

# 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 develop budget-aware decision-making algorithms that approximate optimal decisions in a nonmyopic manner. My current work focuses on developing more expressive measures of uncertainty in experimental design.

## Education

- 2019 – 2024 **Ph.D. in Computer Science**  
*Washington University in St. Louis, St. Louis, MO*  
Dissertation: *Experimental Design for Scientific Discovery* (Turner Ph.D. Dissertation Award)  
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 (selected)

- Aug 2024 to present **Postdoctoral Research Associate** Princeton University  
*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 Aug 2024 **Graduate Research Assistant** Washington University in St. Louis  
*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 Aug 2023 **Student Researcher** Google LLC  
*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

**Quan Nguyen**, Adjı Bousso Dieng. Vendi Information Gain for Active Learning and its Application to Ecology. Preprint, 2025. [Paper](#).

**Quan Nguyen**, Adjı Bousso Dieng. Vendi Information Gain: An Alternative To Mutual Information For Science And Machine Learning. Preprint, 2025. [Paper](#).

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](#).

**Quan Nguyen**, Anindya Sarkar, Roman Garnett. Amortized nonmyopic active search via deep imitation learning. Preprint, 2024. [Paper](#).

Tsung-Wei Liu, **Quan Nguyen**, Adjı Bousso Dieng, Diego Gomez-Gualdron. Diversity-driven, efficient exploration of a MOF design space to optimize MOF properties: application to NH<sub>3</sub> adsorption. *Chemical Science*, 2024. [Paper](#).

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

**Quan Nguyen**. Experimental Design for Scientific Discovery. Ph.D. dissertation, 2024. **Turner dissertation award**. [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.

## Awards & honors

2025	Turner Ph.D. Dissertation Award, Washington University in St. Louis
2024	TRIADS Lightning Talk Award, Washington University in St. Louis
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	Silver Medal, Vietnamese National Mathematical Olympiad

## Talks

Machine learning-aided search for discovery. Invited talk at the Institute for Data Driven Dynamical Design meeting, 2025.

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

Making your experiments count with Bayesian experimental design. TRIADS lightning talk, 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. 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 Bayesian Optimization. Ph.D. qualification exam at *Washington University in St. Louis*, 2021.

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

## Teaching

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

## Services

2025	Workflow Chair, International Conference on Automated Machine Learning
2024	Website Chair, International Conference on Automated Machine Learning
2024	Volunteer Lecturer for Machine Learning, Statistics Without Borders
2021	Student Leadership Council, Harnessing the Data Revolution (HDR) Research Grant
2020	Chair of the Program Committee, PyMCon
2020 – 2021	Lieberman Graduate Advisory Committee, Washington University in St. Louis
2019 – 2020	Graduate Student Association Member, 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

## Peer-reviewing

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

## Trade 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.** Mastering Concurrency in Python: Create faster programs using concurrency, asynchronous, multithreading, and parallel programming. *Packt Publishing Ltd*, 2018. [Book](#).