocities for different bathymetry and BCs with good accuracy, at a computational cost that is significantly lower than the cost of solving the full boundary value problem with traditional methods.



Nonlinear Reduced Order Modelling of Parametrized PDEs using Deep Neural Networks

Theoretical Analysis and Numerical Results



Franco N.R.^[a],
Manzoni A.^[a], Zunino P.^[a]

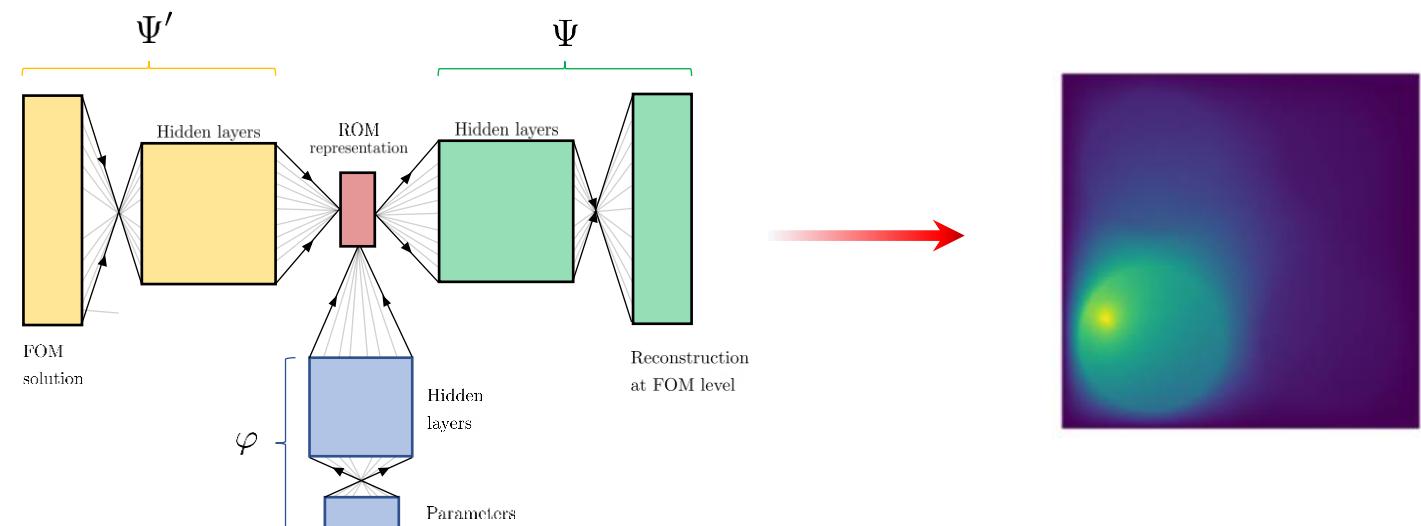
[a] MOX – Modeling and Scientific Computing – Department of Mathematics – Politecnico di Milano (Italy),

About me: PhD student at Politecnico di Milano. Research areas: Numerical Analysis, Machine Learning, Statistics.



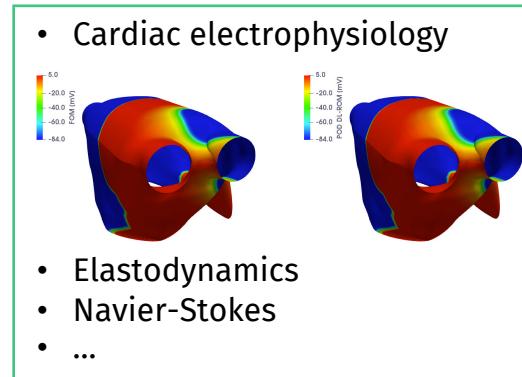
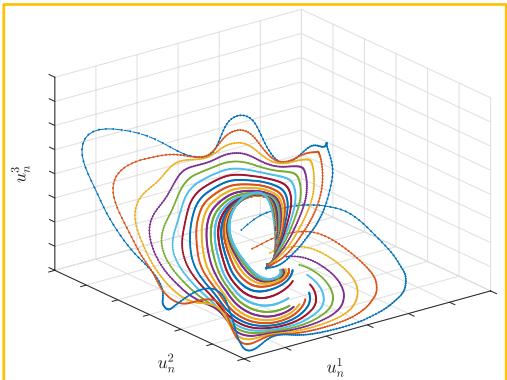
Topic. We consider the problem of **approximating the parameter-to-state map** of a parameter dependent PDE by means of Deep Neural Networks. The research is motivated by the limitations and drawbacks of state-of-the-art algorithms such as the Reduced Basis method. Our construction finds its theoretical fundations in a generalized version of the Kolmogorov n -width.

$$\begin{cases} -\operatorname{div}(\sigma(\mu)\nabla u(\mu)) + \mathbf{b}(\mu) \cdot \nabla u(\mu) = f(\mu) & \text{in } \Omega \\ u(\mu) = 0 & \text{in } \partial\Omega \end{cases}$$



Deep learning-based reduced order models for the real-time approximation of nonlinear time-dependent parametrized PDEs

S. Fresca, A. Manzoni, L. Dedè, A. Quarteroni



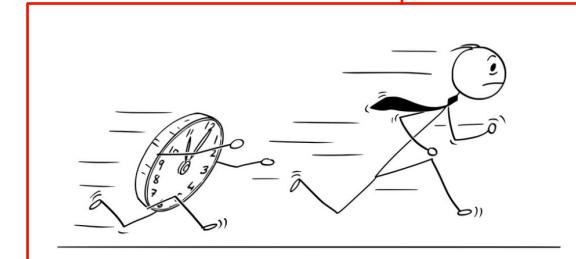
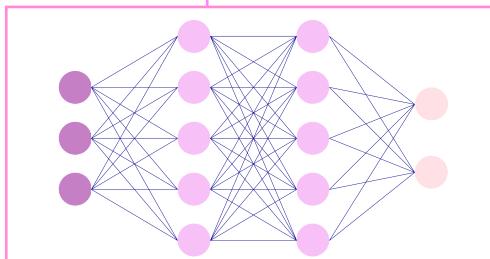
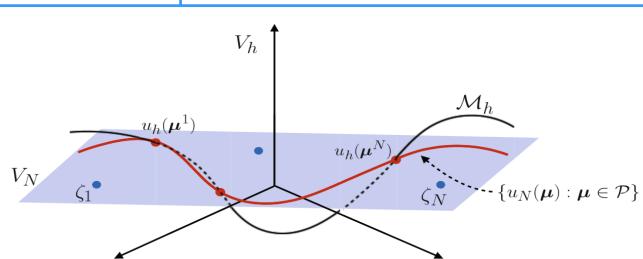
Reduced
order
modeling

New nonlinear
framework

Non-intrusive
deep learning
algorithms

Nonlinear
time-
dependent
parametrized
PDEs

Efficient
training times
and more
than real-time
testing results



Convergence Analysis of the Discovery of Dynamics via Deep Learning

Yiqi Gu

Department of Mathematics,
National University of Singapore
Zoom ID: 640 578 3307

PSU Machine Learning Workshop
Dec. 16, 2020

Robust Data-drive PDE Identification from Single Noisy Trajectory

Poster Presenter: Yuchen He*

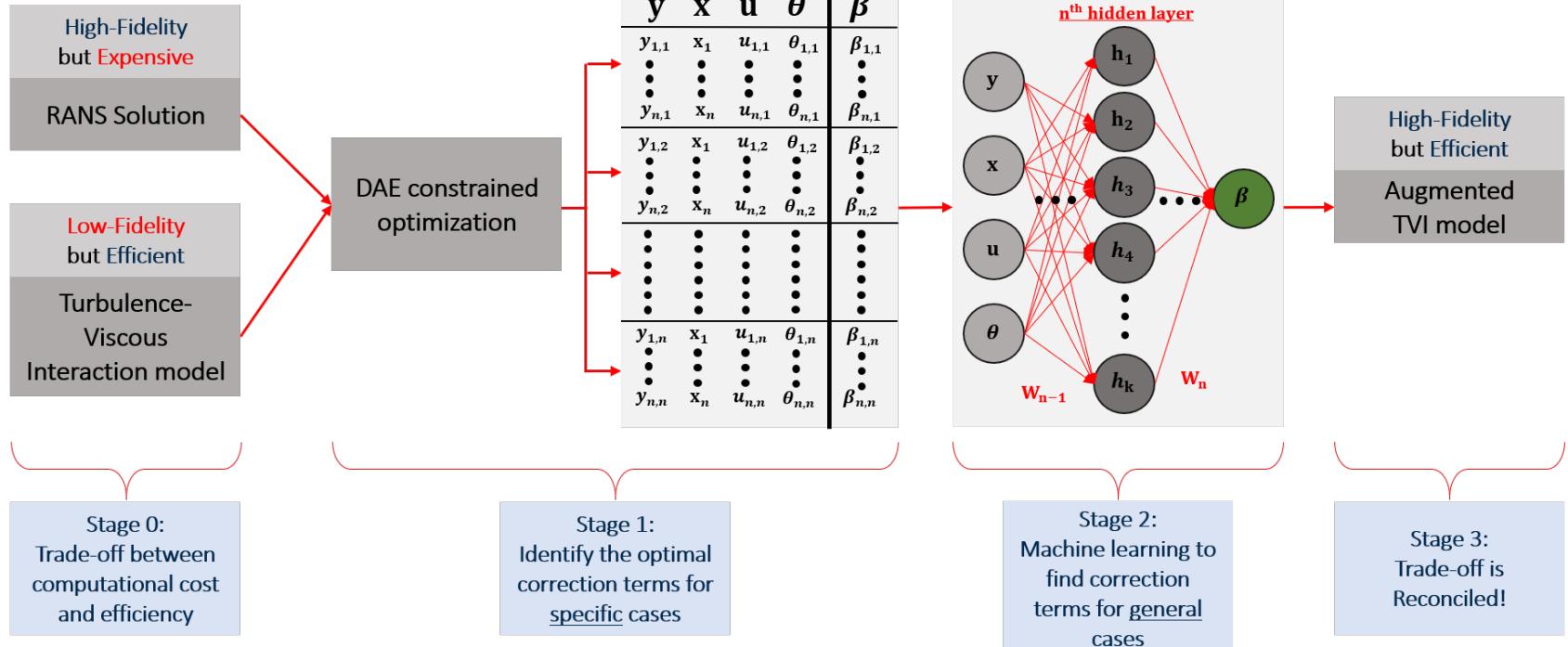
I am a Math Ph.D. student at Georgia Tech advised by Prof. Sung Ha Kang. I am interested in analysis and applications of data-driven mathematical models inspired by problems such as feature identification and dimension reduction. I also enjoy investigating variational analysis, operator splitting, image processing, and computer graphics.

In this poster, on behalf of the coauthors, I present our recent work on data-driven PDE identification focusing on data sampled from single noisy trajectory. To cope with the noise, we proposed several techniques based on principles of numerical PDE approximation and the idea of cross-validation in machine learning. The proposed method successfully automates the PDE modeling from noisy data, which allows easy access to simulation, optimization, prediction, and theoretical analysis. Please join my zoom room if you find this topic interesting. During the poster session, I would also like to share and communicate with the audiences about some existing challenges and exciting future directions.

*Georgia Institute of Technology, School of Mathematics, yhe306@gatech.edu

Resolving Two-Model Problem by Field Inversion and Machine Learning

Carlos Vargas Venegas, Daning Huang.
Penn State Aerospace Engineering



Learning Thermodynamically Stable and Galilean Invariant PDEs for Non-equilibrium Flows

Juntao Huang (MSU), Zhiting Ma, Yizhou Zhou, Wen-An Yong (Tsinghua)*

The Boltzmann equation describe the dynamics of an ideal gas:

$$\frac{\partial f}{\partial t} + \xi \cdot \nabla f_x = \frac{1}{\varepsilon} Q(f), \quad (1)$$

Here $f = f(x, t, \xi)$ is a distribution function with ξ the particle velocity and x the spatial variable.
Knudsen number: $Kn = \varepsilon = \frac{\lambda}{L}$ with λ mean free path, L representative physical length scale

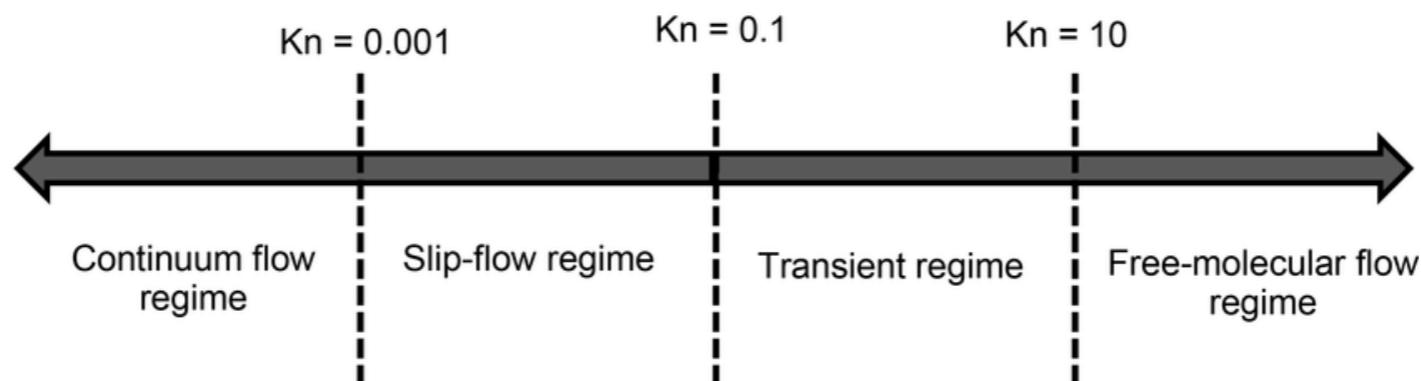


Figure: modeling gas dynamics

What we have done:

- develop a method for learning **thermodynamically stable** and **Galilean invariant** PDEs based on Conservation-dissipation Formalism
- the learned PDEs satisfy the conservation-dissipation principle automatically (**hyperbolic balance laws**)
- our model achieves good accuracy in a wide range of Knudsen numbers

New Potential-Based Bounds for Prediction with Expert Advice

Vladimir Kobzar, NYU Center for Data Science, joint work with Robert Kohn & Zhilei Wang

Prediction with expert advice: At each round, the *player* uses guidance from N experts in order to minimize the difference (*regret*) between the player's loss and that of the best performing expert in hindsight

- ▶ Adversary assigns losses to experts
- ▶ Player strategies often use potentials
- ▶ Adversary strategies are randomized

Our contribution

- ▶ Extend potential-based viewpoint to adversaries, leading to lower bounds
- ▶ More technically: Upper and lower regret bounds \equiv super- and sub-solutions of certain PDEs
- ▶ Practical impact: Understanding how potentials work gives guidance on improving existing bounds as well as designing new strategies/proving new bounds

Why is this approach reasonable?

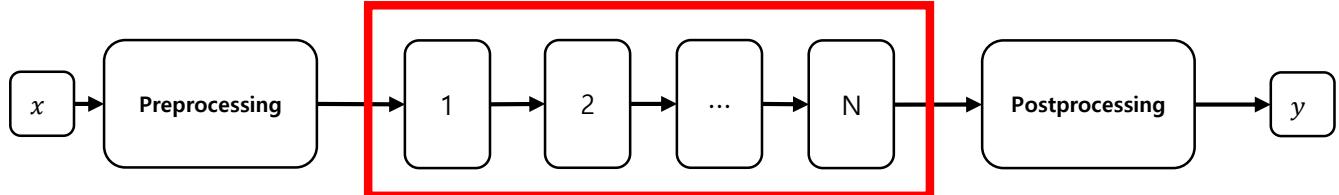
- ▶ Value of a strategy is characterized by a dynamic program
- ▶ It is a discretization of a PDE, which captures the leading order behavior

Youngkyu Lee

Ph. D. Student (Advisor : Prof. Chang-Ock Lee)
 Department of Mathematical Sciences
 KAIST, Korea
 E-mail: lyk92@kaist.ac.kr

Summary of my poster

Feed-forward neural network



Problems

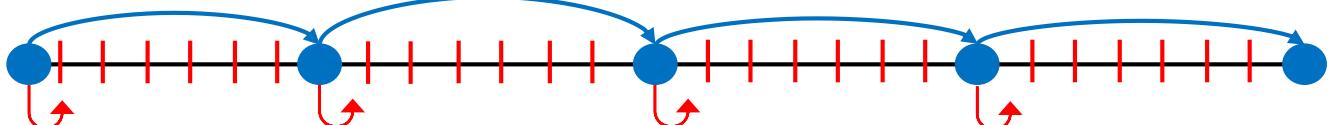
N Subnetworks

- As the depth of network becomes deeper, its training time becomes slower.
- How to accelerating DNN training using multiple GPUs?

Motivation

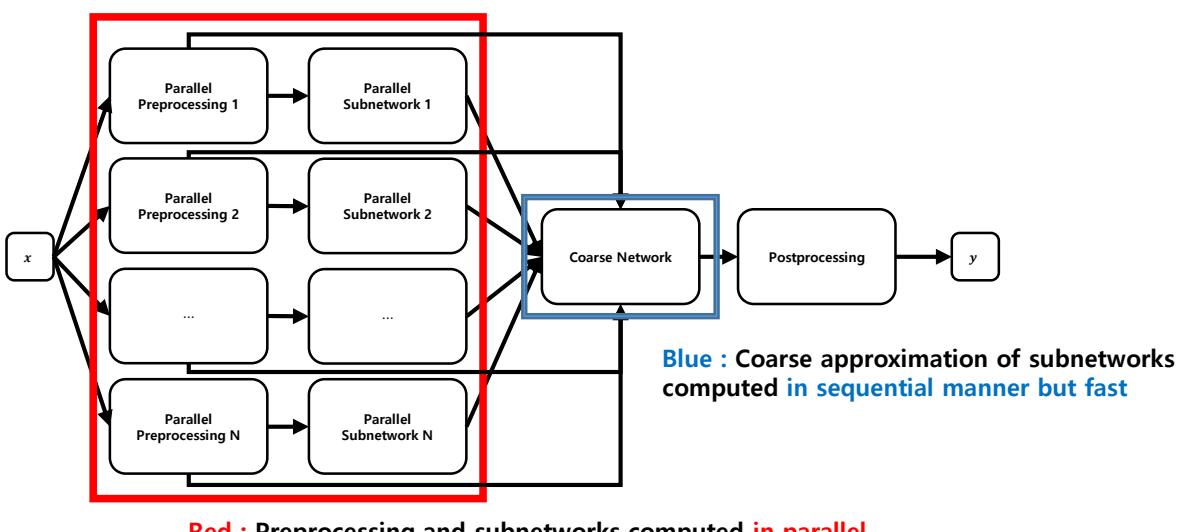
- Lions et al. (2001) – A “parareal” in time discretization of PDE’s

Blue : Coarse approximation of PDE computed in sequential manner but fast



Red : Fine approximation of PDE computed in parallel

Parareal neural network



DeepXDE: A deep learning library for solving differential equations



pypi package 0.9.0

downloads 36k

Anaconda Cloud 0.9.0

downloads 40k

Unstar 322

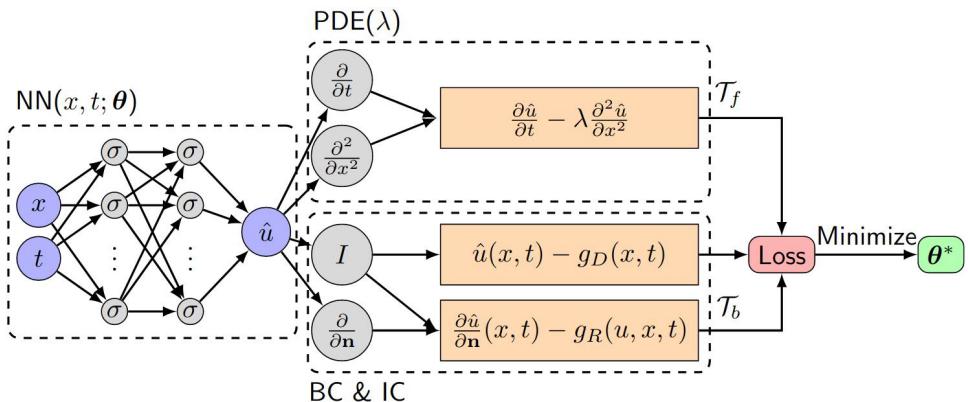
Fork 108



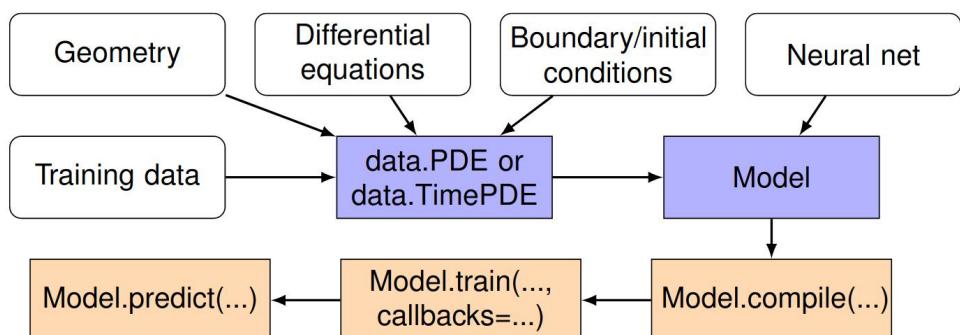
BROWN

Lu Lu, Xuhui Meng, Zhiping Mao, George Karniadakis
Massachusetts Institute of Technology, Brown University, lu_lu@mit.edu

- Physics-informed neural networks (PINNs)



- Flowchart of DeepXDE



Procedure 3: Poisson equation over an L-shaped domain.

1. geometry

```
1 geom = dde.geometry.Polygon(  
2     [[0, 0], [1, 0], [1, -1], [-1, -1], [-1, 1], [0, 1]])
```

2. PDE

```
1 def pde(x, y):  
2     dy_xx = dde.grad.hessian(y, x, i=0, j=0)  
3     dy_yy = dde.grad.hessian(y, x, i=1, j=1)  
4     return -dy_xx - dy_yy - 1
```

3. BC

```
1 def boundary(x, on_boundary):  
2     return on_boundary  
  
3 def func(x):  
4     return np.zeros([len(x), 1])  
  
5 bc = dde.DirichletBC(geom, func, boundary)
```

4. data: geometry + PDE + BC + "training" points

```
1 data = dde.data.PDE(  
2     geom, pde, bc, num_domain=1200, num_boundary=120)
```

5. network

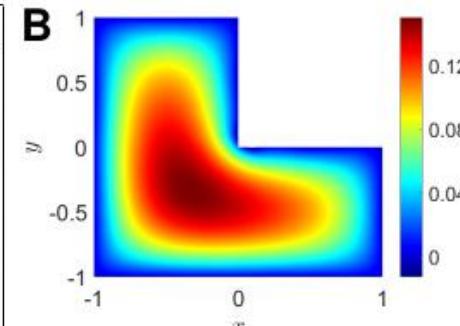
```
1 net = dde.maps.FNN(  
2     [2] + [50] * 4 + [1], "tanh", "Glorot uniform")
```

6. model: data + network

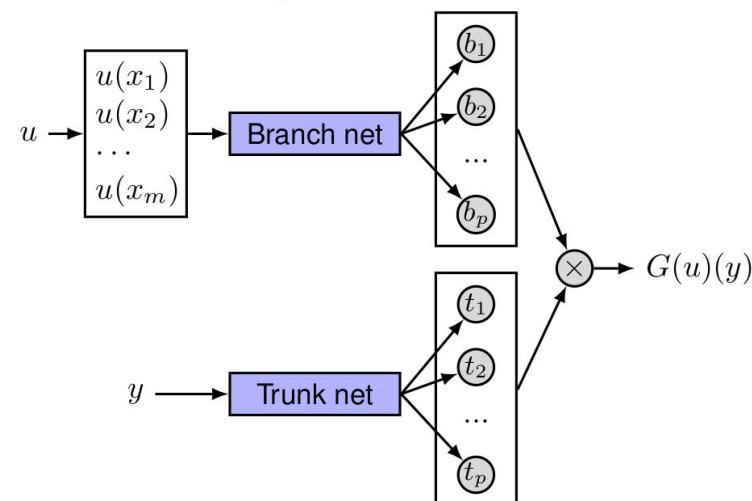
```
1 model = dde.Model(data, net)
```

7. train the model

```
1 model.compile("adam", lr=0.001)  
2 model.train(epochs=50000)
```



- DeepONet: Learning operators (talk by George Karniadakis on Monday)



Hi everyone! I am Yizhou Qian, a third-year PhD at ICME, Stanford. In this presentation we propose several deep learning-based approaches for uncertainty quantification of nearshore bathymetry. Nearshore bathymetry, the topography of the ocean floor in coastal zones, is vital for predicting the surf zone hydrodynamics and for route planning to avoid subsurface features. Hence, it is increasingly important for a wide variety of applications, including shipping operations, coastal management, and risk assessment. However, direct high-resolution surveys of nearshore bathymetry are rarely performed due to budget constraints and logistical restrictions. Another option when only sparse observations are available is to use Gaussian Process regression (GPR), also called Kriging. But GPR has difficulties recognizing patterns with sharp gradients, like those found around sand bars and submerged objects, especially when observations are sparse. In this work, we present several deep learning-based techniques to estimate nearshore bathymetry with sparse, multi-scale measurements. We propose a Deep Neural Network (DNN) to compute posterior estimates of the nearshore bathymetry, as well as a conditional Generative Adversarial Network (cGAN) that samples from the posterior distribution. We train our neural networks based on synthetic data generated from nearshore surveys provided by the U.S.\ Army Corps of Engineer Field Research Facility (FRF) in Duck, North Carolina. We compare our methods with Kriging on real surveys as well as surveys with artificially added sharp gradients. Results show that direct estimation by DNN gives better predictions than Kriging in this application. We use bootstrapping with DNN for uncertainty quantification. We also propose a method, named DNN-Kriging, that combines deep learning with Kriging and shows further improvement of the posterior estimates.

Poster title: Robust learning with implicit residual networks

Authors: Viktor Reshniak (ORNL), Clayton Webster (UTK)

Bio: Viktor Reshniak is a staff mathematician in the Data Analysis and Machine Learning Group at Oak Ridge National Laboratory (ORNL). He received his Ph.D. in Computational Science from Middle Tennessee State University (MTSU) under the supervision of professors Yuri Melnikov and Abdul Khaliq. His work at MTSU was in the field of computational partial differential equations and numerical integration of stiff stochastic systems. After graduating from MTSU in 2017 he started a postdoctoral position in the CAM group at ORNL where he worked with Clayton Webster on several projects in compressed sensing, image processing and machine learning. His current research at ORNL is primarily focused on the design and analysis of new robust machine learning and image processing algorithms.

Brief description: In this effort, we propose a new deep architecture utilizing residual blocks inspired by implicit discretization schemes. As opposed to the standard feed-forward networks, the outputs of the proposed implicit residual blocks are defined as the fixed points of the appropriately chosen nonlinear transformations. We show that this choice leads to the improved stability of both forward and backward propagations, has a favorable impact on the generalization power and allows to control the robustness of the network with only a few hyperparameters. In addition, the proposed reformulation of ResNet does not introduce new parameters and can potentially lead to a reduction in the number of required layers due to improved forward stability. Finally, we derive the memory-efficient training algorithm, propose a stochastic regularization technique and provide numerical results in support of our findings.

CONTACT INFORMATION

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philippe.suennen@tum.de

OUTLINE

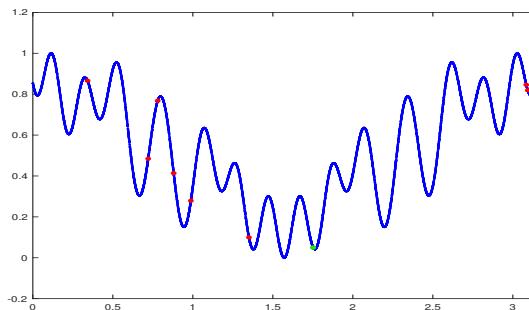
Title: Consensus-based Optimization on Hypersurfaces

Goal: Global optimization of nonconvex functions on hypersurfaces.

Method: System of interacting particles collectively try to find the global minimum of the cost function.

Applications: robust PCA, phase retrieval

Implementation: github.com/PhilippeSu/



REFERENCES

- [1] M. Fornasier, H. Huang, L. Pareschi, P. Sünnen. Consensus-based optimization on hypersurfaces: well-posedness and mean-field limit. Mathematical Models and Methods in Applied Sciences. 2020.
- [2] M. Fornasier, H. Huang, L. Pareschi, P. Sünnen. Consensus based optimization on the sphere: Convergence to global minimizers and machine learning. arXiv:2001.11988. 2020.
- [3] M. Fornasier, H. Huang, L. Pareschi, P. Sünnen. Anisotropic Diffusion in Consensus-based Optimization on the Sphere. in preparation.

Outline of Presentation

Thomas Kofi Torku

Advisor: Dr. Abdul Khaliq

My name is Thomas Kofi Torku, a Ph.D computational science student at Middle Tennessee State University, Tennessee, USA. My research interests include application of deep learning and machine learning models to differential equations (ordinary or partial). In particular, I am interested in **forward and inverse problems** in: **scientific domain problems** such as epidemiology, fluid mechanics, and geophysics; **business-related problems** such as finance and stock market. I am also interested in how to quantify uncertainty in scientific modelling.

In this poster presentation, I worked on the paper.¹ The outline include the following.

1. Dynamical system
2. Residual Network (ResNet) as an Euler Method using one-time stepping.
3. Multi-step recurrent ResNet (RT-ResNet) approximation.
4. Application to Linear and Nonlinear Ordinary Differential equations.
5. Results and Error Analysis.
6. Current and Future Work

¹Tong Qin, Kailiang Wu, Dongbin Xiu, **Data Driven Governing Equations Approximation Using Deep Neural Networks** Journal of Computational Physics 395 (2019): 620-635

Neural network representation of the probability density function of diffusion processes

Wayne Isaac Tan Uy^{1,2} and Mircea Grigoriu²

¹Courant Institute of Mathematical Sciences

²Cornell University Center for Applied Mathematics

Poster outline:

- Introduction to diffusion processes
- PDE for the characteristic function
- PDE for the probability density function (Fokker-Planck equation)
- Physics-informed neural network representation of the pdf and chf
- Applications to Duffing oscillator

IDENTIFYING EIGENFUNCTIONS OF A MARKOV PROCESS USING TRAJECTORY DATA

Robert J. Webber[†]

[†]Courant Institute of Mathematical Sciences

Motivation

- Eigenfunctions are used for reducing dimensionality and analyzing dynamics in biochemistry.
- Monte Carlo methods are needed to estimate eigenfunctions, but these methods have limited accuracy.
- What is driving the error?
- How can we optimize Monte Carlo's efficiency for the future?

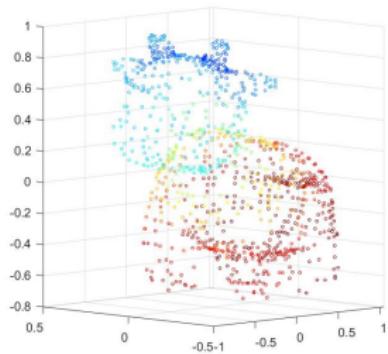
Contributions

- In [2], I proved the convergence of the leading spectral estimation method in biochemistry, called the "variational approach to conformational dynamics" (VAC), and derived detailed error bounds.
- In our follow-up work [1], we extended VAC to make it more robust for applications with limited data and flexible neural network approximation spaces.

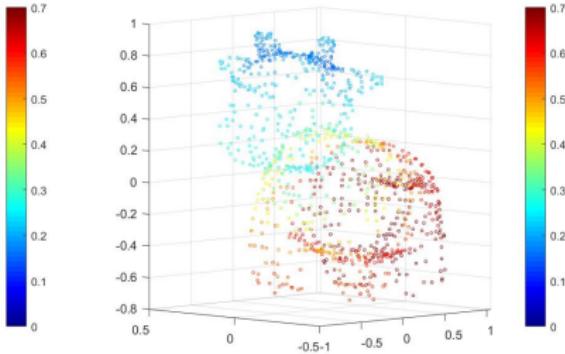
References

- [1] Chatipat Lorpaiiboon et al. "Integrated Variational Approach to Conformational Dynamics: A Robust Strategy for Identifying Eigenfunctions of Dynamical Operators". In: *The Journal of Physical Chemistry B* 124.42 (2020), pp. 9354–9364.
- [2] Robert J Webber et al. "Error bounds for dynamical spectral estimation". In: *SIAM Journal on the Mathematics of Data Science* (2021, to appear).

- ▶ Title: Kernel Methods for Bayesian Elliptic Inverse Problems on Manifolds.
- ▶ Presenter: Ruiyi Yang, University of Chicago.
- ▶ Keywords: Inverse problems, manifold learning, graph Laplacians, Gaussian measures.



Truth.



Reconstruction.

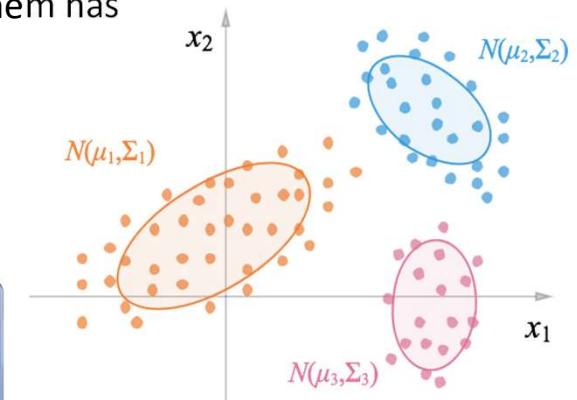
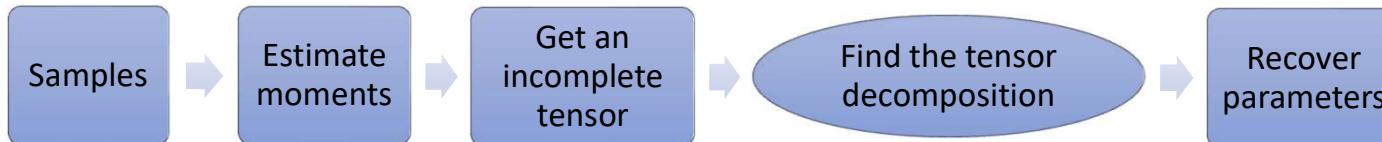
Zi Yang

UC San Diego

- I am a Ph.D student in math at UC San Diego. My research focuses on optimization, tensor computation, and their applications in machine learning.

Learning Gaussian Mixture Models and Tensor Decompositions

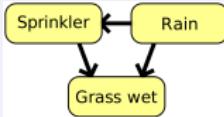
- The Gaussian mixture model is a composition of r Gaussian distributions. Each of them has weight ω_i and distribution $N(\mu_i, \Sigma_i)$.
- We aim to estimate all parameters from given samples.
- An algorithm is proposed to learn the Gaussian mixture model by using tensor decompositions.



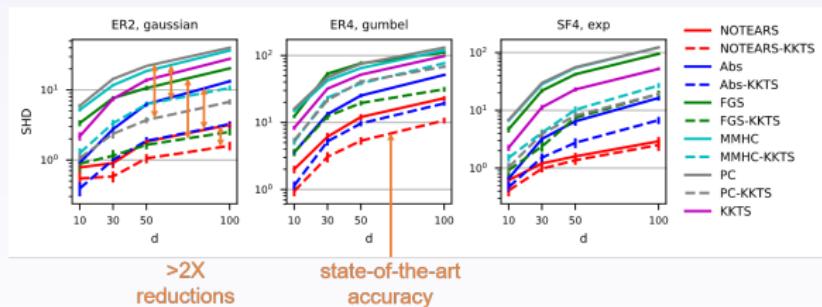
Poster # 28: DAGs with No Fears: A Closer Look at Continuous Optimization for Learning Bayesian Networks

- Problem Settings:

- Given n i.i.d. samples X from an unknown distribution \mathcal{P} of d random variables.
- Our focus is to recover the underlying (causal) directed acyclic graph (DAG) A from X .



- Our Contributions: (1) Found that the KKT condition is not satisfied in the state-of-the-art DAG learning algorithm. (2) Proposed a reformulation and an improved algorithm based on the KKT condition.



Polynomial Based RKHS¹

We focus on a nonparametric density estimator formulated by the kernel embedding of distributions.

Poster Highlights

- We construct the “Mercer-type” kernels based on the classical orthogonal bases defined on non-compact domains.
- By studying the orthogonal polynomial approximation in the RKHS setting, we establish the uniform convergence of the estimator and the connection to Polynomial Chaos Expansion (PCE).
- The algorithm allows one to identify the PCE basis for a consistent estimation through the decay property of the target functions quantified using the available data.

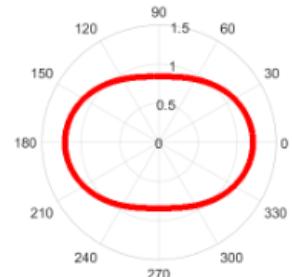
Zoom Link: <https://psu.zoom.us/j/99437721424>

¹Joint work with Prof. John Harlim and Prof. Xiantao Li

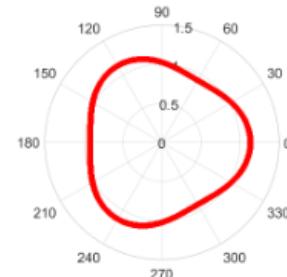
Solving a Free Boundary System by Using Neural Networks

Xinyue (Evelyn) Zhao, Wenrui Hao, Bei Hu

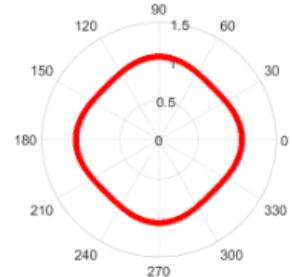
- Verification of the scheme near bifurcation points



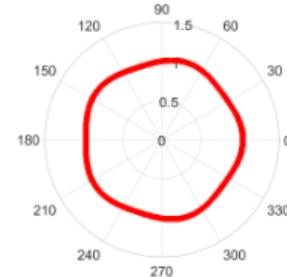
(a) $n = 2$ bifurcation, $\mu = 14.6$.



(b) $n = 3$ bifurcation, $\mu = 28.6$.



(c) $n = 4$ bifurcation, $\mu = 47.0$.

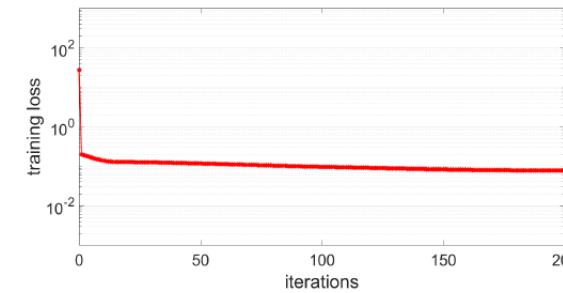


(d) $n = 5$ bifurcation, $\mu = 70.0$.

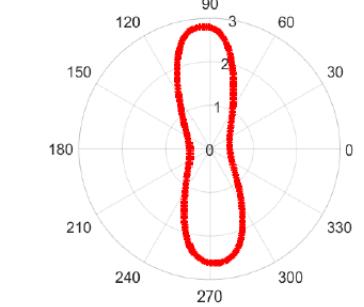
Figure: Contour plot of nonradially symmetric solutions in different bifurcation branches.

Agree well with the theoretical bifurcation results!

- Other non-radially symmetric solutions

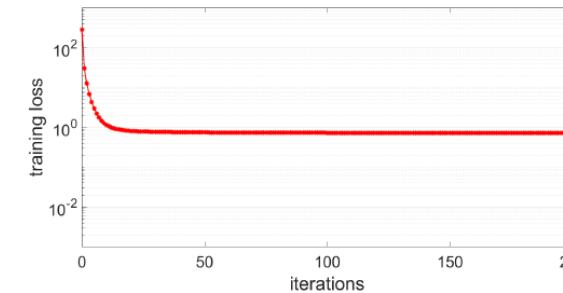


(a) Training loss.

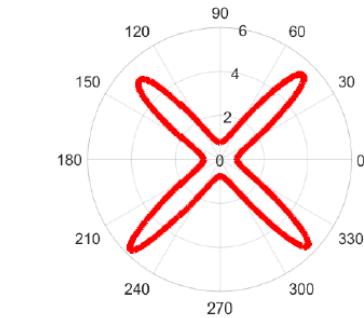


(b) Contour plot.

Figure 3: Non-radially symmetric solution with 2 fingers.



(a) Training loss.



(b) Contour plot.

Figure 4: Non-radially symmetric solution with 4 fingers.