

Nikolaos Karalias

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Research focus

My research is focused on leveraging neural networks to construct general and data-efficient solvers for combinatorial optimization. I place emphasis on designing end-to-end differentiable algorithms that can optimize over discrete structures like graphs and that can guarantee the quality of their solutions.

Academic Positions

Postdoctoral Associate - MIT CSAIL - Stefanie Jegelka Lab	2025-2027
Postdoctoral Fellow - MIT CSAIL - Stefanie Jegelka Lab	
Postdoc Mobility grant awarded by the Swiss National Science Foundation for the project "General neural solvers for combinatorial optimization and algorithmic reasoning"	2023-2025

Education

PhD Thesis: Probabilistic methods for neural combinatorial optimization	2019 – 2023
Supervised by Pierre Vanderghenst at École polytechnique fédérale de Lausanne (EPFL)	
Master's Degree in Informatics Thesis: Spectral Graph Theory and Deep Learning on Graphs	2015 – 2017
Supervised by Anastasios Tefas at Aristotle University of Thessaloniki (AUTH)	
Bachelor's Degree in Informatics Thesis: Graph Spectra and Signal Processing on Graphs	2011 – 2015
Supervised by Ioannis Pitas at Aristotle University of Thessaloniki (AUTH)	

Selected Publications

- Nikolaos Karalias, Saku Peltonen, Nikita Kostin, Stefanie Jegelka. "On the fundamentals of gradient-based SAT solvers." NeurIPS 2026.
- Nikolaos Karalias and Andreas Loukas. "Erdős Goes Neural: an Unsupervised Learning Framework for Combinatorial Optimization on Graphs." NeurIPS 2020 (Oral: Top 1.1% of papers).
- Morris Yau, Nikolaos Karalias, Eric Lu, Jessica Xu, Stefanie Jegelka. "Are Graph Neural Networks Optimal Approximation Algorithms?" NeurIPS 2024 (Spotlight: top 2% of papers).
- Nikolaos Karalias, Akbar Rafiey, Yifei Xu, Zhishang Luo, Behrooz Tahmasebi, Connie Jiang, Stefanie Jegelka. "Geometric Algorithms for Neural Combinatorial Optimization with Constraints". NeurIPS 2025.
- Nikolaos Karalias, Joshua David Robinson, Andreas Loukas, Stefanie Jegelka "Neural Set Function Extensions: Learning with Discrete Functions in High Dimensions." NeurIPS 2022
- Giorgos Bouritsas, Andreas Loukas, Nikolaos Karalias, Michael M. Bronstein. "Partition and Code: learning how to compress graphs." NeurIPS 2021

Academic Honors and Awards

Postdoc Mobility Return Grant - Swiss National Science Foundation	2025
1 year grant from the Swiss National Science Foundation for my research on neural combinatorial solvers.	
Postdoc Mobility Grant - Swiss National Science Foundation	2023
2 year grant by the Swiss National Science Foundation for my research on neural combinatorial solvers.	
Academic Performance Scholarship - AUTH	Fall 2016
Third semester of Master's Degree at Aristotle University of Thessaloniki	

Academic Service

- Co-organizer: NeurIPS 2025 Workshop on Differentiable Learning of Combinatorial Algorithms. I was responsible for organizing the reviewing and decision processes (inviting reviewers, making final paper decisions, etc.) as well as for arranging invited talks and panel discussions.
- Reviewer for Conferences: NeurIPS 2021, ICLR 2022 (Highlighted Reviewer, Top $\sim 10\%$), ICML 2022, NeurIPS 2022 (Top Reviewer, Top $\sim 10\%$), LOG 2022 (One of Top 20 Reviewers), ICML 2023, NeurIPS 2023 (Top Reviewer, Top $\sim 10\%$), ICML 2024 (Top Reviewer, Top $\sim 10\%$), NeurIPS 2024, NeurIPS 2025, LOG 2025, ICML 2025, ICLR 2026, NeurIPS 2026, ICML 2026 (Top/Gold Reviewer).
- Reviewer for Journals: Nature Communications, Journal of Machine Learning Research (JMLR), IEEE Transactions on Neural Networks and Learning Systems, Journal of Optimization Theory and Applications (JOTA).

Invited talks

- LoGaG: Learning on Graphs and Geometry group.
- Cathy Wu group, MIT.
- Tommi Jaakola group, MIT
- Guy Bresler group, MIT.
- Radix Trading.
- Hassini group, McMaster University.

Media coverage and outreach

- MIT CSAIL article features my work on graph neural networks as optimal approximation algorithms: <https://www.csail.mit.edu/news/deep-learning-np-hard-problems>.
- Ozeki podcast on my work on unsupervised learning for combinatorial optimization.

Student Supervision

I have supervised student projects throughout the course of my PhD and Postdoc.

- Master's thesis, Shengzhao Xia, EPFL.
Empirical comparison of autoregressive and one-shot policies for reinforcement learning on classic combinatorial optimization problems.
- Semester Project, Nikita Kostin, TUM.
Neural combinatorial solvers for SAT.
- UROP and Master's Thesis, Connie Jiang, MIT.
Design of novel discrete function extensions based on combinatorial geometry.
- Master's thesis, Nikolaos Efthymiou, EPFL.
Project on combining machine learning models with algorithmic aspects of the Lovász Local Lemma.
- Master's Thesis, Clarise Han, MIT.
Improving reasoning capabilities and compositional generalization of Large Language Models with algorithmic guidance.
- Chenpan Li, TUM.
Studying implicit reasoning budgets in large language models and improving inference efficiency when composing multiple tasks.

Teaching Experience

Teaching Assistant for courses:

- Matrix Analysis EE-312, undergraduate course at EPFL. I taught at practice sessions and I was involved in designing and grading the final exams as well as course assignments. (2023)
- Network Tour of Data Science EE-558, graduate course at EPFL. I designed and graded problem sets, mentored students on projects, and taught at practice sessions. (2019)
- Information, Computation and Communication CS-119, undergraduate course at EPFL. I was in charge of programming and theory sessions. I was also involved in grading projects and exams. (2022)
- Social Media EE-593, undergraduate course at EPFL. Mentored student teams on group projects. I was also involved in grading individual and group projects. (2021)
- Signals and Systems NCO-05-01, undergraduate course at AUTH. I was involved in designing and grading problem sets for exams. I also taught and supervised students at lab sessions. (2016)

List of papers

- Nikolaos Karalias, Saku Peltonen, Nikita Kostin, Stefanie Jegelka. “On the fundamentals of gradient-based SAT solvers.” NeurIPS 2026.
- Chenpan Li, Stefanie Jegelka, Sharut Gupta, Nikolaos Karalias. “When Tasks Compete for Tokens: Implicit Budgeting in Language Models.” (Under Review).
- Nikolaos Karalias, Cameron Diao, Saku Peltonen, Stefanie Jegelka. “How Good Are Masked Discrete Diffusion Models at Constrained Sampling?” (Under Review).
- Nikolaos Karalias, Thien Le, Stefanie Jegelka, Melanie Weber. “Gradient Descent Program: Universality and Landscape.” (Under Review).
- Ashkan Soleymani, Yifei Xu, Nikolaos Karalias, Akbar Rafiey. “Fast and Parallel Algorithm for Neural Combinatorial Optimization with Constraints.” (Under Review).
- Nikolaos Karalias and Andreas Loukas. “Erdős Goes Neural: an Unsupervised Learning Framework for Combinatorial Optimization on Graphs.” NeurIPS 2020 (Oral: Top 1.1% of papers).
- Morris Yau, Nikolaos Karalias, Eric Lu, Jessica Xu, Stefanie Jegelka. “Are Graph Neural Networks Optimal Approximation Algorithms?” NeurIPS 2024 (Spotlight: top 2% of papers).
- Nikolaos Karalias, Akbar Rafiey, Yifei Xu, Zhishang Luo, Behrooz Tahmasebi, Connie Jiang, Stefanie Jegelka. ”Geometric Algorithms for Neural Combinatorial Optimization”. NeurIPS 2025.
- Nikolaos Karalias, Joshua David Robinson, Andreas Loukas, Stefanie Jegelka ”Neural Set Function Extensions: Learning with Discrete Functions in High Dimensions.” NeurIPS 2022
- Giorgos Bouritsas, Andreas Loukas, Nikolaos Karalias, Michael M. Bronstein. “Partition and Code: learning how to compress graphs.” NeurIPS 2021
- Nikolaos Efthymiou, Nikolaos Karalias, ”Probabilistic Loss Functions for Self-Supervised SAT Solvers”. NeurIPS 2025 DiffCOAlg Workshop
- Nikita Kostin, Nikolaos Karalias, Stefanie Jegelka. On the benefits of label preserving augmentations for self-supervised SAT solvers. NeurIPS 2025 DiffCOAlg Workshop

- Yu He, Robert R Nerem, Timo Stoll, Semih Cantürk, Dobrik Georgiev Georgiev, Solveig Wittig, Chendi Qian, Floris Geerts, Stefanie Jegelka, Ellen Vitercik, Yusu Wang, Nikolaos Karalias, Christopher Morris. “Neural Algorithmic Reasoning Must Explain When Neuralization Adds Value.” ICML 2026 AI4Math Workshop (Poster).
- Akbar Rafiey, Yifei Xu, Nikolaos Karalias. “Self-Supervised Combinatorial Optimization with Constraints via Frank–Wolfe.” (Under Review); OPT 2026 Workshop (Poster).
- Nikolaos Karalias, Joshua David Robinson, Andreas Loukas, Stefanie Jegelka. Neural Extensions: Training Neural Networks with Set (Preprint)