Arsenii Ashukha

Home page / Google Scholar / GitHub / Twitter / 📍 London (UK, Global Talent visa)
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I am a Senior Research Scientist at Isomorphic Labs, Alphabet company led by Demis Hassabis, where I work on AI-first drug design. Before joining Isomorphic, I worked at Samsung AI and did my PhD with Dmitry Vetrov, in collaboration with Max Welling. The results of my PhD contributed to sparsification, uncertainty, and generative models.

PROFESSIONAL EXPERIENCE

2022 - now **Isomorphic Labs**

2024 Senior Research Scientist AI. Stealth AI models for drug design.

2022 Research Scientist AI. Stealth AI models for drug design.

2018 - 2022 **Samsung AI**

2021 Deputy Lead of ML Lab. Advised AI projects on applications of generative models and RL.

2018 Research Scientist. Uncertainty generative models (e.g. LaMa inpainting 7.3k github stars).

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

Created *sparse variational dropout, a* method for sparsification of deep neural networks that, for the first time achieved over 250x compression ratio (ICML'17), with the neuron-level sparsity allowed to accelerate inference by 2-5 times (NeurIPS'18). The metod was used for a production image retrieval.

Internships **2016 Yandex** Deep learning based recommendation system for spotify-like music service.
2015 Rambler Recommendation systems for news aggregators.

EDUCATION

2017 - 2022 PhD in Machine Learning, National Research University Higher School of Economics
Title: Prior Knowledge for Deep Learning (link).
Advisor: Dmitry Vetrov.
Committee: Durk Kingma, Karen Ullrich, Jasper Snoek, Yingzhen Li, Sergey Nikolenko.

2015 - 2017 MSc in Computer Science, Moscow Institute of Physics and Technology
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, Aleksei 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, Beam.

CODE

- Research-ready implementations:
  - LaMa Image Inpainting (⭐7.3k)
  - 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).