Kirill Neklyudov

Academic Experience

Vector Institute for Artificial Intelligence — **Nov 2021 – Current**
Postdoctoral Fellow, supervisor: Alireza Makhzani — *Toronto, Canada*
- AI4Science, Generative Modeling, Optimal Transport.

University of Amsterdam — **Sep 2020 – Oct 2021**
Postdoctoral Fellow, supervisor: Max Welling — *Amsterdam, the 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 with honours in Applied Physics and Mathematics — *Dolgoprudny, Russia*

Moscow Institute of Physics and Technology — **Sep 2014 – Jul 2016**
Master degree with honours in Applied Physics and Mathematics — *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*

Publications and Preprints

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

Orbital MCMC — *AISTATS 2022 (oral)*
Kirill Neklyudov, 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

A Computational Framework for Solving Wasserstein Lagrangian Flows — *2023*
Kirill Neklyudov, Rob Brekelmans, Alexander Tong, Lazar Atanackovic, Qiang Liu, Alireza Makhzani

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

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

Deterministic Gibbs Sampling via Ordinary Differential Equations *2019*
Kirill Neklyudov, Roberto Bondesan, 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**

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 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*

Professional Service

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