Zia Ur Rehman

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About Me

I am a PhD researcher in Computational Mathematics at the Technical University of Munich (TUM), supervised by Prof. Dr. Gero Friesecke. My research combines Optimal Transport, Deep Learning, and Molecular Dynamics to develop efficient methods for sampling high-dimensional Boltzmann distributions. I focus on combining mathematical theory with machine learning to develop reliable and computationally efficient methods for molecular simulation.

Research Interests

My research focuses on developing mathematically grounded machine-learning methods for high-dimensional sampling and molecular simulation.

Key Areas

- Optimal Transport and computational mathematics
- Normalizing Flows and generative modeling
- Molecular Dynamics and Boltzmann sampling
- High-dimensional probability and machine learning

Education

Technical University of Munich, Germany
PhD in Computational Mathematics
May 2025 – Present
Advised by Prof. Dr. Gero Friesecke

University of L'Aquila, Italy & Silesian University of Technology, Poland
Double MSc in Mathematics for Real-world Applications (Erasmus Mundus Program)
Graduation: July 2024
Master's Thesis: Generative Adversarial Network Model for Image Input with Noise
Supervised by Prof. Marcin Woźniak (SUT)

Allama Iqbal Open University, Islamabad, Pakistan
Bachelor of Education (B.Ed.)
Graduation: February 2020

University of Peshawar, Pakistan
Bachelor's Studies in Mathematics
Graduation: July 2017

Employment

Technical University of Munich, Germany
Research Associate (Wissenschaftlicher Mitarbeiter), TUM School of Computation, Information and Technology, Department of Mathematics
May 2025 – Present
Full-time position (TV-L E13), funded by the German Research Foundation (DFG), Priority Programme SPP 2298 "Theoretical Foundations of Deep Learning", project no. 543965508

Publications

Sampling Boltzmann distributions via normalizing flow approximation of transport maps
Transactions on Machine Learning Research (TMLR), 2026.
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Enhancing Image Processing with GANs in Noisy Environments
Proceedings of the 29th International Conference Information Society and University Studies (IVUS), Kaunas, Lithuania, May 17, 2024, pp. 310–321.
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Talks & Presentations

Sampling Boltzmann distributions via normalizing flow approximation of transport maps
96th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2026), Stuttgart, Germany, March 16–20, 2026.

Generative Adversarial Network Model for Image Input with Noise
Research Seminar, Technical University of Munich (TUM), Munich, Germany, January 2025.