Kirill Neklyudov (Kyrylo Nekliudov)

Professional Experience

Anthropic — **Jan 2026 – Current**
Member of the Technical Staff

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.

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

- Bayesian Inference, 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.

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.

Education

Moscow Institute of Physics and Technology — **Sep 2010 – Jul 2014**
Bachelor degree in Applied Physics and Mathematics, Graduated with Honors (Red Diploma) — *Dolgoprudny, Russia*

Moscow Institute of Physics and Technology — **Sep 2014 – Jul 2016**
Master degree in Applied Physics and Mathematics, Graduated with Honors (Red Diploma) — *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"),
NeurIPS 2025 Workshop ("Frontiers in Probabilistic Inference: Sampling Meets Learning")
Area Chair at ICLR: 2025, 2026
Reviewer at NeurIPS: 2020, 2021 (outstanding reviewer), 2022, 2023, 2024 (top reviewer), 2025 (top reviewer)
Reviewer at ICLR: 2021, 2022 (highlighted reviewer)
Reviewer at AISTATS: 2021, 2022
Reviewer at TMLR: 2022, 2023, 2024, 2025
Reviewer at JMLR: 2022

Teaching Experience

Université de Montréal (Département de mathématiques et statistique) — **Jan 2025 – Current**
Lecturer — *Montréal, Canada*

- Statistical Learning (in French)
- Advanced Bayesian methods in statistics (github)

Higher School of Economics (CS department) — **Sep 2017 – Apr 2020**
Teaching Assistant — *Moscow, Russia*

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

Yandex School of Data Analysis — **Sep 2017 – Apr 2020**
Teaching Assistant — *Moscow, Russia*

- Bayesian methods in Deep Learning

Higher School of Economics (CS department) — **Sep 2016 – Dec 2018**
Teaching Assistant — *Moscow, Russia*

- Machine Learning

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

Funding

DMS Department Start-up Funds — **Jun 2024, 30k CAD**
Kirill Neklyudov — *Université de Montreal*

IVADO Professor Start-Up — **Jun 2024, 21k CAD**
Kirill Neklyudov — *IVADO*

Generating Rare Samples from Generative Models — **Dec 2024, 50k CAD**
Kirill Neklyudov, Gauthier Gidel, Arnaud Doucet — *Google & Mila*

Closed-loop Training of Molecular Generative Models — **Aug 2025, 88k CAD**
Kirill Neklyudov, Dominique Beaini, Hatem Helal — *IVADO Exploratory Projects*

Ab-initio training of Machine Learning Force Fields (under review) — **Aug 2025**
Kirill Neklyudov, Gauthier Gidel — *Samsung*

Self-improving Monte Carlo algorithms (under review) — **Sep 2025**
Kirill Neklyudov — *FRQNT*

Generative modeling for scientific computing (under review) — **Oct 2025**
Kirill Neklyudov — *NSERC Discovery*

Supervision

Majdi Hassan — **June 2024 - Present**
PhD student in Computer Science — *Université de Montreal*

Simon Paiva — **Jan 2025 - Present**
PhD student in Physics — *Université de Montreal*

Andrés Guzman-Cordero — **Sep 2025 - Present**
PhD student in Statistics — *Université de Montreal*

Chan Gwak — **Jan 2026 - Present**
PhD student in Applied Mathematics — *Université de Montreal*

Jungyoon Lee — **Jan 2026 - Present**
PhD student in Computer Science — *Université de Montreal*

Marta Skreta — **Sep 2025 - Present**
Postdoctoral Researcher, IVADO — *Université de Montreal*

Invited Talks

Monte Carlo Methods In The Age Of Generative Modeling — **Dec 2025**
International Conference on Statistics and Data Science — *ICSDS*

Transferable Monte Carlo Methods via Generative Modeling — **Nov 2025**
Mathematics Department, organizer: Michaël Lalancette — *UQAM*

Repurposing Diffusion Models for Scientific Discoveries — **Jul 2025**
Mathematics Department, organizer: Elina Robeva — *UBC*

Repurposing Diffusion Models for Scientific Discoveries — **Jun 2025**
Molecular Machine Learning Conference 2025 — *Mila*

Self-Refining Training for Amortized Density Functional Theory — **Jun 2025**
Microsoft seminar on sampling and generative modeling, organizer: Carles Domingo-Enrich — *Microsoft New England*

Controlling Diffusion Models at Inference Time (link to recording) — **Apr 2025**
AI4Science Seminar, organizer: Simon Olsson — *Chalmers University*

Controlling Diffusion Models at Inference Time (link to recording) — **Mar 2025**
KAIST Seminar, organizer: Sungsoo Ahn — *KAIST*

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

Wasserstein Lagrangian Flows (link to recording) — **Nov 2023**
Learning on Graphs & Geometry reading group, organizer: Hannes Stärk — *Valence Labs*

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

Publications and Preprints (see Google Scholar)

Foundations of Diffusion Models in General State Spaces: A Self-Contained Introduction *Preprint*
Vincent Pauline, Tobias Höppe, **Kirill Neklyudov**, Alexander Tong, Stefan Bauer, Andrea Dittadi

Wavefunction Flows: Efficient Quantum Simulation of Continuous Flow Models *Preprint*
David Layden, Ryan Sweke, Vojtěch Havlíček, Anirban Chowdhury, **Kirill Neklyudov**

Amortized Sampling with Transferable Normalizing Flows *NeurIPS 2025*
Charlie B. Tan, Majdi Hassan, Leon Klein, Saifuddin Syed, Dominique Beaini,
Michael M. Bronstein, Alexander Tong, **Kirill Neklyudov**

Self-Refining Training for Amortized Density Functional Theory *Preprint*
Majdi Hassan, Cristian Gabellini, Hatem Helal, Dominique Beaini, **Kirill Neklyudov**

Progressive Inference-Time Annealing of Diffusion Models for Sampling from Boltzmann Densities *NeurIPS 2025* (spotlight, 3.17% papers)
Tara Akhound-Sadegh, Jungyoon Lee, Avishek Joey Bose, Valentin De Bortoli,
Arnaud Doucet, Michael M Bronstein, Dominique Beaini, Siamak Ravanbakhsh,
Alexander Tong, **Kirill Neklyudov**

Feynman-Kac Correctors in Diffusion: Annealing, Guidance, and Product of Experts *ICML 2025* (spotlight, 2.59% papers)
Marta Skreta, Tara Akhound-Sadegh, Viktor Ohanesian, Roberto Bondesan, Alán Aspuru-Guzik,
Arnaud Doucet, Rob Brekelmans, Alexander Tong, **Kirill Neklyudov**

The Superposition of Diffusion Models Using the Itô Density Estimator *ICLR 2025* (spotlight, 3.26% papers)
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, 2.08% papers)
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, 3.06% papers)

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*
Kirill Neklyudov, Max Welling (oral, 2.61% papers)

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**