Brenda Nogueira

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Education

University of Notre Dame — *Jan 2024 - Dec 2028*
PhD in Computer Science and Engineering — Notre Dame, IN, United States
Advisors: Prof. Nitesh V. Chawla & Prof. Nuno Moniz

University of Porto — *Sep 2022 - Dec 2024*
Master in Data Science — Porto, Portugal
Advisors: Prof. Nuno Moniz & Prof. Rita Ribeiro

University of Porto — *Sep 2017 - Jun 2022*
Bachelor in Mathematics with Minor in Computer Science — Porto, Portugal

Publications [Google Scholar]

Preprints and Under Submissions

SPECTRA: Spectral Target-Aware Graph Augmentation for Imbalanced Molecular Property Regression (2026)
Brenda Nogueira, Meng Jiang, Nitesh V Chawla, Nuno Moniz.
International Conference on Learning Representations (ICLR)

Rethinking Evaluation in Compound Potency Prediction (2026)
Brenda Nogueira, Nuno Moniz, Connor W. Coley, Nitesh Chawla.
***Journal of Chemical Information and Modeling, JCIM**. ACS Publications*

From Verification Burden to Trusted Collaboration: Design Goals for LLM-Assisted Literature Reviews (2026)
Brenda Nogueira, John Kim, Andrew Andereson, Toby Li, Werner Geyer, Nuno Moniz, Nitesh V. Chawla.
***The Association for the Advancement of Artificial Intelligence (AAAI)**). AI for Scientific Research Workshop*

Peer-Reviewed Publications

Spectral Manifold Harmonization for Graph Imbalanced Regression (2025)
Brenda Nogueira, Gabe Gomes, Meng Jiang, Nitesh V Chawla, Nuno Moniz.
***42nd International Conference on Machine Learning (ICLR)**. DIG-BUGS Workshop*
***31st ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD).** MLoG-GenAI Workshop*

Automated Fish Size Measurement System for Long-Term Growth Studies in the Azores (2025)
Brenda Nogueira, Rita P. Ribeiro, Gui M. Menezes, Nuno Moniz
***European Conference on Machine Learning and Knowledge Discovery (ECML/PKDD**). SoGood Workshop*

Graph-Imbalanced Regression for Rare Phenotypes (2025)
Brenda Nogueira, Nuno Moniz, Nitesh V Chawla.
12th Iberian Conference on Pattern Recognition and Image Analysis (IbPRIA)

Experiential-Informed Data Reconstruction for Fishery Sustainability and Policies in the Azores (2025)
Brenda Nogueira, Gui M. Menezes, Nuno Moniz, Rita P. Ribeiro
***Discover Data**, Springer.*

Dynamics of Fisheries in the Azores Islands: A Network Analysis Approach (2024)
Brenda Nogueira, Ana Torres, Nuno Moniz, Gui M. Menezes.
22nd Portuguese Conference on Artificial Intelligence (EPIA)

Honors and Awards

Scientific Artificial Intelligence Graduate Fellowship — *2025*

NSF Center for Computed Assisted Synthesys Travel Award — *2025*

International Mathematics Without Borders Olympiad Brazilian Section | Gold medal — *2016*

Research Interests

Imbalanced Regression Learning: Designing data-driven solutions to enhance predictive performance in imbalanced and rare-event regression problems.
AI for Science: Applying AI and machine learning to real-world challenges in science and mathematics, including chemistry, biochemistry, and genomics—such as mathematical modeling, molecular design, virtual screening, and drug discovery.
Graph, Generative & Agentic AI: Developing graph-based, generative (VAE, diffusion), and agentic AI systems for synthetic data generation, predictive modeling, and autonomous decision-making.

Experience

Research Assistant *Jan 2024 - Dec 2028 (Expected)*
Lucy Institute for Data & Society
Exploration of Artificial Intelligence with a focus on imbalanced domains and chemistry data.

Research Fellow *July 2023 - Dec 2023*
INESCTEC
Multi-objective optimization of raw material utilization for cutting and packing solutions in industry.

Research Fellow *Oct 2022 - June 2023*
FCUP
Automated email-entity association pipeline using NLP.

Research Initiation Fellow *Aug 2022 - Sept 2022*
INESCTEC
Machine learning for imbalance time series prediction about landings in the OKEANOS dataset.

Intern *March 2022 - June 2022*
INESCTEC
Development of an online platform using Shiny/R for an AutoML solution.

Intern *March 2022 - June 2022*
Ideavity
Development of a sales platform and applications using Outsystems.

Intern *Oct 2021 - Fev 2022*
Evolutio
Website creation using wagtail (based on Django).

Volunteer Intern *July 2021*
INESCTEC
Implementation of real-time face-based sleepiness recognition web-app.

Organizer

Learning on Graphs Conference (**LoG**) Meetup 2025

Mentorship

John Kim, B.E. in Computer Science & Applied Math, University of Notre Dame 2025-Present
C-CAS GUIDE Program 2025-Present

Skills

Programming Languages and Technologies: Python, CUDA, PyTorch, TensorFlow, Deep Learning Frameworks, Scikit-Learn, R, Java.
Areas of Knowledge: Large Language Models, Synthetic Data Generation, Computer Vision, Partial Differential Equations (PDEs), Graph Learning, Contrastive Learning, Natural Language Processing, Time-Series, Generative Models, Statistical Analysis.
Web Technologies: HTML, CSS, JavaScript.