Kirill Neklyudov (Kyrylo Nekliudov)

Academic Experience

Institut Courtois — **Dec 2024 – Current**
Regular Member — *Montreal, Canada*

Mila - Quebec AI Institute — **Jun 2024 – Current**
Core Academic Member — *Montreal, Canada*

Université de Montréal — **Jun 2024 – Current**
Assistant Professor in Machine Learning and Statistics (tenure-track) — *Montreal, Canada*

Vector Institute for Artificial Intelligence — **Nov 2021 – May 2024**
Postdoctoral Fellow, supervisors: Alán Aspuru-Guzik, Alireza Makhzani — *Toronto, Canada*

- AI4Science, Generative Modeling, Optimal Transport.

University of Amsterdam — **Sep 2020 – Oct 2021**
Postdoctoral Fellow, supervisor: Max Welling — *Amsterdam, Netherlands*

- Markov Chain Monte Carlo, Generative Modeling.

Higher School of Economics — **Feb 2018 – Aug 2020**
Researcher, supervisor: Dmitry Vetrov — *Moscow, Russia*

- Bayesian Inference, Markov Chain Monte Carlo, Generative Modeling.

Education

Moscow Institute of Physics and Technology — **Sep 2010 – Jul 2014**
Bachelor degree in Applied Physics and Mathematics, summa cum laude — *Dolgoprudny, Russia*

Moscow Institute of Physics and Technology — **Sep 2014 – Jul 2016**
Master degree in Applied Physics and Mathematics, summa cum laude — *Dolgoprudny, Russia*

Yandex School of Data Analysis — **Sep 2014 – Jun 2016**
Master degree in Machine Learning — *Moscow, Russia*

Higher School of Economics — **Sep 2016 – Nov 2020**
Ph.D. in Computer Science, supervisor: Dmitry Vetrov — *Moscow, Russia*

Professional Service

Organizer: ICML 2024 Workshop ("Structured Probabilistic Inference & Generative Modeling"), ICLR 2025 Workshop ("Frontiers in Probabilistic Inference: Sampling Meets Learning")
Area Chair at ICLR: 2025
Reviewer at NeurIPS: 2020, 2021 (outstanding reviewer), 2022 (top reviewer), 2023, 2024 (top reviewer)
Reviewer at ICLR: 2021, 2022 (highlighted reviewer)
Reviewer at AISTATS: 2021, 2022
Reviewer at TMLR: 2022, 2023, 2024
Reviewer at JMLR: 2022

Teaching Experience

Université de Montréal — **Jan 2025 – Current**
Lecturer — *Moscow, Russia*

- Advanced Bayesian methods in statistics

Higher School of Economics (CS department) — **Sep 2017 – Apr 2020**
Assistant Lecturer (practical courses lecturer) — *Moscow, Russia*

- Bayesian methods in Machine Learning
- Bayesian methods in Deep Learning

Yandex School of Data Analysis — **Sep 2017 – Apr 2020**
Assistant Lecturer (practical courses lecturer) — *Moscow, Russia*

- Bayesian methods in Deep Learning

Higher School of Economics (CS department) — **Sep 2016 – Dec 2018**
Assistant Lecturer (practical courses lecturer) — *Moscow, Russia*

- Machine Learning

Tutor — **Feb 2011 – Dec 2018**
Mathematics and physics tutor for high school students and undergraduate students — *Moscow, Russia*

Invited Talks

Doob's Lagrangian: an Efficient Approach to Transition Path Sampling (link to recording) — **Nov 2024**
Webinar series jointly hosted by Perimeter, IVADO, and Institut Courtois — *Perimeter Institute*

Action Matching (link to recording) — **Oct 2023**
Learning on Graphs & Geometry reading group, organizer: Hannes Stärk — *Valence Labs*

Action Matching — **Aug 2023**
BEEHIVE group, PI: Barbara E Engelhardt — *Stanford University*

Wasserstein Quantum Monte Carlo (link to recording) — **Jun 2023**
Quantum-ML workshop, organizer: Alán Aspuru-Guzik — *Vector Institute*

Introduction to Diffusion Generative Models — **Mar 2023**
PIQuIL Group, PI: Roger Melko — *Perimeter Institute*

Action Matching (link to recording) — **Feb 2023**
Shannon's Bandwagon Seminar, organizer: Alex Alemi — *Google AI*

Fokker-Planck Equation — **Feb 2022**
Guest Lecture, organizer: Greg ver Steeg — *University of Southern California*

Langevin Dynamics for Sampling and Global Optimization (link to recording) — **Aug 2019**
Deep Bayes Summer Schoool, organizer: Dmitry Vetrov — *Higher School of Economics*

Bayesian Sparsification of Deep Neural Networks (link to recording) — **Aug 2018**
Deep Bayes Summer Schoool, organizer: Dmitry Vetrov — *Higher School of Economics*

Open Source Contributions

Superposition of Diffusion Models — **Dec 2024**
https://github.com/necludov/super-diffusion

JAX implementation of Wasserstein Lagrangian Flows — **May 2024**
https://github.com/necludov/wl-mechanics

Contribution of Wasserstein Quantum Monte Carlo to DeepMind FermiNet repository — **Aug 2023**
https://github.com/google-deepmind/ferminet/pull/64

JAX implementation of Wasserstein Quantum Monte Carlo — **May 2023**
https://github.com/necludov/wqmc

JAX implementation of Action Matching — **Feb 2023**
https://github.com/necludov/jam

TensorFlow implementation of Structured Bayesian Pruning — **Dec 2017**
https://github.com/necludov/group-sparsity-sbp

Industry Experience

Samsung AI Center — **Apr 2018 – Aug 2020**
Researcher — *Moscow, Russia*

- Bayesian Inference, Markov Chain Monte Carlo, Generative Modeling.

Yandex Research — **Apr 2017 – Jan 2018**
Researcher — *Moscow, Russia*

- Bayesian Inference, sparsification and acceleration of Deep Neural Networks.

Yandex — **Nov 2013 – Mar 2017**
Data Scientist — *Moscow, Russia*

- Rock Samples Image Segmentation with Deep Learning Methods (I was reproducing U-net when it just appeared).
- Anomaly detection with classic Machine Learning methods.

Publications and Preprints

The Superposition of Diffusion Models Using the Itô Density Estimator *ICLR 2025 (spotlight)*
Marta Skreta, Lazar Atanackovic, Avishek Joey Bose, Alexander Tong, **Kirill Neklyudov**

Efficient Evolutionary Search Over Chemical Space with Large Language Models *ICLR 2025*
Haorui Wang, Marta Skreta, Cher-Tian Ser, Wenhao Gao, Lingkai Kong,
Felix Strieth-Kalthoff, Chenru Duan, Yuchen Zhuang, Yue Yu, Yanqiao Zhu,
Yuanqi Du, Alán Aspuru-Guzik, Chao Zhang, **Kirill Neklyudov**

Meta Flow Matching: Integrating Vector Fields on the Wasserstein Manifold *ICLR 2025*
Lazar Atanackovic, Xi Zhang, Brandon Amos, Mathieu Blanchette, Leo J. Lee,
Yoshua Bengio, Alexander Tong, **Kirill Neklyudov**

Diffusion Models as Constrained Samplers for Optimization with Unknown Constraints *AISTATS 2025*
Lingkai Kong, Yuanqi Du, Wenhao Mu, **Kirill Neklyudov**, Valentin De Bortoli,
Haorui Wang, Dongxia Wu, Aaron Ferber, Yi-An Ma, Carla P. Gomes, Chao Zhang

Doob's Lagrangian: A Sample-Efficient Variational Approach to Transition Path Sampling *NeurIPS 2024 (spotlight)*
Yuanqi Du, Michael Plainer, Rob Brekelmans, Chenru Duan, Frank Noé, Carla P. Gomes,
Alán Aspuru-Guzik, **Kirill Neklyudov**

A Computational Framework for Solving Wasserstein Lagrangian Flows *ICML 2024*
Kirill Neklyudov, Rob Brekelmans, Alexander Tong, Lazar Atanackovic,
Qiang Liu, Alireza Makhzani

Structured Inverse-Free Natural Gradient: Memory-Efficient & Numerically-Stable KFAC *ICML 2024*
Wu Lin, Felix Dangel, Runa Eschenhagen, **Kirill Neklyudov**, Agustinus Kristiadi,
Richard E. Turner, Alireza Makhzani

Wasserstein Quantum Monte Carlo: A Novel Approach for Solving the Quantum Many-Body Schrödinger Equation *NeurIPS 2023 (spotlight)*
Kirill Neklyudov, Jannes Nys, Luca Thiede, Juan Carrasquilla, Qiang Liu,
Max Welling, Alireza Makhzani

Action Matching: Learning Stochastic Dynamics from Samples *ICML 2023*
Kirill Neklyudov, Rob Brekelmans, Daniel Severo, Alireza Makhzani

Quantum HyperNetworks: Training Binary Neural Networks in Quantum Superposition *Preprint 2023*
Juan Carrasquilla, Mohamed Hibat-Allah, Estelle Inack, Alireza Makhzani, **Kirill Neklyudov**,
Graham W. Taylor, Giacomo Torlai

Orbital MCMC *AISTATS 2022 (oral)*
Kirill Neklyudov, Max Welling

Deterministic Gibbs Sampling via Ordinary Differential Equations *Preprint 2021*
Kirill Neklyudov, Roberto Bondesan, Max Welling

Involutive MCMC: a Unifying Framework *ICML 2020*
Kirill Neklyudov, Max Welling, Evgenii Egorov, Dmitry Vetrov

The Implicit Metropolis-Hastings Algorithm *NeurIPS 2019*
Kirill Neklyudov, Evgenii Egorov, Dmitry Vetrov

Variance Networks: When Expectation Does Not Meet Your Expectations *ICLR 2019*

Kirill Neklyudov, Dmitry Molchanov, Arsenii Ashukha, Dmitry Vetrov

Structured Bayesian Pruning via Log-Normal Multiplicative Noise *NeurIPS 2017*
Kirill Neklyudov, Dmitry Molchanov, Arsenii Ashukha, Dmitry Vetrov

Particle Dynamics for Learning EBMs *NeurIPS (Workshop) 2021*
Kirill Neklyudov, Priyank Jaini, Max Welling

MaxEntropy Pursuit Variational Inference *ISNN 2019*
Evgenii Egorov, **Kirill Neklyudov**, Ruslan Kostoev, Evgeny Burnaev

Uncertainty Estimation via Stochastic Batch Normalization *ICLR (Workshop) 2018*
Andrei Atanov, Arsenii Ashukha, Dmitry Molchanov, **Kirill Neklyudov**, Dmitry Vetrov

Predicting Game Outcome from Drafts in Dota 2 *ECML (Workshop) 2016*
Aleksandr Semenov, Peter Romov, Sergey Korolev, Daniil Yashkov, **Kirill Neklyudov**