## Héctor Javier Hortúa

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**Research** interests The research I am currently involved in consists of the application of Deep Learning in several scientific disciplines and real-world scenarios, along with the development of Trustworthy AI models. I have explored this topic based on two pillars: Uncertainty quantification and explainable artificial intelligence (XAI). More specifically, my research falls under two topics: First, the use of neural ensembles, Bayesian neural networks, and Gaussian Processes for modeling uncertainties in Deep learning, which are crucial for making better decisions in real-world applications. Second, the implementation of alternative generalized divergences and Bijectors in VI to improve the inference processes, and be able to obtain well-calibrated neural networks. On the other hand, I have implemented XAI via SHAP and Integrated Gradients, to provide interpretable model decisions and reliable predictions for high-risk applications such as medical diagnosis. I have also worked on the robustness of Bayesian classifiers for detecting adversarial examples through AutoEncoders, and the implementation of stochastic neural networks for Object Detection in computer vision methods. Moreover, I have worked with Graph Neural Networks for building automatizing techniques required by spherical datasets applied to Astrophysics and Chemistry. Finally, I have built different end-to-end data science/ML projects starting from building an ML-focused strategy and progressing into model training, optimization, and productionalization using Google Cloud Platform. Education Universidad Nacional de Colombia Bogotá, Colombia PhD in Physics 04 2019 Universidad Nacional de Colombia Bogotá, Colombia MSc in Astrophysics 07, 2011 Universidad Nacional de Colombia Bogotá, Colombia **BA** in Physics 07, 2008 Honors and scholarships Helmholtz Information & Data Science Academy (HIDA). Visiting Researcher at Deutsches Elektronen-Synchrotron DESY. 2023

Unicore Stipendium der DAAD-Stiftung programme. Visiting Researcher at<br/>Max Planck Institute for Astrophysics, Germany.2022<br/>2022Research credits grant from Google Cloud Research Programme. 2022-2024

	Laureate Distinction: Doctoral Thesis. Universidad Nacional de Colombia. 2020
	Colciencias-Conv. 647, Doctorado Nacional Fellowship 2015
	Meritorious Distinction: Master Thesis. Universidad Nacional de Colombia.
	2011
Internships	Romanian Institute of Science and Technology2018-2019
	Implement supervised and unsupervised techniques in Machine and Deep
	Learning, and the use of TensorFlow and Sonnet for building an end-to-end
	pipeline for big astrophysical datasets.
Research experience	Postdoctoral Research Scientist
	Artificial Intelligence and Data Science Research Centre, Liverpool Centre for
	Cardiovascular Science Liverpool John Moores University 2024-2026
	Design and analysis of novel training algorithms for neural networks in deep
	learning, by applying notions of Riemannian optimization and differential ge- ometry ljmu.
	Long-term visiting researcher at Deutsches Elektronen-Synchrotron DESY
	Zeuthen, Germany 2023-2024
	Applications of Deep Learning and Bayesian recurrent neural nets for the de-
	tection of astrophysical transients via anomaly detection tasks. This project
	framework allows to derive detection prospects of low-luminosity gamma-ray
	bursts for the upcoming Cherenkov Telescope Array.
	Long-term visiting researcher at Max Planck Institute for Astrophysics
	Garching, Germany 2022
	Applications of Deep Learning generative models along with Graph Neural
	Networks to extract underlying spectral information (in the latent space) con-
	tained in Galactic all-sky data covering spectral bands from $\gamma$ -ray to radio waves.
	Postdoctoral Networking in Artificial Intelligence and AI in medicine
	DAAD, Germany 2021-2023
	Initiative funded by the German Federal Ministry of Education and Research to
	scientific talents from all over the world a personalized gateway to the German
	AI research community.
	Postdoctoral Research Scientist
	Romanian Institute of Science and Technology2019-2020
	Design and analysis of novel training algorithms for neural networks in deep
	learning, by applying notions of Riemannian optimization and differential ge-

ometry **RIST**.

#### Argo project

DeepRiemann - Riemannian Optimization Methods for Deep Learning projec	t.
POC 2014-2020	

Argo is a library for deep learning algorithms based on TensorFlow and Sonnet. The library allows you to train different models (feed-forwards neural networks for regression and classification problems, autoencoders and variational autoencoders, Bayesian neural networks, Helmholtz machines, etc) by specifying their parameters as well as the network topologies in a configuration file. The models can then be trained in parallel in presence of multiple GPUs. The library is easy to expand for alternative models and training algorithms, as well as for different network topologies. ARGO

#### Professional Data Science Consultant, University el Bosque

experience

Bogotá, Colombia

2024

Solving scientific and practical questions with data-driven analysis, insight creation, and data science solutions. Responsible for aspects and implementation of medical solutions through data understanding, modeling, and deployment. Application of machine learning, natural language processing, and computer vision. The consultancy is provided to researchers enrolled in the AI for cervical cancer screening project and professors.

#### Data Scientist at Dispell Magic Inc., Competitoor

Dover, County of Kent, Delaware, USA 2021-2023 Stays ahead of the Machine Learning needs by identifying opportunities for improvement modeling tools, processes, and infrastructure. Working on workflow from data access, processing, and modeling, modern software process to develop production.

#### Data Science Researcher at Quaesta AI

Cluj Napoca, Romania

2023

Designing, testing, and employing new AI functionalities for the company goals. Software development and research.

#### Teaching experience

## Teaching associate, Mastría en Estadística Aplicada y Ciencia de Datos,Universidad el Bosque2023-2024

Machine Learning II & Deep Learning II, Supervising master theses. Relevant products:

- Deep Bayesian segmentation for colon polyps: Well-calibrated predictions in medical imaging, arXiv:2407.16608(submitted)

- Trustworthy Bayesian Deep Learning for Pneumonia and COVID-19 diagnosis in 3D medical images. (submitted)

- Forecasting VIX using Bayesian Deep Learning (Int J Data Sci Analysis (2024))

- Adversarial image detection based on Bayesian Neural Layers(submitted)

## Teaching associate, Maestría en Ciencia de Datos, Escuela Colombianade Ingeniería Julio Garavito2022-2024

Hello world!! with Tensorflow 2, an Introduction to Deep Learning & Tensor-Flow 2, Advanced topics& Introduction to Natural Language Processing Relevant products: Jupyter Books and GitHub-classroom repositories.

## Teaching associate, Department of Basic Science and Technology, (UNAD) 2021

Physics, Head and instructor in Data Science specialization program.

Relevant products: Constraining cosmological parameters from N-body simulations with BNNs, results accepted at NeurIPS, Bayesian Deep Learning, 2021 Relevant products: Property estimation method for Terpenes using Machine Learning, ESCAPE32, Toulouse, France, 2022

Relevant products: Un enfoque basado en Machine Learning para estimar el punto de fusión en compuestos químicos, 4ta semana de la Química, Colombia, 2021

### Teaching associate, Department of Basic Science, Universidad Los Libertadores 2011-2014

Physics and Maths

Projects

Relevant products: First Astrostatistics School: Bayesian Methods in Cosmology, held in U. Los Libertadores Bogotá D.C., Colombia. Proceedings Relevant products: IAU Symposium 306: Statistical Challenges in 21st Cosmology Cambridge University Press

### Google Cloud Research Credits Program: Robust Simulation-Based Inference in Cosmology with AI.

Design new ML methods that allow Graph neural networks and Deep models to quantify the uncertainty of its predictions in the cosmological context.

Relevant Products: Bayesian deep learning for cosmic volumes with modified gravity Astronomy& Astrophysics.

Constraining cosmological parameters from N-body simulations with Variational Bayesian Neural Networks Front. Astron. Space Sci. Sec. Astrostatistics. A comprehensive modeling and experimental approach for damped oscillations in U-tubes via Easy JavaScript Simulations Physics Ed.

Seeking Primordial Magnetic Field signals from CMB with Bayesian Graph Deep Neural Networks. Submitted.

Can Multiply Normalizing Flows constrain modified gravity

## Machine Learning-based approaches for estimating melting point in chemical compounds

Design new ML methods based on ensembles, graphs, and BNNs, to determine properties estimation of chemical components.

32nd European Symposium on Computer Aided Process Engineering, ESCAPE 2022, Elsevier, ISBN:9780323958790

### Decomposition of the Galactic multi-frequency sky via Deep Generative Models

Build Variational Autoencoders (VAEs) based graph network for a spherical dataset for detecting the essential spectral information contained in Galactic all-sky data covering all spectral bands.

# Reliable Uncertainties for Bayesian Neural Networks using Alpha divergences

Design new metrics and methods to determine the accuracy in prediction's neural models. Generalized divergences were implemented for different dataset.

Results presented and published at ICML, Uncertainty and Robustness in Deep Learning, 2020.

#### Accelerating MCMC algorithms through Bayesian Deep Networks

New approach to accelerate MCMC techniques by adding covariance matrix from Neural network predictions. It allows to include an optimizing parameter space to be able to speed up the convergence.

Results presented and published at NeurIPS, Machine Learning and Physical Sciences, 2020.

# Constraining the reionization history using Bayesian normalizing flows

Apply Normalized flow in computer vision tasks. Additionally, implement uncertainties in Object detection models to obtain robust vision models. It can be apply to style transfer, segmentation and resolution images.

Results presented and published at Machine Learning Sci.Tech , 2020. and ICLR 2020 workshop Fundamental Artificial Intelligence in science

#### For publications click here.

Conferences IAIFI: NSF Institute for Artificial Intelligence and Fundamental Interactions, virtual, 8 2022 ICTP: Latin American regional workshop on SciTinyML: Scientific Use of Machine Learning on Low-Power Devices, virtual, 7 2022 Conference on Neural Information Processing Systems, NeurIPS, Contribution: "Constraining cosmological parameters from N-body simulations with Bayesian Neural Networks" virtual, 12 2021

Skills	Programming	
	Quantum 2020, The Institute of Physics and IOP Publishing	10 2020
	Microsoft Research Frontiers in Machine Learning	07 2020
Scientific courses	Transylvanian Machine Learning Summer School (TMLSS)	02 2018
	Learn SQL Basics for Data Science, Coursera	08 2020
	Auvanceu Data Science with IDM, Coursera	00 2020
	Advanced Data Science with IBM Converse	10 2020
	TensorFlow: Data and Deployment, Coursera	11 2020
	Machine Learning with 1F on GCP, Coursera	02 2021
	IensorFlow: Advanced Iechniques, Coursera	11 2020
	Advanced Machine Learning on Google Cloud, Coursera	02 2021
Certificated courses	Machine Learning Engineering for Production, Coursera	10 2022
	Artificial Intelligence Technology Certificate, Huawei	02 2021
Certifications	TensorFlow Developer Certificate, Google	01 2021
	land, 06 2019	, 0 11201
	tion: "Estimation of Cosmological Parameters via ConvNets". Ascon	a. Switzer-
	AICosmo2019. Artificial Intelligence Methods in Cosmology	Contribu-
	ral Networks" Paris France 03 2020	ising Neu-
	tribution."Constraining Cosmological Decomptors from CMP many	ves, Con-
	Inference", Virtual, 05 2020	
	Contribution: "Parameters Estimation from the 21 cm signal using V	Variational
	Eighth International Conference on Learning Representation	ns, ICLR,
	divergences", Virtual, 08 2020	s using <i>u</i> -
	Contribution: "Reliable Uncertainties for Bayesian Neural Network	ig, ICML, s using $\alpha_{-}$
	2020	
	BNNs with $\alpha$ -divergences and Normalizing Flows", Les Houches, 1	France, 07
	mation Geometry and Inference for Learning, Contribution: "C	Calibrating
	Joint Structures and Common Foundation of Statistical Physi	cs, Infor-
	izing Flows" virtual, 5 2020	
	Contribution: "Constraining the Reionization History using Bayesia:	n Normal-
	ICTP-SAIFR Latin American Workshop on Observational Co	smology.
	tribution: "Accelerating MCMC algorithms through Bayesian Deep N	Networks"
	Conference on Neural Information Processing Systems, Neur	·IPS, Con-
	with Bayesian Neural Networks" virtual, 12 2021	
	tribution: "Constraining cosmological parameters from N-body si	mulations
	Conference on Neural Information Processing Systems, Neur	·IPS, Con-

Proficient in: Mathematica, C++, Python-libraries, scikit-learn, CUDA, Py-Torch, Pytorch lightning, Tensorflow, Keras, TFProbability, TFX, Pandas ecosystem libraries, Dask, mySQL, GIT, bash, DBeaver, Docker, GCP, Elastic Search, MLflow, Kibana, FastAPI, Django

Familiar with: MPICH2, PyMC, Pystat, Apache Spark, MLlib, Sonnet, dataflow, weaviate, PM2

### OS

Linux

### Editor

⊮T<sub>E</sub>X, Pycharm, Emacs, Atom, Visual Studio

### Languages

Spanish (mother tongue), English (Professional working), German (beginner)