PEINING ZHANG

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Self-Introduction: I'm a Ph.D. student at UConn focusing on applying GenAI—especially diffusion models and large language models—to drug discovery and 3D molecular design. Recently, I developed a 3D molecular diffusion framework that was selected for an Oral presentation at AAAI 2026. With a solid strong academic background and two years of experience at Kuaishou, where I was responsible for developing e-commerce and search engine marketing systems with a daily budget exceeding $1M. I bring a wealth of knowledge in engineering, big data applications, ML strategies, and algorithm iterations.

EDUCATION

University of Connecticut, Connecticut, U.S. 2023 – 2027(expect)

Ph.D. in Computer Science (CS)

Rutgers University, New Jersey, U.S. 2019 – 2021

M.S. in Computer Science (CS)

University of Science and Technology of China (USTC), Anhui, China 2015 – 2019

B.E. in Computer Science (CS)

INDUSTRIAL EXPERIENCE

Kuaishou Technology Co., Ltd Jul. 2021 – May 2023

Software Development Engineer Role: Developing Search Engine and E-commerce Marketing System

- **Real-time API Bidding System**: Designed and developed a purchasing intention model for e-commerce marketing system using Pytorch, boosting e-commerce marketing ROI by 15%.
- **Audience Targeting Shift**: Established a series of dashboards for the new advertising audience, analyzed the reasons for the decline in new users magnitude by sklearn in Python, resulting in a 50% increase in Daily New Users without raising Customer Acquisition Cost.
- **Low-Quality Data Filtering**: Collaborated with media partners to accurately filter cheating traffic, boosting training data for landing page models by 40%. The AUC of the landing page CTR prediction model increased by 2%, and the landing page conversion rate improved by 2.8%.
- **DID Analysis Framework**: Developed a product improvement evaluation framework using **Jupyter** based on Difference-in-Difference (DID) analysis. This framework enabled us assess the effectiveness of over 50 experiments, including those including those beyond the scope of traditional A/B testing.

PROJECTS EXPERIENCE

- **Developing Diffusion Models for Molecule Generation**: Designed and implemented a novel 3D molecular diffusion model by integrating dynamics into the architecture, enhancing conformational validity and accuracy through improved energy relaxation; accepted by *AAAI 2026 (Oral)*. 2024.07–2025.08
- **Reviewing Diffusion models for molecule generation**: Analyzed performance metrics of over 100 diffusion models for molecular generation, published on `Drug Discovery Today`. 2024.02–2024.12
- **Music Comments Generation with GANs**: Led a text generation research project that used GANs in a Seq2Seq manner to generate text guided by music features extracted by WaveNet. paper: `arXiv:2209.01996` (USTC) 2018.02–2020.02
- **Negatively Correlated Search**: Contributed to research improving Negatively Correlated Search for real-parameter optimization, resulting in a published article. (USTC) 2017.05–2018.06

PUBLICATIONS

- *VEDA: 3D Molecular Generation via Variance-Exploding Diffusion with Annealing*, **AAAI 2026 (Oral)**
- *Unraveling the Potential of Diffusion Models in Small Molecule Generation*, **Drug Discovery Today**, 2025
- *Negatively Correlated Search with Asymmetry for Real-Parameter Optimization Problems*, **Journal of Computer Research and Development**, 2019
- *Bridging Music and Text with Crowdsourced Music Comments: A Sequence-to-Sequence Framework for Thematic Music Comment Generation*, **arXiv Preprint**, 2021