Shih-Hsin Wang

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OBJECTIVE

• Aspiring data scientist with a strong foundation in mathematics and experience in geometric deep learning, diffusion 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.

Salt Lake City, UT

Sep. 2016 - June 2020

Taipei, Taiwan

Aug. 2021 – Anticipated May 2026

RESEARCH INTERESTS

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

EDUCATION

•	University of Utah								
	Ph.D.	Candidate	$in \ Mathematics$	(Advisors:	Bao	Wang,	Tommaso	de	Fernex)

• National Taiwan University Bachelor of Science, Mathematics

PUBLICATIONS

* indicates equal contribution

Machine Learning Improving Flow Matching by Aligning Flow Divergence Wang, S. H.*, Huang, Y.*, Transue, T.*, Feldman, W. M., Zhang, H., Wang, B. Under Review, ICML 2025 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 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

University of California, Los Angeles, Mentor: Andrea Bertozzi

• 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 National Laboratory, Mentor: Qi Tang

• 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

Geometric Deep Learning, NSF-supported project, PI: Bao Wang

- 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

University of Utah, Department of Mathematics

- 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

Algebraic Geometry, NSF-supported project, PI: Tommaso de Fernex

• 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

A13 Co., Industry-Academia Cooperation

• 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

Fortunengine.com Corp.

• 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)

Los Angeles, CA Mar. 2025 - Present

Los Alamos, NM May 2024 - Aug. 2024

> Salt Lake City, UT Jan. 2023 - Present

Salt Lake City, UT

Aug. 2024 - Dec. 2024

Salt Lake City, UT May 2022 - Dec. 2022

Taipei, Taiwan May 2018 - Aug. 2019

> Taipei, Taiwan July - Aug. 2017