

# 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

*Investigador Independiente*. National Scientific and Technical Research Council (CONICET). 2022-present.

Principal Data Scientist. [PyMC Labs](#). 2024-present

## Older positions

Postdoc Researcher. Aalto University. 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

## Recent scientific publications

Only last five years, visit [google scholar](#) for the entire 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)

Icazatti A.A, Loyola J.M., Szleifer I, Vila J.A. **Martin O.A.** *Classification of RNA backbone conformations into rotamers using <sup>13</sup>C' chemical shifts: exploring how far we can go*. PeerJ 7, e7904 (2019)

**Martin O.A.** Vorobjev Y, Scheraga HA, Vila JA. *Outline of an experimental design aimed to detect protein A mirror image in solution*. PeerJ Physical Chemistry 1, e2 (2019)

Baldi G, Schauman S.A, Texeira M, Marinaro S, **Martin O.A.**, Gandini P, Jobbágy E.G. *Nature representation in South American protected areas: country contrasts and conservation priorities*. PeerJ 7, e7155 (2019)

Kumar, R. Carroll C, Hartikainen A, **Martin, O.A** *ArviZ a unified library for exploratory analysis of Bayesian models in Python*. The Journal of Open Source Software (2019)

## Preprints

Quiroga M, Garay P. G. ,Alonso J. M. , Loyola J. M., and **Martin O.A.** *Bayesian additive regression trees for probabilistic programming*. ArXiv 2022.

## 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.

## Teaching

Instructor at [Intuitive Bayes](#). Online learning platform for Bayesian statistics.

### 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: Optional 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)

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

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

## Advisor for undergrad and graduate students

Master Advisor: Lic. Miriana Quiroga. *Bayesian additive regression trees: automatic inference, variable selection and interpretability*. National University of San Luis. (2020-2024)

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

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

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

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  $^{13}\text{C}^a$  y  $^{13}\text{C}^b$  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:

[CheShift](#): 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

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