Abhinav K. Adduri, aadduri@andrew.cmu.edu

EDUCATION

Carnegie Mellon University, Advised by Dr. Hosein Mohimani

August 2024

Thesis: Algorithms for Natural Drug Discovery via Machine Learning and Microbial Genome Mining

Ph.D. Computer Science / Computational Biology, GPA: 4.0

Ph.D. Minor Machine Learning, GPA: 4.0

Teaching Assistant: 10-701 Machine Learning, 02-613 Algorithms and Advanced Data Structures

Relevant Graduate Coursework

 $\begin{array}{lll} 10\text{-}701 \; \text{Machine Learning, A} & & 10\text{-}707 \; \text{Advanced Deep Learning, A} \\ 10\text{-}708 \; \text{Probabilistic Graphical Models, A} & 36\text{-}705 \; \text{Intermediate Statistics, A-} \\ 02\text{-}730 \; \text{Cellular \& Systems Modeling, A} & 02\text{-}710 \; \text{Computational Genomics, A+} \end{array}$

10-725 Convex Optimization, A PT-2030 Intro to Computational Structural Biology, A+

University of California, Berkeley

May 2019

B.A. Computer Science, GPA 3.8

B.A. Biochemistry and Molecular Biology, GPA 3.7

Relevant Undergraduate Coursework

CS 170 Efficient Algorithms, ACS 186 Database Systems, A
EE 120 Signals and Systems, A

CS 162 Operating Systems, AMath 110 Linear Algebra, A
EE 123 Digital Signal Processing, A

CS 189 Machine Learning, A EE 126 Probability and Random Processes, A CS 294 Machine Learning in Biology, A- CS 176 Algorithms in Computational Biology, A

Programming

Rust, Python, C++, Typescript / Javascript, HTML, CSS, C, Java

TECHNOLOGIES

Linux, Git, PyTorch, React, Docker

Work Experience

Carnegie Mellon University, Pittsburgh, PA

Ph.D. Candidate

August 2019 - Present

- Developed machine learning methods and graph algorithms to predict novel peptide and polyketide drug structures from microbial genomes
- Discovered a novel antifungal drug which kills the multidrug-resistant pathogen *Candida auris*, which the CDC has labeled as an urgent threat
- \bullet Used protein language models and deep learning to improve small molecule binding prediction for a specific class of proteins. Improved accuracy in generalization benchmark by 20%
- \bullet Developed *Ornaments*, a graph-based alignment tool for unbiased allele-specific read mapping. Improved runtime and accuracy over state of the art by 11.6x / 2x respectively
- Managed over 10 undergrad and Master's students and served on a Master's thesis committee
- Publications and more project details listed below

Square / Caviar, San Francisco, CA

Data Science Engineer Intern

May 2019 - August 2019

- Improved recall / precision of chargeback fraud-detection models by 3.5x / 2.5x respectively
- Improved pre-checkout food delivery ETA predictions for restaurants

Rubrik, Palo Alto, CA

Software Developer Intern

May 2018 - August 2018

- Designed and implemented distributed cache system for filesystems team
- Designed RPCs to expose node cache space to other nodes in the same cluster

Mozilla, Portland, OR

Software Developer Intern

May 2017 - August 2017

- Designed and implemented Firefox Send, a tool for private, end-to-end encrypted file transfer
- $\bullet\,$ Firefox Send was used globally and was covered by news outlets such as Forbes and TechRepublic

PATENTS

Automated Review of Source Code for Style Issues, Rubrik 2018

Honors and Awards CMU-Pitt Ph.D. in Computational Biology: Diversity, Equity and Inclusion Award

CMU SCS Graduate Student Service Award Winner

Publications

Yan, Donghui*, Muqing Zhou*, **Abhinav Adduri***, Mustafa Guler, Sitong Liu, Hyonyoung Shin, Torin Kovach, Gloria Oh, Xiao Liu, Yuting Deng, Liu Cao, Bahar Behsaz, and Hosein Mohimani. Seq2PKS: Discovering Modular Type I Cis-AT Polyketide Natural Products by Integrating Computational Mass Spectrometry and Genome Mining. *Manuscript under review for publication in Nature Communications*.

Adduri, Abhinav, and Seyoung Kim. Ornaments for Accurate and Efficient Allele-Specific Expression Estimation with Bias Correction. bioRxiv (2023): 2023-10. *Manuscript under review for publication in The American Journal of Human Genetics*.

Mongia, Mihir, Romel Baral, **Abhinav Adduri**, Donghui Yan, Yudong Liu, Yuying Bian, Paul Kim, Bahar Behsaz, and Hosein Mohimani. AdenPredictor: accurate prediction of the adenylation domain specificity of nonribosomal peptide biosynthetic gene clusters in microbial genomes. Bioinformatics 39, no. Supplement_1 (2023): i40-i46.

Adduri, Abhinav, and Lee Schruben. The Tao of simulation. In 2017 Winter Simulation Conference (WSC), pp. 607-616. IEEE, 2017.

Adduri, Abhinav. IoT integration in manufacturing Processes. Simulation for Industry 4.0: Past, Present, and Future (2019): 129-139.

Pending Publications Behsaz, Bahar*, **Abhinav Adduri***, Mustafa Guler*, Osama G. Mohamed, Andrés Mauricio Caraballo-Rodríguez, Brendan Duggan, Nirmal Chaudhary, Cameron Miller, Sitong Liu, Benjamin Krummen-acher, Kirk Broders, Daniel Zamith-Miranda, Pamela J. Schultz, David H. Sherman, Jason Clement, Ernesto Nakayasu, Joshua Nosanchuk, Peter C. Dorrestein, Ashootosh Tripathi, and Hosein Mohimani. Pathogen-Oriented Platform for Large-Scale Natural Product Discovery Identifies Novel Antifungal Targeting Drug-Resistant Candidiasis. *Manuscript in preparation for submission to Nature*.

Adduri, Abhinav, Donghui Yan, Mustafa Guler, Chaitanya Suraparaju, Nan Fang, Ashootosh Tripathi, and Hosein Mohimani. (Expected 2024). Seq2Hybrid: Discovering type I polyketide and non-ribosomal peptide hybrid natural products. *Manuscript in preparation for submission to Nature Communications*.

Adduri, Abhinav*, Andrew McNutt*, Chaitanya Suraparaju, Nan Fang, David Koes, and Hosein Mohimani. (Expected 2024). Protein foundation models for accurate and generalizable adenylation domain specificity prediction. *Manuscript in preparation for submission to NeurIPS*.

Ongoing Research

NPDiscover

January 2022 - Present

- Developed machine learning methods and graph algorithms to predict non-ribosomal peptides (NRPs), a type of drug candidate naturally produced by bacteria and fungi
- Developed novel clustering and filtering techniques to reduce the number of predicted drug candidates by 100x while retaining prediction quality
- Used method to discover a novel antifungal drug which kills the multi-drug resistant Candida Auris
- Publication pending preclinical mice model results

Deep AdenPredictor

March 2023 - Present

- Used protein language models as foundation models to improve small molecule binding prediction for adenylation domains, which assemble natural drugs in microbes
- Achieved state of the art performance in normal benchmarks and over 20% improvement over state of the art in generalization benchmarks

Seq2Hybrid

August 2023 – Present

- Expanded previous approaches, which are are restricted to predicting a specific drug class (e.g. peptide drugs), to predict hybrid natural drugs (e.g. peptide + polyketide hybrid drugs)
- Used method to discover a natural producer for immunosuppressants SW-163A and B

Past Projects Seqtools with Nir Yosef - A pipeline for processing ATAC-Seq and RNA-Seq data, 2018 Homolog Identification with Jennifer Doudna - Test and discern evolutionary origin for specific CRISPR mutations, 2017

^{*}Equal contribution.