

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
MSc 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**
Supervisors: Victor Preciado GPA: 3.68/4.00 Dean's List, *magna cum laude*
BSE Thesis: *Motor Task Prediction through fMRI Data*
Minors in Computer Science & Mathematics

PUBLICATIONS

* indicates first authorship. † indicates peer-reviewed conference/journal.

- 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 TBD. 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. 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

- Billy Joe Franks, Moshe Eliasof, **Semih Cantürk**, Guy Wolf, Carola-Bibiane Schönlieb, Sophie Fellenz, Marius Kloft. Should Learnable Positional and Structural Encodings be Integrated Into Graph Foundation Models? *Awaiting review for TMLR*.
- 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

PhD Intern, Physical Simulations Unit

Montreal, QC | Mar-Dec 2024

- 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

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 en Intelligence Artificielle des ESP, Université de Montréal | 2023-2024

Bourse d'exemption, Université de Montréal | 2020-2022 (MSc), 2022-present (PhD)

Societal Impact Award, Penn Department of Electrical & Systems Engineering | 2018

Study In America | Top 25 College Graduates of 2018, Turkey

Learning on Graphs (LoG) | Montréal meetup organizer, 2024

Penn Preceptorials Committee | Chair (2015-2017), Treasurer (2014-2015)

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 the 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.

REVIEWING

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

TALKS

- *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.

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 (B2), French (A2)

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