ANDREW MCNUTT

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EDUCATION

Ph.D. Computational Biology
Expected 2024

Carnegie Mellon University- University of Pittsburgh

B.S. Physics and B.S. Mathematics, Minor: Chemistry
May 2019

Purdue University

RESEARCH EXPERIENCE

Graduate Student Researcher
University of Pittsburgh

Advisor: David Koes

Pittsburgh, PA

Aug 2019 – Current

- Analyzed convolutional neural network (CNN) scoring functions within molecular docking pipeline
- Developed Siamese CNN network to predict relative binding free energy of congeneric series ligands
- Open-sourced a docking pipeline to use pairwise statistics for improved docking performance

Student Intern at Regenstrief Institute
Center for Biomedical Informatics

Mentor: Shaun Grannis

Indianapolis, IN

May 2019 – Aug 2019

- Engineered several machine learning approaches for record-linkage, identifying records that are from the same patient
- Analyzed and compared the performance of record-linkage techniques

Undergraduate Research Assistant at Purdue University
Department of MCMP

Advisor: Markus Lill

West Lafayette, IN

Jan 2017 – December 2018

- Analyzed a novel coarse-grained approach for modeling protein-ligand interaction
- Customized a random forest scoring function for coarse grained modeling of protein-ligand binding
- Enhanced a convolutional neural network with the ability to use probe-protein interaction data to better classify ligand binding poses

Student Intern at Indiana University-Purdue University Indianapolis
Division of Nephrology

Advisor: Tarek M. Ashkar

Indianapolis, IN

May 2018 – Aug 2018

- Researched and determined the strengths and weaknesses of various approaches for clustering and dimensionality reduction
- Collaborated on the development of a full release version of a volumetric cell cytometry software for use on tissue images
- Expanded the capability of the cell cytometry software to include clustering and dimensionality reduction on the data created with the software

Indiana University O'Brien Student Intern
Division of Nephrology

Advisor: Bruce A. Molitoris

Indianapolis, IN

May 2017 – Aug 2017

- Prototyped the merging of a 3D visualization software with an application developed for cell cytometry in tissue images
- Developed procedures for integrating native code into Java applications

SKILLS AND CLASSES

- Python, PyTorch, Pandas, NumPy, Java, Bash, Git
- Deep Learning, Computer Vision, Scalable Machine Learning, Metric Learning
- Molecular Dynamics, Docking, Pharmacophore Modeling
- Linear Algebra, Vector Calculus, Discrete Math, Probability
- Thermal Physics, Computational Physics, Quantum Mechanics
- Biochemistry, Genomics, Systems Biology

PUBLICATIONS

"Improving $\Delta\Delta G$ predictions with a multi-task convolutional Siamese Network" **DOI:**10.1021/acs.jcim.1c01497

McNutt, A. and Koes, D.
Journal of Chemical and Information Modeling (2022)

"GNINA 1.0: molecular docking with deep learning" **DOI:**10.1186/s13321-021-00522-2

McNutt, A.T., Francoeur, P., Aggarwal, R., Masuda, T., Meli, R., Ragoza, M., Sunseri, J. and Koes, D.R.
Journal of Cheminformatics (2021)

"Integrated cytometry with machine learning applied to high-content imaging of human kidney tissue for in-situ cell classification and neighborhood analysis" **DOI:**10.1101/2021.12.27.474025

Winfree, S., **McNutt, A.T.**, Khochare, S., Borgard, T.J., Barwinska, D., Sabo, A.R., Ferkowicz, M.J., Williams, J.C., Lingeman, J.E., Gulbronson, C.J. and Kelly, K.J.,
bioRxiv (2021)

"In situ classification of cell types in human kidney tissue using 3D nuclear staining" **DOI:**10.1002/cyto.a.24274

Woloshuk, A., Khochare, S., Almulhim, A.F., **McNutt, A.T.**, Dean, D., Barwinska, D., Ferkowicz, M.J., Eadon, M.T., Kelly, K.J., Dunn, K.W. and Hasan, M.A.
Cytometry Part A (2021)

PRESENTATIONS

"Open-ComBind: An open-source docking pipeline harnessing pairwise pose statistics"
ACS Spring 2023 ***Mar 2023***

"GNINA 1.0: molecular docking with deep learning"
Broad Institute: Machine Learning in Drug Discovery (Poster) **Oct 2022**
Molecular Machine Learning Conference (Poster) **Oct 2022**
ACS Spring 2021 **April 2021**

"Exploring $\Delta\Delta G$ prediction with Siamese Networks"
Machine Learning for Structural Biology(MLSB) Workshop at NeurIPS (Poster) **Dec 2021**

"Comparison of Supervised Machine Learning and Probabilistic Approaches for Record Linkage"
AMIA Summit 2020 (Not presented due to COVID-19) **March 2020**

MENTORING

Mentoring Master's Student Project

May 2022-Current

University of Pittsburgh **Student: Yanjing Li**

- Advised a Master's student through a neural network knowledge distillation project
- Guided the development of a poster for the PhD program orientation and submitted an abstract to ACS Spring 2023

Summer Research Mentor

Summer 2021

University of Pittsburgh, TECBio Research Experience for Undergraduates **Student: Maddie Bonanno**

- Acted as primary research mentor for an undergraduate student completing graduate-level research in drug discovery
- Advised project to completion; final work presented at university student research symposium

LEADERSHIP

Treasurer

2021-Current

Carnegie Mellon-University of Pittsburgh Computational Biology Graduate Student Association

- Recorded purchases made by the graduate student association
- Budgeted events to fit within our departmental allocations

Senator

2020-2021

Carnegie Mellon-University of Pittsburgh Computational Biology Graduate Student Association

- Organized several in-person and online events for the PhD program
- Assisted in transitioning our PhD program to virtual events during the COVID-19 pandemic

TEACHING

Intro to Computational Structural Biology
Aug 2022-Dec 2022

Graduate Teaching Assistant, University of Pittsburgh

Instructors: David Koes & James Faeder

Scalable Machine Learning for Big Data Biology
Jan 2021-May 2021

Graduate Teaching Assistant, University of Pittsburgh

Instructors: David Koes & Maria Chikina

Modern Mechanics
Jan 2019-May 2019

Undergraduate Teaching Assistant, Purdue University

Electric And Magnetic Interactions
Aug 2016-Nov 2018

Undergraduate Teaching Assistant, Purdue University