

Arsenii Ashukha

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I am a Research Scientist at [Isomorphic Labs](#) where I work on AI-first drug design and digital biology.

Before joining Isomorphic Labs, I was a PhD student at the [Bayesian Methods Research Group](#) and Research Scientist at Samsung AI, where I worked with [Dmitry Vetrov](#). The results of my PhD contributed to sparsification, uncertainty estimation, ensembling, and fundamentals of Bayesian deep learning.

PROFESSIONAL EXPERIENCE

2022 - now **Research Scientist AI, [Isomorphic Labs](#)** (led by [Demis Hassabis](#))

Isomorphic Labs is a new [Alphabet](#) company and commercial venture which aims to reimagine the entire drug discovery process from first principles with an AI-first approach, and, ultimately, to model and understand some of the fundamental mechanisms of life. Using computational advances, we're working at the cutting edge in the new era of 'digital biology'. By significantly increasing the pace of scientific research and efficacy of new medicines, we will be at the forefront of breakthroughs that will benefit millions of people.

2018 - 2022 **Leading Research Scientist AI, Samsung AI Center**

I worked on the development of deep learning algorithms. Specifically, my work is focused on uncertainty estimation, robustness, and fundamentals of Bayesian deep learning. I also contributed to computer vision research e.g., image inpainting. Since Dec of 2020 I served as a Deputy head of Machine Learning Lab, where I co-managed several AI projects.

2016 - 2018 **PhD Candidate, Yandex / University of Amsterdam**

Created *sparse variational dropout*, a method for sparsification of DNNs that, for the first time, allowed to achieve over 250x compression ratio (results published at ICML'17). The modified version of SparseVD with neuron-level sparsity allowed to accelerate inference of a CNN by 2-5 times and was involved in the feature extraction for real image retrieval system (published at NeurIPS).

2016 Summer **Machine Learning Engineer Intern, Yandex**

I worked on feature extraction techniques for music data with convolutional neural networks. I also developed an evaluation of learned representations. The representations were used in the content-based recommendation system for Yandex music.

2015 Summer **Machine Learning Engineer Intern, Rambler**

Worked on recommendation systems. My responsibility included improving the quality and performance of automatic feature extraction algorithms, and recommendation algorithms.

EDUCATION

2017 - 2022 **PhD in Machine Learning, National Research University Higher School of Economics**
Thesis title: Prior Knowledge for Deep Learning Advisor: [Dmitry Vetrov](#)

2015 - 2017 **MSc in Computer Science, Moscow Institute of Physics and Technology** (worked on sparse DNNs) with Distinction (GPA 4.87/5.0)

2011 - 2015 **BSc in Computer Science, Bauman Moscow State Technical University** (worked on language models)

PUBLICATIONS

Google Scholar: scholar.google.com/citations?user=IU-kuP8AAAAJ

* denotes joint first co-authorship

- Resolution-robust Large Mask Inpainting with Fourier Convolutions**, WACV 2022 [arXiv](#) / [code](#)
Roman Suvorov, Elizaveta Logacheva, Anton Mashikhin, Anastasia Remizova, **Arsenii Ashukha**,
Aleksii Silvestrov, Naejin Kong, Harshith Goka, Kiwoong Park, Victor Lempitsky
- Pitfalls of In-Domain Uncertainty Estimation and Ensembling in Deep Learning**, ICLR 2020 [arXiv](#) / [code](#)
Arsenii Ashukha*, Alexander Lyzhov*, Dmitry Molchanov*, Dmitry Vetrov
- Greedy Policy Search: A Simple Baseline for Learnable Test-Time Augmentation**, UAI 2020 [arXiv](#) / [code](#)
Arsenii Ashukha*, Dmitry Molchanov*, Alexander Lyzhov*, Yuliya Molchanova*, Dmitry Vetrov
- The Deep Weight Prior**, ICLR 2019 [arXiv](#) / [code](#)
Arsenii Ashukha*, Andrei Atanov*, Kirill Struminsky, Dmitry Vetrov, Max Welling
- Variance Networks: When Expectation Does Not Meet Your Expectations**, ICLR 2019 [arXiv](#) / [code](#)
Arsenii Ashukha*, Kirill Neklyudov*, Dmitry Molchanov*, Dmitry Vetrov
- Structured Bayesian Pruning via Log-Normal Multiplicative Noise**, NeurIPS 2017 [arXiv](#) / [code](#)
Kirill Neklyudov, Dmitry Molchanov, **Arsenii Ashukha**, Dmitry Vetrov
- Variational Dropout Sparsifies Deep Neural Networks**, ICML 2017 [arXiv](#) / [code](#)
Arsenii Ashukha*, Dmitry Molchanov*, Dmitry Vetrov

TECHNICAL SKILLS

- **Deep Learning, Deep Neural Networks, Machine Learning, Modeling;**
- I'm fluent in **Python** and I used to code in C/C++, Go, language is not a problem after all.
- I'm also fluent with common data science tools such as **NumPy, matplotlib, scikit-learn, and pandas**.
- I'm comfortable with the common data science environment e.g., **bash, git, Linux**.
- Deep learning frameworks: **Jax, PyTorch**, Theano, and TensorFlow.
- Comfortable with **GPU clusters and distributed training**.
- I have experience with MapReduce, Hadoop, Hive, and Spark.

CODE

- **Research-ready implementations:**
 - [LaMa Image Inpainting](#) (★6.2k)
 - [Multi-GPU SimCLRv1](#) closely reproduced results on both CIFAR-10 and ImageNet
 - [Ensembles](#) (Deep ensembles, Snapshot ensembles, cSGLD, FGE, etc.)
- **Simple MVP implementations of ML algorithms:**
 - [Real NVP normalizing flows](#)
 - [Quantile Regression DQN \(Distributional RL\)](#)
 - [Equivariant GNN](#)

THESIS CO-SUPERVISION

- [Alexander Lyzhov](#) (moved to NYU)
 - Deep Neural Network Ensembles: Analysis and Approaches to Diversification (MSc, 2020)

- [Andrei Atanov](#) (moved to EPFL)
 - Effective Learning of Deep Neural Networks Ensembles (BSc, 2018)
 - Learning Deep Models with Small Data (MSc, 2020)
- [Evgenii Nikishin](#) (moved to Mila)
 - Stability Improvement and Knowledge Transfer in Deep Reinforcement Learning (MSc, 2019)

PROGRAM COMMITTEE

- Neural Information Processing Systems, NeurIPS:
 - 2019: top-50% highest-scored reviewers
 - **2021: outstanding reviewer award (top-8%)**
- International Conference on Machine Learning, ICML (2019, 2020)
 - 2020: top-33% highest-scored reviewers
- International Conference on Learning Representations, ICLR (2020, 2021)
- ICML Workshop on Invertible Neural Networks (2019, 2021, invertibleworkshop.github.io)
- Bayesian Deep Learning Workshop (since 2017, bayesiandeeplearning.org)

TEACHING

- Supervisor of reading clubs on machine learning at HSE and Yandex school of data analysis (since 2017)
- A lecture with a practical session on Normalizing Flows at DeepBayes Summer School (2019, links: [1](#), [2](#))
- Lecturer, Moscow Institute of Physics and Technology:
 - A lecturer and a manager of a deep learning part of ML course (ml-mipt.github.io).
 - A lecturer of DL part and an instructor of practical sessions of the *Data Mining in Action* course ([link](#)).