Julien Martinelli

PhD graduate

julien_martinelli@hotmail.com
https://julienmartinelli.github.io/
Born 05/26/1994

Academic background

March 2024 - **Postdoctoral Researcher**, Inria SISTM team, Bordeaux Population Health

Feb. 2022 - Feb. 2024 **Postdoctoral Researcher**, Aalto University, Probabilistic Machine Learning team, Helsinki
Supervised by Samuel Kaski, Markus Heinonen and Vikas Garg

Oct. 2018 - Feb. 2022 **PhD in Computer Science**, *On learning mechanistic models from time series 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^{st}

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*, accepted for publication in *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

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 Seventeeth International Conference on Computational Methods in Systems Biology*, 352-355

Workshop Communications

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 **Preferential Amortized Black-Box Optimization**, *Xinyu Zhang, Daolang Huang, Julien Martinelli and Samuel Kaski*, under review

2024 **Computation-Aware Robust Gaussian Processes**, *Marshal Sinaga, Julien Martinelli and Samuel Kaski*, under review

2024 **Heteroscedastic Preferential Bayesian Optimization with Informative Noise Distributions**, *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 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.*, Analysis 4, Multivariate functions, Université de Paris

2018 – 2019 **Teaching Assistant**, *1st year BSc.*, Mathematics and Calculus 2, Université de Paris

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

Programming skills

Programmation Python, R, Matlab, LaTeX, Shell

Tools GitHub, Vim

Languages

Native French, fluent English