

Andre Ricardo Goncalves

Machine Learning Research Scientist

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Summary

Machine learning research scientist with 15+ years of experience developing statistical learning, optimization, and deep learning methods for biological, clinical, and scientific data. Current work spans antibody design, microbiome modeling, and large-scale clinical foundation models trained on structured electronic health record data. Published in *Nature*, *Science Advances*, *The Lancet Digital Health*, and *JMLR*.

Research Experience

Lawrence Livermore National Laboratory

Oct 2017 – Present

Machine Learning Research Scientist, Machine Learning Group

- Build and lead machine learning efforts across protein design, clinical machine learning, and microbiome research in collaboration with biologists, clinicians, and applied scientists.
- Develop methods for antibody developability prediction, in silico library design, AlphaFold3-based binding estimation, and simulation tools for mutagenesis and experimental design, reducing wet-lab iteration in therapeutic and biomaterials campaigns.
- Train and adapt billion-parameter clinical foundation models on structured event sequences at thousand-GPU scale for biosurveillance, infectious disease detection, and diagnosis prediction, and developed causal ML methods for drug repurposing in ALS.
- Led microbiome disease-prediction work integrating metagenomic profiles with host and protocol metadata across tens of thousands of samples.
- Mentored 10+ undergraduate and graduate students and postdoctoral researchers on interdisciplinary machine learning projects.

Center for Research and Development in Telecommunication (CPqD)

Apr 2015 – Aug 2017

Machine Learning Researcher

- Developed deep learning and machine learning models for voice biometrics and audio processing, including presentation-attack detection using spectral, temporal, and convolutional approaches.
- Contributed to production-oriented speaker recognition systems deployed across multiple companies in Brazil.
- Co-inventor on a Brazilian patent for automatic voice liveness detection.

Doctoral and Graduate Research

2009 – 2016

University of Campinas & University of Minnesota, Twin Cities

- Developed sparse and structural multitask learning methods for high-dimensional prediction problems in climate science and biomedical data, as part of MS and PhD research.
- Conducted 1.5 years of doctoral research at the University of Minnesota (2013–2014) as a Science without Borders visiting scholar.
- Published on multitask learning, structured estimation, and Earth system modeling in venues including *JMLR*, *Computing in Science & Engineering*, *AAAI*, and *CIKM*.

Education

Ph.D. in Electrical and Computer Engineering, University of Campinas and University of Minnesota 2011 – 2016

Thesis: *Sparse and Structural Multitask Learning*

M.S. in Electrical and Computer Engineering, University of Campinas

2009 – 2011

Thesis: *Online Learning in Estimation of Distribution Algorithms for Dynamic Environments*

B.S. in Computer Science, State University of Londrina

2005 – 2008

Undergraduate capstone thesis: *Fundamentals and Applications of Machine Learning*

Honors and Awards

- Director's Science and Technology Award recipient and Director's Award in Publication, Lawrence Livermore National Laboratory, 2022.
- Best Ph.D. Thesis in Computer Engineering, University of Campinas, 2016.
- Science without Borders scholarship for visiting research at the University of Minnesota, 2013–2014.
- Highest GPA in the Computer Science graduating class, State University of Londrina, 2008.

Selected Publications

- Reimer, R. J., Soper, B., Wilson, J. L., **Goncalves, A. R.**, et al. Identification of drug repurposing candidates for amyotrophic lateral sclerosis using electronic health records: A retrospective cohort study. *The Lancet Digital Health*, 2026.
- **Goncalves, A. R.**, Pico, J. C., Hu, Y., Schlessinger, D., Greene, J., O’Suilleabhain, L., et al. AI-enabled diagnostic prediction within electronic health records to enhance biosurveillance and early outbreak detection. *Under Review*, 2026.
- Zhu, F., Rajan, S., Hayes, C. F., Kwong, K. Y., **Goncalves, A. R.**, et al. Preemptive optimization of a clinical antibody for broad neutralization of SARS-CoV-2 variants and robustness against viral escape. *Science Advances*, 2025.
- Desautels, T. A., Arrildt, K. T., Zemla, A. T., Lau, E. Y., Zhu, F., Ricci, D., Cronin, S., **Goncalves, A. R.**, et al. Computationally restoring the potency of a clinical antibody against Omicron. *Nature*, 2024.
- **Goncalves, A. R.**, Ranganathan, H., Valdes, C., Zhu, H., Zhang, B., Kok, C. R., et al. Beyond microbial abundance: Metadata integration enhances disease prediction in human microbiome studies. *Frontiers in Microbiology*, 2025.
- **Goncalves, A. R.**, Ray, P., Soper, B., Stevens, J., Coyle, L., and Sales, A. P. Generation and evaluation of synthetic patient data. *BMC Medical Research Methodology*, 2020.
- **Goncalves, A. R.** and Von Zuben, F. J. Multi-task sparse structure learning with Gaussian copula models. *Journal of Machine Learning Research*, 2016.

Full publication list: [Google Scholar profile](#).

Professional Service and Intellectual Property

Peer reviewer and program committee member for venues including AAAI, SDM, *npj Digital Medicine*, and *PLOS ONE*.
Co-inventor on Brazilian patent BR 10 2015 017556-6, automatic voice liveness detection system.