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# Kilian Fatras

*Senior Machine Learning Research Scientist*

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

## Experiences

04/25–now **Machine Learning Research Scientist** - EvolutionaryScale - New York City, USA
- Leading foundational model research in protein sequence and structure using large-scale protein language models and generative diffusion models.
- Developing scalable architectures for protein-related tasks (motif scaffolding, structure-conditioned sequence generation, binder design, ...).
- Collaborating with wet-lab scientists to validate designed proteins.

06/23–04/25 **Founding Machine Learning Research Scientist** - Dreamfold - Montréal, Canada
- Built and trained generative models for protein design with focus on binder design, motif scaffolding, unconditional generation, and hotspot interactions.
- Led design of multimodal diffusion models conditioned on structure and sequence.
- Contributed to model interpretability, evaluation metrics (pLDDT, pTM), and training infrastructure.

01/22–12/23 **Postdoctoral Fellow on Distribution Shifts and Generative Modelling** - Mila & McGill University
Supervisors: Professor Ioannis Mitliagkas and Professor Adam Oberman
- Published in top ML conferences on flow matching models, optimal transport and distribution shifts.
- Developed and contributed to open-source software that reached thousands of stars on GitHub.

## Education

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

2018 **Master of Science in Machine Learning and Entrepreneurship** – UC Berkeley & Polytechnique

2017 **Master of Engineering in Applied Mathematics and Computer Science** – ENSTA Paris

## Selected Publications and Open-Source Software

1. **Generalizing Flow-Based Generative Models with Optimal Transport** - [URL] - Alex Tong*, **Kilian Fatras***, Nikolay Malkin* et al. - TMLR 2024
2. **SE(3)-Stochastic Flow Matching for Protein Backbone Generation** - [URL] - J. Bose, T. Akhound-Sadegh, G. Huguet, **Kilian Fatras** et al. - ICLR 2024
3. **Sequence-Augmented SE(3)-Flow Matching for Conditional Protein Backbone Generation** - [URL] - Guillaume Huguet*, James Vuckovic*, **Kilian Fatras*** et al. - NeurIPS 2024
4. **Unbalanced Minibatch Optimal Transport; Applications to Domain Adaptation** - [URL] - **Kilian Fatras**, Thibault Séjourné, Nicolas Courty, and Rémi Flamary - ICML 2021
5. **Learning with Minibatch Wasserstein: Asymptotic and Gradient Properties** - [URL] - **Kilian Fatras**, Younes Zine, Rémi Flamary, Rémi Gribonval, and Nicolas Courty - AISTATS 2020
6. **Optimal Transport and Deep Learning: Learning from One Another** - [URL] - Thesis
7. **Conditional Flow Matching** `https://github.com/atong01/conditional-flow-matching`
8. **POT: Python Optimal Transport library** `https://github.com/PythonOT/POT`

## 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