

Buyun Liang

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🎓 Google Scholar

📁 GitHub

EDUCATION

University of Minnesota, Twin Cities

M.Sc in Computer Science | Advisor: Prof. Ju Sun

Minneapolis, MN, USA

Aug 2020 - Jun 2023 (expected)

- GPA: 4.0/4.0

University of Minnesota, Twin Cities

M.Sc in Materials Science (Ph.D. Track) | Advisor: Prof. Ilja Siepmann

Minneapolis, MN, USA

Sep 2018 - Aug 2020

- GPA: 3.66/4.0 | GPA of AI related courses : 4.0/4.0

Nanjing University

B.Sc in Physics (Elite Program)

Nanjing, Jiangsu, China

Sep 2014 - Jul 2018

- GPA: 89.6/100 | Rank: 11/159

RESEARCH INTERESTS

- Optimization for ML & DL [1,2,3,5,6,7]: Optimization software for deep learning with nontrivial constraints
- Robustness in Vision Recognition [2,7]: Reliable and general robust evaluation for DL models against attacks
- AI for Science & Engineering [3,4]: Developing AI for scientific domains (e.g., topology optimization)

PUBLICATIONS

Preprints.....

- [1] **Buyun Liang**, Hengyue Liang, Tim Mitchell, Ying Cui, Ju Sun. NCVX: A General-Purpose Optimization Solver for Machine Learning, and Practical Techniques. Under review at IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI). [[slides](#)][[website](#)][[tutorial proposal 1](#)] [[tutorial proposal 2](#)]
- [2] Hengyue Liang, **Buyun Liang**, Ying Cui, Tim Mitchell, Ju Sun. Optimizers Matter in Adversarial Robustness. Under review at IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI). [[paper](#)][[slides](#)]
- [3] **Buyun Liang**, Ryan de Vera, Hengyue Liang, Tim Mitchell, Ying Cui, Qizhi He, Ju Sun. Deep Structural Optimization with Principled Constrained Optimization. Under review at Transactions on Machine Learning Research (TMLR).
- [4] **Buyun Liang**, Bhargav Joshi, Taihui Li, Roger Rusack, Ju Sun. Using Neural Networks to Predict Radiation Damage to Lead Tungstate Crystals at the CERN LHC. Under review at Nature Machine Intelligence. [[paper](#)]
- [5] **Buyun Liang**, Tim Mitchell, Ju Sun. NCVX: A User-Friendly and Scalable Package for Nonconvex Optimization in Machine Learning. ArXiv preprint arXiv:2111.13984. [[paper](#)]

Conferences & Workshops.....

- [6] **Buyun Liang**, Tim Mitchell, Ju Sun. NCVX: A General-Purpose Optimization Solver for Constrained Machine and Deep Learning. In Neural Information Processing Systems (NeurIPS) Workshop on Optimization for Machine Learning (OPT 2022). [[paper](#)][[poster](#)]
- [7] Hengyue Liang, **Buyun Liang**, Ying Cui, Tim Mitchell, Ju Sun. Optimization for Robustness Evaluation beyond ℓ_p Metrics. In Neural Information Processing Systems (NeurIPS) Workshop on Optimization for Machine Learning (OPT 2022). [[paper](#)][[poster](#)]
- [8] J. Ilja Siepmann, Jingyi L. Chen, **Buyun Liang**, Krishnan Mahesh. Effect of Non-Condensable Gas on the Thermophysical Properties of Bubbly Water and on Bubble Collapse Dynamics Probed by Molecular Simulations. In 33rd Symposium on Naval Hydrodynamics, Osaka, Japan, 18-23 October 2020. [[paper](#)]

RESEARCH EXPERIENCE

Optimization Software for Constrained Machine and Deep Learning.....

NCVX: A General-Purpose Solver for Constrained Deep Learning

Advisors: Prof. Ju Sun, Prof. Tim Mitchell

Apr 2021 - Sep 2022

- Created a software package called NCVX PyGRANSO for constrained optimization in machine & deep learning
- Initiated and hosted multiple interdisciplinary collaborations about robustness in vision recognition and AI for science, where PyGRANSO was served as the backbone method; Published or submitted **6 papers** [1,2,3,5,6,7] based on this solver
- Released a **first author paper** [5] about the software announcement; Published another **first author paper** [6] about the expanded version with detailed examples on constrained deep learning

Constrained Deep Learning & Robustness for Vision Recognition.....

NCVX: A General-Purpose Solver for Machine Learning, and Practical Techniques

Advisors: Prof. Ju Sun, Prof. Tim Mitchell, Prof. Ying Cui

Dec 2021 - Dec 2022

- Proposed practical techniques (e.g., constraints-folding, reformulation, rescaling) to increase the convergence speed of PyGRANSO on large-scale problems
- Achieved state-of-the-art solution quality on a variety of constrained deep learning problems by using PyGRANSO with these practical techniques
- Designed a website <https://ncvx.org> for detailed tutorials to make PyGRANSO friendly to non-experts
- Submitted a **first author paper** [1], an **SDM23 tutorial proposal (accepted)** and an **ICASSP2023 tutorial proposal** based on the improved algorithms and experiments; Designed slides for an **ICCOPT talk**; Contributed to 3 NSF funding proposals and 2 UMII seed grant proposals based on this research

Optimizers Matter in Adversarial Robustness

Advisors: Prof. Ju Sun, Prof. Tim Mitchell, Prof. Ying Cui

Dec 2021 - Dec 2022

- Proposed an algorithmic framework that blends PyGRANSO with constraints-folding to solve both adversarial loss and robustness radius formulation in robust evaluation (RE); Achieved state-of-the-art solution quality on standard RE problems (i.e., ℓ_1 , ℓ_2 and ℓ_∞ metric) by using the new framework
- Generalized RE formulation to include adversarial attack beyond popular ℓ_p metric (e.g., ℓ_8 & LIPIS distance)
- Published a **second author paper** [7] based on the adversarial loss formulation results; Submitted a **second author paper** [2] based on the solution pattern analysis and experimental results from both RE formulations

Constrained Deep Learning & AI for Science and Engineering.....

Deep Structural Optimization with Principled Constrained Optimization

Advisors: Prof. Ju Sun, Prof. Qizhi He, Prof. Tim Mitchell, Prof. Ying Cui

Aug 2022 - Dec 2022

- Applied PyGRANSO to handle constrained optimization in deep structural optimization; Achieved state-of-the-art solution quality on various topology optimization problems by using PyGRANSO
- Submitted a **first author paper** [3] based on the algorithms, practical techniques and experimental results

Machine Learning for High Energy Physics

Advisors: Prof. Ju Sun, Prof. Roger Rusack

May 2022 - Nov 2022

- Proposed a sequence-to-sequence model with teacher forcing strategy to predict laser response in ECAL crystals; Submitted a **co-first author paper** [4] based on the experimental results

Scientific Computing.....

Monte Carlo & Molecular Dynamics Simulation for Multi-Phase Flow

Advisor: Prof. J. Ilja Siepmann

Nov 2018 - Aug 2020

- Performed molecular dynamics simulations to generate trajectories of particles in water-nitrogen mixture systems and calculated the corresponding physical properties (e.g., pressure and viscosity)
- Applied Gibbs Ensemble Monte Carlo methods to simulate nitrogen-water mixture, and determined the nitrogen solubility in the stretched water phase; Published a paper [8] based on the experimental results

EMPLOYMENT HISTORY

University of Minnesota, Twin Cities

Minneapolis, MN

Graduate Research Assistantship from **CS&E**

Jun 2021 - Jan 2022 & May 2022 - Present

Graduate Teaching Assistantship from **CS&E**

Jan 2022 - May 2022

Graduate Research Assistantship from **CEMS**

Sep 2018 - Aug 2020

Graduate Teaching Assistantship from **CEMS**

Jan 2019 - May 2019

TUTORIALS

Deep Learning with Nontrivial Constraints, accepted by **SDM23** [**proposal**]

When Deep Learning Meets Constraints, under review at **ICASSP2023** [**proposal**]

PROFESSIONAL SERVICE

Conference Reviewer for Artificial Intelligence and Statistics (**AISTATS**)

Conference Reviewer for Computer Science and Application Engineering (**CSAE**)

TEACHING EXPERIENCE

Elementary Computational Linear Algebra

University of Minnesota

Graduate Teaching Assistant. Instructors: Prof. Ju Sun, Prof. Carl Sturtivant

Spring 2022

- Organized recitation sessions, designed quizzes, assignments and exams, and hosted office hours.

Introduction to the Science of Engineering Materials

University of Minnesota

Graduate Teaching Assistant. Instructors: Prof. Jeff Schott, Dr. Renee Christensen

Spring 2019

- Led laboratory sessions, hosted office hours, and graded homework assignments and exams.

HONORS AND AWARDS

- UMII Seed Grant Awards, University of Minnesota 2021
- Erling A. Dalaker Fellowship, University of Minnesota 2019
- Outstanding Graduate, Nanjing University 2018
- Aegon-Industrial Fund Management Company Scholarship, Top 2%, Nanjing University 2017
- National Scholarship, Top 2%, Ministry of Education of China 2016
- Elite Program Scholarship×3, Top 4%, Nanjing University 2015, 2016, 2017