Quan Nguyen

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Research interests

I am interested in probabilistic machine learning and decision-making under uncertainty using principled decision theory. Many such problems exist in active learning and in general sample-efficient experimental design, including Bayesian optimization, multi-armed bandits, and active search. I mainly develop budget-aware decision-making policies that approximate optimal decisions in a nonmyopic manner. My current work focuses on enforcing diversity as well as using diversity to measure uncertainty in experimental design.

Education

2019 – 2024   **Ph.D. in Computer Science**
Washington University in St. Louis, St. Louis, MO

Advisor: Roman Garnett

2015 – 2019   **B.A. in Computer Science and Mathematics**
DePauw University, Greencastle, IN

summa cum laude with highest honors, Minor in Philosophy

Advisors: Khadija Stewart, Zhixin Wu, and Ashley Puzzo

Work experiences

Aug 2024 to   **Postdoctoral Research Associate**   Princeton University
present   *Department of Computer Science*

We develop active learning and experimental design algorithms to aid the process of making scientific discoveries. Our focus lies in finding new methods of quantifying uncertainty in machine learning models, leading to more efficient ways to guide the design of experiments.

Aug 2019 to   **Graduate Research Assistant**   Washington University in St. Louis
Aug 2024   *Department of Computer Science & Engineering*

Our research focuses on probabilistic machine learning and experimental design using techniques such as Bayesian optimization, active search, and nonmyopic decision-making. A common application is the acceleration of scientific discovery in e.g. drug and materials science.

Mar 2023 to   **Student Researcher**   Google LLC
Aug 2023   *Google Research*

We design sample-efficient optimization algorithms to calibrate large-scale traffic simulators to match real-life data, leveraging Bayesian optimization techniques. Our approach centers around incorporating prior knowledge into the predictive models that guide decision making.

Academic publications

Andrew Novick, **Quan Nguyen**, Matthew Jankousky, M. Brooks Tellekamp, Eric Toberer, Vladan Stevanović. Basin-Size Mapping: Prediction of Metastable Polymorph Synthesizability Across TaC–TaN Alloys. Journal of the American Chemical Society, 2025. Paper.

Tsung-Wei Liu, **Quan Nguyen**, Adji Bousso Dieng, Diego Gomez-Gualdron. Diversity-driven, efficient exploration of a MOF design space to optimize MOF properties: application to NH_3 adsorption. Chemical Science, 2024. Paper.

Quan Nguyen, Adji Bousso Dieng. Quality-Weighted Vendi Scores And Their Application To Diverse Experimental Design *International Conference on Machine Learning (ICML)*, 2024. Paper.

Andrew Novick, Diana Cai, **Quan Nguyen**, Roman Garnett, Ryan P. Adams, Eric Toberer. Probabilistic Prediction of Material Stability: Integrating Convex Hulls into Active Learning. Materials Horizons, 2024. Paper.

Andrew Novick, **Quan Nguyen**, Roman Garnett, Eric Toberer, Vladan Stevanović. The Mixing Thermodynamics and Local Structure of High-entropy Alloys from Randomly Sampled Ordered Configurations. *Physical Review Materials*, 2023. Paper.

Quan Nguyen, Roman Garnett. Nonmyopic Multiclass Active Search with Diminishing Returns for Diverse Discovery. *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2023. Paper.

Quan Nguyen, Kaiwen Wu, Jacob R. Gardner, Roman Garnett. Local Bayesian optimization via maximizing probability of descent. *Neural Information Processing Systems (NeurIPS)*, 2022. **Oral presentation**. Paper.

Shayan Monadjemi, Sunwoo Ha, **Quan Nguyen**, Henry Chai, Roman Garnett, and Alvitta Ottley. Guided Data Discovery in Interactive Visualizations via Active Search. *IEEE Visualization Conference (VIS)*, 2022. Paper.

Fatemah Mukadum, **Quan Nguyen**, Daniel Adrion, Gabriel Appleby, Rui Chen, Haley Dang, Remco Chang, Roman Garnett, Steven Lopez. Efficient Discovery of Visible Light-Activated Azoarene Photoswitches With Long Half-Lives Using Active Search. *Journal of Chemical Information and Modeling*, 2021. Paper.

Quan Nguyen, Arghavan Modiri, and Roman Garnett. Nonmyopic Multifidelity Active Search. *International Conference on Machine Learning (ICML)*, 2021. Paper.

Quan Nguyen, Sanmay Das, and Roman Garnett. Scarce Societal Resource Allocation and the Price of (Local) Justice. *AAAI Conference on Artificial Intelligence (AAAI)*, 2021. Paper.

Quan Nguyen, Mason Seeger, and Steven Bogaerts. Ensembles of Gradient Boosting Regressors in Housing Price Error Prediction. *Midstates Conference For Undergraduate Research in Computer Science and Mathematics (MCURCSM)*, 2017.

Books & other media

Quan Nguyen. Bayesian Optimization in Action. *Manning Publications, 2023.* (Book.)

Quan Nguyen. Advanced Python Programming, 2nd Edition. *Packt Publishing Ltd, 2022.* Book.

Peter Farrell, Alvaro Fuentes, Ajinkya Sudhir Kolhe, **Quan Nguyen**, Alexander Joseph Sarver, Marios Tsatsos. The Statistics and Calculus with Python Workshop: A comprehensive introduction to mathematics in Python for artificial intelligence applications. *Packt Publishing Ltd, 2020.* Book.

Alessandro Palmas, Emanuele Ghelfi, Alexandra Galina Petre, Mayur Kulkarni, Anand N.S., **Quan Nguyen**, Aritra Sen, Anthony So, Saikat Basak. The Reinforcement Learning Workshop: Learn how to apply cutting-edge reinforcement learning algorithms to a wide range of control problems. *Packt Publishing Ltd, 2020.* Book.

Quan Nguyen. Deep learning with Google Colab: Implementing and training deep learning models in a free, integrated environment. *Udemy, 2019.*

Quan Nguyen. Hands-on Application Development with PyCharm: Accelerate your Python applications using practical coding techniques in PyCharm. *Packt Publishing Ltd, 2019.* Book.

Gabriele Lanaro, **Quan Nguyen**, Sakis Kasampalis. Advanced Python Programming: Build high performance, concurrent, and multi-threaded apps with Python using proven design patterns. *Packt Publishing Ltd, 2019.* Book.

Quan Nguyen. Asynchronous Programming in Python for Web Scraping. *"Learn data science best practices" series of DataScience.com (part of Oracle), 2018.*

Quan Nguyen. Mastering Concurrency in Python: Create faster programs using concurrency, asynchronous, multithreading, and parallel programming. *Packt Publishing Ltd, 2018.* Book.

Presentations & talks

Cost-effective data annotation with Bayesian experimental design. Conference talk at *PyData Global,* 2024.

Diversity-Aware Active Learning for Scientific Discovery. Tutorial at the Institute for Data Driven Dynamical Design meeting, 2024.

Gaussian Processes for Machine Learning. Invited talk at the Data Science School, University of Lagos, 2024.

"But what is a Gaussian process? Regression while knowing how certain you are." Conference talk at *PyData Global,* 2023.

Bayesian Optimization: Fundamentals, Implementation, and Practice. Conference talk at *PyData Global,* 2022.

Local Bayesian Optimization via Maximizing Probability of Descent. **Oral presentation** at *Neural Information Processing Systems (NeurIPS),* 2022.

Local Bayesian Optimization via Maximizing Probability of Descent. Invited talk at the *Information Theory Workshop (ITW)*'s special session on Black-Box Optimization, 2022.

Active Preference Learning and Optimization Under Uncertainty. Conference talk at *PyData Global,* 2021.

Nonmyopic Multifidelity Active Search. Poster presentation at *International Conference on Machine Learning (ICML),* 2021.

Nonmyopic Bayesian Optimization. Ph.D. qualification exam at *Washington University in St. Louis,* 2021.

Scarce Societal Resource Allocation and the Price of (Local) Justice. Poster presentation at *AAAI Conference on Artificial Intelligence (AAAI),* 2021.

Bayesian Machine Learning: A PyMC-Centric Introduction. Conference talk at *PyMCon,* 2020.

Awards & honors

2021 & 2022	Honors Distinction for Outstanding Ph.D. Students, Washington University in St. Louis
2019	Robert J. Thomas Outstanding Senior Award, DePauw University
2019	David Becker Fellow, Information Technology Associates Program, DePauw University
2019	Outstanding Chapter President, DePauw University

2017 – 2019	Perennial Scholarship Recipient, Sigma Nu National Fraternity
2015 – 2019	Science Research Fellow, DePauw University
2019	Phi Beta Kappa, DePauw University
2018	Youngest Published Book Author, Packt Publishing
2018	Wylie Condit Scholarship Recipient, Computer Science Department, DePauw University
2018	Wylie Condit Scholarship Recipient, Mathematics Department, DePauw University
2016	First Place, Michigan Autumn Take-Home (MATH) Mathematics Challenge
2015	Second Place, Vietnamese National Mathematical Olympiad

Peer-reviewing

2022 – 2025	International Conference on Machine Learning (ICML)
2023 & 2024	International Conference on Automated Machine Learning (AutoML)
2021 – 2024	Neural Information Processing Systems (NeurIPS)
2023	Journal of Machine Learning Research
2022 – 2024	International Conference on Artificial Intelligence and Statistics (AISTATS)

Other services

2024	Website Chair, International Conference on Automated Machine Learning
2024	Volunteer Course Designer, Statistics Without Borders
2021	Student Leadership Council, Harnessing the Data Revolution (HDR) Research Grant
2020	Chair of the Program Committee, PyMCon
2020 – 2021	Liberman Advisory Committee, Washington University in St. Louis
2019 – 2020	Graduate Student Association, Washington University in St. Louis
2017 – 2019	Writer for the Python Software Foundation (PSF)
2018 – 2019	President of the DePauw Data Science Group (DPUDS), DePauw University
2018 – 2019	President of the Beta Beta chapter of Sigma Nu fraternity, DePauw University

Teaching experiences

Fall 2023	Instructor, *Introduction to Machine Learning*, Washington University in St. Louis
Spring 2023	Guest lecturer, *Introduction to Machine Learning*, Washington University in St. Louis
Spring 2022	Assistant in instruction, *Machine Learning*, Washington University in St. Louis
Fall 2019	Online instructor, *Deep Learning with Google Colab*, Udemy
Spring 2019	Online instructor, *Python Security*, EC-Council

Technologies

Programming	Python, MATLAB
Machine learning	PyTorch, GPyTorch, BoTorch, TensorFlow, GPFlow, Scikit-learn, JAX
Data engineering	Pandas, NumPy, Jupyter
Collaboration tools	Git, Weights and Biases, Google Colab