





Shih-Hsin Wang

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OBJECTIVE

- Aspiring data scientist with a strong foundation in mathematics and experience in geometric deep learning, generative models, and algebraic geometry. Eager to leverage mathematical rigor to design practical, data-driven solutions. Dedicated to translating complex theoretical frameworks into real-world methodologies that bridge science and industry.

RESEARCH INTERESTS

- Geometric Deep Learning & AI for Science:** *ICLR 2024, ICML 2024, ICLR 2025 Oral*
- Generative (Diffusion & Flow Matching) Models:** *ICML 2025*
- Large Language Models (LLMs)**

EDUCATION

- University of Utah** Salt Lake City, UT
Ph.D. Candidate in Mathematics (Advisors: Bao Wang, Tommaso de Fernex) *Aug. 2021 – Anticipated May 2026*
- National Taiwan University** Taipei, Taiwan
Bachelor of Science, Mathematics *Sep. 2016 – June 2020*

PUBLICATIONS

* indicates equal contribution

Machine Learning **E(3)-Equivariant Fragment-based Graph Neural Networks for Biomolecules**

Wang, S. H., Huang, Y., Transue, T., Baker, J. M., Forstater, J., Strohmer, T., Wang, B.
Under Review

Plug-and-Play Image Restoration with Flow Matching: A Continuous Viewpoint

Jia, F., Huang, Y., **Wang, S. H.**, Garcia-Cardona, C., Bertozzi, A. L., Wang, B.
Under Review

Improving Flow Matching by Aligning Flow Divergence

Huang, Y., Transue, T., **Wang, S. H.**, Feldman, W. M., Zhang, H., Wang, B.
ICML 2025

A Theoretically-Principled Sparse, Connected, and Rigid Graph Representation of Molecules

Wang, S. H.*, Huang, Y.*, Baker, J., Sun, Y. E., Tang, Q., Wang, B.
ICLR 2025

[Oral Presentation]

Learning to Control the Smoothness of Graph Convolutional Networks' Features

Wang, S. H.*, Baker, J.*, Hauck, C. D., Wang, B.
Under Review

An Explicit Frame Construction for Normalizing 3D Point Clouds

Wang, S. H.*, Baker, J.*, de Fernex, T., Wang, B.
ICML 2024

Rethinking the Benefits of Steerable Features in 3D Equivariant Graph Neural Networks

Wang, S. H., Hsu, Y. C., Baker, J., Bertozzi, A. L., Xin, J., Wang, B.
ICLR 2024

Algebraic Geometry **Arcs on Du Val Singularities in Arbitrary Characteristics**

Wang, S. H., de Fernex, T.
In Preparation

Families of Jets of Arc Type and Higher (Co)Dimensional Du Val Singularities

Wang, S. H., de Fernex, T.
C.R. Math. Acad. Sci. Paris, Special Volume in Memory of Jean-Pierre Demailly, arXiv:2306.08291

Other Fields **GenFuzz: GPU-Accelerated Hardware Fuzzing Using Genetic Algorithm with Multiple Inputs**

Lin, D. L., Zhang, Y., Ren, H., Khailany, B., **Wang, S. H.**, Huang, T. W.
ACM/IEEE Design Automation Conference (DAC), 2023

TALKS & PRESENTATIONS

- **ICLR 2025 Oral Presentation:** “A Theoretically-Principled Sparse, Connected, and Rigid Graph Representation of Molecules”
- **JMM 2025:** “Expanding the Mathematical Horizons of Machine Learning: Equivariance and Symmetry”
- **SIAM GL 2023:** “Leveraging Geometric Symmetries with Graph Neural Networks”
- **NCTS Algebraic Geometry Seminar 2023:** “Families of Jets on Higher Du Val Singularities”

WORK EXPERIENCE

- **Visiting Graduate Researcher** Los Angeles, CA
University of California, Los Angeles, Mentor: Andrea Bertozzi Mar. 2025 – Present
 - Initiated a 3D geometric proxy to predict RNA/DNA tertiary structures from secondary structure data, integrating flow-matching models and alignment techniques to enhance folding analysis and downstream property selection
- **Research Intern** Los Alamos, NM
Los Alamos National Laboratory, Mentor: Qi Tang May 2024 - Aug. 2024
 - Established a graph representation that maintains rigidity while reducing edge density by 90% for large disordered proteins, consistently improving model performance in fold classification and ligand-binding affinity prediction
- **Research Assistant** Salt Lake City, UT
Geometric Deep Learning & Generative Models, NSF-supported project, PI: Bao Wang Jan. 2023 - Present
 - Developed a novel normalization for randomly positioned and oriented 3D point clouds using Hopcroft’s algorithm, reducing Wasserstein distance error by 90% compared to existing methods and enabling more accurate downstream tasks
 - Conducted theoretical and empirical analyses on equivariant and invariant graph neural networks, leading to a design strategy for cutting-edge models that boosts accuracy by 50% in classification and enhances efficiency by 30% in regression
- **Undergraduate Instructor** Salt Lake City, UT
University of Utah, Department of Mathematics Aug. 2024 – Dec. 2024
 - Taught and managed a trigonometry course for 58 undergraduates by developing materials and maintaining consistent grading and communication through Canvas
 - Received positive feedback, with students praising clear explanations, structured delivery, and a supportive, engaging teaching style (described as “the GOAT,” “fun,” and “10/10 instructor”)
- **Research Assistant** Salt Lake City, UT
Algebraic Geometry, NSF-supported project, PI: Tommaso de Fernex May 2022 - Dec. 2022
 - Explored connections between Nash components in arc spaces and jet schemes, yielding a generalization of Du Val singularities and resolving the Nash problem for this singularity class
- **Academic Engagement Specialist** Taipei, Taiwan
A13 Co., Industry-Academia Cooperation May 2018 - Aug. 2019
 - Mentored a team of four, including the CEO, in deep learning theory, TensorFlow implementation, and visualization, while advancing face recognition, ranking, and sentence generation projects by refining models and optimizing code for deployment
- **Chatbot Developer Intern** Taipei, Taiwan
Fortunengine.com Corp. July - Aug. 2017
 - Built a Python and SQL-based chatbot, suggesting optimal answers from a Q&A database with 100+ categories, achieving a 74.7% accuracy rate and earning 2nd place in the Civil Affairs ChatBot Competition hosted by the Taipei City Government

ACADEMIC SERVICES

- Reviewer for top-tier ML conferences: **ICLR 2025, ICML 2024, 2025, NeurIPS 2024, 2025, AISTATS 2025**
- Reviewer for journals and reviewing venues: **TMLR, SIAM Journal on Applied Algebra and Geometry, ACM Transactions on Sensor Networks**

PROGRAMMING SKILLS

- Python (Proficient: PyTorch, PyTorch Geometric, Pandas, NumPy, Matplotlib, 3D Visualization), R (Familiar)