Shih-Hsin Wang

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OBJECTIVE

- Focused on developing mathematically rigorous methods that reduce wasted resources and costs by minimizing errors while maximizing efficiency. With expertise in geometric deep learning, generative models, and algebraic geometry, I translate complex theoretical insights into practical solutions for science and industry applications

RESEARCH INTERESTS

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

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

Fast and Guided Multimodal Generation via Mean-Flow Diffusion Coupling
Huang, Y., **Wang, S. H.**, Bertozzi, A. L., Wang, B.
Under Review

Towards Multiscale Graph-based Protein Learning with Geometric Secondary Structural Motifs
Wang, S. H., Huang, Y., Transue, T., Baker, J. M., Forstater, J., Strohmer, T., Wang, B.
NeurIPS 2025

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 Rational Double Points in Arbitrary Characteristic
Wang, S. H., de Fernex, T.
Under Review

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

- **BIRS Workshop 2025 on Efficient and Reliable Deep Learning Methods and their Scientific Applications**
- **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

- **Research Assistant** — Salt Lake City, UT
  Geometric Deep Learning & Generative Models, NSF-supported project, PI: Bao Wang — *Jan. 2023 - Present*
  - Introduced an efficient multiscale graph learning framework for proteins based on secondary structure, achieving nearly 90% memory savings and 2x speedup without compromising accuracy on protein modeling benchmarks
  - Developed a novel normalization method using Hopcroft's algorithm to align 3D point clouds into a consistent canonical frame despite random positions and orientations, reducing Wasserstein distance error by 90% compared to existing methods

- **Visiting Graduate Researcher** — Los Angeles, CA
  University of California, Los Angeles, Mentor: Andrea Bertozzi — *Mar. 2025 – Jun. 2025*
  - 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 hyperparameter-free 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

- **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
  AI3 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, Matplotlib, 3D Visualization), R (Familiar)