Nicholas Ho

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Education

Arizona State University, Tempe, Arizona, USA — August 2019-Present
Computer Science and Mathematics — Graduation: May 2023
GPA: overall 4.0/4.0; CS-only 4.0/4.0; Math-only 4.0/4.0

Skills / Experience

Proficient with Python, C/C++, MatLab, Bash, R, JavaScript, PHP, SQL, Perl, PyTorch, TensorFlow, JAX, Pandas, Numpy.

Experienced and interested in Machine Learning for Healthcare, Geometric Representation Learning, Graph Machine Learning, Multimodal machine learning, Statistical ML, Bayesian Statistics, and Reinforcement Learning.

Publications - Accepted

Nicholas Ho, John Kevin Cava, John Vant, Ankita Shukla, Jacob Miratsky, Pavan Turaga, Ross Maciejewski, Abhishek Singharoy. *Learning Free Energy Pathways through Reinforcement Learning of Adaptive Steered Molecular Dynamics* Machine Learning In Structural Biology (MLSB) Workshop at the 36th Conference on Neural Information Processing Systems (5 Pages)

John Kevin Cava, John Vant, **Nicholas Ho**, Ankita Shukla, Pavan Turaga, Ross Maciejewski, Abhishek Singharoy. *Towards Conditional Generation of Minimal Action Potential Pathways for Molecular Dynamics* ELLIS ML4Molecules Workshop, October 2021, (5 Pages).

Wei Du, Gaoyang Li, **Nicholas Ho**, Landon Jenkins, Drew Hockaday, Jiankang Tan, Huansheng Cao *CyanoPATH: a knowledgebase of genome-scale functional repertoire for toxic cyanobacterial blooms* Briefings in Bioinformatics, Volume 22, Issue 4, July 2021, (12 Pages).

Research Experience

Harvard Medical School Department of Biomedical Informatics with Dr.Marinka Zitnik, June 2022-Present
Conducting research on multimodal geometric representation learning for *Novel Drug-Drug Side Effect Predictions* alongside Yepeng Huang.

- Accepted as a visiting research fellow at Harvard DBMI through a highly competitive application process.
- Currently developing a novel machine learning architecture to deal with missing and imbalanced modalities. Conducted extensive evaluation with dozens of hyperparameter sweeps to benchmark and rigorously validate the model at various points.

ASU Structural Systems Biology Lab in the Biodesign Institute with Dr.Abhishek Singharoy May 2020 - Present
Worked as a Research Associate in the Singharoy Lab. Lead research for my honors thesis to utilize deep ML methods with statistical mechanical methodologies.

- Lead the development of using *reinforcement learning* algorithms alongside NAMD molecular dynamics sims for biologically relevant pathways.
- Enhanced and accelerated the differentiable simulator TorchMD into JAX in order to leverage the JIT computation and ran differentiable simulations on biomolecules. *Up to 20 times computational speedup* even without using the parallelizability on GPU.
- Contributed to developing and testing a Conditional Generative Adversarial Network to generate minimum action pathways for dynamics.
- Implemented and used deep learning models to evolve noisy dynamical molecular systems using Neural SDEs, Graph Neural Networks, Hamiltonian Neural Networks, and more.
- Did extensive testing on the model capacity of LSTMs to be used to evolve a dynamical system.

Carnegie Mellon Statistics and Data Science with Dr. Konstantinos Pelechrinis, Summer 2021
Worked on *An Interpretable Method of Learning Stochastic Game Dynamics* project.

- Accepted as a visiting research fellow in CMU Statistics through a highly competitive summer research program.
- Created and a novel methodology for using stochastic simulators for soccer game predictions. Our method had comparable results to models trained directly on scores.

ASU Cao Lab in the Biodesign Institute with Dr. Huangsheng Cao Sept 2019 - May 2021
Worked under Professor Huangsheng Cao as a Bioinformatician.

- Conducted data engineering and analysis on genomes assembled from a metagenome in order to study the strain level variance within microbiome communities.
- Implemented a web system that highlighted which genes are present in a pathway for a particular cyanobacteria species using PFAM's Hidden Markov Model package, JavaScript, SQL databases, shell and Python. Work published in Briefings in Bioinformatics.

ASU Ferran Pichel Lab in the Biodesign Institute with Dr. Ferran Garcia Pichel May 2020 - May 2021
Worked under professor Ferran Garcia Pichel as an Assistant Research Bioinformatician.

- Developed a Python plugin that interfaced with the Bioinformatics pipeline package Qiime2.

Presentations

Novel Drug Drug Interaction Side Effect Prediction, Harvard Summer Institute of Biomedical Informatics (2022).

An Interpretable Method of Learning Stochastic Game Dynamics [Co-presented]. Carnegie Mellon Sports Analytics Conference, (2021) and Ohio State University Sports Analytics Conference (2021).

Towards autoregressive generation of steered MD simulations [Co-presented]. NAMD Developer Workshop at Urbana Champaign (2021).

Concordia International IOT Environmental Sensors and Data Analysis at the International Conference on Big Data and Education, (ICBDE 2018).

Significant Course Projects

CSE485 Computer Science Capstone with Dr. Ross Maciejewski Fall 2021 -Spring 2022

- Lead project developer, using the agile workflow to develop an improved data visualization dashboard for CSRankings of universities.

APM541 Graduate Stochastic Processes and Biology with Dr. Nicolas Lanchier Fall 2021

- My final project was *Particle System Dynamics for Compromised Social Networks* where I extended and implemented the infinite graph contact process for Facebook graphs to simulate and visualize the stability of compromised accounts. Code available on github.

PHY598 Graduate Data Driven Inference and Stochastic Processes with Dr. Steve Presse Spring 2021

- Implemented various Bayesian algorithms from scratch such as the Viterbi Algorithm for Hidden Markov Models, Gaussian processes, and the Gibbs Sampling algorithm. Code available per request.

APM598 Graduate Introduction to Deep Learning with Dr. Sebastian Motsch Spring 2022

- Lead a team where our final project was analyzing the capacity for a U-net autoencoder for coloring images.

Industry Experience

Western Tool and Supply June 2019 - July 2019, June 2020 - July 2020
Summer Software Developer Intern

- Successfully integrated and programmed Bluetooth LE between microcontrollers and Google Chrome into their IOT interfaced storage system.

IOT Environmental Sensors for Concordia Intl' School Shanghai Jan 2018 - May 2019

- Built, programmed, and deployed 30 microcontroller sensors capable of streaming air quality data. Data was recorded and the effect on student health was presented at ICBDE conference.
- Developed and programmed the full stack air quality monitor system and SQL databases on local servers from scratch.

Awards

2022 Wojcik Family Research Fellowship – $4,500
2022 ON Semiconductor Engineering Scholarship – $2,338
2019-2023 President's Award - New American University – $7,750 each semester

Community Involvement

Machine Learning Club, *Eboard Member, Technical Advisor* 2022
Arizona State University Fulton Student Council *Student Volunteer* August 2019 - 2020

References

Dr. Marinka Zitnik
Assistant Professor at Harvard Department of Biomedical Informatics, **Email:** Marinka@hms.harvard.edu
Dr. Ross Maciejewski
Professor at ASU in the School of Computing and Augmented Intelligence, **Email:** rmacieje@asu.edu