Kilian Fatras

Senior machine learning research scientist

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Scholar
Website

Research Interests: Generative Models, Protein Design, Optimal Transport, Distribution Shifts

Positions

04/25–now **Machine Learning Research Scientist** - EvolutionaryScale

06/23–04/25 **Founding Machine Learning Research Scientist** - Dreamfold

12/2023 **Postdoctoral Fellow on Distribution Shifts and Generative Modelling** - Mila and McGill University - Supervisors: Professor Ioannis Mitliagkas & Professor Adam Oberman

Education

2021 **PhD in Computer Science: "Optimal Transport & Deep Learning: Learning from One Another"**- Inria - Supervisors: Professor Nicolas Courty & Professor Rémi Flamary

2018 **Master of Science in Machine Learning** - UC Berkeley & Polytechnique

2018 **Engineering Diploma in Applied Mathematics and Computer Science** - ENSTA Paris

2015 **Bachelor in Mathematics and Physics (Double Major)** - University of Western Brittany

Research Summary

As a research scientist, I develop novel generative models for geometric data with a current focus on protein backbones. In particular, I have developed a strong expertise in Flow Matching, a recent framework for training normalizing flows akin to diffusion models, through my PhD and postdoctoral research. During my PhD, I led the theoretical analysis of minibatch optimal transport, a crucial element for using optimal transport with deep learning methods. During my postdoc, I co-developed an optimal transport-based flow matching method for Euclidean data, such as images. These works lay the foundation for my most recent project: developing a SE(3)-Flow Matching method to generate protein backbone designs that can be conditioned on amino acid sequences using large language models.

Selected Publications

1. **Generalizing Flow-Based Generative Models with Optimal Transport** - [URL] - Alex Tong*, **Kilian Fatras***, Nikolay Malkin* et al. - TMLR 2024
2. **Simulation-Free Schrödinger Bridges via Score and Flow Matching** - [URL] - Alex Tong*, Nikolay Malkin*, **Kilian Fatras*** et al. - AISTATS 2024
3. **SE(3)-Stochastic Flow Matching for Protein Backbone Generation** - [URL] - J. Bose, T. Akhound-Sadegh, G. Huguet, **Kilian Fatras** et al. - ICLR 2024
4. **Sequence-Augmented SE(3)-Flow Matching for Conditional Protein Backbone Generation** - [URL] - Guillaume Huguet*, James Vuckovic*, **Kilian Fatras*** et al.
5. **Generating and Imputing Tabular Data via Diffusion and Flow-based Gradient-Boosted Trees** - [URL] - Alexia Jolicoeur-Martineau, **Kilian Fatras**, Tal Kachman - AISTATS 2024
6. **Unbalanced Minibatch Optimal Transport; Applications to Domain Adaptation** - [URL] - **Kilian Fatras**, Thibault Séjourné, Nicolas Courty, and Rémi Flamary - ICML 2021
7. **Learning with Minibatch Wasserstein: Asymptotic and Gradient Properties** - [URL] - **Kilian Fatras**, Younes Zine, Rémi Flamary, Rémi Gribonval, and Nicolas Courty - AISTATS 2020
8. **Optimal Transport and Deep Learning: Learning from One Another** - [URL] - Thesis

Open Source Software

- Conditional Flow Matching `https://github.com/atong01/conditional-flow-matching`
- POT: Python Optimal Transport library `https://github.com/PythonOT/POT`
- A Reproducible and Realistic Evaluation of Partial Domain Adaptation Methods `https://github.com/kilianFatras/BenchmarkPDA`

- Unbalanced minibatch Optimal Transport; applications to Domain Adaptation https://github.com/kilianFatras/JUMBOT
- Learning with minibatch Wasserstein: asymptotic and gradient properties https://github.com/kilianFatras/minibatch_Wasserstein

Research Internships

May 2018 **Research Assistant - University of British Columbia, Vancouver**

During this 6-month research internship, I focused on optimization for optimal transport and the generation of adversarial examples. I worked under the supervision of Professor Mark Schmidt.

08/17–12/17 **Research Assistant - University of California, Berkeley**

During this 8-month research project, my goal was to develop and improve the analysis of sparse distributed variance reduction algorithms. I worked under the supervision of Fabian Pedregosa.

Seminar Organisation

2022-2023 Co-organisation of the Montréal Optimization (MtL-OPT) Seminar

11/18/2021 Co-organisation of the GDR-ISIS-MIA workshop on Optimal Transport in Machine Learning

2018-2021 Co-organisation of INRIA Panama team seminar

2018-2021 Co-organisation of IRISA Obelix team seminar

Selected invited talks

03/10/24 Xaira Therapeutics: Sequence-Augmented SE(3)-Flow Matching for Protein Backbone Generation

17/09/24 EvolutionaryScale: Sequence-Augmented SE(3)-Flow Matching for Protein Backbone Generation

11/04/23 FAIR Lab (Montréal): Designing and evaluating new domain adaptation methods

28/02/23 Microsoft AI Lab (Montréal) seminar: Optimal transport and deep partial domain adaptation

08/12/22 Huawei (Noah's Ark Lab, Paris) seminar: Optimal transport and deep partial domain adaptation

04/12/22 Canadian Mathematical Society winter meeting: Minibatch optimal transport distances in deep learning

25/11/22 LITIS seminar: Optimal transport and deep partial domain adaptation

04/04/22 DS4DM Coffee Talks Polytechnique Montréal: Unbalanced minibatch Optimal Transport

14/02/22 Gauthier Gidel's group: Adversarial examples meet optimal transport

01/09/21 CMAP Ecole Polytechnique: Unbalanced minibatch optimal transport; applications to domain adaptation

28/04/21 Mila-MLOpt - Unbalanced minibatch optimal transport; applications to domain adaptation

09/07/19 GDR-ISIS: Optimal transport in statistical learning - Wasserstein adversarial regularization for label noise

Teaching and co-supervision

2022/2023 Co-supervision of Hiroki Naganuma on Out-Of-Distribution samples with Professor Ioannis Mitliagkas

2021/2022 Introduction to Optimal Transport - Guest lecturer - UniversitÃĭ de MontrÃĭal and McGill University

2020/2021 Introduction to Deep Learning - Co-organizer and lecturer - Erasmus Mundus master in Digital Earth at University of Southern Brittany

2019/2020 Co-supervision of Jean-Christophe Burnel on Generating natural adversarial Remote Sensing Images

Community service

Reviewer for JMLR, JOTA, ICML, ECML, IEEE TGRS, AIStats, NeurIPS, ICLR (best reviewer 2022)

Languages

French (Native), **English** (Fluent/ TOEIC 975/990)

References

- Ioannis Mitliagkas (Google DeepMind, Mila, Université de Montréal) - ioannis@mila.quebec
- Rémi Flamary (CMAP, École Polytechnique de Paris) - remi.flamary@polytechnique.edu
- Fabian Pedregosa (Google DeepMind) - pedregosa@google.com
- Nicolas Courty (IRISA, Université de Bretagne-Sud) - nicolas.courty@irisa.fr