Alex Morehead

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Machine Learning • Deep Learning • Computational Biology • High-Performance Computing

Education

University of Missouri — Columbia, Missouri
Ph.D. Computer Science — Aug 2020 - Present
- *Dissertation Advisor*: Prof. Jianlin Cheng
- *Cumulative GPA*: 4.0/4.0
- *Relevant Coursework*: Computational Intelligence, Machine Learning/Pattern Recognition, Deep Learning, NLP, Computer Vision, Unsupervised Learning, Computational Systems Biology, Design & Analysis of Algorithms

Missouri Western State University — St. Joseph, Missouri
B.S. Computer Science — Aug 2016 - May 2020
- *Minor*: Mathematics
- *Cumulative GPA*: 4.0/4.0 with General Studies Honors

Professional Experience

University of Missouri Bioinformatics & Machine Learning Lab — Columbia, Missouri
Graduate Research Assistant | Advisor: Jianlin Cheng — Aug 2020 – Present
- Research and develop novel geometric deep learning algorithms applicable to computational biology
- Authored and published at ICLR 2022 the Geometric Transformer architecture within DeepInteract, a state-of-the-art geometric deep learning pipeline for predicting protein interface contacts
- Published the Geometry-Complete Perceptron Network model for representation learning of 3D molecular graphs

University of Missouri Allen Angel Capital Education Program — Columbia, Missouri
Investment Analyst | Advisor: William (W.D) Allen — Aug 2022 – Present
- Cultivate deal flow for identifying promising technology start-ups
- Pitched several technology companies to the fund, a subset of which have made it to due diligence

Absci AI Research Lab — New York City, New York
AI Scientist Intern | Manager: Joshua Meier — Jun 2022 – Aug 2022
- Researched and built deep learning algorithms for antibody design

Altec Information Services — Saint Joseph, Missouri
Software Development Intern | Advisor: Dan White — Aug 2018 – Aug 2020
- Reduced miscommunication between service centers globally by engineering over 5 new Angular web applications
- Built more than 6 secure backend APIs with the Spring framework in an agile development setting
- Collaborated closely with business stakeholders and analysts to understand data and problems needing to be solved

NSF Research Experience for Undergraduates in Data Science of Risk and Human Activity — Indianapolis, Indiana
Undergraduate Research Assistant | Program Directors: George Mohler, Mohammad Al Hasan — Jun 2019 - Aug 2019
- Authored an ensemble pipeline of 3 convolutional neural networks trained to detect gunshot sounds in the vicinity
- Deployed the pipeline to a cluster of Raspberry Pi 3 Model B+ microcomputers and evaluated its performance in real-world settings in collaboration with Indianapolis public safety officials
- Published as a manuscript and orally presented the gunshot sound detection project's results at the 2019 IEEE International Conference on Big Data

NSF Research Experience for Undergraduates in Synthetic Biology — St. Joseph, Missouri
Undergraduate Research Assistant | Program Directors: Todd Eckdahl, Jeffrey Poet — May 2018 - Aug 2018
- Investigated applications of combinatorial optimization to model lab experiments performed by synthetic biologists
- Produced Variant Sampler, a Java application for modeling the sample space of in vitro experiments
- Published results of the Variant Sampler project in the American Journal of Undergraduate Research

Center for Academic Support — St. Joseph, Missouri
Computer Science Content Tutor | Manager: Karen Luke — Feb 2017 - Aug 2018
- Tutored a total of 5 undergraduate students, 2 being from underrepresented groups
- Spent up to 1 hour with each student per week, reviewing data structures and object-oriented programming

Publications

• *Accepted/Published* •

Geometry-Complete Perceptron Networks for 3D Molecular Graphs — AAAI '23 – Graph Deep Learning Workshop
A. Morehead, J. Cheng — Washington D.C.

3D-Equivariant Graph Neural Networks for Protein Model Quality Assessment — Bioinformatics '23
C. Chen, X. Chen, **A. Morehead**, T. Wu, J. Cheng — Journal

A Region-Based Deep Learning Approach to Automated Retail Checkout — CVPR '22 – AI City Workshop
M. Shoman, A. Aboah, **A. Morehead**, Y. Duan, A. Daud, Y. Adu-Gyamfi — New Orleans, LA

Geometric Transformers for Protein Interface Contact Prediction — ICLR '22
A. Morehead, C. Chen, J. Cheng — (Virtual)

High-Performance Deep Learning Toolbox for Genome-Scale Prediction of Protein Structure and Function — IEEE SuperComputing '21 St. Louis, MO
M. Gao, P. L. Andersen, **A. Morehead**, S. Mahmud, C. Chen, X. Chen, N. Giri, R. Roy, F. Quadir, T. C. Effler, R. Prout, S. Abraham, W. Elwasif, J. Skolnick, J. Cheng, A. Sedova

Synthetic Biology Bicistronic Designs Support Gene Expression Equally Well in vitro and in vivo — AJUR '20 Journal
O. Koucky, J. Wagner, S. Aguilera, B. Bashaw, Q. Chen, A. Eckdahl, E. Edman, P. Gomez, N. Hanlan, N. Kempf, D. Mattoon, S. McKlin, C. Mazariegos, **A. Morehead**, S. Q. Ong, A. Peterson, M. Rojas, K. Roland, K. Schildknecht, H. Seligmann, K. Slater, A. Tauchen, R. Tittor, T. Travieso, D. Urban, C. Willis, J. Zhou, N. L. Snyder, L. J. Heyer, J. L. Poet, T. T. Eckdahl, A. M. Campbell

Low Cost Gunshot Detection using Deep Learning on the Raspberry Pi — IEEE BigData '19
A. Morehead, L. Ogden, G. Magee, R. Hosler, B. White, G. Mohler — Los Angeles, CA

• *Under Review* •

DRLComplex: Reconstruction of protein quaternary structures using deep reinforcement learning — arXiv '22
E. Soltanikazemi, R. S. Roy, F. Quadir, N. Giri, **A. Morehead**, J. Cheng — Under Review

DProQ: A Gated-Graph Transformer for Protein Complex Structure Assessment — arXiv '22
X. Chen, **A. Morehead**, J. Liu, J. Cheng — Under Review

EGR: Equivariant Graph Refinement and Assessment of 3D Protein Complex Structures — arXiv '22
A. Morehead, X. Chen, T. Wu, J. Liu, J. Cheng — Under Review

• *Preprint* •

Semi-Supervised Graph Learning Meets Dimensionality Reduction — arXiv '22
A. Morehead, W. Chantapakul, J. Cheng — Preprint Archive

DIPS-Plus: The Enhanced Database of Interacting Protein Structures for Interface Prediction — arXiv '21 Preprint Archive
A. Morehead, C. Chen, A. Sedova, J. Cheng

Presentations

Neural Diffusion Models: Next-Generation Generative Deep Learning — University of Missouri – Deep Learning F22
A. Morehead — Columbia, Missouri

A Region-Based Deep Learning Approach to Automated Retail Checkout — CVPR '22 – AI City Workshop
A. Morehead, M. Shoman, A. Aboah — New Orleans, Lousiana

Geometric Transformers for Protein Interface Contact Prediction — ICLR '22
A. Morehead — (Virtual)

Geometric Transformers for Protein Interface Contact Prediction — Shandong University '22
A. Morehead — Qingdao, Shandong Province, China (Virtual)

High-Performance Toolbox for Deep Learning of Protein Structure and Function — IEEE SuperComputing '21
A. Morehead, A. Sedova, M. Gao — St. Louis, Missouri (Virtual)

Low Cost Gunshot Detection using Deep Learning on the Raspberry Pi — IEEE BigData '19
A. Morehead, L. Ogden, G. Magee — Los Angeles, California

Low Cost Gunshot Detection using Deep Learning on the Raspberry Pi — IUPUI Student Summer Poster Symposium
A. Morehead, L. Ogden, G. Magee — Indianapolis, Indiana

Variant Sampling in vitro with a Scheduling Twist — Alpha Chi National Convention '19
A. Morehead — Cleveland, Ohio

Variant Sampling in vitro with a Scheduling Twist — MWSU PORTAL Summer Research Showcase '18
A. Morehead — St. Joseph, Missouri

Predicting Game Genres by Analyzing Code Structure — CSCC Central Plains Conference '18
S. Frazier, **A. Morehead**, S. Prine — Maryville, Missouri

Predicting Game Genres by Analyzing Code Structure — MWSU Multidisciplinary Research Day '18
S. Frazier, **A. Morehead**, S. Prine — St. Joseph, Missouri

Leadership Activities

ICLR Volunteer — Apr 2022
NeurIPS Reviewer — Sep 2021 – Present
Upsilon Pi Epsilon (ΥΠΕ) | University of Missouri Chapter — Aug 2020 - Present
Alpha Chi (AX) | Missouri Western State University Chapter — Mar 2018 – May 2020
Kappa Mu Epsilon (KME) | Missouri Western State University Chapter — Mar 2018 – May 2020

Awards & Grants

CVPR Travel Grant — *Jun 2022*
XSEDE Startup Hardware Grant — *Dec 2021*
Dean's Engineering Excellence Fellowship — *Aug 2020*
James W. and Joan M. O'Neill Graduate Fellowship in Engineering — *Aug 2020*
MWSU Outstanding Graduating Computer Science Student Award — *May 2020*
MWSU President's Honor Roll — *May 2020*
Floyd Tesmer/Strayer University Prize in Computer Science and Engineering — *Apr 2019*
Alpha Chi Region IV Scholarship — *Apr 2019*
Grand Midwest Asynchronous Programming Contest 3rd Place Prize — *Apr 2017*
East Side Lions Club Scholarship — *May 2016*

Projects

PyTorch Lightning (20k+ Stars) | GitHub: https://github.com/Lightning-AI/lightning — October 2022 – Present
- Work as a Lightning League Ambassador to ensure the quality of PyTorch Lightning code

BioPython (3k+ Stars) | GitHub: https://github.com/biopython/biopython — Apr 2022 – Present
- Created functionality to remove large feature generation temporary files after all processing completes
- Collaborated with senior project developers to ensure proposed solution matched existing code standards

Graphein (300+ Stars) | GitHub: https://github.com/a-r-j/graphein — Apr 2022 – Present
- Added workflow to catch elusive OS errors when executing external programs
- Worked with senior project developer to ensure workflow matched existing code standards

EGNN-PyTorch (150+ Stars) | GitHub: https://github.com/lucidrains/egnn-pytorch — Apr 2021 – Present
- Noticed the omission of an important geometric unit test for this neural network architecture
- Developed and validated the code to test for node-wise permutation equivariance within the network

AMG-List (80+ Stars) | GitHub: https://github.com/amorehead/awesome-molecular-generation July 2022 – Present

- Curated an open-source list of machine learning research papers related to molecular generation
- Through pull requests, collaborate with other researchers to maintain the quality of papers presented

DeepInteract (40+ Stars) | GitHub: https://github.com/BioinfoMachineLearning/DeepInteract Oct 2021 – Present

- Designed and developed a state-of-the-art geometric deep learning pipeline for predicting protein interface contacts
- Maintain project by addressing bug fixes, feature requests, and future planning

DIPS-Plus (20+ Stars) | GitHub: https://github.com/BioinfoMachineLearning/DIPS-Plus June 2021 – Present

- Curated (to date) the largest molecular dataset for machine learning of protein interface contacts
- Work to ensure ease of use and adoption by responding to feature requests and open issues

Technical Skills

Programming: Python 3 • Java • Angular 2+ • C/C++ • HTML/CSS • SQL • C# • R • MATLAB

Tools/Frameworks: PyTorch • TensorFlow • NumPy • Pandas • Spring Boot • NodeJS • Docker • AWS • Google Cloud

Methodologies: RESTFUL APIs • Version Control {Git} • Agile Development

News & Media Outreach

[1] MU Engineering. (2020, October 27). *Alex Morehead*. University of Missouri College of Engineering. https://engineering.missouri.edu/alex-morehead/.

[2] MU Engineering. (2021, October 18). *New protein prediction tool could accelerate biological discoveries*. University of Missouri College of Engineering. https://engineering.missouri.edu/new-protein-prediction-tool-could-accelerate-biological-discoveries/.

[3] ORNL. (2021, January 10). *Summit Powers Novel Protein Function Prediction Work*. Oak Ridge National Laboratory. https://www.ornl.gov/news/scientists-use-summit-supercomputer-deep-learning-predict-protein-functions-genome-scale/.

[4] HPCwire. (2021, January 13). *Summit Powers Novel Protein Function Prediction Work*. HPCwire. https://www.hpcwire.com/2022/01/13/summit-powers-novel-protein-function-prediction-work/.

[5] MarkTechPost. (2022, January 18). *Researchers Introduce High-Performance Deep Learning Toolbox for Genome-Scale Prediction of Protein Structure and Function*. MarkTechPost Tech News – AI Paper Summary. https://www.marktechpost.com/2022/01/18/researchers-introduce-high-performance-deep-learning-toolbox-for-genome-scale-prediction-of-protein-structure-and-function/.