ALEX MOREHEAD

PhD Researcher

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EXPERIENCE

Graduate Research Assistant
University of Missouri

Aug 2020 – Ongoing | Missouri, USA

- Research **geometric deep learning** and **generative modeling** methods for bioinformatics, to date yielding **15+ academic works**.
- Developed **two state-of-the-art protein representation learning methods** along with the **first** geometric diffusion model to successfully generate large, stable 3D molecules. **My GitHub**.

Geometric deep learning | Graph neural networks | Equivariance | Generative modeling | Computational biology

Research Intern
Profluent Bio

May 2023 – Aug 2023 | California, USA

- Created **MMDiff**, the first SE(3) diffusion model for joint sequence-structure generation of DNA, RNA, and proteins, which achieved a **9% nucleic acid design success rate**. **Paper** and **Code**.

Diffusion modeling | Prototyping | Google Cloud

Research Intern
Absci

Jun 2022 – Apr 2023 | New York, USA

- Collaboratively attained a **0.1%** *de novo* antibody binder design success rate using deep learning, **a first-of-its-kind result**. **Paper** and **Code**.

Protein design | Data science | Kubernetes

Software Development Intern
Altec

Aug 2018 – Aug 2020 | Missouri, USA

- Reduced miscommunication between service centers globally by engineering over **5 new Angular web applications** and **6 secure Spring backend APIs** in a Scrum environment.

Software development | Version control

Undergraduate Research Assistant
IUPUI

Jun 2019 – Aug 2019 | Indiana, USA

- Invented and deployed a convolutional neural network pipeline that yielded a **98% F-1 score** for gunshot sound detection.
- **Published** and orally presented one corresponding manuscript **at IEEE Big Data (2019)**. **Paper** and **Code**.

Artificial intelligence | Machine learning | Data mining

EDUCATION

PhD in Machine Learning and Computational Biology
University of Missouri | O'Neill and College of Engineering Dean's Graduate Fellow

Aug 2020 - Ongoing

- **Geometric Deep Learning** and **Generative Modeling** for Structural Bioinformatics

B.S. in Computer Science
Missouri Western State University | General Studies and Outstanding Graduate Honors

Aug 2016 – May 2020

- Graduated **top of class** among all 2020 graduates in computer science, mathematics, and physics.

SKILLS

PyTorch | PyTorch Lightning | PyG | NumPy/SciPy | Git/GitHub

Python | Java | JavaScript | C

Programming | Operating systems

English | Teamwork | Collaboration

ACHIEVEMENTS

LoG Top-10 Reviewer
• Awarded monetary prize for being a *top-3%* reviewer for the 2023 Learning on Graphs (LoG) conference.

Dean's Engineering Excellence and O'Neill Graduate Fellowships
• Won *two* competitive graduate fellowships for first-year PhD students.

Region IV Scholarship and Floyd Tesmer/Strayer University Prize in Computer Science and Engineering
• Earned *two* awards for innovative computer science research.

Proven peer review experience
• Peer-reviewed 10+ academic submissions for *prestigious* venues such as NeurIPS, Nature Machine Intelligence, LoG, as well as IEEE TNNLS.

PUBLICATIONS

Conference Proceedings

[1] M. Gao, P. Lund-Andersen, **A. Morehead**, *et al.*, "High-performance deep learning toolbox for genome-scale prediction of protein structure and function," in *2021 IEEE/ACM MLHPC Workshop*.

[2] A. R. Jamasb*, **A. Morehead***, Z. Zhang*, *et al.*, "Evaluating representation learning on the protein structure universe," in *NeurIPS MLSB Workshop*, Under review with ICLR 2024.

[3] **A. Morehead**, L. Ogden, G. Magee, R. Hosler, B. White, and G. Mohler, "Low cost gunshot detection using deep learning on the raspberry pi," in *2019 IEEE International Conference on Big Data*.

[4] X. Chen*, **A. Morehead***, J. Liu, and J. Cheng, "A gated graph transformer for protein complex structure quality assessment and its performance in casp15," in *ISMB*, 2023.

[5] **A. Morehead**, A. Bhatnagar, J. A. Ruffolo, and A. Madani, "Towards joint sequence-structure generation of nucleic acid and protein complexes," in *NeurIPS MLSB Workshop*, 2023.

[6] **A. Morehead**, W. Chantapakul, and J. Cheng, "Semi-supervised graph learning meets dimensionality reduction," in *2023 22nd IEEE International Conference on Machine Learning and Applications*, 2023.

[7] **A. Morehead** and J. Cheng, "Geometry-complete diffusion for 3d molecule generation," in *ICLR MLDD Workshop*, Under review with Nature Communications, 2023.

[8] **A. Morehead** and J. Cheng, "Geometry-complete perceptron networks for 3d molecular graphs," in *AAAI Workshop on Deep Learning on Graphs: Methods and Applications*, Finalizing review with Bioinformatics, 2023.

[9] E. Soltanikazemi, R. S. Roy, F. Quadir, N. Giri, **A. Morehead**, and J. Cheng, "Drlcomplex: Reconstruction of protein quaternary structures using deep reinforcement learning," in *International Conference on Intelligent Biology and Medicine*, 2023.

[10] **A. Morehead**, C. Chen, and J. Cheng, "Geometric transformers for protein interface contact prediction," in *International Conference on Learning Representations (ICLR)*, 2022.

Journal Articles

[11] C. Chen, X. Chen, **A. Morehead**, T. Wu, and J. Cheng, "3d-equivariant graph neural networks for protein model quality assessment," *Bioinformatics*,

[12] M. F. Lensink, G. Brysbaert, N. Raouraoua, *et al.*, "Impact of alphafold on structure prediction of protein complexes: The casp15-capri experiment," *Proteins: Structure, Function, and Bioinformatics*, 2023.

[13] **A. Morehead**, C. Chen, A. Sedova, and J. Cheng, "Dips-plus: The enhanced database of interacting protein structures for interface prediction," *Scientific Data*, 2023.

[14] **A. Morehead** and J. Cheng, "Protein structure accuracy estimation using geometry-complete perceptron networks," 2023, Under review with Protein Science.

[15] A. Shanehsazzadeh, S. Bachas, M. McPartlon, *et al.*, "Unlocking de novo antibody design with generative artificial intelligence," *bioRxiv*, 2023.

[16] O. Kouckya, J. Wagnerb, S. Aguilerab, *et al.*, "Synthetic biology bicistronic designs support gene expression equally well in vitro and in vivo," *AJUR*, 2020.

MY LIFE PHILOSOPHY

"The cure for boredom is curiosity. There is no cure for curiosity." - Dorothy Parker

INVITED TALKS

A Gated Graph Transformer for Protein Complex Structure Quality Assessment

ISMB - 3DSIG

Jul 2023 — Lyon, FR

- Introduced the new Gated-Graph Transformer architecture published **at ISMB 2023**.

Presentation | Graph transformers

Geometry-Complete Perceptron Networks for 3D Molecular Graphs

AAAI-AI2ASE

Feb 2023 — Washington D.C., USA

- Contributed an **oral presentation** on the new GCPNet architecture **at the 2023 AAAI-AI2ASE workshop**.

Communication | Geometric deep learning

Neural Diffusion Models: Next-Generation Generative Deep Learning

University of Missouri Deep Learning Course

Nov 2022 — Missouri, USA

- Taught a **graduate-level seminar on** latest advances in **diffusion probabilistic models**.

Teaching | Diffusion modeling

Geometric Transformers for Protein Interface Contact Prediction

Shandong University

May 2022 — Zoom

- Showcased the new Geometric Transformer architecture **published at ICLR 2022**.

Discussion | Geometric graph learning