Ilia 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 - Present **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 - Present **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

Feb 2021 - Present **Research Intern**, **Laboratoire Jean Kuntzmann**, *Grenoble, France*.
Supervisor: Dr. Sergei Grudinin
- I am working on a 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**, 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.

[2] **Ilia Igashov**, Nikita Pavlichenko, Sergei Grudinin. "Spherical convolutions on molecular graphs for protein model quality assessment". *Accepted at Machine Learning: Science and Technology*. 2020. arXiv: 2011.07980.

Professional Experience

May 2020 - Present **Data Science Team Leader**, **PeakData**, *Remote*.
- NLP startup in healthcare domain aimed to gather and process information on medical topics.
- My team consists of five people, and my core responsibilities are product planning, team management, and writing code.

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

Feb 2021 - Present **Academic course "My first scientific paper" at MIPT**, *Mentor*.
- Supervising 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 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.

Dec 2019 **Tsukuba University - UGA Computer Science Workshop, Grenoble**, *Speaker*.
- Report "Graph convolutional networks in Structural Biology".

Oct 2018 **Vk Hackathon, Saint Petersburg**, *Participant*.
- Created an Android application for recognition composers on wall posters (Moscow Philharmonia project).

Feb 2018 - May 2018 **DeepPavlov**, *Contributor*.
- Took part in building an active-learning process for training a model for NER in Russian language.

Technical Skills

Programming	Python, C/C++, Java, SQL
Frameworks	PyTorch, TensorFlow, Keras
Utilities	Git, Docker, Jupyter, Postgres, MySQL, MongoDB
Language	English (TOEFL iBT: 106), French (A2), Russian (Native)