ANDREW MCNUTT

@ E-mail: and.mcnutt@pitt.edu Phone: (317) 509-1583 drewnutt.github.io drewnutt

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

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
- 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
- Adapted 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

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

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

Indianapolis, IN — May 2017 – Aug 2017

- Attempted to merge a 3D visualization software with an application developed for cell cytometry in tissue images
- Developed procedures for integrating native code into Java applications

PUBLICATIONS

"Improving $\Delta\Delta G$ predictions with a multi-task convolutional Siamese Network"
McNutt, A. and Koes, D.
ChemRxiv(2021) **DOI:**10.26434/chemrxiv-2021-vcmzz

"GNINA 1.0: molecular docking with deep learning"
McNutt, A.T., Francoeur, P., Aggarwal, R., Masuda, T., Meli, R., Ragoza, M., Sunseri, J. and Koes, D.R.
Journal of Cheminformatics(2021) **DOI:**10.1186/s13321-021-00522-2

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

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) **DOI:**10.1101/2021.12.27.474025

"In situ classification of cell types in human kidney tissue using 3D nuclear staining"

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) **DOI:**10.1002/cyto.a.24274

PRESENTATIONS

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

"Gnina 1.0: Molecular docking with deep learning"
ACS Spring 2021 **April 2021**

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

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 program to virtual events

Summer Research Mentor — Summer 2021

University of Pittsburgh, TECBio Research Experience for Undergraduates

- 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

SKILLS AND CLASSES

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