

KIRILL NEKLYUDOV (KYRYLO NEKLIUDOV)

ACADEMIC EXPERIENCE

Institut Courtois <i>Regular Member</i>	Dec 2024 – Current Montreal, Canada
Mila - Quebec AI Institute <i>Core Academic Member</i>	Jun 2024 – Current Montreal, Canada
Université de Montréal <i>Assistant Professor in Machine Learning and Statistics (tenure-track)</i>	Jun 2024 – Current Montreal, Canada
Vector Institute for Artificial Intelligence <i>Postdoctoral Fellow, supervisors: Alán Aspuru-Guzik, Alireza Makhzani</i> <ul style="list-style-type: none">AI4Science, Generative Modeling, Optimal Transport.	Nov 2021 – May 2024 Toronto, Canada
University of Amsterdam <i>Postdoctoral Fellow, supervisor: Max Welling</i> <ul style="list-style-type: none">Markov Chain Monte Carlo, Generative Modeling.	Sep 2020 – Oct 2021 Amsterdam, Netherlands
Higher School of Economics <i>Researcher, supervisor: Dmitry Vetrov</i> <ul style="list-style-type: none">Bayesian Inference, Markov Chain Monte Carlo, Generative Modeling.	Feb 2018 – Aug 2020 Moscow, Russia

EDUCATION

Moscow Institute of Physics and Technology <i>Bachelor degree in Applied Physics and Mathematics, summa cum laude</i>	Sep 2010 – Jul 2014 Dolgoprudny, Russia
Moscow Institute of Physics and Technology <i>Master degree in Applied Physics and Mathematics, summa cum laude</i>	Sep 2014 – Jul 2016 Dolgoprudny, Russia
Yandex School of Data Analysis <i>Master degree in Machine Learning</i>	Sep 2014 – Jun 2016 Moscow, Russia
Higher School of Economics <i>Ph.D. in Computer Science, supervisor: Dmitry Vetrov</i>	Sep 2016 – Nov 2020 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
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 <i>Lecturer</i> <ul style="list-style-type: none">Statistical Learning (in French)Advanced Bayesian methods in statistics (github)	Jan 2025 – Current Montréal, Canada
Higher School of Economics (CS department) <i>Assistant Lecturer (practical courses lecturer)</i> <ul style="list-style-type: none">Bayesian methods in Machine LearningBayesian methods in Deep Learning	Sep 2017 – Apr 2020 Moscow, Russia
Yandex School of Data Analysis <i>Assistant Lecturer (practical courses)</i> <ul style="list-style-type: none">Bayesian methods in Deep Learning	Sep 2017 – Apr 2020 Moscow, Russia

Higher School of Economics (CS department)

Assistant Lecturer (practical courses)

- Machine Learning

Sep 2016 – Dec 2018

Moscow, Russia

Tutor

Mathematics and physics tutor for high school students and undergraduate students

Feb 2011 – Dec 2018

Moscow, Russia

INVITED TALKS

Repurposing Diffusion Models for Scientific Discoveries

Mathematics Department, organizer: Elina Robeva

Jul 2025

UBC

Repurposing Diffusion Models for Scientific Discoveries

Molecular Machine Learning Conference 2025

Jun 2025

Mila

Controlling Diffusion Models at Inference Time ([link to recording](#))

AI4Science Seminar, organizer: Simon Olsson

Apr 2025

Chalmers University

Controlling Diffusion Models at Inference Time ([link to recording](#))

KAIST Seminar, organizer: Sungsoo Ahn

Mar 2025

KAIST

Doob's Lagrangian: an Efficient Approach to Transition Path Sampling ([link to recording](#))

Webinar series, joint organizers: Perimeter, IVADO, Institut Courtois

Nov 2024

Perimeter Institute

Wasserstein Lagrangian Flows ([link to recording](#))

Learning on Graphs & Geometry reading group, organizer: Hannes Stärk

Nov 2023

Valence Labs

Action Matching ([link to recording](#))

Learning on Graphs & Geometry reading group, organizer: Hannes Stärk

Oct 2023

Valence Labs

Action Matching

BEEHIVE group, PI: Barbara E Engelhardt

Aug 2023

Stanford University

Wasserstein Quantum Monte Carlo ([link to recording](#))

Quantum-ML workshop, organizer: Alán Aspuru-Guzik

Jun 2023

Vector Institute

Introduction to Diffusion Generative Models

PIQuLL Group, PI: Roger Melko

Mar 2023

Perimeter Institute

Action Matching ([link to recording](#))

Shannon's Bandwagon Seminar, organizer: Alex Alemi

Feb 2023

Google AI

Fokker-Planck Equation

Guest Lecture, organizer: Greg van Steeg

Feb 2022

University of Southern California

Langevin Dynamics for Sampling and Global Optimization ([link to recording](#))

Deep Bayes Summer School, organizer: Dmitry Vetrov

Aug 2019

Higher School of Economics

Bayesian Sparsification of Deep Neural Networks ([link to recording](#))

Deep Bayes Summer School, organizer: Dmitry Vetrov

Aug 2018

Higher School of Economics

OPEN SOURCE CONTRIBUTIONS

Superposition of Diffusion Models

<https://github.com/necludov/super-diffusion>

Dec 2024

JAX implementation of Wasserstein Lagrangian Flows

<https://github.com/necludov/wl-mechanics>

May 2024

Contribution of Wasserstein Quantum Monte Carlo to DeepMind FermiNet repository

<https://github.com/google-deepmind/ferminet/pull/64>

Aug 2023

JAX implementation of Wasserstein Quantum Monte Carlo

<https://github.com/necludov/wqmc>

May 2023

JAX implementation of Action Matching

<https://github.com/necludov/jam>

Feb 2023

TensorFlow implementation of Structured Bayesian Pruning

<https://github.com/necludov/group-sparsity-sbp>

Dec 2017

INDUSTRY EXPERIENCE

Samsung AI Center

Researcher

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

Apr 2018 – Aug 2020

Moscow, Russia

Yandex Research

Researcher

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

Apr 2017 – Jan 2018

Moscow, Russia

Yandex

Data Scientist

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

Nov 2013 – Mar 2017

Moscow, Russia

PUBLICATIONS AND PREPRINTS (SEE [GOOGLE SCHOLAR](#))

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)

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)

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)

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, Ling kai 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**