Ilia Igashov

+41 76 706 83 01
ilia.igashov@gmail.com
igashov.github.io

Research Interests

Machine Learning, Geometric Learning, Representation Learning for Graphs and 3D data, and its applications in scientific domains, e.g., Biology and Chemistry.

Education

2020 - 2021 **Université Grenoble Alpes**, *Grenoble, France*,
Master of Science in Industrial and Applied Mathematics, GPA: 15.13/20.
Thesis: Geometric learning for 3D shapes and structural bioinformatics.

2019 - 2021 **Moscow Institute of Physics and Technology**, *Moscow, Russia*,
Master of Science in Computer Science, GPA: 4.32/5.
Thesis: Graph neural networks for model protein quality assessment.

2015 - 2019 **Moscow Institute of Physics and Technology**, *Moscow, Russia*,
Bachelor of Science in Applied Mathematics and Physics, GPA: 4.53/5.
Thesis: Application of multi-armed bandits in Yandex.Radio.

Research Experience

Oct 2021 - Present **École Polytechnique Fédérale de Lausanne**, *Lausanne, Switzerland*,
PhD in Computational and Quantitative Biology.
Thesis directors: Bruno Correia, Michael Bronstein

Feb 2021 - Jul 2021 **Research Intern**, **Laboratoire Jean Kuntzmann**, *Grenoble, France*.
Supervisor: Dr. Sergei Grudinin
- Developed rotation-invariant deep learning approach for predicting chemo-physical properties of small organic molecules.

Nov 2019 - May 2020 **Research Intern**, **Inria**, Nano-D Team, *Grenoble, France*.
Supervisor: Dr. Sergei Grudinin
- Created methods VoroCNN and Spherical Graph Convolutional Network (S-GCN) for the protein model quality assessment problem.

Feb 2018 - May 2018 **Undergraduate Research Project**, **MIPT**, *Moscow, Russia*.
- Built a hybrid model with SVM and linear regression components for predicting the type of conformation and the value of binding energy of protein-ligand complexes.

Publications

[1] **Ilia Igashov**, Ilia Igashov, Hannes Stärk, Clément Vignac, Victor Garcia Satorras, Pascal Frossard, Max Welling, Michael Bronstein, Bruno Correia. "Equivariant 3D-conditional diffusion models for molecular linker design". *Under review*. arXiv:2210.05274, 2022.

[2] **Ilia Igashov**, Kliment Olechnovič, Maria Kadukova, Česlovas Venclovas, Sergei Grudinin. "VoroCNN: Deep convolutional neural network built on 3D Voronoi tessellation of protein structures". *Bioinformatics*. 2021. btab118, https://doi.org/10.1093/bioinformatics/btab118.

[3] **Ilia Igashov**, Nikita Pavlichenko, Sergei Grudinin. "Spherical convolutions on molecular graphs for protein model quality assessment". *Machine Learning: Science and Technology*. 2020. https://doi.org/10.1088/2632-2153/abf856.

[4] Dmitrii Zhemchuzhnikov, **Ilia Igashov**, Sergei Grudinin. "6DCNN with roto-translational convolution filters for volumetric data processing". *Preprint*. 2021. arXiv:2107.12078.

Professional Experience

Nov 2022 - present **Research Intern**, **Monte Rosa Therapeutics**, *Basel*.
- Working on deep learning methods for design of molecular glue degraders.

May 2020 - August 2021 **Data Science Team Leader**, **PeakData**, *Remote*.
- NLP startup in healthcare domain aimed to gather and process information on medical topics.

Sep 2018 - Oct 2019 **Software Developer**, **Yandex.Music**, Recommendation Team, *Moscow, Russia*.
- Launched three smart playlists based on personal recommendation algorithms.
- Implemented Multi-Armed Bandits algorithm for optimal recommendation of radio stations for new users.
- Created personal recommendations of podcasts and promotions.

July 2017 - Aug 2017 **Summer Intern**, **Intel**, *Nizhny Novgorod, Russia*.
- Implemented and integrated additional split criteria in Decision Tree algorithm for Intel DAAL.

Teaching & Mentorship

Oct 2021 **Université Paris Saclay Thematic School 2021: Graph as models in life sciences: Machine learning and integrative approaches**, *Teacher*.
- Tutorial on geometric deep learning in structural bioinformatics

Oct 2021 **YSDA Machine Learning course**, *Teacher*.
- Seminar on graph neural networks

Feb 2021 - May 2021 **Academic course "My first scientific paper" at MIPT**, *Mentor*.
- Supervised a MIPT student in research project on application of pre-trained transformers in the protein classification task.

Feb 2020 - May 2020 **Academic course "My first scientific paper" at MIPT**, *Mentor*.
- Supervised a MIPT student in research project on spherical convolutions for molecular graphs.

July 2019 - Aug 2019 **Sberbank Machine Learning Course, Moscow**, *Lecturer*.
- Taught introductory Python and Machine Learning courses for Sberbank employees.

Projects & Activities

Dec 2022 **Learning on Graphs (LoG) Conference**, *Organizer*.

Mar 2022 **AMLD EPFL, AI & the Molecular World**, *Organizer*.

Jul 2021 **ICML 2021 Workshop on Computational Biology**, *Speaker*.
- Highlight presentation "VoroCNN: Deep Convolutional Neural Network Built on 3D Voronoi Tessellation of Protein Structures".

Jul 2021 **Maths & AI: MIPT-UGA young researchers workshop**, *Speaker*.
- Report "Graph Convolutional Networks for Protein Model Quality Assessment".

Dec 2020 **Critical Assessment of protein Structure Prediction: CASP14 Conference**, *Poster session*.
- Posters with VoroCNN and S-GCN.

May 2020 - Aug 2020 **Critical Assessment of protein Structure Prediction: CASP14 Challenge**, *Participant*.
- S-GCN is in the top-1 by MCC(40) on CAD-score and in the top-5 by AUC on CAD-score.
- VoroCNN is in the top-2 by MCC(40) on CAD-score and in the top-7 by AUC on CAD-score.

Apr 2020 - May 2020 **Critical Assessment of protein Structure Prediction: COVID-19**, *Participant*.
- 2 variations of VoroCNN participated in CASP_Commons, COVID-19.