

Daniel Augusto de Souza

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About

I am a final-year Ph.D. student at UCL, advised by Prof. Marc Deisenroth, with a focus on probabilistic machine learning and Gaussian processes. I am particularly interested in their applications to climate modeling and material discovery. Beyond research, I am passionate about translating academic insights into deployable solutions, which has led me to multiple roles in industrial research, DevOps, and software engineering.

Skills

Programming Python, C/C++ (Linux), Java, C#, SQL, Docker, Git, Bash.
Packages TensorFlow, BoTorch, PyTorch, HuggingFace Transformers, Stan.
Languages Portuguese (native), English (proficient, TOEFL iBT: 110/120), Japanese (basic)

Education

Ph.D. in Computer Science

London, UK

UNIVERSITY COLLEGE LONDON (UCL) ADVISED BY PROF. MARC DEISENROTH

Sep. 2021 - Now

Research interests: deep Gaussian processes for compact manifolds; interpretability of DGP layers and physical priors, applications to climate problems.

MSc project supervision: on the use of inter-domain inducing variables in Gaussian processes to speed up the gridding of weather observations from sparse satellite observations tracks.

M.Sc. in Computer Science (GPA: 9.22/10)

Fortaleza, Brazil

UNIVERSIDADE FEDERAL DO CEARÁ (UFC) ADVISED BY PROF. JOÃO PAULO PORDEUS AND PROF. CÉSAR LINCOLN

Feb. 2018 - Sep. 2020

Dissertation: "Contributions on latent projections for Gaussian process modeling"

📄 URL

Resulted in publication (AISTATS, 2021): "Learning GPLVM with arbitrary kernels using the unscented transformation"

B.Sc. in Computer Science (GPA: 8.86/10)

Fortaleza, Brazil

UNIVERSIDADE FEDERAL DO CEARÁ (UFC)

Apr. 2013 - Aug. 2017

Covered a broad range of courses in mathematics and theoretical computer science. Including elective classes in formal logic, formal software verification, number theory, and neural networks.

Awarded two research scholarships by the CAPES Foundation. Teaching assistant for Introduction to Logic and Theory of Computation.

Undergraduate international exchange

Bellingham, US

WESTERN WASHINGTON UNIVERSITY (WWU)

Fall 2015 - Spring 2016

Awarded by the Brazil Scientific Mobility Program with funding from the Federal Government of Brazil.

Took classes in robotics, embedded AI programming, abstract algebra, and graph theory.

Honors & Awards

2021-2025	Ph.D. Studentship, DeepMind Chair Endowment (approx. 200,000£)
2019	M.Sc. Travel grant, Federal University of Ceará
2018	M.Sc. State Scholarship, FUNCAP [Declined]
2018	M.Sc. Federal Scholarship, CAPES Foundation/CNPq [Declined]
2015	International undergraduate exchange (USA), Brazil Scientific Mobility Program - CAPES Foundation/CNPq
2015	B.Sc. Travel grant, NAT@Logic and 10th LSFA - Federal University of Rio Grande do Norte
2014	B.Sc. Scholarship, Institutional Scientific Initiation Scholarship Program (PIBIC) - CAPES Foundation
2013	B.Sc. Undergraduate research award, Young Talents for Science - CAPES Foundation

Experience

Matterhorn Studio

Oxford, UK

MACHINE LEARNING LEAD

Jun. 2022 - Now

A startup focused in democratizing material discovery using Bayesian optimization.

🌐 Web page

As part of the founding team, I developed a custom Bayesian optimisation solution algorithm for their specific manufacturing process for a world-leading producer of after-glow material.

Dell LEAD

AI PROGRAMMER

Worked on a whole-chat textual time series classification project for Dell Support.

Fortaleza, Brazil

Jun. 2021 - Oct. 2021

Delfos Intelligent Maintenance

GRADUATE PART-TIME RESEARCHER

Joint project between Universidade Federal do Ceará, Delfos Intelligent Maintenance and Fundação ASTEF.
Funded by Delfos Intelligent Maintenance.

Researched machine learning models for fault detection and process monitoring for wind turbines and hydroelectric plants.

Fortaleza, Brazil

May 2019 - Sep. 2020

GreenMile LLC

JUNIOR SOFTWARE ENGINEER

Worked on the DevOps team, developing and maintaining internal tools for product support and software delivery in Python, Node.JS and React. After being transferred to the Architecture and Microservices team, I focused on dockerizing old microservices and setting up them on Amazon's ECS.

Alongside these projects, I developed a Bayesian regression model and implemented it as a microservice in Java and Stan.

Fortaleza, Brazil

Aug. 2017 - Sep. 2018

Deals Only WebStore

SUMMER INTERN

Refactored and optimized legacy PHP and Javascript code related to the shop front-end and internal staff tooling.

Bellingham, US

Jun. 2016 - Jul. 2016

Undergraduate research assistant (Universidade Federal do Ceará)

LOGIA (GROUP OF LOGIC AND ARTIFICIAL INTELLIGENCE) ADVISED BY PROF. CARLOS BRITO

Researched about Shannon's classical information theory and how it plays with physical systems.

After this first project, our focus shifted to connections between kinds of typed lambda calculi with logic systems and how proof assistants can help mathematicians and computer scientists.

Fortaleza, Brazil

Sep. 2013 - Sep. 2015

Work in progress

Infinite Neural Operators: Gaussian processes on functions

AUTHORS: **DANIEL AUGUSTO DE SOUZA**, YUCHEN ZHU, HARRY JAKE CUNNINGHAM, YURI SAPORITO, DIEGO MESQUITA, MARC PETER DEISENROTH.

In progress

We characterize the distribution and show the conditions for the existence of two-layer neural operators (NOs) with infinitely many hidden channels. We propose methods of computing the infinite limit of Fourier NOs and a proposed architecture based on Matérn kernels. These limits are compared to their finite counterparts in distribution at initialization and their performance in Bayesian operator learning.

Guaranteed Reward Hacking Mitigation for Large Language Models

AUTHORS: YUCHEN ZHU, ZHENGYAN SHI, **DANIEL AUGUSTO DE SOUZA**, MENGYUE YANG, PASQUALE MINERVINI, ALEXANDER NICHOLAS D'AMOUR, MATT KUSNER.

In progress

We address the problem of reward hacking, where maximizing a proxy reward reduces true reward, in large language models (LLMs) fine-tuned using reinforcement learning from human feedback. We describe weak assumptions under which reward hacking can be avoided with access to proxy feedback and sparse true feedback. We propose a new LLM parameterization that has provably improved sample complexity under this scenario. We believe this work provides the first convergence guarantees for LLM fine-tuning with RLHF.

Publications

Streaming Bayes GFlowNets

AUTHORS: TIAGO SILVA, **DANIEL AUGUSTO DE SOUZA**, DIEGO MESQUITA.

Dec. 2024

In proceedings: **37th Advances in Neural Information Processing Systems (NeurIPS 2024)**

We propose a two training losses and a corresponding provably correct algorithm enabling the training of GFlowNets in a streaming data setting, without the need to revisit past data. These are then used to devise an alternative VI algorithm employing low-variance gradient estimators. Our proposals are backed by theoretical and empirical analysis.

Interpretable deep Gaussian processes for geospatial tasks

AUTHORS: **DANIEL AUGUSTO DE SOUZA**, DANIEL GILES, MARC PETER DEISENROTH.

Apr. 2024

Extended abstract presented in: **Climate Informatics 2024**

We re-analyse the interpretability of hidden layers in different architectures of deep Gaussian processes. By focusing on the prior covariance of the output gradient, we show that it is a better tool of analysis than lengthscale fields due to its direct physical meaning and by being architecture independent.

Thin and Deep Gaussian Processes

[Blog](#)

AUTHORS: **DANIEL AUGUSTO DE SOUZA**, ALEXANDER NIKITIN, S. T. JOHN, MAGNUS ROSS, MAURICIO A. ÁLVAREZ,
MARC PETER DEISENROTH, JOÃO P. P. GOMES, DIEGO MESQUITA, CÉSAR LINCOLN MATTOS.

Dec. 2023

In proceedings: **36th Advances in Neural Information Processing Systems (NeurIPS 2023)**

We propose a new architecture of deep Gaussian processes (DGP) with a focus on supervised dimensionality reduction and interpretability. Our architecture merges the best properties of compositional DGPs with lengthscale mixture DGPs allowing our method to both be described in terms of latent spaces, like traditional DGPs, and in terms of varying lengthscale fields.

Actually Sparse Variational Gaussian Processes

[URL](#)

AUTHORS: HARRY JAKE CUNNINGHAM, **DANIEL AUGUSTO DE SOUZA**, SO TAKAO, MARK VAN DER WILK, MARC PETER DEISENROTH

Apr. 2023

In proceedings: **26th International Conference on Artificial Intelligence and Statistics (AISTATS 2023)**

We propose a highly scalable method for low-dimensional (≤ 4) Gaussian process regression. By exploiting the properties of B-splines, we use them to define a compact basis for a inter-domain inducing point solution which turns most covariance matrices sparse and allows the use of band-diagonal matrix computation.

Parallel MCMC Without Embarrassing Failures

[URL](#)

AUTHORS: **DANIEL AUGUSTO DE SOUZA**, DIEGO MESQUITA, SAMUEL KASKI, LUIGI ACERBI

Apr. 2022

In proceedings: **25th International Conference on Artificial Intelligence and Statistics (AISTATS 2022)**

We show three pathologies that most embarrassingly parallel MCMC algorithms are susceptible to. We present a scalable solution that can overcome these failures using Gaussian process surrogate modelling and active learning.

Learning GPLVM with arbitrary kernels using the unscented transformation

[URL](#)

AUTHORS: **DANIEL AUGUSTO DE SOUZA**, DIEGO MESQUITA, CÉSAR LINCOLN C. MATTOS, JOÃO PAULO GOMES

Apr. 2021

In proceedings: **24th International Conference on Artificial Intelligence and Statistics (AISTATS 2021)**

In this article, we investigated the unscented transformation as a parameter-less alternative to Gauss-Hermite quadrature and Monte Carlo integration for arbitrary kernel Gaussian process latent variable models. We illustrate the applicability of our method with experiments on dimensionality reduction and multistep-ahead prediction with uncertainty propagation.

No-PAS-BO: Normalized Portfolio Allocation Strategy for Bayesian Optimization

[URL](#)

AUTHORS: THIAGO DE P. VASCONCELOS, **DANIEL A. R. M. DE SOUZA**, CÉSAR L. C. MATTOS AND JOÃO P. P. GOMES

Nov. 2019

In proceedings: **IEEE 31st International Conference on Tools with Artificial Intelligence (ICTAI 2019)**

Part of the joint project with Delfos Intelligent Maintenance.

I helped the main author with the technical aspects of the experimental section of the paper, mostly related with computer infrastructure and code.