

## Academic background

- March 2024 - **Postdoctoral Researcher**, Inria SISTM team, Bordeaux Population Health
- 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. 2018 **Summer Intern**, *Learning mechanistic models from time series data*, Inria Saclay,  
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 2017 **Summer Intern**, *Random matrix theory, Application to community detection within networks*, Laboratoire MAP5, Université de Paris  
Supervised by Manon Defosseux
- 2016 – 2017 **First year of Masters in Applied Mathematics**, Université de Paris  
ranked 1<sup>st</sup>
- 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*

- 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

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**
- July 2024 **European Conference on Mathematical and Theoretical Biology**, *Toledo*
- June 2024 **Journées Maths-Bio-Santé**, *Nantes*
- May 2024 **Public Seminar**, *TU Hamburg*
- May 2024 **Monthly seminar BIOS-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 BIOS-IA**, *Remote*
- May 2019 **BIOS-IA Days**, *Laboratoire d'Informatique Fondamentale d'Orléans*
- December 2018 **BIOS-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*, Bayesian Experimental Design  
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 AISTATS, ICML, NeurIPS, ICLR, 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

Programming Python, R, Matlab,  $\text{\LaTeX}$ , Shell

Tools GitHub, Vim

## Languages

Native French, fluent English