llia Igashov

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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 protein model 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 École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland, Present PhD in Computational and Quantitative Biology. Thesis directors: Bruno Correia, Michael Bronstein
- Feb 2021 Research Intern, Laboratoire Jean Kuntzmann, Grenoble, France.
- Jul 2021 Supervisor: Dr. Sergei Grudinin • Developed rotation-invariant deep learning approach for predicting chemo-physical properties of small organic
- Nov 2019 Research Intern, Inria, Nano-D Team, Grenoble, France.
- May 2020 Supervisor: Dr. Sergei Grudinin

molecules.

- Created methods VoroCNN and Spherical Graph Convolutional Network (S-GCN) for the protein model quality assessment problem.
- Feb 2018 Undergraduate Research Project, MIPT, Moscow, Russia.
- May 2018 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

- 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] Arne Schneuing, Yuanqi Du, Charles Harris, Arian Jamasb, Ilia Igashov, Weitao Du, Tom Blundell, Pietro Lió, Carla Gomes, Max Welling, Michael Bronstein, Bruno Correia. "Structure-based Drug Design with Equivariant Diffusion Models". Under review. arXiv:2210.13695, 2022.
- [3] Ilia Igashov, Arian Jamasb, Ahmed Sadek, Freyr Sverrisson, Arne Schneuing, Tom Blundell, Pietro Liò, Michael Bronstein, Bruno Correia. "Decoding Surface Fingerprints for Protein-Ligand Interactions". *ICLR 2022 MLDD Workshop.* https://doi.org/10.1101/2022.04.26.489341, 2022.
- [4] Dmitrii Zhemchuzhnikov, **Ilia Igashov**, Sergei Grudinin. "6DCNN with roto-translational convolution filters for volumetric data processing". *AAAI 2022*. arXiv:2107.12078.

- [5] Ilia Igashov, Kliment Olechnovič, Maria Kadukova, Česlovas Venclovas, Sergei Grudinin. "VoroCNN: Deep convolutional neural network built on 3D Voronoi tessellation of protein structures". *Bioinfor-matics*. 2021. btab118, https://doi.org/10.1093/bioinformatics/btab118.
- [6] 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.

Professional Experience

- Nov 2022 Research Intern, Monte Rosa Therapeutics, Basel.
 - Jan 2023 Deep learning methods for design of molecular glue degraders.
- May 2020 Data Science Team Leader, PeakData, Remote.
- August 2021 NLP startup in healthcare domain aimed to gather and process information on medical topics.
- Sep 2018 Software Developer, Yandex. Music, Recommendation Team, Moscow, Russia.
 - Oct 2019 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 Summer Intern, Intel, Nizhny Novgorod, Russia.
- Aug 2017 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 Academic course "My first scientific paper" at MIPT, Mentor.
- May 2021 Supervised a MIPT student in research project on application of pre-trained transformers in the protein classification task.
- Feb 2020 Academic course "My first scientific paper" at MIPT, Mentor.
- May 2020 Supervised a MIPT student in research project on spherical convolutions for molecular graphs.
- July 2019 Sberbank Machine Learning Course, Moscow, Lecturer.
- Aug 2019 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 & Al: MIPT-UGA young researchers workshop, Speaker.
 o 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 Critical Assessment of protein Structure Prediction: CASP14 Challenge, Participant.
 - Aug 2020 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 Critical Assessment of protein Structure Prediction: COVID-19, Participant.
- May 2020 2 variations of VoroCNN participated in CASP_Commons, COVID-19.