Ali Khodabandeh Yalabadi

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Summary

Ph.D. candidate and AI researcher with a strong focus on computational drug discovery, machine learning, and data science. Experienced in developing advanced AI models for drug-target interaction prediction, generative molecular design, and algorithmic fairness. Proficient in statistics, data analysis, and predictive modeling, with publications in top-tier venues. Adept at leading projects and managing cross-functional collaborations, combining technical expertise with business acumen. Background in industrial engineering, applying optimization and data-driven strategies to real-world AI challenges.

Skills

Programming Languages: Python, SQL, R, MATLAB

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

Tools: Git, HTML, CSS, LATEX, Tableau, Minitab, MSP, GAMS, NetLogo, R-Studio, Microsoft Office

Quantitative Research: Machine Learning Methods, Artificial Intelligence, Generative AI, Drug Discovery, Graph Neural Networks, Transformers, Mathematical Optimization, Mathematical Modeling

Soft Skills: Leadership & Mentorship, Scientific Communication, Strategic & Analytical Thinking, Global & Multicultural Collaboration, Adaptability & Self-Driven Learning, Professional Engagement

Education

University of Central Florida *Aug 2022 – Aug 2026*
PhD in Industrial Engineering
- GPA: 4.0/4.0

Sharif University of Technology *Sept 2017 – Jan 2020*
MS in Industrial Engineering
- GPA: 3.27/4.0

Sharif University of Technology *Sept 2013 – Aug 2017*
BS in Industrial Engineering
- GPA: 3.34/4.0

Research Experience

Graduate Research Assistant *Orlando, FL*
University of Central Florida *Aug 2022 – present*
- Conducted advanced research in **drug-target interaction** prediction and **algorithmic fairness**.
- Designed and implemented machine learning models using **Transformers**, **Graph Neural Networks**, and other AI architectures.
- Contributed to **interdisciplinary projects**, advancing AI applications in drug discovery and molecular modeling.
- Published in top-tier journals and presented findings at **international conferences**.
- Developed and optimized models using **PyTorch** and **Scikit-learn** for improved performance.
- Performed in-depth data analysis and fine-tuned models to improve **predictive accuracy** and **computational scalability**.
- Mentored students, fostering academic growth and collaborative research.

Selected Publications

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 (Submitted to ISMB 2025)

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)

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)

Enhancing supply chain resilience under disruption: analysis of the farmed data by Monte Carlo simulation 2024

Ali Khodabandeh-Yalabadi, Mohammad Sheikhalishahi, Seyed Ali Torabi, Mohsen Naderpour, AmirHossien Radmankian

10.1080/23302674.2024.2398573 (International Journal of Systems Science: Operations & Logistics)

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)

Controlling the misinformation diffusion in social media by the effect of different classes of agents 2023

Ali Khodabandeh Yalabadi, Mehdi Yazdani-Jahromi, Sina Abdidizaji, Ivan Garibay, Ozlem Ozmen Garibay

10.48550/arXiv.2401.11524 (The Computational Social Science Society of the Americas Annual Conference)

Agent-Based Modeling of C. Difficile Spread in Hospitals: Assessing Contribution of High-Touch vs. Low-Touch Surfaces and Inoculations' Containment Impact 2023

Sina Abdidizaji, **Ali Khodabandeh Yalabadi**, Mehdi Yazdani-Jahromi, Ozlem Ozmen Garibay, Ivan Garibay

10.48550/arXiv.2401.11656 (The Computational Social Science Society of the Americas Annual Conference)

Teaching Experience

Teaching Assistant *June 2023 – present*

University of Central Florida

- Machine Learning, Spring 2025
- Data Preparation, Fall 2024
- Computational Analysis of Social Complexity, Fall 2023
- Data mining II, Summer 2023

Work Experience

Data Engineer & Analytics Specialist *Jan 2021 – June 2022*

Keyashian, Tehran, Iran

- Engineered efficient data pipelines and workflows.
- Automated business processes for operational efficiency.

- Optimized data strategies for cost-effective insights.
- Conducted data analysis to support decision-making.

Junior Data Scientist *Jan 2020 – Jan 2021*
KIT, Tehran, Iran
- Integrated Instagram data via APIs.
- Applied image processing for age and gender detection.
- Preprocessed data using Python for analysis.

Head of Business Planning & Supervision *Jan 2018 – Jan 2020*
Farda Digital Transformation Studio, Tehran, Iran
- Developed business models, strategies, and feasibility studies using BP and Canvas frameworks.
- Conducted financial forecasting, valuation, and investor materials (pitch decks, tear sheets).
- Supervised marketing analytics, hiring processes, and operational oversight.

Founder & CEO *Aug 2018 – Dec 2019*
Mr.Zorro Startup, Tehran
- Led UI/UX design and ensured seamless website and app functionality.
- Built strategic partnerships and assembled a high-performing team.
- Managed fundraising, budget planning, and financial execution.
- Drove innovation, differentiation, and customer-centric strategies.

Awards

Invited to Golden Key International Honor Society *2022*

Outstanding Graduate Fellowship University of Central Florida *2022*

Ranked 7th among 2000 competitors in Iranian national entrance exam for Ph.D. of industrial engineering *2020*

Ranked 6th among 25000 competitors in Iranian national entrance exam for M.Sc. of industrial engineering *2017*

Accepted in first round of IOI (Iran Olympiad in Informatics) *2011*

Ranked 1st in Robocop (Iran student's maze runner robots) *2010*

Projects

Statistical Labeling: Cluster-based Approach for Improving Minority Detection in Unbalanced Datasets
- Developed a novel approach to improve **minority class detection** in **unbalanced datasets**.
- Introduced **cluster-based classification**, separating majority and minority classes for better performance.
- Calculated **probability distributions** of classifier predictions within each cluster.
- Labeled test data **statistically** based on the candidate cluster and its probability distribution.

Certificates

Digital transformation *2019*
- Sharif University of Technology

References

Dr. Ozlem Ozmen (Advisor)
- Assistant Professor at University of Central Florida Email

Dr. Ivan Garibay
- Associate Professor at University of Central Florida Email