

Semih Cantürk

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EDUCATION

PhD in Computer Science Mila & Université de Montréal	2022–Present
Supervisor: Guy Wolf GPA: 4.30/4.30	
Visiting researcher at RWTH Aachen, LOG Group with Christopher Morris in Fall 2025	
MSc in Computer Science Mila & Université de Montréal	2020–2022
Supervisor: Guy Wolf GPA: 4.30/4.30	
Thesis: <i>Taxonomy of Datasets in Graph Learning: A Data-Driven Approach to Improve GNN Benchmarking</i>	
BSE in Systems Science & Engineering University of Pennsylvania	2014–2018
Supervisor: Robert Ghrist GPA: 3.68/4.00 Dean's List, <i>magna cum laude</i>	
Minors in Computer Science & Mathematics Thesis: <i>Motor Task Prediction through fMRI Data</i>	

PUBLICATIONS

* indicates first authorship.

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- **Semih Cantürk***, Thomas Sabourin*, Frederik Wenkel, Michael Perlmutter, Guy Wolf. Can Computational Reducibility Lead to Transferable Models for Graph Combinatorial Optimization? *Proceedings of the 43rd International Conference on Machine Learning (ICML)*. Seoul, South Korea. July 6-11, 2026.
 - Yu He, Robert R. Nerem, Timo Stoll, **Semih Cantürk**, Dobrik Georgiev, Chendi Qian, Solveig Wittig, Floris Geerts, Stefanie Jegelka, Ellen Vitercik, Yusu Wang, Nikolaos Karalias, Christopher Morris. Neural Algorithmic Reasoning Must Explain When Neuralization Adds Value. *3rd AI for Math Workshop @ ICML 2026*. Seoul, South Korea. July 6-11, 2026.
 - Billy Joe Franks, Moshe Eliasof, **Semih Cantürk**, Guy Wolf, Carola-Bibiane Schönlieb, Sophie Fellenz, Marius Kloft. Towards Graph Foundation Models: A Study on the Generalization of Positional and Structural Encodings. *Transactions in Machine Learning Research (TMLR)*. February 20, 2025.
 - Frederik Wenkel*, **Semih Cantürk***, Michael Perlmutter, Guy Wolf. Towards a General Recipe for Combinatorial Optimization with Multi-Filter GNNs. *Proceedings of the Third Learning on Graphs Conference (LoG, Spotlight)*. PMLR 269. Virtual, November 26–29, 2024.
 - **Semih Cantürk***, Renming Liu*, Olivier Lapointe-Gagné, Vincent Létourneau, Guy Wolf, Dominique Beaini, Ladislav Rampásek. Graph Positional and Structural Encoder. *Proceedings of the 41st International Conference on Machine Learning (ICML)*, PMLR 235. Vienna, Austria. July 21-27, 2024.
 - Renming Liu*, **Semih Cantürk***, Frederik Wenkel, Sarah McGuire, Xinyi Wang, Anna Little, Leslie O'Bray, Michael Perlmutter, Bastian Rieck, Matthew Hirn, Guy Wolf, Ladislav Rampásek. Taxonomy of Benchmarks in Graph Representation Learning. *Proceedings of the First Learning on Graphs Conference (LoG, Spotlight)*. PMLR 198. Virtual, December 9–12, 2022.
 - Renming Liu*, **Semih Cantürk***, Frederik Wenkel, Dylan Sandfelder, Devin Kreuzer, Anna Little, Sarah McGuire, Leslie O'Bray, Michael Perlmutter, Bastian Rieck, Matthew Hirn, Guy Wolf, Ladislav Rampásek. Towards a Taxonomy of Graph Learning Datasets. *Data Centric AI (DCAI) workshop at NeurIPS*. December 14, 2021.

Preprints & Under Review

- **Semih Cantürk***, Arman Mielke*, Andrei Manolache, Chendi Qian, Antoine Siraudin, Christopher Morris, Mathias Niepert, Guy Wolf. GraIP: A Benchmarking Framework for Neural Graph Inverse Problems. *Under review*.
- Lydia Mezrag*, **Semih Cantürk***, Bastian Rieck, Guy Wolf. Path Laplacian Encodings for Directed Graphs. *Under review*.
- **Semih Cantürk***, Yimeng Min, Frederik Wenkel, Michael Perlmutter, Guy Wolf. Avoiding the Oversmoothing Versus Underreaching Tradeoff in Graph Convolutional Networks via Hybrid Scattering Networks. *Under review*.
- Cristian Gabellini, Nikhil Shenoy, Stephan Thaler, **Semih Cantürk**, Daniel McNeela, Dominique Beaini, Michael Bronstein, Prudencio Tossou. OpenQDC: Open Quantum Data Commons. *ArXiv preprint*. November 29, 2024.
- **Semih Cantürk***, Aman Singh*, Patrick St-Amant & Jason Behrmann. Machine-Learning Driven Drug Repurposing for COVID-19. *ArXiv preprint*. June 25, 2020.

WORK EXPERIENCE

Valence Labs

Montreal, QC | Mar-Dec 2024

PhD Intern, Physical Simulations Unit

- Developed an equivariant GNN-based delta-learning framework for molecular dynamics (MD) systems, enabling the use of smaller MLIPs without sacrificing simulation accuracy.
- Contributed to the development of OpenQDC, an open source library of QM datasets and MLIPs. Main contributions were on extending experimentations and developing visualizations.

Zetane Systems

Montreal, QC | 2019–2024

Researcher and Software Developer, Machine Learning

- Responsible for development of the ML explainability module (XAI) in the *Zetane Engine* for computer vision problems through approaches such as class-activation mapping (CAM) methods, as well as game-theoretic or surrogate approaches such as SHAP and LIME.
- Develop the dataset augmentation and model explainability (XAI) modules of *Zetane Protector* for object classification, object detection and semantic segmentation.
- Lead and support machine learning projects with industry partners in robotics, energy, construction and automotive industries.

University of Pennsylvania

Philadelphia, PA | 2018–2020

Undergraduate Researcher, supervised by Victor Preciado & Cassiano Becker

- Built an ML pipeline that predict motor tasks from fMRI data using signal processing and LSTMs, which won the Penn Engineering Societal Impact Award.
- After graduation, extended the project to use mesh-based learning and GNNs.

InfoTRON

Istanbul, Turkey | 2017–2018

Software Development Intern

- Built an ML framework using ARToolkit and OpenCV to recognize and classify CAD models in AR/VR environments.

Imperial College

London, UK | Summer 2016

Undergraduate Researcher

- Awarded a £3,000 research stipend, built a distributed system to run acute3D, a 3D-modeling software, in the Imperial College Data Observatory.

SAS Analytics

Istanbul, Turkey | Summer 2016

Data Scientist Intern

- Worked on fraud detection projects with global industry partners in insurance sector.
- Completed training on SAS language, SAS Enterprise Guide & SAS Enterprise Miner

TEACHING

Mila & Université de Montréal

Montréal, QC | Fall 2021-2023

Teaching Assistant

MAT 6495: Spectral Graph Theory/Théorie spectrale des graphes, Guy Wolf. Fall 2021, 2022, 2024.

MAT 6493: Geometric Data Analysis/Analyse géométrique de données, Guy Wolf. Fall 2023.

University of Pennsylvania

Philadelphia, PA | Fall 2016

Teaching Assistant

ESE 210: Introduction to Dynamical Systems, Robert Ghrist

AWARDS & LEADERSHIP

- **Bourse de fin d'études doctorales.** Université de Montréal, 2026-2027
- **Top/Gold Reviewer Award.** ICML 2026, ICLR 2026.
- **Mitacs Globalink Research Award (GRA).** Mitacs, 2025
- **Bourse d'excellence du département d'informatique et de recherche opérationnelle (DIRO).** Université de Montréal, Hiver/Winter 2025.
- **Bourse en Intelligence Artificielle des ESP.** Université de Montréal, 2023-2024
- **Bourse d'exemption, PhD.** Université de Montréal, 2022-present
- **Bourse d'exemption, MSc.** Université de Montréal, 2020-2022
- **Societal Impact Award.** U. of Pennsylvania, Dept. of Electrical & Systems Engineering, 2018
- **Top 25 College Graduates of 2018, Turkey.** Study In America e-Newsletter, 2018
- **Research Stipend.** Imperial College Data Science Institute, 2016

TUTORIALS & TALKS

- Tutorial: *Geometric and Topological Representation Learning*. IEEE International Workshop on Machine Learning for Signal Processing (MLSP). Istanbul/Turkey, August 31-September 3, 2025.
- *Towards a General Recipe for Combinatorial Optimization with Multi-Filter GNNs*. LoG 2024 Montréal Meetup, Mila — Quebec AI Institute, November 25, 2024.
- *Graph Representation Learning*. A gentle introduction & new perspectives. Université de Montréal, September 25, 2024.
- *Graph Representation Learning*. A gentle introduction & new perspectives. Concordia University, March 27, 2024.
- *Graph Positional and Structural Encoder*. LoG 2023 Montréal Meetup, Mila — Quebec AI Institute, December 4, 2023.
- *Graph Representation Learning*. Université de Montréal, November 9, 2023.
- *Graph Representation Learning*. Concordia University, March 3, 2023.

REVIEWING

- International Conference on Machine Learning (ICML). 2026 (**Gold reviewer**)
- International Conference on Learning Representations (ICLR). 2025, 2026 (**Top reviewer**)
- Learning on Graphs (LoG) conference. 2022, 2025
- NeurIPS Workshop on Symmetry and Geometry in Neural Representations (NeurReps). 2023, 2025

- IEEE Transactions on Neural Networks and Learning Systems (TNNLS) Regular Papers, 2024, 2023; Special Issue: Graph Learning, 2023
- Workshop on Topology, Algebra and Geometry in Data Science (TAG-DS). ICML 2023, NeurIPS 2025
- ICLR Workshop on Geometrical and Topological Representation Learning, 2022

OTHER ACADEMIC SERVICES

- Organizer of the Graph Signal Processing (GSP) Workshop, 8th Edition, 2025
- Organizer of the Learning on Graphs (LoG) conference Montréal meetup, 2024
- Chair (2015-2017) and Treasurer (2014-2015) of the Penn Preceptorials Committee

Penn Preceptorials is a student-run organization that creates seminars, talks and other events in collaboration with the University of Pennsylvania faculty to encourage intellectual development in the student community.

- As Chair, led the Preceptorials governing board, overseeing all committee activities.
- As Treasurer, was responsible for the planning and accounting of \$28K budget.

SKILLS

Programming: Python, Java, C++, C#, JavaScript, Matlab, HTML, CSS, SQL, SAS, Swift

ML Libraries & Software: PyTorch, PyTorch Geometric, DGL, Lightning, Hydra, Optuna, HPC/SLURM, TensorFlow, Spark, Hadoop, SAS Enterprise Guide & Miner

Computer Vision & Graphics: OpenCV, WebGL, ARToolkit

3D Graphics & CAD Software: AutoCAD, Rhinoceros 3D, AVEVA, acute3D

Languages: Turkish (Native), English (Fluent), Spanish (B2), Greek (B1), French (A2)

Hobbies: Tennis, football, skiing, guitar, literature, languages, history & anthropology