

# Buyun Liang

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🏠 buyunliang.org

🎓 Google Scholar

📁 GitHub

## EDUCATION

### University of Minnesota, Twin Cities

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

◦ GPA: 4.0/4.0

Minneapolis, MN, USA

Sep 2020 - Jun 2023 (expected)

### University of Minnesota, Twin Cities

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

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

Minneapolis, MN, USA

Sep 2018 - Aug 2020

### Nanjing University

B.Sc in Physics (Elite Program)

◦ GPA: 89.6/100

Nanjing, Jiangsu, China

Sep 2014 - Jun 2018

## RESEARCH INTERESTS

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

## PUBLICATIONS

Publications are actively updated. See my website [buyunliang.org](http://buyunliang.org) for the latest versions.

### Optimization for Machine and Deep Learning.....

- [1] **Buyun Liang**, Hengyue Liang, Tim Mitchell, Ying Cui, Ju Sun. NCVX: A General-Purpose Optimization Solver for Machine Learning, and Practical Techniques. In preparation for IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI). [[paper](#)][[slides](#)][[website](#)][[SDM2023 tutorial](#)] [[ICASSP2023 tutorial](#)]
- [2] **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](#)]
- [3] **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](#)]

### Adversarial Robustness of Vision Recognition.....

- [4] Hengyue Liang, **Buyun Liang**, Le Peng, Ying Cui, Tim Mitchell, Ju Sun. Optimization for Adversarial Robustness Evaluations and Implications from the Solution Patterns. Under review at International Journal of Computer Vision (IJCV). [[paper](#)][[slides](#)]
- [5] Hengyue Liang, **Buyun Liang**, Ying Cui, Tim Mitchell, Ju Sun. Optimization for Robustness Evaluation beyond  $\ell_p$  Metrics. In Neural Information Processing Systems (NeurIPS) Workshop on Optimization for Machine Learning (OPT 2022). [[paper](#)][[poster](#)]

### AI for Science and Engineering.....

- [6] **Buyun Liang**, Ryan de Vera, Hengyue Liang, Tim Mitchell, Ying Cui, Qizhi He, Ju Sun. Neural Topology Optimization with Principled Constrained Optimization. In preparation for Transactions on Machine Learning Research (TMLR). [[paper](#)]
- [7] **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](#)]

### Scientific Computing.....

- [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** [1,2,3,4,5,6] based on this solver
- Released a **first-author paper** [3] about the software announcement; Published another **first-author paper** [2] 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 and implemented practical techniques (e.g., constraints-folding, reformulation, rescaling) to accelerate the convergence of PyGRANSO on large-scale problems
- Achieved state-of-the-art (SOTA) solution quality (i.e., lower objective value in minimization and better feasibility) on a variety of constrained deep learning problems by using PyGRANSO with practical techniques
- Designed a website <https://ncvx.org> for detailed tutorials to make PyGRANSO friendly to non-experts
- Prepared a **first-author manuscript** [1] (this paper is in the final polishing stage); Submitted 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, 1 NIH funding proposal, 1 approved CISCO fund, and 3 UMII seed grant proposals (one was approved) based on this framework.

#### Optimizers Matter in Adversarial Robustness

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

Dec 2021 - Dec 2022

- Proposed and implemented a novel algorithmic framework that blends PyGRANSO with constraints-folding to solve both adversarial loss and robustness radius formulation in robust evaluation (RE)
- Achieved SOTA adversarial loss and minimal radius with great feasibility on standard RE problems (i.e.,  $\ell_1$ ,  $\ell_2$  and  $\ell_\infty$  metric) by using the new framework
- Generalized RE formulation to include adversarial attacks on non- $\ell_p$  metrics (e.g., perceptual metrics)
- Published a **second-author paper** [5] based on the adversarial loss formulation results; Submitted a **second-author paper** [4] based on the solution pattern analysis and experimental results from both RE formulations

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

#### Neural Topology Optimization with Principled Constrained Optimization

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

Aug 2022 - Dec 2022

- Proposed and implemented a novel neural-reparameterized topology optimization computing framework that could handle implicit physical constraints, combinatorial constraints, and nonlinear physical constraints
- Achieved SOTA compliance (i.e., the objective function in TO) and guaranteed feasibility on various design problems including multi-story buildings and supporting bridges
- Prepared a **co-first-author manuscript** [6] based on algorithms, practical techniques, and experiments

#### Machine Learning for High Energy Physics

Advisors: Prof. Ju Sun, Prof. Roger Rusack

May 2022 - Nov 2022

- Proposed and implemented a sequence-to-sequence model with teacher forcing strategy to predict laser response in ECAL crystals; Submitted a **co-first-author paper** [7] 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

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### University of Minnesota, Twin Cities

Graduate Research Assistantship from **CS&E**  
Graduate Teaching Assistantship from **CS&E**  
Graduate Research Assistantship from **CEMS**  
Graduate Teaching Assistantship from **CEMS**

### Minneapolis, MN, USA

Jun 2021 - Jan 2022 & May 2022 - Present  
Jan 2022 - May 2022  
Sep 2018 - Aug 2020  
Jan 2019 - May 2019

## TUTORIALS

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

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

## PROFESSIONAL SERVICE

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### Review for Conferences

- Artificial Intelligence and Statistics (**AISTATS**)
- International Conference on Acoustics, Speech, and Signal Processing (**ICASSP**)
- Computer Science and Application Engineering (**CSAE**)

## TEACHING EXPERIENCE

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### Elementary Computational Linear Algebra

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

### University of Minnesota

Spring 2022

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

### Introduction to the Science of Engineering Materials

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

### University of Minnesota

Spring 2019

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

## HONORS AND AWARDS

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- UMII Seed Grant Awards, University of Minnesota  
(Drafted the funding proposal; Received the approved fund of \$10,000 as Research Assistantship) 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

## REFERENCES

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- Tim Mitchell**  
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