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Aleksei G Sorokin

Background

Research Interests Scientific Machine Learning, Gaussian Processes, Quasi-Monte Carlo, Probabilistic Numerics

Programming Python (PyTorch, GPyTorch, pandas, Matplotlib), Julia, C, MATLAB, R, SQL, Wolfram

Tools AWS (SageMaker, EC2), GitHub (general, actions, pages), LaTeX, Docker

Education

2021 - 2026 **PhD in Applied Math.** Illinois Institute of Technology (IIT). GPA $3.89/4$.

2017 - 2021 **Master of Data Science.** IIT. Summa cum laude. GPA $3.94/4$.

2017 - 2021 **B.S. in Applied Math, Minor in Computer Science.** IIT. Summa cum laude. GPA $3.94/4$.

Experiences

Summer 2024 **Scientific Machine Learning Researcher** at **FM (Factory Mutual Insurance Company).** I built SciML models including Physics Informed Neural Networks (PINNs) and Deep Operator Networks (DeepONets) for solving Radiative Transport Equations (RTEs). These deep learning models were trained on large scale GPUs and used to speed up CFD fire dynamics simulations. Resulted in publication of "A neural surrogate solver for radiation transfer".

Summer 2023 **Graduate Intern** at **Los Alamos National Laboratory.** I modeled the solution processes of PDEs with random coefficients using efficient and error aware Gaussian processes. Resulted in publication of "Computationally efficient and error aware surrogate construction for numerical solutions of subsurface flow through porous media".

Summer 2022 **Givens Associate Intern** at **Argonne National Laboratory**. I researched methods to efficiently estimate failure probability using Monte Carlo with non-parametric importance sampling. Resulted in publication of *Credible Intervals for Probability of Failure with Gaussian Processes*.

Summer 2021 **ML Engineer Intern** at **SigOpt, an Intel Company**. I developed novel meta-learning techniques for model-aware hyperparameter tuning via Bayesian optimization. In a six person ML engineering team, I contributed production code and learned key elements of the AWS stack. Resulted in publication of "SigOpt Mulch: An intelligent system for AutoML of gradient boosted trees".

2021 - 2024 **Teaching Assistant** at **IIT**. I lead review sessions for PhD qualifying exams in applied math.

Projects

Fast Gaussian Processes with Derivatives for Solving PDEs The cost of Gaussian process regression can be reduced from $\mathcal{O}(n^3)$ to $\mathcal{O}(n \log n)$ when one has control over the design of experiments. This is achieved by pairing quasi-random sampling with matching kernels to induce structure in the kernel matrix. My PhD research studies generalizations for quickly incorporating gradient information into the ML model and using these efficient strategies to solve PDEs with either random or deterministic coefficients.

QMCPy Software I lead development of the open source project QMCPy, a Quasi-Monte Carlo Python Library. This package provides high quality quasi-random sequence generators, automatic variable transformations, adaptive stopping criteria algorithms, and diverse use cases. Over the past five years, this project has grown to dozens of collaborators and [5, 6, 7, 8]. See *qmcpy.org* for more information.

Argonne: AI on Supercomputers I studied *AI Driven Science on Supercomputers* during my time at *Argonne National Laboratory*. Key topics included handling large scale data pipelines and parallel training for neural networks.

Awards

2024 **DOE SCGSR Fellow in Applied Mathematics**, Sandia National Laboratory at Livermore.

2024 **Teaching Assistant Award**, IIT.

2023 **Outstanding Math Poster**, Los Alamos National Laboratory.

2020 **Karl Menger Student Award for Exceptional Scholarship**, IIT.

Publications

[1] Aleksei Sorokin, Xiaoyi Lu, and Yi Wang. "A neural surrogate solver for radiation transfer". In: *NeurIPS 2024 Workshop on Data-driven and Differentiable Simulations, Surrogates, and Solvers*. 2024. URL: https://openreview.net/forum?id=SHidR8UMKo.

[2] Aleksei G. Sorokin, Aleksandra Pachalieva, Daniel OMalley, James M. Hyman, Fred J. Hickernell, and Nicolas W. Hengartner. "Computationally efficient and error aware surrogate construction for numerical solutions of subsurface flow through porous media". In: *Advances in Water Resources* 193 (2024), p. 104836. ISSN: 0309-1708. DOI: https://doi.org/10.1016/j.advwatres.2024.104836. URL: https://www.sciencedirect.com/science/article/pii/S0309170824002239.

[3] Aleksei G. Sorokin and Vishwas Rao. *Credible Intervals for Probability of Failure with Gaussian Processes*. 2023. arXiv: 2311.07733 [stat.ME].

[4] Aleksei G. Sorokin, Xinran Zhu, Eric Hans Lee, and Bolong Cheng. "SigOpt Mulch: An intelligent system for AutoML of gradient boosted trees". In: *Knowledge-Based Systems* (2023), p. 110604. ISSN: 0950-7051. DOI: https://doi.org/10.1016/j.knosys.2023.110604. URL: https://www.sciencedirect.com/science/article/pii/S0950705123003544.

[5] Sou-Cheng T Choi, Yuhan Ding, Fred J Hickernell, Jagadeeswaran Rathinavel, and Aleksei G Sorokin. "Challenges in Developing Great Quasi-Monte Carlo Software". In: *International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing*. Springer. 2022, pp. 209–222.

[6] Sou-Cheng T. Choi, Fred J. Hickernell, Rathinavel Jagadeeswaran, Michael J. McCourt, and Aleksei G. Sorokin. "Quasi-Monte Carlo Software". In: *Monte Carlo and Quasi-Monte Carlo Methods*. Ed. by Alexander Keller. Cham: Springer International Publishing, 2022, pp. 23–47. ISBN: 978-3-030-98319-2.

[7] Aleksei G Sorokin and Jagadeeswaran Rathinavel. "On Bounding and Approximating Functions of Multiple Expectations Using Quasi-Monte Carlo". In: *International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing*. Springer. 2022, pp. 583–599.

[8] Aleksei G. Sorokin, Fred J. Hickernell, Sou-Cheng T. Choi, Michael J. McCourt, and Rathinavel Jagadeeswaran. "(Quasi-)Monte Carlo Importance Sampling with QMCPy". In: *IIT Undergraduate Research Journal* (2021), pp. 49–54. URL: http://urj.library.iit.edu/index.php/urj/article/view/48.