Marcos López De Castro

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Birthplace: Salamanca, Spain. **Birthdate**: 08/09/1998.
Languages: Spanish(Native), English(C1).

Current position: Research Scientist at University of Navarra.
Center: Institute of Data Science and Artificial Intelligence (DATAI), University of Navarra.

Experience

AI Research Scientist, DATAI – Institute of Data Science and Artificial Intelligence. Dec 2022 – Now
Pamplona, Navarra, Spain

- Working on distribution-free uncertainty quantification in machine learning models and knowledge discovery.

Visiting Scientist, Ghent University. Sept 2025 – Dec 2025
Ghent, Belgium

- Predoctoral research stay.
- Advisor: Yvan Saeys, PhD.

Research Technician, BCAM – Basque Center for Applied Mathematics. Nov 2021 – Dec 2022
Bilbao, Basque Country, Spain

- Data analysis of stochastic processes through ensemble forecasting techniques, statistics and advanced modelization.
- Advisor: Gianni Pagnini, PhD.

Research Intern, BCAM – Basque Center for Applied Mathematics. Aug 2021 – Oct 2021
Bilbao, Basque Country, Spain

- A technological solution was developed, based on AI, to predict fuel type maps from remote sensing data.
- Advisor: Gianni Pagnini, PhD; Maria Isabel Asensio Sevilla, PhD.

Education

PhD in Applied Engineering, TECNUN School of Engineering, University of Navarra. Dec 2022 – Nov 2026

- Thesis title: "Advances in distribution free uncertainty quantification" (Mark:).
  - Advisors: Rubén Armañanzas Arnedillo, PhD; Jesús López Fidalgo, PhD.

MSc in Mathematical Modelling, University of Salamanca. Oct 2020 – July 2021

- TFM: "Design of an individual combat model" (Mark: 9/10).

BSc in Physics, University of Salamanca. Sep 2016 – July 2020

- TFG: "Charm baryon spectra" (Mark: 9.8/10).

Teaching

Lecturer at *Master in Real Estate*, Faculty of Architecture, University of Navarra. Winter 2026

- Data managment and data analysis. Python. Applied data science.

Lecturer at *BSc in Applied Management*, ISSA School for Applied Management, University of Navarra. Spring 2025, 2026.

- Introduction to data analysis with excel and Python. Applied data science.

Advisoring: Final Master thesis (TFM). *Master in Big data Science*, University of Navarra.

- *Herramienta Estratégica para la Optimización de la Coordinación Multifuncional del Espacio Aéreo.* (2024).
- *Uncertainty Quantification of Mutual Information Estimates.* (2025).
- *Benchmark comparativo de modelos de Machine Learning para predicción de churn*. (2026).

Selected Scientific Contributions

- ***M.López-De-Castro***, A.García-Galindo, R.Armañanzas. (2025). Conformal Inference for Reliable scRNA-seq Annotation, *bioinformatics*, 41(10), btaf521, /10.1093/bioinformatics/btaf521
- ***M.López-De-Castro***, A.García-Galindo, R.Armañanzas. (2025). Enhanced Feature Selection via Strangeness Minimization and Conditional Mutual Information Maximization, UNDER-REVIEW .
- ***M.López-De-Castro***, A.García-Galindo, R.Armañanzas. (2025). Conformal Recursive Feature Elimination, UNDER-REVIEW , https://arxiv.org/abs/2405.19429
- ***M.López-De-Castro***, A.Trucchia, U.Morra-di-Cella, *et al*. (2024). Fire-spotting modelling in operational wildfire simulators based on Cellular Automata: A comparison study, *Agric. For. Meteorol.*,350,109989, 10.1016/j.agrformet.2024.109989.
- ***M.López-De-Castro***, D.Prieto-Herráez, MI.Asensio-Sevilla, G Pagnini. (2022). A high-resolution fuel type mapping procedure based on satellite imagery and neural networks: Updating fuel maps for wildfire simulators, *Remote. Sens. Appl.*,27, 100810, 10.1016/j.rsase.2022.100810.

Other publications/scientific work

- ***M.López-De-Castro***, J. González-Gomariz, A.García-Galindo, K.Ni, B. Haibe-Kains, R.Armañanzas. (2026). Bidirectional Floating Feature Selection Guided by Uncertainty Quantification, *24th Internationa Conference on Artificial Intelligence in Medicine 2026 (AIME2026)*.
- A.García-Galindo, ***M.López-De-Castro***, R.Armañanzas. (2025). Fair prediction sets through multi-objective hyperparameter optimization, *Mach. Learn.*, 114(27), 10.1007/s10994-024-06721-w.
- F.A.Aghababazadeh, L.Alonso, ***M.López-De-Castro***, *et al*. (2024). 1197 Harnessing the cancer immunity cycle via machine learning models to generate novel strategies for personalized cancer therapy, *J. immunotherap. cancer*, 12, 10.1136/jitc-2024-SITC2024.1197.
- ***M.López-De-Castro***, A.García-Galindo, R.Armañanzas. (2024). Conformal Stability Measure for Feature Selection Algorithms, *In: Proceedings of the 13th Symposium on Conformal and Probabilistic Prediction with Applications*, PMLR, v230/lopez-de-castro24a.html
- A.García-Galindo, ***M.López-De-Castro***, R.Armañanzas. (2024). Multi-Class Classification With Reject Option and Performance Guarantees Using Conformal Prediction, *In: Proceedings of the 13th Symposium on Conformal and Probabilistic Prediction with Applications*, PMLR, v230/garcia-galindo24a.html
- A.García-Galindo, ***M.López-De-Castro***, R.Armañanzas. (2023). An uncertainty-aware sequential approach for predicting response to neoadjuvant therapy in breast cancer, *In: Proceedings of the 12th Symposium on Conformal and Probabilistic Prediction with Applications*, PMLR, v204/garcia-galindo23a.html

Software developed

- https://github.com/digital-medicine-research-group-UNAV/CRFE
- https://github.com/digital-medicine-research-group-UNAV/MaxRel_MinRed_MinStra
- https://github.com/digital-medicine-research-group-UNAV/conformalized_single_cell_annotator
- https://github.com/digital-medicine-research-group-UNAV/conformalized_single_cell_annotator
- https://github.com/digital-medicine-research-group-UNAV/Conformal-BFS