

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

- AI4Science, Generative Modeling, Optimal Transport.

Nov 2021 – May 2024

Toronto, Canada

University of Amsterdam

Postdoctoral Fellow, supervisor: Max Welling

- Markov Chain Monte Carlo, Generative Modeling.

Sep 2020 – Oct 2021

Amsterdam, the Netherlands

Higher School of Economics

Researcher, supervisor: Dmitry Vetrov

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

Feb 2018 – Aug 2020

Moscow, Russia

EDUCATION

Moscow Institute of Physics and Technology

Bachelor degree with honours in Applied Physics and Mathematics

Sep 2010 – Jul 2014

Dolgoprudny, Russia

Moscow Institute of Physics and Technology

Master degree with honours in Applied Physics and Mathematics

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

PUBLICATIONS AND PREPRINTS

A Computational Framework for Solving Wasserstein Lagrangian Flows

Kirill Neklyudov, Rob Brekelmans, Alexander Tong, Lazar Atanackovic, Qiang Liu, Alireza Makhzani

ICML 2024

Wasserstein Quantum Monte Carlo: A Novel Approach for Solving the Quantum Many-Body Schrödinger Equation

Kirill Neklyudov, Jannes Nys, Luca Thiede, Juan Carrasquilla, Qiang Liu, Max Welling, Alireza Makhzani

NeurIPS 2023 (spotlight)

Action Matching: Learning Stochastic Dynamics from Samples

Kirill Neklyudov, Rob Brekelmans, Daniel Severo, Alireza Makhzani

ICML 2023

Orbital MCMC

Kirill Neklyudov, Max Welling

AISTATS 2022 (oral)

Involutive MCMC: a Unifying Framework

Kirill Neklyudov, Max Welling, Evgenii Egorov, Dmitry Vetrov

ICML 2020

The Implicit Metropolis-Hastings Algorithm

Kirill Neklyudov, Evgenii Egorov, Dmitry Vetrov

NeurIPS 2019

Variance Networks: When Expectation Does Not Meet Your Expectations

Kirill Neklyudov, Dmitry Molchanov, Arsenii Ashukha, Dmitry Vetrov

ICLR 2019

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

NeurIPS 2017

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

2023

Particle Dynamics for Learning EBMs
Kirill Neklyudov, Priyank Jaini, Max Welling

NeurIPS (Workshop) 2021

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

2019

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

TEACHING EXPERIENCE

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

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 van Steeg

University of Southern California

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

Aug 2019

Deep Bayes Summer School, organizer: Dmitry Vetrov

Higher School of Economics

Bayesian Sparsification of Deep Neural Networks (link to recording)

Aug 2018

Deep Bayes Summer School, organizer: Dmitry Vetrov

Higher School of Economics

PROFESSIONAL SERVICE

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

ICLR Reviewer: 2021, 2022 (highlighted reviewer)

AISTATS Reviewer: 2021, 2022

TMLR Reviewer: 2022, 2023

JMLR Reviewer: 2022

OPEN SOURCE CONTRIBUTIONS

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.