Noah J. Wichrowski

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Education

Johns Hopkins University, Baltimore, MD

- **Ph.D. Candidate, Applied Mathematics and Statistics**
- **M.S.E., Applied Mathematics and Statistics**, May 2020
- Dissertation: *Data-Driven Dimensionality Reduction: Manifold Learning for Optimization*
- Adviser: Dr. Ioannis G. "Yannis" Kevrekidis
- Research Interests: Data Science, Optimization, Stochastic Processes, Machine Learning

University of Maryland, College Park, MD

- **B.S., Chemical Engineering**, *summa cum laude*, May 2017
- **B.S., Mathematics**, *summa cum laude*, May 2017

Research Experience

Johns Hopkins University, Baltimore, MD

Graduate Research Assistant, May 2018–Present

- *Parameter Nonidentifiability:* data-driven model order reduction, parameter estimation, prediction
  - Discovered reduced sets of effective parameters with which to describe dynamic models.
  - Confirmed equivalence of data-driven parameters to analytical expressions proposed by experts.
  - Used reduced representations to predict unseen system behaviors and parameter values.
  - Implemented conformal autoencoders to disentangle effective from redundant parameters.
- *Machine Learning for Materials Science:* parameterizing structure-process-property relations in data
  - Constructed machine learning models of zeolite catalyst properties from small data set.
  - Used models to propose new synthesis conditions that improved catalytic performance.
  - Co-developed an active learning scheme for exploration of high-entropy alloy lattice space.
  - Including dimensionality reduction and comparing performance to composition-based approach.
- *Data-Driven Optimization:* manifold learning for accelerated solution of high-dimensional problems
  - Analyzed trajectories of simulated annealing as time series from Langevin dynamics.
  - Combined diffusion maps with SDE parameter inference to inform larger, coarse-grained steps.
  - Achieved convergence with fewer objective evaluations than standard simulated annealing.
  - Extending approach to Bayesian optimization on reduced space of diffusion coordinates.

University of Maryland, College Park, MD

Gemstone Honors Research Program, September 2013–May 2017

- Team MagNET: Magnetic Non-mechanical Energy Transfer
- Thesis: Magnetic Field Manipulation as a Means of Stabilization
  - Contributed to design and construction of prototype device for levitating, moving, and rotating magnetic payload without physical contact, via an electromagnetically-based control system.
  - Aided development of control structure for microcontroller implementation of device.
  - Developed mathematical model to describe experimental magnetic field data.

Work Experience

Johns Hopkins University, Baltimore, MD

AMS Teaching Fellow, January 2020–Present

Apprentice Teaching Fellow, January 2019–January 2020

Graduate Teaching Assistant, August 2017–January 2019

- Lead weekly recitation sections and office hours; respond to students' emails.
- Interview candidates for grader positions; coordinate grading duties.
- Write problems and solutions for homework and exams; proctor exams.
- Create and present material for review sessions and coding tutorials.

U.S. Food and Drug Administration, Silver Spring, MD
ORISE Research Intern, May 2017–August 2017

- Conducted quantitative characterization of methods and operations of drug substance manufacturing processes in recently FDA-approved drug applications.
- Contributed to published technical report about drug substance manufacturing project.
- Collaborated on internal report assessing the drug quality review of orphan drug applications.

Naval Air Warfare Center, Patuxent River, MD
Pathways Intern, June 2014–August 2016

- Applied chemical kinetic theory to derive mathematical model describing electrochemical impedance spectroscopy and galvanic corrosion.
- Performed and implemented model evaluation on basis of experimental data.
- Conducted data analysis to predict metal corrosion rate from environmental conditions.
- Collected and analyzed data for experiments investigating chloride diffusion in metals.
- Designed improvement of experimental apparatus for chloride diffusion experiments.
- Contributed to declassified technical report on ionic transport through organic coatings.

Technical Skills

Programming Languages

- Python: Autograd/Jax, Jupyter, Matplotlib, NumPy, Pandas, Pyomo, PyTorch, Scikit-learn, SciPy
- MATLAB/Octave
- Some experience with C++, Fortran, Java

Computational Techniques

- Dimensionality reduction: autoencoders, diffusion maps, principal component analysis
- Optimization: simulated annealing, Bayesian optimization, stochastic approximation, recursive least squares, line search, trust region
- Regression: Gaussian processes, geometric harmonics, heteroscedastic GPR, neural networks
- Classification: nearest neighbors, random forest, support vector machines

Software

- Typesetting: LaTeX, Beamer, TikZ
- MS Office: Excel, Word, PowerPoint
- Dynamical Systems: AUTO, Scigma
- Development: Git, Markdown

Publications

- X. Li*, H. Han*, N. Evangelou*, **N. J. Wichrowski***, and nine others, "Machine-Learning Assisted Crystal Engineering of a Zeolite," **2022**. [Under review]
- N. Evangelou*, **N. J. Wichrowski***, and five others, "On the Parameter Combinations That Matter and on Those That do Not," *arXiv preprint arXiv:2110.06717*, **2022**. [Under review]
- D. Pozharskiy, **N. J. Wichrowski**, and three others, "Manifold Learning for Accelerating Coarse-Grained Optimization", *J. Comput. Dyn.*, **2020**, *7*(2), 511–536.
- **N. J. Wichrowski**, A. C. Fisher, N. S. Arden, X. Yang, "An Overview of Drug Substance Manufacturing Processes," *AAPS PharmSciTech*, **2020**, *21*(7), 1–6.
- B. Mobley, **N. Wichrowski**, and four others, "Ionic Transport Through Metal-Rich Organic Coatings," *Report No. NAWCADPAX/TIM-2016/54*, Patuxent River, MD: U.S. Department of the Navy, Naval Air Warfare Center Aircraft Division, **2016**.

* Equal contribution

Affiliations

Graduate Student Member, Society for Industrial and Applied Mathematics
Knights of Columbus, Ss. Philip and James Council, #14102