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, Java, Kotlin, Javascript, C/C++ (Linux), 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
Fortaleza, Brazil

AI PROGRAMMER
Jun. 2021 - Oct. 2021

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

Delfos Intelligent Maintenance
Fortaleza, Brazil

GRADUATE PART-TIME RESEARCHER
May 2019 - Sep. 2020

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.

GreenMile LLC
Fortaleza, Brazil

JUNIOR SOFTWARE ENGINEER
Aug. 2017 - Sep. 2018

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.

Deals Only WebStore
Bellingham, US

SUMMER INTERN
Jun. 2016 - Jul. 2016

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

Undergraduate research assistant (Universidade Federal do Ceará)
Fortaleza, Brazil

LOGIA (GROUP OF LOGIC AND ARTIFICIAL INTELLIGENCE) ADVISED BY PROF. CARLOS BRITO
Sep. 2013 - Sep. 2015

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.

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

AUTHORS: **DANIEL AUGUSTO DE SOUZA**, ALEXANDER NIKITIN, S. T. JOHN, MAGNUS ROSS, MAURICIO A. ÁLVAREZ,

Dec. 2023

MARC PETER DEISENROTH, JOÃO P. P. GOMES, DIEGO MESQUITA, CÉSAR LINCOLN MATTOS.

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

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

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

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-Hemite 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-PASt-BO: Normalized Portfolio Allocation Strategy for Bayesian Optimization

AUTHORS: THIAGO DE P. VASCONCELOS, **DANIEL A. R. M. A. 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.