Senwei Liang

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Google scholar: NLNoSBsAAAAJ | Github: https://github.com/LeungSamWai

Research interests

My research interest spans several topics:

Scientific machine learning: Modeling dynamical systems; Solving high-dimensional PDEs; Symbolic regression; Neural network approximation; Activation function.

Interdisciplinary study: Transitional path sampling in chemical reaction; Rare events; Reinforcement learning-based optimization.

Deep learning algorithm: Regularization methods; Classification models; Foundation models; Explainable models; Graph neural networks; Network slimming; Diffusion models.

Education

Purdue University — West Lafayette, IN
Doctor of Philosophy. Advisor: Prof. Haizhao Yang — Dec 2019 – 2022
Thesis: *Learning and Solving Differential Equations With Deep Learning*

National University of Singapore — Singapore
Master of Science. Advisor: Prof. Haizhao Yang — Aug 2017 – 2019

Sun Yat-Sen University — Guangzhou, China
Bachelor of Science. Advisor: Prof. Lihua Yang — Aug 2013 – 2017

Positions

Lawrence Berkeley National Laboratory — Berkeley, CA
Postdoc. Advisors: Profs. Chao Yang and Lin Lin — Aug 2022 – Present

Argonne National Laboratory — Lemont, IL
Wallace Givens Associate. Advisors: Dr. Hong Zhang — May – Aug 2021

Computational Medical Imaging Laboratory — Guangzhou, China
Research assistant. Advisor: Prof. Yao Lu — Jun 2016 – 2017

Journal publications

[12] Artificial-Intelligence-Driven Shot Reduction in Quantum Measurement — 2024
S Liang, L Zhu, C Yang and X Li
Chemical Physics Reviews, accepted [PDF] [Code]

[11] A Generic Shared Attention Mechanism for Various Backbone Neural Networks — 2024
Z Huang, ***S Liang***, M Liang
Neurocomputing, Volume 611, 128697 [PDF] [Code]

[10] Optimizing Shot Assignment in Variational Quantum Eigensolver Measurement — 2024
L Zhu, ***S Liang***†, C Yang and X Li († joint first author)
Journal of Chemical Theory and Computation, 20, 6, 2390-2403 [PDF] [Code]

[9] Solving PDEs on Unknown Manifolds with Machine Learning — 2024
S Liang, SW Jiang, J Harlim and H Yang
Applied and Computational Harmonic Analysis, Volume 71, 101652 [PDF] [Code]

[8] Reproducing Activation Function for Deep Learning — 2024
S Liang, L Lyu, C Wang and H Yang
Communications in Mathematical Sciences, 22 (2), 285 – 314 [PDF] [Code]

[7] Learning Nonlinear Integral Operators via Recurrent Neural Networks and Its Application 2024
H Bassi, Y Zhu, ***S Liang***, J Yin, CC Reeves, V Vlček and C Yang
Machine Learning with Applications 15, 100524 [PDF]

[6] Probing Reaction Channels via Reinforcement Learning 2023
S Liang, AN Singh, Y Zhu, DT Limmer and C Yang
Machine Learning: Science and Technology 4 (4) [PDF] [Code]

[5] On Fast Simulation of Dynamical System with Neural Vector Enhanced Numerical Solver 2023
Z Huang, ***S Liang***†, H Yang, L Lin († Joint first author)
Scientific reports 13 (1), 15254 [PDF][Code]

[4] Stationary Density Estimation of Ito Diffusions Using Deep Learning 2023
Y Gu, J Harlim, H Yang and ***S Liang**** (* Corresponding author)
SIAM Journal on Numerical Analysis 61 (1), 45-82 [PDF]

[3] Quantifying Spatial Homogeneity of Urban Road Networks via Graph Neural Networks 2022
J Xue, N Jiang, ***S Liang***, Q Pang, T Yabe, SV Ukkusuri and J Ma
Nature Machine Intelligence 4 (selected as cover paper)[PDF] [Code]

[2] Machine Learning for Prediction with Missing Dynamics 2021
J Harlim, SW Jiang, ***S Liang*** and H. Yang (Alphabetical order)
Journal of Computational Physics 428, 109922 [PDF] [Code]

[1] Drop-Activation: Implicit Parameter Reduction and Harmonic Regularization 2021
S Liang, Y Khoo and H Yang
Communications on Applied Mathematics and Computation 3, 293-311 [PDF] [Code]

Conference proceedings

[6] Altersgd: Finding Flat Minima for Continual Learning by Alternative Training 2025
Z Huang, M Liang, ***S Liang*** and S Zhong
Accepted by Multimedia Modeling 2025 [PDF]

[5] Lottery Ticket Hypothesis for Attention Mechanism in Residual Convolutional Neural Net. 2024
Z Huang, ***S Liang***†, M Liang, W He, H Yang and L Lin († joint first author)
IEEE International Conference on Multimedia & Expo [PDF] [Code]

[4] Stiffness-aware Neural Network for Learning Hamiltonian Systems 2022
S Liang, Z Huang and H Zhang
International Conference on Learning Representations [PDF]

[3] Blending Pruning Criteria for Convolutional Neural Networks 2021
W He, Z Huang, M Liang, ***S Liang*** and H Yang
International Conference on Artificial Neural Networks [PDF]

[2] DIANet: Dense-and-Implicit Attention Network 2020
Z Huang, ***S Liang***†, M Liang and H Yang († joint first author)
Proceedings of the AAAI Conference on Artificial Intelligence [PDF] [Code]

[1] Instance Enhancement Batch Normalization: An Adaptive Regulator for Batch Noise 2020
S Liang, Z Huang, M Liang and H Yang
Proceedings of the AAAI Conference on Artificial Intelligence [PDF] [Code]

Manuscripts & Ongoing research

[7] Solving High-Dim. Partial Integral Differential Equations with Finite Expression Method 2024
G Hardwick, ***S Liang*** and H Yang
arxiv: 2410.00835 [PDF]

[6] Learning Biological Systems with Finite Expression Method 2024
J Du, ***S Liang*** and C Wang
In preparation [PDF]

[5] Learning Hamiltonian with Finite Expression Method 2024
J Lai, ***S Liang*** and C Wang
In preparation

[4] QuGStep: Refining Step Size Selection for Gradient-Based Quantum Optimization 2024
S Liang, L Zhu, X Li and C Yang
In preparation

[3] Piecewise Local PCA for Nonlinear Embedding and Collective Variables 2024
S Liang and C Yang
In preparation

[2] Effective Many-body Interactions in Reduced-Dimensionality Spaces through Neural Nets 2024
S Liang, K Kowalski, C Yang and NP Bauman
arXiv:2407.05536 [PDF]

[1] Finite Expression Method for Solving High-Dimensional Partial Differential Equations 2022
S Liang and H Yang
arXiv:2206.10121 [PDF] [Code]

Awards

- Travel Award, SIAM Northern and Central California Sectional Meeting 2024
- Travel Award, International Congress on Industrial and Applied Mathematics 2023
- Outstanding Reviewer, Computer Vision and Pattern Recognition Conference 2022
- Grad Student Travel Grant, American Mathematical Society 2022
- Ross-Lynn Fellowship, Purdue University 2021 – 2022
- Top Graduate Tutors, Department of Mathematics, National University of Singapore 2020
- Thirty-fourth AAAI Conference Scholarship 2020
- Samsung Scholarship, Samsung 2015 – 2016
- Outstanding Student Scholarship, Sun Yat-sen University 2013 – 2017
- National Scholarship, Ministry of Education of China 2013 – 2014

Invited Presentation in Conference and Workshop

- Studying rare chemical reactions via deep learning, Postdoc Symposium, Berkeley lab 2024
- Identifying reaction channels via reinforcement learning, ICIAM, Waseda University 2023
- Identifying reaction channels via reinforcement learning, Postdoc Symposium, Berkeley lab 2023
- Solving PDEs on unknown manifolds with machine learning, AMS Sectional meeting, Purdue University 2022
- Solving PDEs on unknown manifolds with machine learning, Joint Mathematics Meetings, Seattle WA 2022
- Solving PDEs on unknown manifolds with machine learning, 4th Annual Meeting of the SIAM Texas-Louisiana Section, South Padre Island, Texas 2021
- Solving PDEs on Unknown Manifolds with Machine Learning, SIAM Southeastern Atlantic Section Conference, Auburn University 2021
- Solving PDEs on Unknown Manifolds with Machine Learning, IMA Workshop on the Mathematical Foundation and Applications of Deep Learning, Purdue University 2021
- Regularization Methods of Deep Learning for Image Classification, Workshop on “High-Dimensional Learning and Computation in Physics", National University of Singapore 2019

Developed Software Package

Deep Attention Neural Networks: A collection of popular self-attention neural networks for image classification, boasting over 160 stars on GitHub. [Link]

Finite Expression Method: The implementation of the finite expression method for a variety of problems, including solving high-dimensional PDEs, eigenvalue problems, and more. [Link]

Academic Service

Conference reviewer:

- NeurIPS Workshop FM4Science (Foundation Models for Science) 2024
- Conference on Neural Information Processing Systems (NeurIPS) 2023
- International Conference on Computer Vision (ICCV) 2023
- European Conference on Computer Vision (ECCV) 2023
- Conference on Computer Vision and Pattern Recognition (CVPR) 2023, 2022
- AAAI Conference on Artificial Intelligence 2021
- International Conference on Artificial Neural Networks (ICANN) 2021, 2022

Journal reviewer:

- Journal of Scientific Computing (JOMP)
- Journal of Vibration and Control

Organizer:

- Symposium at SIAM Conference on Computational Science and Engineering 2025
- Symposium at AMS Sectional meeting, Purdue University 2022
- Symposium at 4th Annual Meeting of the SIAM Texas-Louisiana Section 2021

Professional References

Prof. Haizhao Yang (PhD supervisor)

- Associate Professor at University of Maryland College Park
- hzyang@umd.edu

Dr. Chao Yang (Postdoc supervisor)

- Senior Scientist at Lawrence Berkeley National Laboratory
- cyang@lbl.gov

Prof. Harlim John (Collaborator)

- Professor at Penn State University
- jharlim@psu.edu

Dr. Hong Zhang (Intern mentor)

- Principle Mathematics Specialist at Argonne National Laboratory
- hongzhang@anl.gov

Prof. Xiaosong Li (Collaborator)

- Larry R. Dalton Endowed Professor at University of Washington
- xsli@uw.edu

Dr. Karol Kowalski (Collaborator)

- Scientist at Pacific Northwest National Laboratory
- karol.kowalski@pnnl.gov

Prof. Kim-Chuan Toh (Teaching)

- Professor at National University of Singapore
- mattohkc@nus.edu.sg