PUBLICATIONS

Some of the material, including figures, tables, concepts, and ideas, presented in this thesis have previously appeared in the following works (co-)authored during the course of the PhD degree:

[1] Pantelis Elinas, Edwin V Bonilla, and Louis C Tiao. "Variational Inference for Graph Convolutional Networks in the Absence of Graph Data and Adversarial Settings". In: *Advances in Neural Information Processing Systems*. Ed. by H. Larochelle, M. Ranzato, R. Hadsell, M.F. Balcan, and H. Lin. Vol. 33. Curran Associates, Inc., 2020, pp. 18648–18660. URL: https://bit.ly/elinas2020variational. **(Accepted as *Spotlight* presentation).**

[2] Aaron Klein, Louis C Tiao, Thibaut Lienart, Cedric Archambeau, and Matthias Seeger. "Model-based Asynchronous Hyperparameter and Neural Architecture Search". In: *arXiv preprint arXiv:2003.10865* (2020).

[3] Rafael Oliveira, Louis C Tiao, and Fabio T Ramos. "Batch Bayesian Optimisation via Density-Ratio Estimation with Guarantees". In: *Advances in Neural Information Processing Systems*. Ed. by S. Koyejo, S. Mohamed, A. Agarwal, D. Belgrave, K. Cho, and A. Oh. Vol. 35. Curran Associates, Inc., 2022, pp. 29816–29829. URL: https://bit.ly/oliveira2022batch.

[4] Louis C Tiao. "Numerical Methods for Improved Decoupled Sampling of Gaussian Processes". In: *Secondmind Labs Technical Reports* (2021).

[5] Louis C Tiao, Edwin V Bonilla, and Fabio T Ramos. "Cycle-Consistent Adversarial Learning as Approximate Bayesian Inference". In: *ICML 2018 Theoretical Foundations and Applications of Deep Generative Models*. Stockholm, Sweden, July 2018. **(Accepted as *Oral* presentation).**

[6] Louis C Tiao, Vincent Dutordoir, and Victor Picheny. "Spherical Inducing Features for Orthogonally-Decoupled Gaussian Processes". In: *Proceedings of the 40th International Conference on Machine Learning*. Ed. by Andreas Krause, Emma Brunskill, Kyunghyun Cho, Barbara Engelhardt, Sivan Sabato, and Jonathan Scarlett. Vol. 202. Proceedings of Machine Learning Research. PMLR, July 2023, pp. 34143–34160. URL: https://proceedings.mlr.press/v202/tiao23a.html. **(Accepted as *Oral* presentation).**

[7] Louis C Tiao, Aaron Klein, Matthias W Seeger, Edwin V Bonilla, Cedric Archambeau, and Fabio T Ramos. "BORE: Bayesian Optimization by Density-Ratio Estimation". In: *Proceedings of the 38th International Conference on Machine Learning*. Ed. by Marina Meila and Tong Zhang. Vol. 139. Proceedings of Machine Learning Research. PMLR, July 2021, pp. 10289–10300. URL: https://proceedings.mlr.press/v139/tiao21a.html. **(Accepted as *Oral* presentation).**

AUTHORSHIP ATTRIBUTION STATEMENT. The contents of this thesis relate more precisely to the works listed above as follows:

- Chapter 3 corresponds to the work published as [6], which was a continuation of the research initiated while a student researcher at Secondmind Labs in Cambridge, UK. I developed the methodology, including mathematical derivation and analyses, in conjunction with V. Dutordoir. I implemented the core methodology, carried out the experiments, analysed the empirical results, and wrote the drafts of the manuscript. V. Dutordoir provided source code and ongoing technical guidance for numerical calculations relating to the spherical harmonics in high dimensions and the Fourier analysis of the spherical NN activations. In addition, each co-author provided advisory and editorial contributions that helped refine the final manuscript.

- Chapter 4 corresponds to the work published as [5]. I developed the methodology, including mathematical derivation and analyses, in conjunction with E. Bonilla. I implemented the core methodology, carried out the experiments, analysed the empirical results, and wrote the drafts of the manuscript, which were refined through careful editing by E. Bonilla. Each co-author provided advisory and editorial contributions that helped refine the final manuscript.

- Chapter 5 corresponds to the work published as [7]. I developed the methodology with the help of A. Klein, who provided a continuous stream of invaluable suggestions since its early infancy, and M. Seeger, who contributed insightful mathematical derivations and analyses. I implemented the initial prototype of the method variant based on multi-layer perceptron (MLP) classifiers and carried out toy experiments on synthetic problems. A. Klein implemented the remaining variants based on tree-based ensembles and carried out large-scale experiments on a diverse range of challenging problems. Finally, I wrote the drafts of the manuscript, which were refined through careful editing by F. Ramos and C. Archambeau. Each co-author provided advisory and editorial contributions that helped refine the final manuscript.

- Appendix A corresponds to the ongoing work listed as [4], which was primarily carried out while a student researcher at Secondmind Labs. I developed the methodology at the suggestion of V. Dutordoir and V. Picheny. I implemented the methodology, carried out the experiments, analysed the empirical results, and wrote the drafts of the manuscript. In addition, each co-author provided advisory contributions that helped refine the manuscript.

- The work listed as [2] was jointly led by A. Klein and myself and initiated in my capacity as an Applied Science intern at Amazon Web Services in Berlin, Germany. The core methodology, including its mathematical derivations and analyses, was developed principally by M. Seeger, with contributions from A. Klein and myself. M. Seeger implemented early prototypes of the method, later refined by A. Klein and myself, who also carried out large-scale experiments on a diverse range of challenging problems. Since the conclusion of my internship, A. Klein, T. Lienart, and David Salinas have dedicated considerable effort to expanding the experimental analysis. In addition, each co-author provided advisory and editorial contributions that helped refine the final manuscript. While this work touches upon the central themes of this thesis, specifically in its development of multi-output GPs for asynchronous multi-fidelity BO (in turn for the tuning of deep learning models), this thesis' focus rather lies in devising new deep-learning-based approximation techniques for the GP and BO frameworks themselves. As such, while still relevant, this work is arguably tangential to the core topic and has thus been excluded.

- The work published as [1] was principally led by P. Elinas and E. Bonilla and initiated in my part-time capacity as a research software engineer at CSIRO's Data61 in Sydney, Australia. I had a role in implementing initial prototypes, carrying out toy experiments on synthetic problems, writing early drafts of the manuscript, and helping to refine directions and ideas. This work is relevant to the central themes of this thesis insofar as it develops a VI approach for an unwieldy class of probabilistic models, in particular, deep learning models of graph data that contain discrete hidden variables representing links. However, beyond the formative stages of this project, my contributions to this work were marginal, so it has been excluded from this thesis.

- The work published as [3] is a follow-up to [7], intending to address some of the questions left unresolved from the earlier work. It was principally led by R. Oliveira, and I had a role in implementing early prototypes, carrying out toy experiments on

synthetic problems, and helping to refine directions and ideas. Beyond this, my contributions to this work were insignificant, so it has been excluded from this thesis.

In addition to the statements above, in cases where I am not the corresponding author of a published item, permission to include the published material has been granted by the corresponding author.

Sep 2023

Louis Chi-Chun Tiao

As supervisor for the candidature upon which this thesis is based, I can confirm that the authorship attribution statements above are correct.

Sep 2023

Fabio T. Ramos