Dilip Krishnamurthy

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Interests

Physics-Informed Machine Learning, Deep Learning, Artificial Intelligence, Computational Material Design, Automotive Engineering, Next-Generation Batteries and Fuel Cells, Density Functional Theory (DFT) Simulations

Education

Carnegie Mellon University (CMU) — Pittsburgh, PA
Doctor of Philosophy (Ph.D.) in Mechanical Engineering [GPA: 4.0/4.0] — Spring 2021 (expected)
Advisor: Prof. Venkat Viswanthan

Indian Institute of Technology Madras (IIT-Madras) — Chennai, India
Bachelor of Tech. (Hons) and Master of Tech. in Engg. Design (Automotive Engg.) [GPA: 9.35/10] — June 2015

Skills

Programming/Tools	Python, MATLAB, C++, Bash, SQL, LaTeX, Unix, Git
Machine Learning	TensorFlow, DeepChem, PyTorch
Materials Simulation	DFT packages (GPAW, VASP), Molecular Dynamics (LAMMPS)

Research Experience

Ph.D. Candidate, Carnegie Mellon University (Aug 2015 – present) — Pittsburgh, PA

- **Deep Learning to Discover Materials for Electrochemical Ammonia Production**
  - Developed a material-to-performance mapping and identified a novel material that beats the state-of-the-art.
  - Built supervised learning (classification) models trained on experimental data including logistic regression, (kernel) support vector machines (SVMs), decision trees, naive Bayes classifiers and random forest classifiers.
  - Built and optimized the architecture of a deep learning model using TensorFlow to predict KT parameters.
  - Led the closed-loop material design between computation and experiments (Manthiram Group, MIT) and identified 9 novel materials of which 1 material surpasses the Faradaic efficiencies of all reported materials.

- **Prediction of Transition Temperature of Liquid Crystals through a Deep Learning Approach**
  - Curated a dataset of liquid crystals and the associated transition temperatures between various phases.
  - Built an approach to create the input dataset for a classifier given a temperature and a material of interest.
  - Found extended connectivity fingerprints as optimal for classification (crystalline, smectic, nematic, isotropic).
  - Developed and optimized the architecture of a deep learning classifier using TensorFlow to predict the phase of a liquid crystal at a given temperature (accurate within 10° C) based on molecular-scale input features.

- **Engineering the Composition of Solid Electrolyte Interface (SEI) in Li-Metal Batteries**
  - Developed a mechanistic understanding of two high-performing electrolytes (FEC and DFEC) to demonstrate that small structural variations can lead to different decomposition products, and thereby the nature of the SEI.
  - Performed DFT calculations to find two different initial bond-breaking mechanisms between FEC and DFEC.
  - Proposed that the formation of oligomers instead of long polymers may lead to compact SEIs.

- **Computational Design of Cathode Materials for Batteries With Higher Energy Density**
  - Performed atomic-scale (density functional theory) simulations to understand the energetics of several materials to enable rechargeable chemistry and realize the theoretical energy density of lithium-oxygen batteries.
  - Screened through transitional metals for selectivity towards lithium peroxide, the preferred discharge product.
  - Identified 2 noble metals and 1 material from the MXene family of materials that were computed to facilitate rechargeable chemistry with $<$0.2 V overpotential (voltage loss).

- **Machine Learning to Identify Low-Cost (Platinum-Group Metal Free) Materials for Fuel Cells**
  - Developed a neural-network machine learning model to learn the mapping from atomic-scale structure of the catalyst site to the performance. Inverted the machine learning model to identify favorable reaction sites.
  - Identified the nature of active sites where the oxygen reduction reaction occurs on metal sulfide surfaces: 3 sulfur nearest neighbors for Ni-S, similarly for each class of transition metal sulfide.
  - Found that the neural network model and a k-nearest neighbors regression model both perform equally well.
  - Collaborated with experimentalists to successfully test surfaces with higher density of identified optimal sites.
- **Machine Learning Expertise Through Pet Projects and Courses**
  - Developed a spam classifier by automatically extracting features and using kernel support vector machines.
  - Build a recommender system for movies based on ratings by utilizing collaborative filtering.
  - Implemented a deep convolutional generative adversarial networks (DC-GAN) to generate emojis from samples of random noise. Built a Cycle-GAN to convert between Apple-style and Windows-style emojis.
  - Implemented in OpenAI Gym Markov decision processes (MDPs) for reinforcement learning of agent motion.

Master's Thesis, Indian Institute of Technology Madras (Jan 2015 – Aug 2015) Chennai, India

- **Estimation of spatially varying elasto-plastic parameters of structural materials**
  - Performed uniaxial tension tests on specimens sliced out of cylindrical welded stainless steel rods.
  - Imaged specimens during displacement and obtained strain fields through digital image correlation.
  - Computed spatially-varying parameters using the inversion technique of virtual fields method.
  - Correlated the computed parameters with the microstructure of the welded material. Performed principal component analysis (PCA) of the displacement and strain fields to reveal primary deformation patterns.

Industry Experience

MRF Tires, Intern (Jan 2014 – Jan 2015) Chennai, India

- **Mechanical characterization and compositional optimization of tires**
  - Developed a computational method for mechanical characterization (hyperelasticity) of carbon-filled rubbers.
  - Performed experiments to capture 3-Dimensional displacement data using Digital Image Correlation (DIC).
  - Designed and optimized a novel specimen to obtain heterogeneous strains using a planar test setup.
  - The developed model is being used to further optimize the material composition of tires for heavy-duty trucks.

Select Publications

D. Krishnamurthy, N. Lazouski, M.L. Gala, K. Manthiram, V. Viswanathan, "Closed-Loop Design of Hydrogen Donors for Lithium-Mediated Ammonia Production With Interpretable Models and Molecular Machine Learning", preprint (2020).

D. Krishnamurthy, H. Weiland, A.B. Farimani, E. Anton, J. Green, and V. Viswanathan, "Accelerating Energy Materials Discovery and Optimization through Machine Learning based Approaches", ACS Energy Lett. (2018)

Book

D. Krishnamurthy, B. Ramsundar, V. Viswanathan, "Machine Learning for Physical Systems." (in preparation)

Community Building for Scientific Machine Learning

I organize and moderate webinar sessions on scientific machine learning (https://www.cmu.edu/aced/sciML.html) to bring together industry leaders, academic researchers and venture capitalists to cross-pollinate ideas across domains.

Select Awards & Honors

Presidential Fellow at Carnegie Mellon University, the highest fellowship at the university level	2019–present
Bradford & Diane Smith Fellowship, awarded to a department-nominated Ph.D. candidate	2018–2019
Kokes Award, awarded by the North American Catalysis Society (NACS)	2017
Neil & Jo Bushnell Fellowship, awarded to one department-nominated Ph.D. candidate	2017–2018
Sundback Graduate Fellowship, awarded to one department-nominated Ph.D. candidate	2016–2017
Institute Merit Prizes, the best academic record across the department at IIT Madras	2014 & 2012