MARIYA POPOVA

+1 (919) 869-63-13
mariewelt@gmail.com
mpopova@andrew.cmu.edu

SUMMARY

I am a 4th year PhD student at Carnegie Mellon University advised by prof. Olexandr Isayev. My thesis research focuses on applications and development of deep learning methods for computational chemistry and drug design. I am developing deep learning algorithms to solve computational chemistry problems such as generation of novel molecules with desired properties and prediction of a synthesis path for a given chemical compound. My broader scientific interests include various applications of Deep Learning for solving real-life problems.

EDUCATION

Carnegie Mellon University, School of Computer Science, Pittsburgh, PA **Expected May 2022**
PhD, Computational Biology

University of North Carolina at Chapel Hill, Chapel Hill, NC **Transferred to CMU starting Jan 2020**
PhD, Bioinformatics and Computational Biology

- Selected coursework: Structural Bioinformatics, Sequence Modelling, Mathematical Modelling

Moscow Institute of Physics and Technology, Moscow, Russia **July 2017**
Master of Science (with honors), Applied Mathematics and Physics (double degree program)

- Thesis project: Generative and Predictive models for producing novel molecular compounds
- Selected coursework: Image Processing and Recognition,
  Signals and Multidimensional Data Processing, Regression Analysis

Skolkovo Institute of Science and Technology, Moscow, Russia **June 2017**
Master of Science (with honors), Mathematics and Computer Science (double degree program)

- Thesis project: Deep Reinforcement Learning for de-novo drug design
- Academic excellence award
- Selected coursework: Numeric Linear Algebra, Optimization Methods, Machine Learning,
  Deep Learning, Bayesian Methods – Advanced Machine Learning, Probabilistic Graphical Models

Moscow Institute of Physics and Technology, Moscow, Russia
Bachelor of Science (with honors), Applied Mathematics and Physics **July 2015**

- Thesis project: Selection of an optimal neural network model for multi-class time series classification

SKILLS

Programming/Scripting Languages: Python, Java, Matlab, R
Frameworks and Tools: PyTorch, PyMol, PyRosetta

TEACHING

Automation of Scientific Research (02750) **Spring 2020**
Carnegie Mellon University

- Teacher Assistant: prepared and graded homework assignments, answered students' questions

Tutorial "Generation of molecular libraries with reinforcement learning" **November 2019**
University of Maryland

- *Gave a 3 hours tutorial as a part of workshop on Machine Learning and Chemistry*

Mathematical Modeling of Biological Processes (BCB 715) **Fall 2018**
University of North Carolina at Chapel Hill

- Teacher Assistant: graded homework assignments, answered student questions
- Gave a lecture "Application of Deep Learning for Mathematical Modeling in Life Sciences"

EXPERIENCE

Machine Learning Research Intern **June 2020 – August 2020**
Pfizer

- Worked on developing deep generative model for 3D molecular graphs

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Research Intern **September 2019 – December 2019**

NVIDIA Corporation

- Worked on developing deep generative model for designing selective kinase inhibitors

Deep Learning Software Engineer Intern **Summer 2019**

NVIDIA Corporation

- Developed novel algorithm for correction of automatic speech recognition

Deep Learning Software Engineer Intern **Summer 2018**

NVIDIA Corporation

- Developed an open-source Deep Learning toolkit for Computational Chemistry and Drug Design

Visiting Research Scholar

University of North Carolina at Chapel Hill **Oct 2016 – Mar 2017**

- Developed a Deep Learning model (Python + Lasagne) for computational design of chemical compounds with optimized properties

Research Intern **June 2016 – August 2016**

Yandex LLC CERN Research Group, Moscow, Russia

- Developed a Reinforcement Learning prototype for treatment optimization of patients with liver disease

SELECTED PROJECTS

OpenChem: Deep Learning toolkit for Computational Chemistry and Drug Design

NVIDIA Corporation, University of North Carolina at Chapel Hill

- Toolkit for Computational Chemistry with PyTorch backend aimed to make Deep Learning models an easy-to-use tool for Computational Chemistry and Drug Design Researchers
- Available at https://github.com/Mariewelt/OpenChem

De Novo Drug Design with Deep Reinforcement Learning

University of North Carolina at Chapel Hill

- Deep learning library with Pytorch backend for generation of ligands with target-biased properties
- Available at https://github.com/isayev/ReLeaSE
- Patent pending

HONORS AND AWARDS

NVIDIA GTC 2020 Best Poster Award **2020**

- Awarded to the winner of best poster contest at NVIDIA GTC.

NVIDIA Graduate Fellowship **2019/2020**

- Awarded to Ph.D. students involved in GPU computing research

Molecular Sciences Software Institute (MolSSI) Seed Software Fellowship **2019**

- Awarded to graduate students and postdocs pursuing the development of software infrastructure, middleware, and frameworks that will benefit the broader field of computational molecular sciences

SELECTED PUBLICATIONS

1. **M. Popova**, O. Isayev, A. Tropsha, Deep reinforcement learning for de novo drug design. *Science Advances.* 4 (2018), doi:10.1126/sciadv.aap7885.
2. **Popova, Mariya**, et al. "MolecularRNN: Generating realistic molecular graphs with optimized properties." *arXiv preprint arXiv:1905.13372* (2019).
3. Oleksii Hrinchuk, **Mariya Popova***, and Boris Ginsburg. "Correction of Automatic Speech Recognition with Transformer Sequence-to-sequence Model." *arXiv preprint arXiv:1910.10697* (2019). **(ICASSP 2020)**
4. Cichonska A, Ravikumar B, Allaway RJ, Park S, Wan F, Isayev O, Li S, Mason MJ, Lamb A, Jeon M, Kim S., **Popova M**, Capuzzi S, Zeng J, Dang K. Crowdsourced mapping of unexplored target space of kinase inhibitors. bioRxiv. 2020 Jan 1:2019-12.
5. **Popova, Mariya**, et al. "Openchem: deep learning toolkit for computational chemistry and drug design." (2020).