Alejandro García Castellanos

Ph.D. Candidate Machine Learning
AMLab, University of Amsterdam

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Research Interests

Applying topology, geometry, and algebra to the representation learning and generative modeling of shapes for enhanced human-AI collaboration.

Experience

Ph.D. Candidate — Feb. 2024 – Present
AMLab (Amsterdam Machine Learning Lab), UvA — *Amsterdam, Netherlands*

- Under the supervision of Erik Bekkers (UvA) and co-supervision of Daniël Pelt (ULEI)
- Sponsored by The Hybrid Intelligence Centre
- Geometry-informed machine learning techniques for collaborative human-computer image annotation

Research Engineer — Mar. 2023 – Feb. 2024
RPL (Division of Robotics, Perception and Learning), KTH — *Stockholm, Sweden*

- Under the supervision of Danica Kragic
- Metric learning in generative models
- Hierarchy discovery in Hyperbolic geometry

Trainee Internship — Sep. 2020 – Jan. 2021
MEDAL laboratory, CTB (Center of Biomedical Technology) — *Madrid, Spain*

- Under the supervision of Ernestina Menasalvas
- Development of new techniques for information recognition in medical corpus
- Fine-tuning an LLM in breast and lung cancer's clinical notes

Education

MSc in Machine Learning — Sep. 2021 – Oct. 2023
KTH Royal Institute of Technology — *Stockholm, Sweden*

- Average grade: 4.00 GPA
- Applied Mathematics elective track: Topological Data Analysis, Regression Analysis, Time Series Analysis
- Thesis in *"Topological regularization and relative latent representations"*

B.S. in Mathematics and Computer Science — Sep. 2017 – Jul. 2021
Universidad Politécnica de Madrid — *Madrid, Spain*

- Average grade: 9.78/10.0 (4.00 GPA)
- Best academic record amongst all programs at the ETSIINF (Higher Technical School of Computer Engineers) of the promotion 2020/2021
- Honours granted by UPM in 29 courses
- Three Scholarships for Academic Excellence granted by the Community of Madrid
- Thesis in *"Robustness of Persistent Homology: the Stability Theorem"*

Skills

Programming: Python, Java, C, R, SQL, MATLAB, Maple, Prolog, Bash

ML Frameworks: PyTorch, PyTorch Lightning, JAX, TensorFlow

Tools: LaTeX, Git, Microsoft Office, Keynote, Pages, Adobe Photoshop, Adobe Lightroom

Soft Skills: public speaking, written communication, teamwork, project and time management, critical thinking, analytical skills, research skills, creativity, strategic thinking

Teaching & Supervision

Reinforcement Learning 2025, 2026
Teaching assistant *Master In Artificial Intelligence, UvA*

Deep Learning 2 2024, 2025
Teaching assistant and project supervisor *Master In Artificial Intelligence, UvA*

Master Thesis Supervisor 2025
Thesis: "Persistent Homology Go Combinatorial" *Master In Artificial Intelligence, UvA*

Research Publications

NeurIPS '25 **A. García-Castellanos**, D. R. Wessels, N. J. Berg, R. Duits, D. M. Pelt, E. J. Bekkers (2025). "*Equivariant Eikonal Neural Networks: Grid-Free, Scalable Travel-Time Prediction on Homogeneous Spaces*". In: *Advances in Neural Information Processing Systems (NeurIPS)*.

ALENEX '25 **A. García-Castellanos***, A. A. Medbouhi*, G. L. Marchetti, E. J. Bekkers, D. Kragic (2025). "*Hypersteiner: Computing heuristic hyperbolic steiner minimal trees*". In: *2025 Proceedings of the Symposium on Algorithm Engineering and Experiments (ALENEX)*.

TAG-DS '25 Oral O. Boufalis*, J. Carrasco-Pollo*, J. Rosenthal*, E. Terres-Caballero*, **A. García-Castellanos** (2025). "*Symmetry-Aware Graph Metanetwork Autoencoders: Model Merging through Parameter Canonicalization*". In: *Proceedings of the 1st Conference on Topology, Algebra, and Geometry in Data Science (TAG-DS)*. **Oral presentation**.

UniReps '24 **A. García-Castellanos**, G. L. Marchetti, D. Kragic, M. Scolamiero (2024). "*Relative representations: Topological and geometric perspectives*". In: *Proceedings of the II edition of the Workshop on Unifying Representations in Neural Models (UniReps)*.

Preprints & Manuscripts

UniReps '25 (Ext. Abs.) B. Kuipers*, F. Byrman*, D. Uyterlinde* **A. García-Castellanos** (2025). "*Symmetry-Aware Fully-Amortized Optimization with Scale Equivariant Graph Metanetworks*". In: *Extended Abstract track of the III edition of the Workshop on Unifying Representations in Neural Models (UniReps)*.

ArXiv '25 (Preprint) **A. García-Castellanos***, A. A. Medbouhi*, G. L. Marchetti, D. M. Pelt, E. J. Bekkers, D. Kragic (2025). "*Randomized HyperSteiner: A Stochastic Delaunay Triangulation Heuristic for the Hyperbolic Steiner Minimal Tree*".

GRaM '24 (Blog Post) D. Canez*, N. Midavaine*, T. Stessen*, J. Fan*, S. Arias*, **A. García-Castellanos** (2024). "*Effect of equivariance on training dynamics*". In: *Workshop Blog track at the I edition of the Workshop on Geometry-grounded Representation Learning and Generative Modeling (GRaM)*.

GRaM '24 (Blog Post) M. Carrasco*, A. Berentzen*, **A. García-Castellanos** (2024). "*Applications of TopoX to Equivariant Topological Networks*". In: *Workshop Blog track at the I edition of the Workshop on Geometry-grounded Representation Learning and Generative Modeling (GRaM)*.

Invited Talks

4th workshop on Mathematics and AI June 2025
Tilburg, Netherlands

Learning on Graphs Conference November 2024
Amsterdam, Netherlands

Community Service

Reviewer 2025
NeurIPS Proceedings

Reviewer 2025
NeurReps Workshop

Reviewer 2024
UniReps Workshop

Reviewer 2024
ICML Proceedings

Languages

English: Advanced level (C1), CAE by Cambridge English

Spanish: Native language

German: Low Beginner Level