

KIRILL NEKLYUDOV (KYRYLO NEKLIUDOV)

ACADEMIC EXPERIENCE

Mila - Quebec AI Institute

Core Academic Member

Jun 2024 – Current

Montreal, Canada

Université de Montréal

Assistant Professor in Machine Learning and Statistics (tenure-track)

Jun 2024 – Current

Montreal, Canada

Vector Institute for Artificial Intelligence

Postdoctoral Fellow, supervisors: Alán Aspuru-Guzik, Alireza Makhzani

Nov 2021 – May 2024

Toronto, Canada

- AI4Science, Generative Modeling, Optimal Transport.

University of Amsterdam

Postdoctoral Fellow, supervisor: Max Welling

Sep 2020 – Oct 2021

Amsterdam, Netherlands

- Markov Chain Monte Carlo, Generative Modeling.

Higher School of Economics

Researcher, supervisor: Dmitry Vetrov

Feb 2018 – Aug 2020

Moscow, Russia

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

EDUCATION

Moscow Institute of Physics and Technology

Bachelor degree in Applied Physics and Mathematics, summa cum laude

Sep 2010 – Jul 2014

Dolgoprudny, Russia

Moscow Institute of Physics and Technology

Master degree in Applied Physics and Mathematics, summa cum laude

Sep 2014 – Jul 2016

Dolgoprudny, Russia

Yandex School of Data Analysis

Master degree in Machine Learning

Sep 2014 – Jun 2016

Moscow, Russia

Higher School of Economics

Ph.D. in Computer Science, supervisor: Dmitry Vetrov

Sep 2016 – Nov 2020

Moscow, Russia

PROFESSIONAL SERVICE

Organizer of ICML Workshop: 2024 ("[Structured Probabilistic Inference & Generative Modeling](#)")

Area Chair at ICLR: 2025

Reviewer at NeurIPS: 2020, 2021 (outstanding reviewer award), 2022 (top reviewer), 2023, 2024

Reviewer at ICLR: 2021, 2022 (highlighted reviewer)

Reviewer at AISTATS: 2021, 2022

Reviewer at TMLR: 2022, 2023, 2024

Reviewer at JMLR: 2022

TEACHING EXPERIENCE

Higher School of Economics (CS department)

Assistant Lecturer (practical courses lecturer)

Sep 2017 – Apr 2020

Moscow, Russia

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

Yandex School of Data Analysis

Assistant Lecturer (practical courses lecturer)

Sep 2017 – Apr 2020

Moscow, Russia

- Bayesian methods in Deep Learning

Higher School of Economics (CS department)

Assistant Lecturer (practical courses lecturer)

Sep 2016 – Dec 2018

Moscow, Russia

- Machine Learning

Tutor

Mathematics and physics tutor for high school students and undergraduate students

Feb 2011 – Dec 2018

Moscow, Russia

INVITED TALKS

Action Matching (link to recording) <i>Learning on Graphs & Geometry reading group, organizer: Hannes Stärk</i>	Oct 2023 <i>Valence Labs</i>
Action Matching <i>BEEHIVE group, PI: Barbara E Engelhardt</i>	Aug 2023 <i>Stanford University</i>
Wasserstein Quantum Monte Carlo (link to recording) <i>Quantum-ML workshop, organizer: Alán Aspuru-Guzik</i>	Jun 2023 <i>Vector Institute</i>
Introduction to Diffusion Generative Models <i>PIQuIL Group, PI: Roger Melko</i>	Mar 2023 <i>Perimeter Institute</i>
Action Matching (link to recording) <i>Shannon's Bandwagon Seminar, organizer: Alex Alemi</i>	Feb 2023 <i>Google AI</i>
Fokker-Planck Equation <i>Guest Lecture, organizer: Greg van Steeg</i>	Feb 2022 <i>University of Southern California</i>
Langevin Dynamics for Sampling and Global Optimization (link to recording) <i>Deep Bayes Summer School, organizer: Dmitry Vetrov</i>	Aug 2019 <i>Higher School of Economics</i>
Bayesian Sparsification of Deep Neural Networks (link to recording) <i>Deep Bayes Summer School, organizer: Dmitry Vetrov</i>	Aug 2018 <i>Higher School of Economics</i>

OPEN SOURCE CONTRIBUTIONS

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 <i>Researcher</i> <ul style="list-style-type: none">Bayesian Inference, Markov Chain Monte Carlo, Generative Modeling.	Apr 2018 – Aug 2020 <i>Moscow, Russia</i>
Yandex Research <i>Researcher</i> <ul style="list-style-type: none">Bayesian Inference, sparsification and acceleration of Deep Neural Networks.	Apr 2017 – Jan 2018 <i>Moscow, Russia</i>
Yandex <i>Data Scientist</i> <ul style="list-style-type: none">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 <i>Moscow, Russia</i>

- 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, Alan Apsuru-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
- Meta Flow Matching: Integrating Vector Fields on the Wasserstein Manifold** *Preprint 2024*
Lazar Atanackovic, Xi Zhang, Brandon Amos, Mathieu Blanchette, Leo J. Lee, Yoshua Bengio, Alexander Tong, **Kirill Neklyudov**
- Efficient Evolutionary Search Over Chemical Space with Large Language Models** *Preprint 2024*
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**
- Diffusion Models as Constrained Samplers for Optimization with Unknown Constraints** *Preprint 2024*
Ling kai Kong, Yuanqi Du, Wenhao Mu, **Kirill Neklyudov**, Valentin De Bortoli, Haorui Wang, Dongxia Wu, Aaron Ferber, Yi-An Ma, Carla P. Gomes, Chao Zhang
- 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

Kirill Neklyudov, Priyank Jaini, Max Welling

NeurIPS (Workshop) 2021

MaxEntropy Pursuit Variational Inference

Evgenii Egorov, **Kirill Neklyudov**, Ruslan Kostoev, Evgeny Burnaev

ISNN 2019

Uncertainty Estimation via Stochastic Batch Normalization

Andrei Atanov, Arsenii Ashukha, Dmitry Molchanov, **Kirill Neklyudov**, Dmitry Vetrov

ICLR (Workshop) 2018

Predicting Game Outcome from Drafts in Dota 2

Aleksandr Semenov, Peter Romov, Sergey Korolev, Daniil Yashkov, **Kirill Neklyudov**

ECML (Workshop) 2016