Buyun Liang

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EDUCATION

University of Minnesota, Twin Cities — **Minneapolis, MN, USA**
M.Sc in Computer Science | *Advisor: Prof. Ju Sun* — *Aug 2020 - Jun 2023 (expected)*
- GPA: 4.0/4.0

University of Minnesota, Twin Cities — **Minneapolis, MN, USA**
M.Sc in Materials Science (Ph.D. Track) | *Advisor: Prof. Ilja Siepmann* — *Sep 2018 - Aug 2020*
- GPA: 3.66/4.0 | GPA of AI-related courses: 4.0/4.0

Nanjing University — **Nanjing, Jiangsu, China**
B.Sc in Physics (Elite Program) — *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` 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 of 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*