

ELISA GÓMEZ DE LOPE

elisa.gdelope@gmail.com | elisagdelope.rbind.io | github.com/elisagdelope | [LinkedIn](#)

Hello! I'm excited about applying ML methods to biomedical challenges, with a particular interest on graph representation learning. My background blends bioinformatics & ML.

EDUCATION

2020–2023	PhD – Biomedical Data Science Group, LCSB, University of Luxembourg Thesis: <i>Interpreting Omics Data in Parkinson's Disease: A Statistical, Machine Learning, and Graph Representation Learning Approach</i> Supervisor: Professor Enrico Glaab, LCSB, University of Luxembourg.
2022-2023	Visiting PhD - University of Cambridge, UK Supervisor: Prof. Pietro Lió, Department of Computer Science and Technology
2023	MIT Catalyst Fellowship – Massachusetts Institute of Technology (MIT), USA Supervisor: Professor Martha Gray, MIT, MIT SLOAN, linQ, IMES
2019-2020	Postgraduate course – Data science and big data, Universitat de Barcelona Project: Histopathological cancer detection with CNNs
2017-2018	MSc. Bioinformatics – Universitat Autònoma de Barcelona Thesis: <i>A Parametrized Approach to LogP-based Hydrophobic Descriptors in Virtual Screening with Pharmscreen®</i> Supervisors: Professor F. Javier Luque and Dr. Enric Herrero
2013-2017	BSc. (Comp.) Biotechnology – Universidad Politécnica de Madrid Thesis: <i>Inferring population structure from ancient DNA of the Tollense battlefield</i> Specialization: Computation (Programming, databases, ML, structural bioinformatics) Supervisors: Prof. Daniel Wegmann (University of Fribourg), Prof. Pablo R. Palenzuela
2017	Visiting Student – University of Fribourg (Switzerland) Supervisor: Prof. D. Wegmann, Statistical and Computational Evolutionary Biology

RESEARCH & WORK EXPERIENCE

Open source contributor DeepChem library , Bharath Ramsundar Integrate Hugging Face pLM ESM-2 in DeepChem open source library for predicting protein binding sites. Production-level coding and tutorials. Proposal accepted (13.4% ratio).	2024 - Present
Postdoctoral researcher Dept. of Engineering , University of Luxembourg (Prof. Stephane Bordas) Graph representation learning for modelling omics data (extension of PhD project).	2024 - Present

MIT Catalyst Fellow

2023 - Present

[*Massachusetts Institute of Technology, Catalyst Fellowship \(linQ\)*](#)

Validated a clinical unmet need and built a prototype for connecting wearables data to guide treatment of sleep disturbance in PTSD.

Advisors: Prof. Martha Gray (MIT), Dr. Anne Quaadgras (MIT Sloan), and Nancy R. Steele.

Visiting researcher

2022 - 2023

[*The Computer Laboratory*](#) (CS department), University of Cambridge (Prof. Pietro Lio)

Applications of graphs and GNNs for modeling omics data in neurodegeneration.

Co-supervised a MSc Student at the University of Cambridge.

Doctoral researcher

2020 - 2023

[*Biomedical Data Science*](#), University of Luxembourg (Prof. Enrico Glaab)

Statistics, ML models and networks for modelling of omics data in Parkinson's disease (PD):

- [*Cross-sectional and longitudinal profiling of PD transcriptomics and metabolomics*](#).
- [*NestedCV class*](#): Nested cross-validation class compatible with the scikit-learn extensions suite
- Interpretable machine learning for [*omics biomarker discovery in PD*](#) and for the study of [*UPDRS III prognosis*](#).
- Graph representation learning for the study of omics data in Parkinson's disease. A comparative study using [*sample similarity networks*](#) versus [*molecular interaction networks*](#).

Advisor, data scientist and bioinformatician

2021 - 2022

[*Farmelody*](#)

Built the prototype of a dashboard, management and predictive system of industrial dairy farms, pre-seed stage.

Data Scientist & consultant

2019 - 2020

[*Accenture Applied Intelligence*](#)

- Computer vision: OCR detection from labels.
- Sales forecast: Time-series auto-regressive and ML models for sales prediction.
- Fraud detection: Statistics for anomaly detection in insurance claims.

[*Capgemini*](#)

2018

Data extraction, transformation & analysis. ETL and database migration.

Bioinformatics intern & MSc Thesis

Spring & Summer 2018

[*Pharmacelera SL*](#)

Developed a [*pipeline*](#) for the parametrization of molecular hydrophobicity descriptors based on atom types, reaching speedup x30 with no loss of accuracy in virtual screening tool Pharmscreen.

Visiting undergraduate research assistant & BSc Thesis

Spring 2017

[*Statistical and Computational Evolutionary Biology*](#), University of Fribourg (Prof. D. Wegmann)

Inferring population structure from ancient DNA of the Tollense battlefield:

- Comparison of ATLAS base quality scores recalibration methods (BQSR vs. Recal)
- Population genetics and statistics: The Hardy-Weinberg equilibrium in Tollense

SKILLS SUMMARY

Programming languages: Python, R, Bash, Perl, Matlab, HTML, CSS, javascript

Data: SQL, SAS, Google Cloud Platform

Libraries/modules: PyTorch, Pytorch geometric, Scikit-learn suite, deepchem; caret, tidyverse

Bioinformatics: ATLAS, VCFtools, SAMtools, RDKit, Pymol, swisspdbviewer

Other tools: Git, HPC slurm, Blender, Visual Basic, Google Cloud Platform

Languages: Spanish, English & French (fluent); Italian, Catalan (conversational)

CONTRIBUTIONS AND DISSEMINATION

Packages

- [NestedCV](#) (scikit-learn suite): Streamlines nested cross-validation with scikit learn models.
- [funOmics](#) (accepted in Bioconductor): Aggregate omics data into higher level, functional representations.
- [DeepChem](#): contributions on tutorials & integration of protein language models.

Journal publications

- [Gómez de Lope E](#), Deshpande S, Vinas Torne R, Lio P, Glaab E, Bordas S. Graph Representation Learning Strategies for Omics Data: A Case Study on Parkinson's Disease. <https://arxiv.org/abs/2406.14442>, 2024
- [Gómez de Lope E](#), Loo R, Rauschenberger A, Ali M, Pavelka L, Marques T, Gomes C, Rejko Krüger, Glaab E. Comprehensive blood metabolomics profiling of Parkinson's disease reveals coordinated alterations in xanthine metabolism. <https://www.nature.com/articles/s41531-024-00671-9>, 2024
- Diaz-Uriarte R, [Gómez de Lope E](#), Giugno R, Fröhlich H, Nazarov PV, Nepomuceno-Chamorro IA, Rauschenberger A, Glaab E. [Ten quick tips for biomarker discovery and validation analyses using machine learning](#). PLoS Computational Biology 2022
- [Gómez de Lope E](#) et al. Carnitine shuttle alterations in Parkinson's disease -in preparation

Conferences

- ISMB/ECCB 2023 ([poster](#)): Graph neural networks for investigating complex diseases: A case study on Parkinson's Disease. [Gómez de Lope E](#), Vinas Torne R, Lio P, Glaab E
- RISP 2023 ([talk](#)): Unravelling Inflammatory Pathways in Parkinson's Disease: Insights from Pathway-Based Machine Learning Analysis of Transcriptomics Data.
- ECCB 2022 ([talk](#), [poster](#)): Machine learning to identify pathways in Parkinson Disease? [Gómez de Lope E](#), Glaab E
- ICSB 2022 (talk, [poster](#)): Machine learning based pathway deregulation analysis of metabolomics data for Parkinson's Disease. [Gómez de Lope E](#), Glaab E

- Cambridge Trustworthy AI for Medical and Health Research Workshop: Machine learning applied to higher order functional representations of omics data reveals biological pathways associated with Parkinson's Disease. [Gómez de Lope E](#), Glaab E

AWARDS & ACHIEVEMENTS

- Google Summer of Code 2024 grant
- London Geometry and Machine Learning 2024
- 2023 MIT Catalyst Fellowship
- LCSB-RIKEN grant for RISP 2023
- Invited at Excellerator Leadership Summit 2023
- 2022 Elected Doctoral Program representative at University of Luxembourg
- 2021 Pelican Award Grant by Fondation de Luxembourg
- 2020 Marie Slodowska-Curie Fellowship
- Pytorch DL Scholarship Challenge by Facebook, Inc & Udacity 2018
- Third prize winner in MIT Critical Care Unit Datathon Tarragona 2018
- 2013 Spanish Academic Excellence Scholarship. Awarded to undergraduate students with outstanding academic records.
- 2011 St. Viator National Research Award in Science for the project "Un cacao de disoluciones"

VOLUNTEERING, AFFILIATIONS

2024 Co-host of [University of Luxembourg Machine Learning seminar](#).

2022 Journal club of the Luxembourg Center of Systems Biomedicine co-organizer & speaker.

2020 – 2022 Board member at [ISCB](#) Luxembourg's Regional Student Group. Organization of workshops, talks and events around hot topics in the field of bioinformatics and ML.

2021 – Present Global Shaper at [Global Shapers](#) Luxembourg hub. Projects for social good, initiative by the [World Economic Forum](#) (Geneva).

2019 [Pint of Science](#) Barcelona Co-organizer. Pint of Science is a scientific festival, my role was contact, management, and logistics of speakers and presenting the sessions.

2019 [Biotechnology Annual Congress](#) of Spain Co-organizer. My role was related to the congress' website management.

2013 – 2017 Leisure activities instructor at [CAL](#) – Madrid. Instructor at a youth association

MENTORING, NON-ACADEMIC CONTRIBUTIONS

Talk: [AI Saturdays](#) bootcamp kick off 2021: *Ethics & AI*.

Talk: [AI Saturdays AlxFP](#) program 2020: *Etica & Inteligencia Artificial*.

[Girls in tech by Accenture](#) 2019/2020: Teaching programming bases (pseudocode, scratch) to 9 year old girls to initiate and encourage them into coding and careers in STEM.

[AI Saturdays](#) mentor Barcelona 2019/2020: Teaching the basics of ML to study groups.

School support teacher 2013-2017: Freelance tutor for teenagers with scholar needs.