

Academic background

- Apr. 2025 - **Research Fellow**, Aalto University, Finnish Center for Artificial Intelligence
- Mar. 2024 - **Postdoctoral Researcher**, Inria SISTM team, Bordeaux Population Health
Mar. 2025
- Feb. 2022 - **Postdoctoral Researcher**, Aalto University, Probabilistic Machine Learning team,
Feb. 2024 Helsinki
Supervised by Samuel Kaski, Markus Heinonen and Vikas Garg
- Oct. 2018 - **PhD in Computer Science**, *On learning mechanistic models from time series*
Feb. 2022 *data with applications to personalised chronotherapies*, Inria Saclay, Institut Curie
Saint-Cloud, École polytechnique
Supervised by François Fages and Annabelle Ballesta
- Apr.-Sept. **Summer Intern**, *Learning mechanistic models from time series data*, Inria Saclay,
2018 Lifeware Team
Supervised by François Fages
- 2017 – 2018 **Masters in Random Modelling, Finance and Data Science, M2MO**, *Data Science track*, Université de Paris
- May-July **Summer Intern**, *Random matrix theory, Application to community detection*
2017 *within networks*, Laboratoire MAP5, Université de Paris
Supervised by Manon Defosseux
- 2016 – 2017 **First year of Masters in Applied Mathematics**, Université de Paris
ranked 1st
- 2012 – 2015 **BSc. Mathematics**, Université de Paris

Publications

Journal Articles

- 2024 **Human-in-the-loop active learning for goal-oriented molecule generation**, Yasmine Nahal, Janosch Menke, Julien Martinelli, Markus Heinonen, Mikhail Kabeshov, Jon Paul Janet, Eva Nittinger, Ola Engkvist and Samuel Kaski, *Journal of Chemoinformatics*
- 2022 **Accelerating metabolic models evaluation with statistical metamodels: application to Salmonella infection models**, Clémence Frioux, Sylvie Huet, Simon Labarthe, Julien Martinelli, Thibault Malou, David Sherman, Marie-Luce Taupin, Pablo Ugalde-Salas, *ESAIM Proceedings & Surveys*
- 2021 **A mathematical model of the circadian clock and drug pharmacology to optimize irinotecan administration timing in colorectal cancer**, Janina Hesse, Julien Martinelli, Ouda Aboumanify, Annabelle Ballesta and Angela Relógio, *Computational and Structural Biotechnology*
- 2021 **Model learning to identify systemic regulators of the peripheral circadian clock**, Julien Martinelli, Xiao-Mei Li, Sandrine Dulong, Sylvain Soliman, Francis Lévi, François Fages and Annabelle Ballesta, *Bioinformatics*

Proceedings

- 2025 **Preferential Amortized Black-Box Optimization**, Xinyu Zhang, Daolang Huang, Samuel Kaski and Julien Martinelli, *Proceedings of The 13th International Conference on Learning Representations (spotlight)*

- 2024 **Bayesian Active Learning in the Presence of Nuisance Parameters**, Sabina J. Sloman, Ayush Bharti, Julien Martinelli and Samuel Kaski, *Proceedings of The 40th International Conference on Uncertainty in Artificial Intelligence* (oral)
- 2024 **Learning relevant contextual variables within Bayesian optimization**, Julien Martinelli, Ayush Bharti, Armi Tiihonen, S.T. John, Louis Filstroff, Sabina J. Sloman, Patrick Rinke and Samuel Kaski, *Proceedings of The 40th International Conference on Uncertainty in Artificial Intelligence*
- 2023 **Multi-Fidelity Bayesian Optimization with Unreliable Information Sources**, Petrus Mikkola, Julien Martinelli, Louis Filstroff and Samuel Kaski, *Proceedings of The 26th International Conference on Artificial Intelligence and Statistics*, 7425-7454
- 2019 **On Inferring Reactions from Data Time Series by a Statistical Greedy Heuristics**, Julien Martinelli, Jeremy Grignard, Sylvain Soliman and François Fages, *Proceedings of the Seventeenth International Conference on Computational Methods in Systems Biology*, 352-355

Workshop Communications

- 2024 **Computation-Aware Robust Gaussian Processes**, Marshal Sinaga, Julien Martinelli and Samuel Kaski, *NeurIPS 2024 Workshop on Bayesian Decision-making and Uncertainty*
- 2024 **Challenges in interpretability of additive models**, Xinyu Zhang, Julien Martinelli and S.T. John, *IJCAI 2024 Workshop on Explainable Artificial Intelligence (XAI)*
- 2023 **Preferential Heteroscedastic Bayesian Optimization with Informative Noise Priors**, Marshal Sinaga, Julien Martinelli and Samuel Kaski, *NeurIPS 2023 Workshop on Adaptive Experimental Design and Active Learning in the Real World*
- 2023 **Learning relevant contextual variables within Bayesian optimization**, Julien Martinelli, Ayush Bharti, Armi Tiihonen, Louis Filstroff, S.T. John, Sabina J. Sloman, Patrick Rinke and Samuel Kaski, *NeurIPS 2023 Workshop on Adaptive Experimental Design and Active Learning in the Real World*
- 2023 **Leveraging expert feedback to align proxy and ground truth rewards in goal-oriented molecular generation**, Julien Martinelli, Yasmine Nahal, Duong Lê, Ola Engkvist and Samuel Kaski, *NeurIPS 2023 Workshop on New Frontiers of AI for Drug Discovery and Development*
- 2019 **A statistical unsupervised learning algorithm for inferring reaction networks from time series data**, Julien Martinelli, Jeremy Grignard, Sylvain Soliman and François Fages, *ICML 2019-Workshop on Computational Biology*

Preprints

- 2024 **Proxy-informed Bayesian transfer learning with unknown sources**, Sabina J. Sloman, Julien Martinelli and Samuel Kaski, under review
- 2024 **Heteroscedastic Preferential Bayesian Optimization with Kernel Density Based User Modelling**, Marshal Sinaga, Julien Martinelli, Vikas Garg and Samuel Kaski, under review
- 2022 **Reactmine: a search algorithm for inferring chemical reaction networks from time series data**, Julien Martinelli, Jeremy Grignard, Sylvain Soliman, Annabelle Ballesta and François Fages

Oral Communications

Invited Talks

July 2024 **European Conference on Mathematical and Theoretical Biology**, Toledo

- February 2023 **Biostatistics Seminar**, *Bordeaux Population Health Center*
- January 2023 **Public Seminar - CRiStAL team**, *Université de Lille*
- November 2022 **AI Day**, *Helsinki*
- July 2022 **Workshop on Hybrid models and methods in systems medicine**, *Institut Curie, Paris*
- Talks**
- March 2025 **DataIA Workshop Mathematical Foundations of AI**, *Paris*
- June 2024 **Journées Maths-Bio-Santé**, *Nantes*
- May 2024 **Public Seminar**, *TU Hamburg*
- May 2024 **Monthly seminar BIoSS-IA**, *Remote*
- November 2023 **Public Seminar - SISTM team**, *Bordeaux Population Health Center*
- May 2023 **Machine Learning Coffee Seminar**, *Helsinki*
- August 2022 **Finnish Center for Artificial Intelligence - Get together**, *Helsinki*
- August 2021 **CEMRACS - Data Assimilation and Reduced Modeling for High Dimensional Problems**, *Luminy*
- July 2021 **Twentieth European Conference on Computational Biology**, *Remote*
- June 2021 **Tenth biennial of the Society of Applied and Industrial Mathematics (SMAI)**, *La Grande Motte*
- May 2021 **Workshop Modelling Heterogeneous populations with applications in biology**, *Remote*
- April 2021 **Monthly seminar BIoSS-IA**, *Remote*
- May 2019 **BIoSS-IA Days**, *Laboratoire d'Informatique Fondamentale d'Orléans*
- December 2018 **BIoSS-IA Days**, *Pasteur Institute, Paris*

Poster Sessions

- July 2024 **UAI 2024**, *Barcelona*
- December 2023 **NeurIPS 2023 Workshops**, *New Orleans*
- September 2023 **ELLIS Robust ML Workshop**, *Helsinki*
- April 2023 **AISTATS 2023**, *València*
- July 2021 **JOBIM 2021**, *Remote*
- January 2021 **Winter school AI4Health**, *Remote*
- June 2019 **Summer School Formal Modeling of Biological Regulatory Networks**, *Porquerolles*

Teaching

- 2022 – 2023 **Teaching Assistant**, *MSc.*, Machine Learning: Advanced Probabilistic Methods, Aalto University
- 2019 – 2021 **Teaching Assistant**, *2nd year BSc.*, Real Analysis, Multivariate functions, Université Paris Cité
- 2018 – 2019 **Teaching Assistant**, *1st year BSc.*, Mathematics and Calculus 2, Université Paris Cité

Supervision and Advising

- February 2024 - August 2024 **Xinyu Zhang**, *Master Thesis*, 2nd year MSc. student, Amortized Bayesian Optimization
 Joint supervision with Daolang Huang
- September 2023 – January 2024 **Xinyu Zhang**, *Research Assistant*, 2nd year MSc. student, Probabilistic Neural Additive Models for Interpretable Machine Learning
 Joint supervision with S.T. John
- June 2023 – **Marshal Sinaga**, *PhD Student*, Integrating Robustness and Human-Centric Perspectives in Bayesian Optimization
 Advisor (Supervisor: Samuel Kaski)
- June – August 2023 **Duong Le**, *Summer Intern*, 3rd year BSc. student, Benchmarking Human-In-The-Loop and active learning strategies for molecular generation
 Joint supervision with Yasmine Nahal
- June – August 2023 **Xinyu Zhang**, *Summer Intern*, 1st year MSc. student, Probabilistic Neural Additive Models for Interpretable Machine Learning
 Joint supervision with S.T. John
- June – August 2023 **Kaul Rajat**, *BSc Thesis supervision*, 3rd year BSc. student, Learning Biological ODE models from time series data

Other key academic merits

- Reviewing service NeurIPS, ICML, ICLR, AISTATS, UAI, JMLR, PAMI, TCBB, Communications Biology, ECCB, CMSB
- Research funding and grants Contributed to the preparation of an European Research Council Advanced Grant currently under review (PI Samuel Kaski). I specifically contributed to the topics of domain expert involvement in out-of-distribution regimes and active robustness for out-of-distribution generalization.
- Membership European Laboratory for Learning and Intelligent Systems Society (ELLIS)

Programming skills

- Programmation Python, Stan, R, Matlab, \LaTeX , Shell
 Tools GitHub, Vim

Languages

- Native French, fluent English