Georgios (George) Dasoulas

Senior Machine Learning Scientist

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Research Interests

Geometric Deep Learning, Foundation Models, Multimodal Learning, Knowledge Graphs, Graph Machine Learning, Generative Models, Evaluation and Benchmarking, AI for Science, AI for Biology.

Professional Experience

March 2025 - Today

Merck & Co, Cambridge, Massachusetts,USA

- Senior Machine Learning Research Scientist @ Merck Research Laboratories.
- Single-cell Foundation Models for target discovery.
- Geometric deep learning for gene regulatory network inference.
- Multimodal learning for spatial transcriptomics and H&E imaging.

July 2022 - February 2025

Harvard University, Boston, Massachusetts, USA

- Harvard Data Science Initiative Postdoctoral Research Fellow.
- Appointment: Blavatnik Institute, Department of Biomedical Informatics, Harvard Medical School.
- Hosting Labs: 1) Marinka Zitnik's Lab @ DBMI,
  2) Francesca Dominici's Lab @ HDSI.
- Research focus: a) Geometric deep learning for 3D biomolecular structure representation and design.
  b) Multimodal Foundation Models for therapeutics.
  c) Equivariant message passing for spatiotemporal modeling.

October 2018 - April 2022

Huawei Technologies, Paris, France

- Doctoral research scientist in graph machine learning.
- Laboratory: Noah's Ark Lab, AI department of Huawei R&D.
- Research focus: Representation learning algorithms for static and dynamic networks, specialized in telecommunications.

June 2017 - January 2018

TWT GmbH Science & Innovation, Stuttgart, Germany.

- MSc Thesis research in machine learning for prediction-based optimization.
- ML-powered recommender system for short-term prediction and decision-making on optimal refueling.

October 2013 - February 2016

Software Engineering Laboratory at National Technical University of Athens, Greece

- Laboratory Assistant for computer programming courses.
- Tasks: Teaching assistant, and laboratory supervisor.

Education

April 2019 - March 2022	**École Polytechnique**, Palaiseau, Paris, France. • Ph.D. student in computer science. • Laboratory: Data Science and Mining Team, LIX, École Polytechnique. • Funding: CIFRE PhD Collaboration with Huawei Technologies, France. • Thesis: *"Towards Expressive Graph Neural Networks: Theory, Algorithms, Applications"*. • Supervisor: Prof. Michalis Vazirgiannis (DaSciM). • External advisors: Dr. Aladin Virmaux (Huawei), Dr. Kevin Scaman (INRIA Paris). • Graduation date: 21st March 2022.
October 2012 - February 2018	**National Technical University of Athens**, Athens, Greece. • BSc & MSc in Electrical and Computer Engineering (5-year joint degree; 300 ECTS) – Order of Entrance: 10th among undergraduate students – Overall GPA: 9.06/10 (Excellent). Top 3% among graduate class – Specialization: Computer Science (Major), Mathematics, Networks (Minor) • Thesis : *"Predictive Refueling - Combining machine learning algorithms with optimization calculations for operations planning"*. Grade: 10/10. • Thesis supervision: Prof. Nectarios Koziris (National Technical University of Athens), Dr. Florian Mittag (TWT GmbH Science & Innovation).
July 2012	Nationwide University Entrance Examination score : 19.676/20.000 (top 1% nationwide).

Honors & Awards

July 2023	**Wojcicki Troper postdoctoral fellowship**. Named fellowship funded by Harvard Data Science Initiative for outstanding early-career researchers (awarded for 2nd year).
July 2022	**Wojcicki Troper postdoctoral fellowship**. Named fellowship funded by Harvard Data Science Initiative for outstanding early-career researchers (awarded for 1st year).
November 2020	**Eleftheria Barka scholarship**. Scholarship for graduation excellence and pursuit of doctoral studies for the academic year 2020-2021.
November 2019	**Eleftheria Barka scholarship**. Scholarship for graduation excellence and pursuit of doctoral studies for the academic year 2019-2020.
December 2015	**Papakyriakopoulos award**. Award of excellence in Mathematics (corresponding subjects in Mathematics).
March 2014	**Silver medal** in South Eastern Mathematical Olympiad for university students (aka. Seemous), Iasi, Romania.
October 2013	Participation in the IEEExtreme 24-Hour Programming Competition.
September 2012	**"The Great Moment of Education" award – scholarship** by Eurobank EFG, for excellency in national qualifications exams.
May 2010	**Certificate** for the theoretical and practical educational seminar for C.P.R - F.B.A.O - A.E.D knowledge, Red Cross, Greece.
March 2009	**Bronze Medal** in National Mathematical Olympiad for high school students in Athens.

Publications & Patents

Preprints

1. ProCyon: A multimodal foundation model for protein phenotypes, 2025.

Conferences

2. Alexis Chevalier, Soumya Ghosh, Urvi Awasthi, James Watkins, Julia Bieniewska, Nichita Mitrea, Olga Kotova, Kirill Shkura, Andrew Noble, Michael J. Steinbaugh, Vijay Sadashivaiah, George Dasoulas, Julien Delile, Christoph Meier, Leonid Zhukov, Iya Khalil, Srayanta Mukherjee, Judith Mueller. TEDDY: A Family Of Foundation Models For Understanding Single Cell Biology. In *ICML 2025 Generative AI and Biology (GenBio) Workshop*, 2025.

3. Claudio Battiloro, Ege Karaismailoglu, Mauricio Tec, George Dasoulas, Michelle Audirac, Francensca Dominici. E(n) Topological Neural Networks. In *International Conference on Learning Representations (ICLR)*, 2025.

4. Tina Vartziotis, Ippolyti Dellatolas, George Dasoulas, Maximilian Schmidt, Florian Schneider, Tim Hoffmann, Sotirios Kotsopoulos, Michael Keckeisen. Learn to Code Sustainably: An Empirical Study on LLM-based Green Code Generation. In *the First International Workshop on Large Language Models for Code (LLM4Code)*, 2024.

5. Jiali Cheng, George Dasoulas, Huan He, Chirag Agarwal, Marinka Zitnik. GNNDelete: A General Unlearning Strategy for Graph Neural Networks. In *International Conference on Learning Representations (ICLR)*, 2023.

6. Michalis Chatzianastasis, Johannes Lutzeyer, George Dasoulas, Michalis Vazirgiannis. Graph Ordering Attention Networks. In *AAAI Conference on Artificial Intelligence (AAAI)*, 2023.

7. George Dasoulas, Kevin Scaman, Aladin Virmaux. Lipschitz Normalization for Self-Attention Layers with Application to Graph Neural Networks. In *International Conference on Machine Learning (ICML)*, 2021.

8. Michail Chatzianastasis, George Dasoulas, Georgios Siolas, Michalis Vazirgiannis. Graph-based Neural Architecture Search with Operation Embeddings. In *Neural Architectures: Past, Present and Future Workshop for International Conference on Computer Vision (ICCV)*, 2021.

9. George Dasoulas, Johannes Lutzeyer, Michalis Vazirgiannis. Learning Parametrised Graph Shift Operators. In *International Conference on Learning Representations (ICLR)*, 2021.

10. George Dasoulas, Giannis Nikolentzos, Kevin Scaman, Aladin Virmaux, Michalis Vazirgiannis. Ego-based Entropy Measures for Structural Representations on Graphs. In *International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, 2021.

11. George Dasoulas, Ludovic Dos Santos, Kevin Scaman, Aladin Virmaux. Coloring graph neural networks for node disambiguation. In *International Joint Conference on Artificial Intelligence (IJCAI)*, 2020.

12. Stratis Limnios, George Dasoulas, Dimitrios M. Thilikos, Michalis Vazirgiannis. Hcore-Init: A graph-based initialization method for neural networks. In *International Conference of Pattern Recognition (ICPR)*, 2020.

Journals

13. Lev Telyatnikov, Guillermo Bernardez, Marco Montagna, Mustafa Hajij, Martin Carrasco, Pavlo Vasylenko, Mathilde Papillon, Ghada Zamzmi, Michael T. Schaub, Jonas Verhellen, Pavel Snopov, Bertran Miquel-Oliver, Manel Gil-Sorribes, Alexis Molina, Victor Guallar, Theodore Long, Julian Suk, Patryk Rygiel, Alexander Nikitin, Giordan Escalona, Michael Banf, Dominik Filipiak, Max Schattauer, Liliya Imasheva, Alvaro Martinez, Halley Fritze, Marissa Masden, Valentina Sánchez,

Manuel Lecha, Andrea Cavallo, Claudio Battiloro, Matt Piekenbrock, Mauricio Tec, George Dasoulas, Nina Miolane, Simone Scardapane, Theodore Papamarkou. TopoBench: A Framework for Benchmarking Topological Deep Learning, *Journal of Data-centric Machine Learning Research (DMLR)*, 2025.

14. George Dasoulas*,Dimitris Vartziotis*, Florian Pausinger. Learn2Extend: Extending sequences by retaining their statistical properties with mixture models. *Experimental Mathematics*, 2024.
15. George Dasoulas*, Yasha Ektefaie*, Ayush Noori, Maha Farhat, Marinka Zitnik. Multimodal representation learning with graphs, *Nature Machine Intelligence*, 2023.
16. Giannis Nikolentzos, George Dasoulas, Michalis Vazirgiannis. Permute Me Softly: Learning Soft Permutations for Graph Representations, *IEEE Transactions on Pattern Analysis and Machine Intelligence (PAMI)*, 2022.
17. Guillaume Salha-Galvan, Johannes Lutzeyer, George Dasoulas, Romain Hennequin, Michalis Vazirgiannis. Modularity-Aware Graph Autoencoders for Joint Community Detection and Link Prediction, *Neural Networks*, June 2022.
18. Giannis Nikolentzos, George Dasoulas, Michalis Vazirgiannis. k-hop Graph Neural Networks. *Neural Networks*, Volume 130, Pages 195-205, October 2020.

Patents

19. Aladin Virmaux, George Dasoulas, Kevin Scaman. Normalization scheme for self-attention neural networks. US2023/0385615 A1. November 2023.
20. Aladin Virmaux, George Dasoulas, Kevin Scaman. A normalization scheme for self-attention neural networks. WO2022167077 A1 International Publication Number. August 2022.
21. George Dasoulas, Ludovic Dos Santos, Kevin Scaman, Aladin Virmaux. Node Disambiguation. US 2022/0215260 A1 . July 2022.
22. George Dasoulas, Ludovic Dos Santos, Kevin Scaman, Aladin Virmaux. Node Disambiguation. WO 2021/058096 A1 International Publication Number. April 2021.

Skills

Deep Learning Frameworks:	Pytorch, TensorFlow, Keras, Pyro, Huggingface
Programming Languages:	Python, R, C++, OCaml, MATLAB, bash, Latex.
Tools & Platforms:	Git, Jira, AWS, SageMaker, Cuda, GNU/Linux, Windows, MacOS.

Societies & Affiliations

- **Conference Reviewer:** NeuRIPS 2022, NeurIPS 2023, NeurIPS 2024, ICLR 2022, ICLR 2023, ICLR 2024, ICML 2022, ICML 2024, AAAI 2021, AAAI 2022, AAAI 2023, IJCAI 2021, ISMB/ECCB 2023.
- **Program Committee:** ISMB/ECCB 2023.
- **Journal Reviewer:** 1) Elsevier's Neural Networks Journal 2021-Today, 2) IEEE Transactions on Neural Networks and Learning Systems 2020-Today, 3) IEEE Transactions on Pattern Analysis and Machine Intelligence 2023-Today.
- **Member:** IEEE Computer Society 2013-2014.

Test Scores

- General GRE: Quantitative Score: 167/170, Verbal Score: 157/170, Essay: 4/6.
- TOEFL iBT : 100/120.

Languages

- **Greek** (Native speaker)
- **English** (Excellent - CEF:C2) : Examination for the Certificate of Proficiency in English (ECPE)
- **German** (Very good command - CEF :C1) : Goethe-Zertificat B1, TestDAF Level C1
- **French** (Intermediate)