Mehdi Yazdani-Jahromi

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Summary

AI Research Scientist and Ph.D. candidate specializing in computational drug discovery and machine learning, with proven expertise in developing novel architectures for Transformers and Graph Neural Networks. Led groundbreaking research at Johnson & Johnson, developing HELM, the first mRNA antibody language model. Published extensively in top-tier venues with focus on algorithmic fairness, drug-target interaction prediction, and innovative AI methodologies. Demonstrated track record of translating complex research into practical applications, combining deep technical knowledge with strong collaborative abilities across academic and industry settings. Proficient in large-scale distributed systems and experienced in implementing production-ready AI solutions.

Skills

Programming Languages: Python, Dart, JavaScript, C++, C#, SQL, Solidity, MATLAB

Python Packages: Pytorch, Numpy, Pandas, Keras, TensorFlow, Scikit-learn, Scipy, Networkx, iGraph, dgl, matplotlib, seaborn

JavaScript Frameworks: Vue.js, Electron, NativeScript

Tools: Kubernetes, Docker, Git, HTML, CSS, LATEX, AWS, Slurm

Quantitative Research: Machine Learning Methods, Artificial Intelligence, Large Language Models, Generative AI, Genomics Sequence Modeling, Drug Discovery, Graph Neural Networks, Transformers, Recurrent Neural Networks, LSTMs, Mathematical Optimization, Mathematical Modeling

Soft Skills: Research team coordination, Student mentoring, Technical writing, Conference presentations, Resource allocation, Strategic planning, Analytical thinking, Complex problem resolution, International team collaboration, Multicultural communication, Self-directed learning, Professional networking

Education

University of Central Florida *Jan 2021 – Oct 2025*
PhD in Computer Science
- GPA: 3.94/4.0

University of Central Florida *Jan 2021 – Aug 2023*
MS in Computer Science
- GPA: 3.9/4.0

Sharif University of Technology *Sept 2017 – Dec 2019*
MS in Industrial Engineering
- GPA: 3.88/4.0

Research Experience

AI Research Scientist Intern, Bio-LLMs *Redmond, WA*
Microsoft *June 2025 – Sept 2025*
- Built a novel agent orchestration system for planning, tool use, and judgment.
- Explored agentic AI on deidentified clinical datasets with end to end experiments and evaluation.
- Developed a RAG retrieval stack with hybrid dense and sparse search, reranking, and citation attribution.
- Contributed to the development of evaluation metrics and benchmarks for agentic AI systems.

Graduate Research Assistant *Orlando, FL*
University of Central Florida *Aug 2021 – present*

- Conducted advanced research in computational drug discovery, focusing on drug-target interaction and algorithmic fairness.
- Developed and implemented machine learning models, including Transformers and Graph Neural Networks, for computer vision applications.
- Collaborated on multiple interdisciplinary projects, contributing to the advancement of AI methodologies in drug discovery.
- Published research findings in reputable journals and presented them at international conferences.
- Utilized tools such as Pytorch, TensorFlow, and Scikit-learn to develop and evaluate innovative algorithms.
- Engaged in data analysis and model optimization to enhance prediction accuracy and computational efficiency.
- Assisted in mentoring undergraduate and graduate students and contributed to the academic community through collaborative efforts and knowledge-sharing sessions.

Data Science Intern, AI/ML for Drug Discovery *May 2024 – Nov 2024*
Johnson & Johnson (Janssen R&D)

- Developed and trained HELM (Hierarchical Encoding for mRNA Language Modeling), the first mRNA antibody language model, achieving up to 8% increase in prediction accuracy and enabling the generation of more diverse and biologically plausible sequences.
- Explored alternative attention architectures such as Mamba and Hyena, enhancing transformer model efficiency and effectiveness in processing mRNA sequences.
- Implemented large-scale distributed training on Kubernetes, resulting in significant reduction in training time for LLMs on extensive datasets, optimizing resource utilization and scalability.
- Collaborated with cross-functional teams to refine and deploy advanced LLM architectures, enhancing model accuracy and efficiency for large-scale data processing tasks.

Selected Publications

Equi-mRNA: Protein Translation Equivariant Encoding for mRNA Language Models 2025
Mehdi Yazdani-Jahromi, Ali Khodabandeh Yalabadi, Ozlem Ozmen Garibay
10.48550/arXiv.2508.15103 (Neurips 2025)

BoKDiff: Best-of-K Diffusion Alignment for Target-Specific 3D Molecule Generation 2025
Ali Khodabandeh Yalabadi, **Mehdi Yazdani-Jahromi**, Ozlem Ozmen Garibay
10.48550/arXiv.2501.15631 (Advances in Bioinformatics)

HELM: Hierarchical Encoding for mRNA Language Modeling 2024
Mehdi Yazdani-Jahromi, Mangal Prakash, Tommaso Mansi, Artem Moskalev, Rui Liao
10.48550/arXiv.2410.12459 (ICLR 2025, Neurips 2024 Workshop on AI for New Drug Modalities)

Fair Bilevel Neural Network (FairBiNN): On Balancing fairness and accuracy via Stackelberg Equilibrium 2024
Mehdi Yazdani-Jahromi, Ali Khodabandeh Yalabadi, AmirArsalan Rajabi, Aida Tayebi, Ivan Garibay, Ozlem Ozmen Garibay
10.48550/arXiv.2410.16432 (Neurips 2024)

Learning Fair Representations: Mitigating Statistical Dependencies 2024
Aida Tayebi, **Mehdi Yazdani-Jahromi**, Ali Khodabandeh Yalabadi, Niloofar Yousefi, Ozlem Ozmen Garibay
10.1007/978-3-031-60611-3_8 (HCII conference 2023 Oral Presentation)

FragXsiteDTI: an interpretable transformer-based model for drug-target interaction prediction 2024

Ali Khodabandeh Yalabadi, **Mehdi Yazdani-Jahromi**, Niloofar Yousefi, Aida Tayebi, Sina Abdidizaji, Ozlem Ozmen Garibay
10.1007/978-1-0716-3989-4_5 (Recomb 2024 (Oral), Neurips 2023 Workshop on New Frontiers of AI for Drug Discovery and Development)

Through a fair looking-glass: on mitigating bias in image datasets 2023
Amirarsalan Rajabi, **Mehdi Yazdani-Jahromi**, Ozlem Ozmen Garibay, Gita Sukthankar
10.1007/978-3-031-35891-3_27 (HCII conference 2023 (Oral), AAAI 2023 Workshop on Representation Learning for Responsible Human-Centric AI)

BindingSiteAugmented DTA to enable A Next-Generation Pipeline for Interpretable Prediction Models in Drug-Repurposing 2023
Niloofar Yousefi, **Mehdi Yazdani-Jahromi**, Aida Tayebi, Elayaraja Kolanthai, Craig J Neal, Tanumoy Banerjee, Agnivo Gosai, Ganesh Balasubramanian, Sudipta Seal, Ozlem Ozmen Garibay
10.1093/bib/bbad136 (Briefings in Bioinformatics)

AttentionSiteDTI: Attention Based Model for Predicting Drug-Target Interaction Using 3D Structure of Protein Binding Sites 2022
Mehdi Yazdani-Jahromi, Niloofar Yousefi, Aida Tayebi, Elayaraja Kolanthai, Craig J Neal, Sudipta Seal, Ozlem Ozmen Garibay
10.1093/bib/bbac272 (Briefings in Bioinformatics)

UnbiasedDTI: Mitigating Real-World Bias of Drug-Target Interaction Prediction 2022
Aida Tayebi, Niloofar Yousefi, **Mehdi Yazdani-Jahromi**, Elayaraja Kolanthai, Craig J Neal, Sudipta Seal, Ozlem Ozmen Garibay
10.3390/molecules27092980 (MDPI Molecules)

Academic Services

Reviewer of Journal Briefings in Bioinformatics

Reviewer of Computational and Structural Biotechnology Journal

Reviewer of IEEE Transactions on Neural Networks and Learning Systems Journal

Program Committee Member of AAAI Artificial Intelligence for Social Impact 2025 & 2026.

Reviewer of Neurips 2025 (The Thirty-Ninth Annual Conference on Neural Information Processing Systems)

Developement Experience

Blockchain Developer *June 2020 – Dec 2020*
ZTech Team
- Developed blockchain applications on the Ethereum network using **Solidity**, including implementing ERC20 token standards and smart contracts for financial ICOs.

Lead Software Developer *Jan 2019 – Dec 2020*
BerimCafe
- Developed software for cafe and restaurant management with **Django** and **Flutter**.

Lead Software Developer *Jan 2019 – Mar 2020*
TAEPO
- Created TOEFL Online Practice and Exam Platform using **Django**, **Vue.js**, and **Electron.js**.

Lead Software Developer *Feb 2018 – Dec 2019*
MrZoro.ir
- Developed an automated solution for reserving meals in university, a **Django** based project.

Awards

Received 30000 dollar Amazon Research Credit Award *2023*

Nominated for Order of Pegasus award *2023*

Invited to Golden Key International Honor Society *2022*

Outstanding Graduate Fellowship University of Central Florida *2021*

Ranked 1st among 25000 competitors in Iranian national entrance exam for M.Sc. of industrial engineering *2017*

Ranked 2nd in "Kharazmi" national Prize for Programming *2012*

Projects

DeepDrugDomain: Easy-to-use drug-target affinity/interaction prediction package for architecture design

- Developed an open source **Python package** for drug-target affinity/interaction prediction using deep learning models, including **transformers** and **graph neural networks**, for computational drug discovery.
- Implemented a user-friendly API for easy-to-use drug-target affinity/interaction prediction.
- Published on GitHub

COVID-19 Data Collection and Screening Project

- Initiated and led an open-source, pro bono project for COVID-19 data collection and screening, utilizing technologies such as **Python**, **Django**, and **PostgreSQL** for *backend* development link, and **JavaScript**, **Vue js** for *frontend* development link, to support public health efforts during the pandemic.

Cache Simulator

- Developed a cache simulator to evaluate the performance of different cache management strategies, including LRU, FIFO, and LFU. Implemented in **C++**.

Certificates

Machine Learning Specialization *2024*

- Stanford University and DeepLearning.AI - link

Python Fundamentals *2018*

- Tehran University - link

Advanced Python *2018*

- Maktabkhooneh - link

References

Dr. Ozlem Ozmen (Advisor)

- Assistant Professor at University of Central Florida Email

Dr. Mangal Prakash

- Senior Scientist, AI/ML at Johnson & Johnson (Janssen R&D) Email

Dr. Artem Moskalev

- Research Scientist at Johnson & Johnson (Janssen R&D) Email

Dr. Ivan Garibay

- Associate Professor at University of Central Florida Email