CURRICULUM VITAE

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Academic Background

PhD in Biology. *Chemical Shifts-Driven Monte Carlo Simulations*. National University of San Luis. 2007-2012.

Current positions

Principal Data Scientist. PyMC Labs. February 2024-present Lecturer Bayesian Statistics. Universidad Nacional de San Martín. June 2024-present

Older positions

Investigador Independiente. National Scientific and Technical Research Council (CONICET). April 2022 - June 2024.

Postdoc Researcher. (Prof. Dr. Vehtari), Aalto University. Finland. March 2021 – April 2022 Investigador Adjunto. National Scientific and Technical Research Council (CONICET). 2017-2021 Investigador Asistente. National Scientific and Technical Research Council (CONICET). 2014-2017

All publications in the last 5 years (Visit google scholar or ORCID for the full list)

Abril-Pla O, Andreani V, Carroll C, Dong L, Fonnesbeck CJ, Kochurov M, Kumar R, Lao J, Luhmann CC, **Martin O.A.**, Osthege M, Vieira R, Wiecki T, Zinkov R. *PyMC: A modern, and comprehensive probabilistic programming framework in Python*. PeerJ Computer Science 9:e1516. 2023.

Icazatti A, Abril-Pla O, Klami A. Martin O.A. PreliZ: A tool-box for prior elicitation. The Journal of Open Source Software. 2023.

Niborski M.J.; **Martin, O.A.**; Murray F.; Jobbágy EG; Nosetto MD; Paez RA; Magliano PN *Modeling Rainwater Harvesting and Storage Dynamics of Rural Impoundments in Dry Chaco Rangelands*. Water. 2023.

Mikkola, P. **Martin, O.A.** Chandramoul, S. Hartmann, M. Abril-Pla, O. Thomas, O. Pesonen. Corander, J. Vehtari, Aki. Kaski S. Bürkner, PC. Klami A. *Prior knowledge elicitation: The past, present, and future*. Bayesian Analysis. 2023.

Capretto, T. Piho, C. Kumar, R. Westfall, J. Yarkoni, Tal. **Martin O.A.** *Bambi: A simple interface for fitting Bayesian linear models in Python*. Journal of Statistical Software. 2022.

Martin O.A, ; Teste F.P. A call for changing data analysis practices: from philosophy and comprehensive reporting to modeling approaches and back. Plant and Soil. 2022.

Arroyuelo, A. Vila, J.A. **Martin O.A.** *Exploring the quality of protein structural models from a Bayesian perspective.* Journal of Computational Chemistry. 2021.

Martin O.A, Vila J.A. *The Marginal Stability of Proteins: How Jiggling and Wiggling of Atoms are Connected to Neutral Evolution*. Journal of molecular evolution. 2020.

Arroyuelo A., **Martin, O.A** Scheraga H.A. Vila, J. A. *Assessing the One-Bond Ca-H Spin-Spin Coupling Constants in Proteins: Pros and Cons of Different Approaches*. The Journal of Physical Chemistry B. 2020.

Preprints

Quiroga M, Garay P. G. , Alonso J. M., Loyola J. M., and Martin O.A. Bayesian additive regres-

Books

Bayesian Analysis with Python. **Martin O.A**. Packt Publishing. Third Edition. ISBN-13: 978-1805127161. 2024.

Bayesian Modeling and Computation in Python. **Martin O.A**. Kumar R, Lao J. CRC press. ISBN 978-0367894368. 2021.

Online courses

Practical MCMC. <u>Intuitive Bayes</u>. Online learning platform for Bayesian statistics. (paid) Exploratory Analysis of Bayesian Models <u>https://arviz-devs.github.io/Exploratory-Analysis-of-Bayesian-Models/</u> (free)

Modelado Bayesiano https://gmp.net.ar/modelado bayesiano/ (free, Spanish)

Past teaching experience

Lecturer

Bayesian Modeling. UNSL. Hourly credit 60 hours. 2022, 2023

Bayesian data analysis. UNT. Second week March 2020

Bayesian data analysis. UNSL. First week December 2019

Advanced methods in statistics and data analysis UNSL October-December 2019

Postgraduate Refresher Program UNSL: Introduction to Data Science.

- Introduction to data science. Hourly credit 60 hours. February-March 2018.
- Bayesian data analysis. Hourly credit 60 hours. August-September 2018.

Bayesian data analysis UNSL: Postgraduate course. Hourly credit 90 hours. February 2015.

Teaching Assistant

Bayesian Data Analysis. Aalto University. 2021

Structural Bioinformatics: Elective course for the Bachelor's Degree in Molecular Biology. Hourly credit 90 hours. 2013-2016.

Algorithms in bioinformatics: Postgraduate course. Hourly credit 80 hours. February 2015.

Research projects funding as main researcher/principal investigator

Bayesian additive regression trees: automatic inference, variable selection, and interpretability. FONCYT (2023-2024)

Dashboard-assisted exploratory analysis of Bayesian models. NumFOCUS small development grants. (2023)

Jax SMC samplers for PyMC. NumFOCUS small development grants. (2022)

Fine tuning the Bayesian Additive Regression Trees implementation in PyMC. NumFOCUS small development grants. (2021)

Improving and expanding the implementation of Approximate Bayesian Computation. NumFOCUS small development grants. (2020)

Create educational material and give workshops related to exploratory analysis of Bayesian models with ArviZ. NumFOCUS small development grants. (2019)

Probabilistic programming for Structural Bioinformatics FONCYT. PICT-Joven (2017-2019)

Advisor for undergrad and graduate students

PhD Advisor: Lic Agustina Arroyuelo. *Structural determination of biomolecules by statistical inference*. National University of San Luis. (2016-2021). Approved.

Co-advisor Phd Thesis: Alejandro Icazatti. *Validation and determination of the structure of nucleic acids*. National University of San Luis. (2014-2019). Approved

Co-advisor Phd Thesis: Pablo Garay. *CheSweet: Determination and validation of glycans and glycoproteins*. National University of San Luis. (2013-2017). Approved

Advisor BSc Thesis: Agustina Arroyuelo. *Development of a software application for creating, viewing and analyzing models of macromolecules.* Thesis to get the degree of Bachelor in Molecular Biology. National University of San Luis. Approved September 2019.

Advisor BSc Thesis: Pedro Ramírez. *Protein structure refinement guided by* ¹³C^a y ¹³C^b chemical shifts. Thesis to get the degree of Bachelor in Molecular biology. National University of San Luis. Approved December 2014.

Co-advisor BSc Thesis: Ezequiel Frigini. *Is the cell membrane, permeable to the diffusion of glyphosate?* Thesis to get the degree of Bachelor in Molecular biology. National University of San Luis. Approved December 2014.

Software development

Core developer of:

ArviZ. Exploratory analysis of Bayesian models

Bambi. Bayesian Model-Building Interface in Python.

Kulprit. Kullback-Leibler projections for Bayesian model selection

PreliZ. A tool-box for prior elicitation

PyMC. Probabilistic Programming in Python

PyMC-BART. Bayesian Additive Regression Trees for Probabilistic programming

Older projects:

<u>CheShift</u>: A web-server for protein-structure validation.

PyMOL Plugins: PyMOL is a molecular visualization system

Synergistic activities

Member of the PhD in Biology Committee. National University of San Luis. 2019-2021.

Head of the organizing committee of Argentinean workshop of scientific computation, San Luis, Argentina 2019.

Head of the organizing committee of PyData, San Luis, Argentina 2017. This was the first PyData in Latin-America. Member of the PyData San Luis chapter.

Co-host La Búsqueda, popular science radio-show and podcast. Radio UNSL 2008-2009. Radio Ciudad 2010