# SHREYAS PADHY

PhD Candidate | Machine Learning Group | University of Cambridge (sp2058@cam.ac.uk) | (shreyaspadhy.github.io)

#### **EDUCATION**

University of Cambridge

October 2021 - July 2025 (expected)

PhD in Engineering

Supervised by Dr. Jose Miguel Hernández-Lobato

Johns Hopkins University

August 2017 - May 2019

MSE in Biomedical Engineering

Overall GPA: 4.0

Indian Institute of Technology Delhi

July 2013 - May 2017

B.Tech in Engineering Physics

Overall GPA: 8.871/10 (Department Rank 4)

### **EMPLOYMENT**

# ML Scientist, Atinary Technologies

November 2024 - current

50% position (Lausanne, Switzerland)

· Fundamental ML Research in Bayesian Optimisation and Molecular Discovery

# Research Scientist Intern, Meta Reality Labs

June 2024 - October 2024

Under mentorship of Michael Paskett and Allen Yin (Burlingame, CA)

· Worked on generative models for improved data efficiency in training and personalization of wrist-wearable neural interfaces.

#### Research Intern, Microsoft Research

May 2023 - August 2023

Under mentorship of James Hensman and John Winn (Cambridge, UK)

- · Developed time-series Gaussian Process models for sparse, discrete count data using negative binomial likelihoods.
- · Developed temporal models of source information for large-scale, distributed knowledge graph databases using INFER.net and Bayesian linear models.

# AI Resident, Google Brain

August 2019 - August 2021

Under mentorship of Balaji Lakshminarayanan and Jasper Snoek (Cambridge, MA)

- · Published research in *NeurIPS 2020* and *JMLR 2023* on Spectral-normalized Neural Gaussian Process (SNGP), a competitive single-model approach on prediction, calibration and out-of-domain detection.
- · Core contributor for the Uncertainty Baselines open-source library in Python, Jax, and Tensorflow.
- · Published multiple topics of research in *ICML Workshops* on one-vs-all losses, Mahalanobis distance for OOD detection, and batch normalisation for improved predictive uncertainty.

#### SELECTED PUBLICATIONS

#### CONFERENCES

- · DEFT: Efficient Finetuning of Conditional Diffusion Models by Learning the Generalised h-transform. Shreyas Padhy\*, Alexander Denker\*, Francisco Vargas\*, Kieran Didi\*, Simon Mathis\* et al. (NeurIPS 2024)
- · Improving Linear System Solvers for Hyperparameter Optimisation in Iterative Gaussian Processes.

  Jihao Andreas Lin, Shreyas Padhy, Bruno Mlodozeniec, et al. (NeurIPS 2024) arxiv.
- $\cdot$  A Generative Model of Symmetry Transformations.

James Allingham, Bruno Mlodozeniec, Shreyas Padhy, Javier Antorán, David Krueger, Richard E. Turner, Eric Nalisnick, José Miguel Hernández-Lobato. (NeurIPS 2024) arxiv.

· Stochastic Gradient Descent for Gaussian Processes Done Right.
Shreyas Padhy\*, Jihao Andreas Lin\*, Javier Antoran\*, Austin Tripp, Alexander Terenin, Csaba Szepesvari, José

Miguel Hernández-Lobato, David Janz. (ICLR 2024) arxiv.

- · Transport Meets Variational Inference: Controlled Monte Carlo Diffusions.

  Shreyas Padhy\*, Francisco Vargas\*, Denis Blessing, Nikolas Nüsken. (ICLR 2024) arxiv.
- · Sampling from Gaussian Process Posteriors using Stochastic Gradient Descent

  Shreyas Padhy\*, Jihao Andreas Lin\*, Javier Antoran\*, David Janz, José Miguel Hernández-Lobato, Alexander Terenin. (NeurIPS 2023 (Oral)) arxiv.
- · Sampling-based inference for large linear models, with application to linearised Laplace.

  Shreyas Padhy\*, Javier Antoran\*, Riccardo Barbano, Eric Nalisnick, David Janz, and José Miguel Hernández-Lobato. (ICLR 2023).
- · Simple & principled uncertainty estimation with deterministic deep learning via distance awareness. Jeremiah Zhe Liu, Zi Lin, Shreyas Padhy, Dustin Tran, Tania Bedrax-Weiss, and Balaji Lakshminarayanan.

  (NeurIPS 2020)

## **PREPRINTS**

· Kernel Regression with Infinite-Width Neural Networks on Millions of Examples. Ben Adlam, Jaehoon Lee, Shreyas Padhy, Zachary Nado, Jasper Snoek. arxiv.

#### **JOURNALS**

· A Simple Approach to Improve Single-Model Deep Uncertainty via Distance-Awareness.

Jeremiah Liu\*, Shreyas Padhy\*, Jie Ren\*, Zi Lin, Yeming Wen, Ghassen Jerfel, Zack Nado, Jasper Snoek, Dustin Tran, and Balaji Lakshminarayanan. (JMLR 2023).arxiv

#### WORKSHOPS

- Warm Start Marginal Likelihood Optimisation for Iterative Gaussian Processes.

  Jihao Andreas Lin, Shreyas Padhy, Bruno Mlodozeniec, José Miguel Hernández-Lobato. Approximate Advances in Bayesian Inference, 2024. arxiv
- · Learning Generative Models with Invariance to Symmetries.

  James Allingham, Javier Antoran, Shreyas Padhy, Eric Nalisnick, and José Miguel Hernández-Lobato.

  NeurReps Workshop at NeurIPS 2022.
- · A Simple Fix to Mahalanobis Distance for Improving Near-OOD Detection.

  Jie Ren, Stanislav Fort, Jeremiah Liu, Abhijit Guha Roy, Shreyas Padhy, and Balaji Lakshminarayanan. ICML

  2021 Workshop on Uncertainty and Robustness in Deep Learning.
- · Evaluating prediction-time batch normalization for robustness under covariate shift.

  Zachary Nado, Shreyas Padhy, D. Sculley, Alexander D'Amour, Balaji Lakshminarayanan, and Jasper Snoek.

  ICML 2020 Workshop on Uncertainty and Robustness in Deep Learning.
- · Revisiting One-vs-All Classifiers for Predictive Uncertainty and OOD Detection in Neural Networks.

  Shreyas Padhy, Zachary Nado, Jie Ren, Jeremiah Liu, Jasper Snoek, and Balaji Lakshminarayanan.

  ICML 2020 Workshop on Uncertainty and Robustness in Deep Learning.
- · Uncertainty Baselines: Benchmarks for Uncertainty & Robustness in Deep Learning. Zachary Nado et. al., Bayesian Deep Learning Workshop, 2021. arxiv &

#### AWARDS AND ACHIEVEMENTS

- · Qualcomm Innovation Fellowship 2023: Among 11 finalists invited for the online finals.
- · Qualcomm Innovation Fellowship 2022: Among 12 finalists invited to Amsterdam.
- · Trinity-Henry Barlow Scholarship 2021: Awarded by Trinity College, University of Cambridge.
- · Harding Distinguished Postgraduate Scholars Programme 2021: Awarded by the Harding Foundation.
- · Outstanding Reviewer Award at ICML 2024.
- · Outstanding Reviewer Award at ICML 2022.
- · Summer Undergraduate Research Award 2015: For undergraduate research in microwave imaging.
- Top 7% GPA Merit Scholarship: In 2013, 2014, 2015, and 2016 Fall Semesters for exceptional performance at the Indian Institute of Technology Delhi.

#### PROFESSIONAL ENGAGEMENTS

#### **Talks**

- · Invited Talk on Stochastic Gradient Descent for Bayesian ML at SIAM UQ, Trieste, March 2024
- · Guest Lecture on Conditioning in SDEs, Advanced Machine Learning course, Cambridge February 2024 .
- · Invited Talk on Stochastic Gradient Descent for GPs at Atinary Technologies, Lausanne, February 2024
- · Invited Talk on Stochastic Gradient Descent for GPs at NeurIPS@Cambridge, December 2023.
- · Invited Talk on Stochastic Gradient Descent for GPs at Microsoft Research Cambridge, October 2023.
- · SDEs and Schrodinger Bridges, presented at the Cambridge MLG Reading Group, July 2023.
- · Invited Talk on Sampling-Based Inference, at NeurIPS @ Cambridge, December 2022.
- · Out-of-Distribution Generalisation, presented at the Cambridge MLG Reading Group, October 2022.
- · Optimal Transport Metrics, presented at the Cambridge MLG Reading Group, February 2022.

## **Reviewing And Organisation**

- · Area Chair for AISTATS 2024.
- Reviewer for NeurIPS (2023, 2022, 2021), ICML (2024, 2023, 2022), ICLR (2023), AISTATS (2023), AAAI (2024, 2023).

#### **TEACHING**

Machine Learning for Signal Processing, Fall 2018: Graduate Course, by Dr. Najim Dehak, JHU Developing weekly assignments and homeworks, and grading for 50+ students.

Intro. to Computational Medicine, Fall 2018: Graduate Course, by Dr. Michael Miller, JHU Developing homeworks and course notes, extended codebase to Python, and grading for 60+ students. Gateway Computing: Python, Spring 2019: Undergraduate Course, by Dr. Kwame Kutten, JHU Developing homeworks, weekly assignments and programming assignments in Python.

## TECHNICAL PROJECTS

Uncertainty Baselines (7)

Core contributor, Google Brain

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UNet-Zoo (7)
Maintainer and developer

#### TECHNICAL STRENGTHS

DL Frameworks

Jax (Flax, Optax, Haiku, Numpyro, Blackjax), Tensorflow, PyTorch (Pyro), Keras

Computer Languages

Python, C++, Verilog

Medical Imaging TOAST++, FSL, SPM, Freesurfer