

# Ali Khodabandeh Yalabadi

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## Summary

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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

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**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

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**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

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**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

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**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](https://arxiv.org/abs/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](https://doi.org/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](https://arxiv.org/abs/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](https://doi.org/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](https://arxiv.org/abs/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](https://arxiv.org/abs/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](https://arxiv.org/abs/10.48550/arXiv.2401.11656)  (The Computational Social Science Society of the Americas Annual Conference)

## Teaching Experience

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### 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

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### 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

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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

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### 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

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### Digital transformation

2019

- Sharif University of Technology

## References

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### Dr. Ozlem Ozmen (Advisor)

- Assistant Professor at University of Central Florida [Email](#) [🔗](#)

### Dr. Ivan Garibay

- Associate Professor at University of Central Florida [Email](#) [🔗](#)