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

MSc in Computer Science | Mila & Université de Montréal **2020–2022**
Supervisor: Guy Wolf GPA: 4.30/4.30
Thesis: *Taxonomy of Datasets in Graph Learning: A Data-Driven Approach to Improve GNN Benchmarking*

BSE in Systems Science & Engineering | University of Pennsylvania **2014–2018**
Supervisor: Robert Ghrist GPA: 3.68/4.00 Dean's List, *magna cum laude*
Minors in Computer Science & Mathematics Thesis: *Motor Task Prediction through fMRI Data*

PUBLICATIONS

* indicates first authorship.

- 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. *Accepted to 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 Rampášek. 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 Rampášek. 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 Rampášek. Towards a Taxonomy of Graph Learning Datasets. *Data Centric AI (DCAI) workshop at NeurIPS*. December 14, 2021.

Preprints & Under Review

- **Semih Cantürk***. GraIP: A Benchmarking Framework for Neural Graph Inverse Problems. Under review for the International Conference on Learning Representations 2026.
- 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 to leverage the correlated nature of sequential states of 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 machine learning 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 a machine learning 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 a machine learning framework using ARToolkit and OpenCV to recognize and classify CAD models in AR/VR environments.

Imperial College **London, UK | Summer 2016**

Undergraduate Researcher

- Built a distributed system that runs acute3D, a 3D-modeling software, in the Imperial College Data Observatory, the largest data visualization studio of its kind in Europe.

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 Institute & Université de Montréal **Montréal, QC | Fall 2021-2023**

Teachning 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**

Teachning Assistant

ESE 210: Introduction to Dynamical Systems, Robert Ghrist

AWARDS & LEADERSHIP

- **Mitacs Globalink Research Award (GRA).** Mitacs, 2025
- **Bourse d'excellence du département d'informatique et de recherche opérationnelle (DIRO).** Université de Montréal, 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 Learning Representations (ICLR). 2025, 2026
- 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. Also managed communications between Preceptorials and Penn administration for budgeting.

SKILLS

Programming: Python, Java, C++, C#, JavaScript, Matlab, HTML, CSS, SQL, SAS, Swift
ML Libraries & Software: PyTorch, 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