Nikola B. Kovachki

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EDUCATION

California Institute of Technology, Pasadena, CA, USA

- Ph.D. in Applied and Computational Mathematics — Oct 2016 – Present
  - Cumulative GPA: 4.0/4.0
  - Adviser: Prof. Andrew M. Stuart
- B. Sc. in Mathematics — Oct 2012 – Jun 2016
  - Cumulative GPA: 3.9 / 4.0

RESEARCH EXPERIENCE

California Institute of Technology, Pasadena, CA, USA — Oct 2016 – Present

- Research Assistant
- Teaching Assistant

My Ph.D. research is at the intersection of inverse problems, data assimilation, numerical PDEs, and deep learning, drawing on ideas from these fields for their mutual advancement. My work pursues the development and application of methods from mathematical modeling and machine learning to help accelerate scientific progress. I have worked on a variety of both theoretical and application-based topics with my major contributions outlined below.

- **Operator Learning:** I pioneered the concept of operator leaning using deep neural networks [3]. In particular, I developed models that, with the same set of parameters, produce consistent answers given any discretization (resolution) of the input and output space. I am a co-inventor of the ”Neural Operator” paradigm [6,15] and of the now widely adopted Fourier Neural Operator [5], having written the original PyTorch implementation. I developed a universal approximation theory for the method, constituting some of the first results on learning maps that act between general Banach spaces [10,11,13]. I have further worked on the application of operator learning methods to fluid flows [9,12] and materials modeling [1,2], demonstrating substantial speed-ups in physical simulations that can help revolutionize scientific inquiry. Current work constitutes applications to climate modeling and computer vision tasks.
- **Conditional Sampling:** I developed a technique capable of sampling arbitrary conditionals by learning a transport map (GAN) for a joint distribution [14]. The method allows for characterizing the epistemic uncertainty in supervised learning tasks and for efficiently solving Bayesian inverse problems. Applications to complex systems and the development of an approximation theory for the method are a current work in progress.
- **Molecular Prediction:** Collaborating with computational chemists, I developed novel machine learning techniques to accurately predict the activation energy of molecules, providing many orders of magnitude speed-up over conventional methods [7]. Applications of such techniques have the potential to greatly accelerate progress in drug discovery. I continued this work during an internship at the Series A funded start-up company Entos, Inc.
- **Optimization:** I have developed novel methods for optimizing neural networks that are easily parallelizable and derivative-free, showing tremendous promise for models like RNNs [8]. I have also worked on the continuous-time analysis of momentum-based gradient methods, elucidating their inner-workings through the method of modified equations and the theory of invariant manifolds [4].

Entos Inc., Los Angeles, CA, USA — May 2020 – Aug 2020

- Machine Learning Researcher (Intern)

Modeling many molecular properties using traditional techniques from quantum chemistry is often infeasible due to either a lack of understanding of the complex, multi-scale physics or due to the exponentially scaling computational cost. I worked on developing novel graph neural network models capable of processing arbitrarily large molecules for the task of predicting various molecular properties relevant to drug discovery applications. These models have shown tremendous success with the ability to solve problems that were previously considered intractable. I further developed representation learning techniques which improved the models' generalization capabilities, allowing more efficient exploration of chemical space. My work has been part of two patents delineating this new technology.

PUBLICATIONS

PUBLISHED

[1] Kovachki N. B., Liu B., Sun X., Zhou H., Bhattacharya K., Ortiz M., Stuart A. M., "Multiscale Modeling of Materials: Computing, Data Science, Uncertainty and Goal-oriented Optimization," Accepted: *Mechanics of Materials*, (2022).

[2] Liu B., Kovachki N.B., Li Z., Azizzadenesheli K., Stuart A.M., Bhattacharya K., Anandkumar A., "A Learning-based Multiscale Method and its Application to Inelastic Impact Problems," *Journal of the Mechanics and Physics of Solids*, vol. 158, (2022).

[3] Bhattacharya K., Hosseini B., Kovachki N.B., Stuart A.M., "Model Reduction and Neural Networks for Parametric PDE(s)," *The SMAI journal of computational mathematics*, vol. 7, (2021).

[4] Kovachki N.B., Stuart A.M., "Continuous Time Analysis of Momentum Methods," *Journal of Machine Learning Research*, vol. 22, no. 17, (2021)

[5] Li Z., Kovachki N.B., Azizzadenesheli K., Liu B., Stuart A.M., Bhattacharya K., Anandkumar A., "Fourier Neural Operator for Parametric Partial Differential Equations," *9th International Conference on Learning Representations (ICLR)*, (2021).

[6] Li Z., Kovachki N.B., Azizzadenesheli K., Liu B., Stuart A.M., Bhattacharya K., Anandkumar A., "Multipole graph neural operator for parametric partial differential equations," *Advances in Neural Information Processing Systems 33*, (2020).

[7] Cheng L., Kovachki N.B., Welborn M., and Miller T.F. III, "Regression-clustering for improved accuracy and training cost with molecular-orbital-based machine learning," *J. Chem. Theory Comput.*, vol. 15, no. 6668, (2019).

[8] Kovachki N.B., Stuart A.M., "Ensemble Kalman Inversion: A Derivative-Free Technique For Machine Learning Tasks," *Inverse Problems*, vol. 35, no. 9, (2019).

PREPRINTS

[9] Li Z., Zheng H., Kovachki N.B., Jin D., Chen H., Liu B., Azizzadenesheli K., and Anandkumar A., "Physics-Informed Neural Operator for Learning Partial Differential Equations," Submitted: *ICLR 2022*, arXiv: 108.12515, (2021).

[10] Hoop M.V., Kovachki N.B., Nelsen N.H., and Stuart A.M., "Convergence Rates for Learning Linear Operators from Noisy Data," Submitted: *SIAM JUQ*, arXiv: 108.12515, (2021).

[11] Kovachki N.B., Li Z., Liu B., Azizzadenesheli K., Bhattacharya K., Stuart A.M., and Anandkumar A., "Neural Operator: Learning Maps Between Function Spaces," Submitted: *JMLR*, arXiv: 2108.08481, (2021).

[12] Li Z., Kovachki N.B., Azizzadenesheli K., Liu B., Stuart A.M., Bhattacharya K., Anandkumar A., "Markov Neural Operators for Learning Chaotic Systems," arXiv: 2106.06898, (2021).

[13] Kovachki N.B., Lanthaler S., Mishra S., "On Universal Approximation and Error Bounds for Fourier Neural Operators," Submitted: *JMLR*, arXiv: 2107.07562, (2021).

[14] Kovachki N.B., Baptsita R., Hosseini B., Marzouk Y., "Conditional Sampling With Monotone GANs," arXiv:2006.06755, (2020).

[15] Li Z., Kovachki N.B., Azizzadenesheli K., Liu B., Stuart A.M., Bhattacharya K., Anandkumar A., "Neural Operator: Graph Kernel Network for Partial Differential Equations," arXiv:2003.03485, (2020).

PATENTS

- U.S. Patent 16/817,489: "Systems and Methods for Determining Molecular Structures with Molecular-Orbital-Based Features," *Filled* September 17, 2020.
- U.S. Patent 62/817,344: "Harvesting, Databasing, And Regressing Molecular-Orbital-Based Features For Accelerating Quantum Chemistry," *Filled* March 12, 2019.

AWARDS

- Amazon AI4Science Fellowship 2020 – 2021
- Computing and Mathematical Sciences First Year Graduate Student Fellowship 2016 – 2017

INVITED TALKS & PRESENTATIONS

Deep Learning on Function Spaces

- Rough Paths Interest Group. *Talk* (Virtual). Nov 2021
- Deep Learning and Inverse Problems (INI MDLW02). *Talk*. Sep 2021
- Computation and Learning in High Dimensions (MFO). *Talk*. Aug 2021
- Foundations of Bayesian Inference for Complex Statistical Models (MFO). *Talk* (Virtual). May 2021
- The Aerospace Corporation. *Talk* (Virtual). Dec 2020
- SIAM Conference on Mathematics of Data Science (MDS20). *Talk* (Virtual). Jun 2020
- MEDE-ARL Fall Meeting. *Poster*. Oct 2019
- MEDE-ARL Fall Meeting. *Poster*. Oct 2018

Conditional Sampling via Measure Transport

- Second Symposium on Machine Learning and Dynamical Systems. *Talk* (Virtual). Sep 2020
- SIAM Conference on Imaging Science (IS20). *Talk* (Virtual). Jul 2020

Understanding Momentum through Continuous Time Analysis

- International Congress on Industrial and Applied Mathematics (ICIAM). *Talk*. Jul 2019
- Applied Inverse Problems (AIP). *Talks*. Jul 2019
- Inverse Problems and Machine Learning (IPML). *Talk*. May 2019
- SIAM Conference on Applications of Dynamical Systems (DS19). *Talk*. May 2019

Regression Clustering for Molecular Predictions

- CMS 273 (Schmidt Futures). *Talk*. Mar 2019

Ensemble Kalman Inversion for Machine Learning

- International Congress on Industrial and Applied Mathematics (ICIAM). *Talk*. Jul 2019
- Applied Inverse Problems (AIP). *Talks*. Jul 2019
- SIAM Conference on Computational Science and Engineering (CSE19). *Talk*. Feb 2019
- Southern California Applied Mathematics Symposium (SOCAMS). *Poster*. Apr 2018
- UQ for Inverse Problems in Complex Systems (INI UNQW04). *Poster*. Apr 2018
- Inverse Problems and Machine Learning (IPML). *Talk*. Feb 2018

ORGANIZING

- SIAM Conference on Uncertainty Quantification (UQ22) Apr 2022
  Minisymposium: *Operator Learning in PDEs, Inverse Problems, and UQ*

TEACHING

TEACHING ASSISTANTSHIP

- Clustering and Classification on Graphs (ACM 270-2) 2020
- Linear Analysis with Applications (CMS/ACM/IDS 107) 2019
- Linear Analysis with Applications (CMS/ACM/IDS 107) 2018
- Linear Analysis with Applications (CMS/ACM/IDS 107) 2017
- Introduction to Probability Models (ACM/EE 116) 2016
- Technical Seminar Presentations (E 10) 2016

REVIEWING

JOURNALS

- Journal of Computational Physics 2021 – Present
- Quantum 2021 – Present
- Neural Networks 2021 – Present
- Inverse Problems 2020 – Present
- Constructive Approximation 2020 – Present
- SIAM Journal on Scientific Computing 2020 – Present

CONFERENCES

- International Conference on Learning Representations (ICLR) 2022
- International Conference on Learning Representations (ICLR) 2021
- Neural Information Processing Systems (NeurIPS) 2021
- Mathematical and Scientific Machine Learning (MSML2021) 2021
- International Conference on Machine Learning (ICML) 2021
- International Conference on Learning Representations (ICLR) 2020
- Mathematical and Scientific Machine Learning (MSML2020) 2020

PROGRAMMING

- Python (numpy, scipy, sklearn, pytorch, pytorch-geometric)
- Linux/Unix
- MATLAB
- Mathematica
- Julia
- C/C++

LANGUAGES

English (fluent), Bulgarian (native).

REFERENCES

- **Professor Andrew M. Stuart**
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  California Institute of Technology
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