I. <u>PERSONAL DETAILS</u>

Prof. Gilles Louppe

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Education and key qualifications

2010–2014	Ph.D., Computer Science
	University of Liège, Belgium
	Supervisor: Prof. Pierre Geurts
	Thesis: Understanding Random Forests – From Theory to Practice
2008–2010	M.Sc., Computer Science (Summa Cum Laude)
	University of Liège, Belgium
2005–2008	B.Sc., Computer Science (Summa Cum Laude)
	University of Liège, Belgium

Current position(s)

2023–Present	Professor (Professeur)
	Faculty of Applied Sciences, University of Liège, Belgium

Previous position(s)

Assistant Professor (Chargé de cours)
Faculty of Applied Sciences, University of Liège, Belgium
Postdoctoral Associate
Center for Data Science, New York University, USA
Center for Cosmology and Particle Physics, New York University, USA
Marie-Curie Research Fellow
CERN, Switzerland
FRS-FNRS Research Fellow
Faculty of Applied Sciences, University of Liège, Belgium

II. RESEARCH ACHIEVEMENTS AND PEER RECOGNITION

Research achievements

Trained as a computer scientist, I view and investigate AI as a way to understand the world around us. In pursuit of this objective, my research efforts have been focused on deep generative models, approximate Bayesian inference, and applications thereof in the physical sciences. I am at the origin of a new generation of algorithms for simulation-based inference based on deep neural networks and have been developing and leading this research track ever since. The methodology we have built and improved over the years has been successfully validated on a range of scientific problems, through international collaborations with domain scientists in particle physics, astrophysics, astronomy, biophysics, and neuroscience. The next frontier of my research work is to scale up these methods to high-dimensional inference problems found in Earth and climate sciences.

<u>Selected publications</u> The publications selected below are representative of my research efforts over the last years, acting for all of them as the, or one, of the principal investigators. The exhaustive list of my publications is available at <u>https://bit.ly/3MzUfXQ</u>.



- (1) François Rozet and <u>Gilles Louppe</u>. "Score-based Data Assimilation." In Advances in Neural Information Processing Systems 37 (2023). <u>https://doi.org/10.48550/arXiv.2306.10574</u> In this paper; we present a novel data assimilation method based on score-based deep generative models. We demonstrate promising results on high-dimensional geophysical dynamical systems. This work illustrates some of our recent work on high-dimensional Bayesian inference and diffusion models, with direct potential applications in the geosciences.
- (2) Malavika Vasist, François Rozet, Olivier Absil, Paul Mollière, Evert Nasedkin, <u>Gilles Louppe</u>. "Neural posterior estimation for exoplanetary atmospheric retrieval." In Astronomy and Astrophysics 672 (2023): A147. <u>https://doi.org/10.1051/0004-6361/202245263</u> This work demonstrates the potential of simulation-based inference for exoplanetary atmospheric retrieval. It illustrates one of our successful collaborations with astronomers (University of Liège, Belgium; MPI for Astronomy, Germany).
- (3) Arnaud Delaunoy, Joeri Hermans, François Rozet, Antoine Wehenkel, <u>Gilles Louppe</u>. "Towards reliable simulation-based inference with balanced neural ratio estimation." In Advances in Neural Information Processing Systems 36 (2022). <u>https://doi.org/10.48550/arXiv.2208.13624</u> *This paper introduces BNRE, a variation of NRE (see (8)) designed to produce posterior approximations that are robust to false discoveries and therefore more reliable for scientific usage.*
- Joeri Hermans, Arnaud Delaunoy, François Rozet, Antoine Wehenkel, Volodimir Begy, Gilles Louppe. (4) "A Crisis In Simulation-Based Inference? Beware, Your Posterior Approximations Can Be Unfaithful." In Transactions Machine Learning Research on (2022). https://openreview.net/forum?id=LHAbHkt6Aq In this work, we present extensive empirical evidence showing that Bayesian simulation-based inference algorithms can produce computationally unfaithful posterior approximations. This study was motivated by the strict requirements of scientific applications, where posterior approximations can be used for claiming discoveries or for making decisions with potentially far-reaching consequences.
- (5) Kyle Cranmer, Johann Brehmer, and <u>Gilles Louppe</u>. "The frontier of simulation-based inference." Proceedings of the National Academy of Sciences 117, no. 48 (2020): 30055-30062. <u>https://www.pnas.org/content/117/48/30055.short</u> In this paper, we review the rapidly developing field of simulation-based inference and identify the forces giving additional momentum to the field. In recent years, this paper has become the go-to reference for an introduction and overview to the topic of simulation-based inference.
- (6) Johann Brehmer, <u>Gilles Louppe</u>, Juan Pavez, and Kyle Cranmer. "Mining gold from implicit models to improve likelihood-free inference." Proceedings of the National Academy of Sciences 117, no. 10 (2020): 5242-5249. <u>https://www.pnas.org/content/117/10/5242.short</u> We show that information that characterizes the latent data generation process can be extracted from scientific simulators and used for training surrogate models. This paper illustrates how techniques from probabilistic programming can drastically improve sample efficiency in simulation-based inference algorithms.
- (7) Joeri, Hermans, Nilanjan Banik, Christoph Weniger, Gianfranco Bertone, and <u>Gilles Louppe</u>. "Towards constraining warm dark matter with stellar streams through neural simulation-based inference." In Monthly Notices of the Royal Astronomical Society 507, no. 2 (2021). <u>https://doi.org/10.1093/mnras/stab2181</u> We apply NRE (see (8)) to the statistical analysis of the observed perturbations in the density of stellar streams, which can in principle set stringent constraints on the mass function of dark matter subhaloes, and in turn can be used to constrain the mass of the dark matter particle. This study is another example of a successful collaboration with astrophysicists (University of Amsterdam, Netherlands).
- (8) Joeri Hermans, Volodimir Begy, and <u>Gilles Louppe</u>. "Likelihood-free MCMC with amortized approximate ratio estimators." In International Conference on Machine Learning, pp. 4239-4248. PMLR, 2020. <u>http://proceedings.mlr.press/v119/hermans20a</u> This work introduces Neural Ratio Estimation (NRE), a novel approach for Bayesian inference with scientific simulators. NRE is now well-established and is one of the reference algorithms in simulation-based inference.

- (9) Kyle Cranmer, Juan Pavez, and <u>Gilles Louppe</u>. "Approximating likelihood ratios with calibrated discriminative classifiers." (2015) <u>https://doi.org/10.48550/arXiv.1506.02169</u> We show that discriminative classifiers can be used to approximate the generalized likelihood ratio statistic when only a generative model for the data is available. This paper sparked my research work on simulation-based inference. It has initiated a new generation of approximate inference algorithms based on deep neural networks.
- (10) <u>Gilles Louppe</u>. "Understanding random forests: From theory to practice." (2014) <u>https://arxiv.org/abs/1407.7502</u> This publication is my PhD thesis on the analysis of random forests. Although I am no longer doing research on this topic, my thesis and its related publications have proven to be helpful to many machine learning scientists or practitioners.

<u>Summary of my track record.</u> 59 refereed publications in international conference proceedings or in journals, 30 refereed publications in international workshops, and 98 publications overall (including pre-prints). My h-index is 33, my i10-index is 57, and my citations count is above 90000 (Google Scholar, December 2023).

<u>Publication strategy.</u> In artificial intelligence and machine learning, publications at international conferences are the main form of dissemination. The main conferences (incl. NeurIPS, ICML or ICLR) are among the most impactful venues across all scientific disciplines [<u>https://bit.ly/4a4k4cI</u>]. They are highly competitive, with acceptance rates of 25% or less, and only publish peer-reviewed papers presenting original research. The main conferences are complemented by workshops, which are less selective and publish papers that are not necessarily peer-reviewed with the same level of scrutiny. Machine learning journals are less common and typically focus on longer publications exceeding 25 pages.

My publication strategy aims to prioritize conference papers as they offer a prime opportunity to present innovative research, undergo rigorous peer review, and gain visibility within the ML community. By targeting tier-1 conferences, I can ensure that my work receives the recognition and scrutiny necessary for establishing credibility and advancing knowledge in the field. Since 2017, I primarily assume the position of the last author, as I prioritize the front-line involvement of my researchers and PhD students. I co-design, guide, and supervise their research work and co-write their papers, allowing them to gain valuable experience and recognition for their contributions while fostering a collaborative research environment.

Peer recognition

<u>Invited talks</u> The exhaustive list of my talks (99 in total) is available at <u>https://bit.ly/4a09KTa</u>. Among those, 5 notable invited talks are:

- (1) <u>G. Louppe</u>. "Simulation-based inference: Proceed with caution!." CAP-RFIAP 2022 (Conférence Française sur l'Apprentissage Machine), Vannes, France, July 2022. Keynote speaker.
- (2) <u>G. Louppe</u>. "The frontier of simulation-based inference." AIMS Seminar Series. Oxford, UK, February 12, 2021. <u>http://hdl.handle.net/2268/256816</u>
- (3) <u>G. Louppe</u>. "Neural Likelihood-free Inference." GRAPPA colloquium. Amsterdam, The Netherlands, November 19, 2019. <u>http://hdl.handle.net/2268/241474</u>
- (4) <u>G. Louppe.</u> "Adversarial Games for Particle Physics." Deep Learning for Physical Sciences workshop, NeurIPS 2018. Los Angeles, USA, December 8, 2017. <u>http://hdl.handle.net/2268/226455</u>
- (5) <u>G. Louppe</u>. "Teaching Machines to Discover Particles." Nikhef Colloquium. Amsterdam, The Netherlands, September 29, 2017. <u>http://hdl.handle.net/2268/226452</u>

Fellowships and memberships

- 2023–Present Member of the "Société Royale des Sciences de Liège"
- 2021–Present Board member of the "Benelux Association for Artificial Intelligence" (BNVKI)
- 2021–Present President of the scientific advisory board of the "Trusted AI Labs Institute" (TRAIL)
- 2018–Present Member of the "ELLIS Society"

III. ADDITIONAL INFORMATION

Close scientific collaborators

<u>Particle physics:</u> Kyle Cranmer (New York University, 2015-2021), Johann Brehmer (New York University, 2017-2020), Michael Kagan (SLAC, 2016-2021), David Rousseau (Université Paris-Saclay, 2018-Present), Tilman Plehn (2023-Present), Fabio Maltoni (2023-Present); <u>Astrophysics:</u> Siddharth Mishra-Sharma (MIT, 2019-2020), Christoph Weniger (University of Amsterdam, 2020-Present), Joshua Bloom (UC Berkeley, 2023-Present); <u>Astronomy:</u> Olivier Absil (ULiège, 2019-Present); <u>Biophysics:</u> Namid Stillman (University College London, 2022-Present); <u>Geoscience:</u> Marilaure Grégoire (ULiège, 2023-Present).

Engagement in the research system

Conference and workshop co-organizer

2020-2023	Machine Learning and the Physical Sciences, NeurIPS workshop.
2023	Synergy of Scientific and Machine Learning Modeling, ICML workshop.
2019	Advanced Workshop on Accelerating the Search for Dark Matter with ML.
2016	Data Science @ HEP at the Simons Foundation.
2015	Data Science @ LHC Workshop.

Program committees

2022–Present	Recurrent area chair-for NeurIPS, ICML, ICLR and AISTATS.
2014–2022	Recurrent peer-reviewer for NeurIPS, ICML, ICLR and AISTATS.

Dissertation committees

Member of the evaluation committee of 20 PhD theses, both locally and internationally.

Academic supervision

PhD Students

2017-2022	Joeri Hermans, "Advances in Simulation-based inference"
2018-2022	Antoine Wehenkel, "Inductive bias in deep probabilistic modelling"
2018–Present	Norman Marlier, "Simulation-based inference for robotic grasping"
2019–Present	Maxime Quesnel, "Deep learning-based wavefront sensing for exoplanet imaging"
2019–Present	Malavika Vasist, "Simulation-based inference for exoplanet characterization"
2020–Present	Arnaud Delaunoy, "Reliable simulation-based inference"
2021–Present	François Rozet, "Simulation-based inference for large-scale dynamical systems"
2021–Present	Omer Rochman, "Scientific emulators with deep neural networks"
2023–Present	Gérome Andry, "Overcoming model misspecification with deep learning"
2023–Present	Victor Mangeleer, "Understanding submesoscale oceanic processes with deep learning"
2023–Present	Sacha Lewin, "Infinite-dimensional deep generative models for spatiotemporal data"

<u>MSc Students</u> Since 2017, I have supervised 46 MSc students on various topics in deep learning and approximate Bayesian inference. The exhaustive list is available at <u>https://bit.ly/3SpWOzC</u>.

Teaching

Course development and multi-year teaching of "Introduction to AI", "Foundations of Data Science", "Deep Learning" and "Advanced Machine Learning". Pedagogical materials are all open source and publicly available at https://glouppe.github.io/teaching.

Software

Core developer of the <u>Scikit-Learn</u> library for machine learning in Python, from 2010 to 2015. This library is now the most popular machine learning library in Python, with more than <u>1.5M</u> downloads per day.