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 local Bayesian optimization of expensive blackbox objective functions.

Education

2019 – present
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 2019 – present
Graduate Research Assistant — Washinton University in St. Louis, MO
McKelvey School of 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.

May 2022 – Aug 2022
Data Science Intern — Micron Technology, Inc., Boise, ID
R&D Department

We modeled performance metrics in the semiconductor production line using Bayesian linear regression models, which allowed incorporating informative priors and quantifying predictive uncertainty. We then applied Bayesian optimization to optimize these metrics of interest.

Aug 2017 – May 2019
Research Assistant — DePauw University, Greencastle, IN
Computer Science Department

We developed robust ensemble models and an efficient hyperparameter tuning scheme. Our work was presented at MCURCSM 2017. Our solution finished in 15th place (2.5%) of Kaggle's DonorsChoose competition.

Academic publications

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.

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. *arXiv preprint*, 2022. Paper.

Quan Nguyen, Roman Garnett. Nonmyopic Multiclass Active Search for Diverse Discovery. *arXiv preprint*, 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.* (In preparation.)

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

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

Activities

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	Present of the Beta Beta chapter of Sigma Nu fraternity, DePauw University