Derek Jones

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Education

University of Kentucky

M.S., 3.70

Major: Computer Science

Advisors: Dr. Nathan Jacobs & Dr. Sally R. Ellingson

University of Kentucky

B.S., 3.09 Major: Computer Science & Mathematical Economics

Experience

Data Scientist ATOM Consortium

ChemBio Data Scientist

Lawrence Livermore National Laboratory

Data Science Summer Institute

Lawrence Livermore National Laboratory

Intern

Lawrence Berkeley National Laboratory

Research Assistant

Markey Cancer Center

Teaching Assistant

Department of Computer Science, University of Kentucky

Technical Experience

Proficient:

• Python, C/C++

o PyTorch, Keras, Sci-kit learn, Pandas, Numpy, HDF5, PyCharm

Experienced:

• Matlab, R

• Tensorflow, Multiprocessing, Git

Publications

Conference Papers

Lexington, KY

Lexington, KY

August 2011 - May 2016

August 2016 - May 2018

San Francisco, CA

September 2018 - Present

Livermore, CA

September 2018 - Present

Livermore, CA

June 2018 - September 2018

Berkeley, CA

June 2017 - August 2017

Lexington, KY

January 2017 - May 2018

Lexington, KY

August 2016 - May 2017

Derek Jones, Jeevith Bopaiah, Fatemah Alghamedy, Nathan Jacobs, Heidi L Weiss, W A de Jong, and Sally R Ellingson. Polypharmacology within the full kinome: a machine learning approach. In *AMIA 2018 Informatics Summit*, 2018.

Fatemah Alghamedy, Jeevith Bopaiah, Derek Jones, Xiaofei Zhang, Heidi L Weiss, and Sally R Ellingson. Incorporating protein dynamics through ensemble docking in machine learning models to predict drug binding. In *AMIA 2018 Informatics Summit*, 2018.

Poster Sessions

Derek Jones, Nathan Jacobs, and Sally Ellingson. Learning deep feature representations for kinase polypharmacology. In *ACM Richard Tapia Celebration of Diversity in Computing*, 2018.

Derek Jones, Sally R Ellingson, and W A de Jong. How low can you go? feature selection for drug discovery. In *Commonwealth Computational Summit*, 2017.

Talks

Derek Jones. Leveraging large scale molecular dynamics simulations and deep learning for binding activity models. SIAM 2019 Conference on Computational Science and Engineering, 2019.

Theses

Derek Jones. Scalable feature selection and extraction with applications in kinase polypharmacology. Master's thesis, University of Kentucky, 2018.

Grants and Awards

- 2018 ACM Student Reserch Competition (SRC) Travel Award
- 2018 ACM Richard Tapia 2018 Travel Scholarship
- 2018 UK CS Departmental travel grant
- 2017 Supercomputing (SC) 2017 Student Volunteer Travel Award
- 2017 CRA Computing Sciences Research Pathways Fellowship (LBNL)
- 2017 Lyman T. Johnson Diversity Fellowship
- 2017 AAAI 2017 Scholarship
- 2017 AAAI 2017 Diversity Workshop travel award
- 2017 UK CS Departmental travel grant

Volunteering Experience

- 2017 Supercomputing (SC) 2017 Student Volunteer
- 2017 AAAI 2017 Student Volunteer

Organizations

2016-present Association for Computing Machinery (ACM)