

# Buyun Liang

MSc Student in CS @ UMN

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🏠 [buyunliang.org](http://buyunliang.org)

🎓 [Google Scholar](#)

📁 [GitHub](#)

## EDUCATION

**University of Minnesota, Twin Cities**

*M.Sc in Computer Science*

**Minneapolis, MN, USA**

*Aug 2020 - Jun 2023 (expected)*

◦ GPA: 4.0/4.0

◦ Research Focus: **Optimization for ML & DL, Robustness in Vision, AI for Science** (Advisor: Prof. Ju Sun)

**University of Minnesota, Twin Cities**

**Minneapolis, MN, USA**

*M.Sc in Materials Science (Ph.D. Track)*

*Sep 2018 - Aug 2020*

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

◦ Research Focus: Monte Carlo & Molecular Dynamics Simulation (Advisor: Prof. Ilja Siepmann)

**Nanjing University**

**Nanjing, Jiangsu, China**

*B.Sc in Physics (Elite Program)*

*Sep 2014 - Jul 2018*

◦ GPA: 89.6/100 | Rank: 11/159

◦ Research Focus: Soft Matter Physics (Advisor: Prof. Yi Cao)

## PUBLICATIONS

### Preprints.....

- [1] **Buyun Liang**, Hengyue Liang, Tim Mitchell, Ying Cui, Ju Sun. *Constrained Optimization in Machine and Deep Learning with NCVX and Its Practical Tricks*. Under review at IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI). [[slides](#)][[website](#)][[tutorial proposal](#)]
- [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). [[slides](#)]
- [3] **Buyun Liang**, Ryan de Vera, Hengyue Liang, Tim Mitchell, Ying Cui, Qizhi He, Ju Sun. *On optimization and Optimizers in Neural Structural Optimization*. In preparation for International Conference on Acoustics, Speech, and Signal Processing (ICASSP 2023).
- [4] Bhargav Joshi<sup>†</sup>, **Buyun Liang**<sup>†</sup>, Taihui Li<sup>†</sup>, Roger Rusack<sup>†</sup>, Ju Sun<sup>†</sup>. *Using Neural Networks to Predict Radiation Damage to Lead Tungstate Crystals at the CERN LHC*. Under review at Nature Machine Intelligence. (<sup>†</sup> Equal contributors) [[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*. NeurIPS Workshop on Optimization for Machine Learning (OPT 2022). [[paper](#)]
- [7] Hengyue Liang, **Buyun Liang**, Ying Cui, Tim Mitchell, Ju Sun. *Optimization for Robustness Evaluation beyond  $\ell_p$  Metrics*. NeurIPS Workshop on Optimization for Machine Learning (OPT 2022). [[paper](#)]
- [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*. 33rd Symposium on Naval Hydrodynamics, Osaka, Japan, 18-23 October 2020. [[paper](#)]

## RESEARCH EXPERIENCE

### Optimization Software for Constrained Deep Learning .....

#### Constrained Optimization in Machine & Deep Learning with NCVX and Its Practical Tricks

Research Assistant. Advisors: Prof. Ju Sun, Prof. Tim Mitchell, Prof. Ying Cui Dec 2021 - Present

- Provided practical tricks to speed up the convergence of PyGRANSO on large scale problems.
- Introduced constraints folding to reduce the cost of auto-differentiation and quadratic programming.
- Created reformulation for  $\ell_\infty$  constraint to avoid slow convergence caused by sparse gradients.
- Applied rescaling strategy for objective and constraint functions to avoid extreme values in penalty parameter.
- Benchmarked the performance of PyGRANSO on constrained deep learning problems.
- The algorithms and experiments led to [paper \[1\]](#), an [ICCOPT talk](#), and a [SDM23 tutorial proposal](#).

#### NCVX PyGRANSO: A General-Purpose Solver for Constrained Deep Learning

Research Assistant. Advisors: Prof. Ju Sun, Prof. Tim Mitchell Apr 2021 - Sep 2022

- Created a software package for constrained optimization problem in machine & deep learning.
- Improved GRANSO package by introducing auto-differentiation, GPU support and tensor inputs.
- Created and maintained a website <https://ncvx.org> for detailed documentation and tutorials.
- The software announcement led to [paper \[5\]](#); the expanded version with detailed examples on constrained deep learning led to [paper \[6\]](#).

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

#### Optimizers Matter in Adversarial Robustness

Research Assistant. Advisors: Prof. Ju Sun, Prof. Tim Mitchell, Prof. Ying Cui Dec 2021 - Dec 2022

- Proposed an algorithmic framework that blends PyGRANSO With Constraint-Folding (PWCF) to solve both adversarial loss and robustness radius formulation in robust evaluation (RE).
- Benchmarked performance of PWCF on standard RE problems (i.e.,  $\ell_1$ ,  $\ell_2$  and  $\ell_\infty$  metric).
- Solved RE problems beyond popular  $\ell_p$  metric (e.g.,  $\ell_{1.5}$ ,  $\ell_8$  and LIPIS distance) by using PWCF.
- Improved success rates of SOTA RE packages like AutoAttack by introducing PWCF as a reliable supplement.
- Explored the distinct solution patterns found by various combination of losses, model and algorithms.
- The experimental results from adversarial loss formulation led to [paper \[7\]](#). The solution pattern analysis and experimental results from both RE formulations led to [paper \[2\]](#).

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

#### Neural Structural Optimization with General Physical Constraints

Research Assistant. Advisors: Prof. Ju Sun, Prof. Qizhi He, etc Aug 2022 - Present

- Customized PyGRANSO to handle constrained optimization in neural topology optimization, which is over-parameterized by using a deep-image-prior (DIP) structure.
- Introduced step functions in DIP architecture to promote binary value solutions.
- Benchmarked performance of PyGRANSO on standard neural topology optimization problems.
- Explored general nonlinear physical constraints in neural topology optimization by using PyGRANSO.
- The algorithms, practical tricks and experimental results led to [paper \[3\]](#).

#### Machine Learning for High Energy Physics

Research Assistant. Advisors: Prof. Ju Sun, Prof. Roger Rusack May 2022 - Nov 2022

- Applied sequence-to-sequence model with teacher forcing strategy to predict laser response in ECAL crystals. The experimental results led to [paper \[4\]](#).

### Computational Science .....

#### Monte Carlo & Molecular Dynamics Simulation for Multi-Phase Flow

Research Assistant. 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. The experimental results led to [paper \[8\]](#).

## TUTORIALS

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Deep Learning with Nontrivial Constraints, *under review at SDM23* [proposal]

When Deep Learning Meets Constraints, *under review at ICASSP2023*

## PROFESSIONAL SERVICE

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Conference Reviewer for Artificial Intelligence and Statistics (AISTATS)

Nov 2022

Conference Reviewer for Computer Science and Application Engineering (CSAE)

Aug 2022

## TEACHING EXPERIENCE

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Elementary Computational Linear Algebra

University of Minnesota

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

Spring 2022

- Led recitation sessions; designed quizzes, assignments and exams; 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; graded homework assignments and exams.

## HONORS AND AWARDS

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- 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

## ACADEMIC APPOINTMENTS

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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