Derek Jones

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wderekjones

Education

Aug. 2020 – present **Ph.D**, *University of California - San Diego*, La Jolla, CA.
Major: Computer Science
Advisor: Dr. Tajana Rosing

Aug. 2016 - May. 2018 **M.Sc.**, *University of Kentucky*, Lexington, KY, 3.70.
Major: Computer Science
Advisors: Dr. Nathan Jacobs & Dr. Sally R. Ellingson

Aug. 2011 - May. 2016 **B.S.**, *University of Kentucky*, Lexington, KY, 3.09.
Major: Computer Science & Mathematical Economics
Advisor: Dr. Judy Goldsmith

Experience

Sept. 2018 - Pres. **Data Scientist**, *ATOM Consortium*, San Francisco, CA.
Contributing machine learning and generative modeling expertise on behalf on Lawrence Livermore National Laboratory to develop an open source framework for automated, data-driven, chemical design of disease therapeutics. Specifically developing models and software to enable scalable training and analysis for massive chemical libraries.

Sept. 2018 - Pres. **Research Data Scientist**, *Lawrence Livermore National Laboratory*, Livermore, CA.
Working as part of an inter-disciplinary team to develop structure based deep learning models to augment physics-based simulation pipelines to drive more effective exploration of protein-ligand binding dynamics.

Jun. 2018 - Sept. 2018 **Summer Intern**, *Lawrence Livermore National Laboratory*, Livermore, CA.
Developed spatial graph deep learning technique to model protein-ligand interactions, presenting a poster covering a series of transfer learning experiments. Supervised by Dr. Jonathan E. Allen.

Jun. 2017 - Aug. 2017 **Summer Intern**, *Lawrence Berkeley National Laboratory*, Berkeley, CA.
Conducted research with the Computational Chemistry, Materials, and Climate group in the Computational Research Division of LBNL. Applied machine learning and HPC resources to process high dimensional biochemical data for drug discovery and develop a novel random-forest based feature selection algorithm. Supervised by Dr. Bert de Jong.

Jan. 2017 - May. 2018 **Grad. Research Assistant**, *University of Kentucky - Markey Cancer Center*, Lexington, KY.
Worked as part of an interdisciplinary team to study the prediction of potential off-target effects of candidate cancer therapeutics. Developed data processing pipeline and feature selection algorithms to aid in the understanding of important properties of selectivity in the kinase class of proteins.

Aug. 2016 - May. 2017 **Grad. Teaching Assistant**, *University of Kentucky - Department of Computer Science*, Lexington, KY.

Lab instructor for "Introduction to Programming Design and Abstraction" course, taught in C++. Led 90 minute lab sessions, held office hours to consult with students outside of class, and graded lab assignments, programming assignments, and exams.

Industry Knowledge

∘ Deep Learning ∘ High-Performance Computing (HPC) ∘ Statistical Data Analysis ∘ Sequence Modeling ∘ Message Passing Neural Networks (MPNNs) ∘ Graph Convolution Neural Networks (GCNNs) ∘ Convolutional Neural Networks (CNNs) ∘ Mathematics ∘ Research Projects ∘ Bioinformatics ∘ Computational Biology ∘ Drug Discovery ∘ Computer Science ∘ Programming ∘ Statistical Modeling ∘ Machine Learning ∘ Data Analysis ∘ Statistics ∘ Data Visualization

Tools & Technologies

∘ Python ∘ C++ ∘ C ∘ Matlab ∘ R ∘ STATA ∘ Linux ∘ PyTorch ∘ Keras ∘ Tensorflow ∘ Numpy ∘ Pandas ∘ Matplotlib ∘ Scipy ∘ Git ∘ LaTeX ∘ MySQL ∘ SLURM ∘ LSF ∘ POWER architecture ∘ Microsoft Office

Soft Skills

∘ Inter-personal communication ∘ Inter-disciplinary collaboration ∘ Teamwork ∘ Leadership ∘ Public speaking on technical subjects ∘ Presentation of complex analysis for general audiences

Publications

Journals

Sam Ade Jacobs, Tim Moon, Kevin McLoughlin, Derek Jones, David Hysom, Dong H. Ahn, John Gyllenhaal, Pythagoras Watson, Felice C. Lightstone, Jonathan E. Allen, Ian Karlin, and Brian Van Essen. Enabling rapid covid-19 small molecule drug design through scalable deep learning of generative models. *International Journal of High Performance Computing Applications*, March 2021.

Derek Jones, Hyojin Kim, Xiaohua Zhang, Adam Zemla, Garrett Stevenson, William D Bennett, Dan Kirshner, Sergio Wong, Felice Lightstone, and Jonathan E Allen. Improved protein-ligand binding affinity prediction with Structure-Based deep fusion inference. *J. Chem. Inf. Model.*, March 2021.

W F Drew Bennett, Stewart He, Camille L Bilodeau, Derek Jones, Delin Sun, Hyojin Kim, Jonathan E Allen, Felice C Lightstone, and Helgi I Ingólfsson. Predicting small molecule transfer free energies by combining molecular dynamics simulations and deep learning. *J. Chem. Inf. Model.*, September 2020.

Fangqiang Zhu, Xiaohua Zhang, Jonathan E Allen, Derek Jones, and Felice C Lightstone. Binding affinity prediction by pairwise function based on neural network. *J. Chem. Inf. Model.*, 60(6):2766–2772, June 2020.

Conference Papers

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.

Preprints

Derek Jones, Hyojin Kim, Xiaohua Zhang, Adam Zemla, Garrett Stevenson, William D Bennett, Dan Kirshner, Sergio Wong, Felice Lightstone, and Jonathan E Allen. Improved protein-ligand binding affinity prediction with Structure-Based deep fusion inference. May 2020.

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. Fusion of structure based deep learning to accelerate molecular docking predictions. 5th Computational Approaches for Cancer Workshop at SC19, 2019.

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

2020 Lawrence Livermore Physical and Life Sciences Summer Directorate Award
2020 Lawrence Livermore Computing Directorate Noteworthy Achievement Award
2020 Alfred P. Sloan Foundation Graduate Fellowship
2018 ACM Student Research 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)