

# Ilia Igashov

+7-916-812-38-80  
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

- Feb 2021 - **Research Intern, Laboratoire Jean Kuntzmann, Grenoble, France.**  
Jul 2021 Supervisor: Dr. Sergei Grudin  
  - I am working on a rotation-invariant deep learning approach for predicting chemo-physical properties of small organic molecules.
- Nov 2019 - **Research Intern, Inria, Nano-D Team, Grenoble, France.**  
May 2020 Supervisor: Dr. Sergei Grudin  
  - 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

- [1] **Ilia Igashov**, Kliment Olechnovič, Maria Kadukova, Česlovas Venclovas, Sergei Grudin. "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 Grudin. "Spherical convolutions on molecular graphs for protein model quality assessment". *Machine Learning: Science and Technology*. 2020. <https://doi.org/10.1088/2632-2153/abf856>.
- [3] Dmitrii Zhemchuzhnikov, **Ilia Igashov**, Sergei Grudin. "6DCNN with roto-translational convolution filters for volumetric data processing". *Preprint*. 2021. arXiv:2107.12078.

## Professional Experience

- 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
  - o Launched three smart playlists based on personal recommendation algorithms.
  - o Implemented Multi-Armed Bandits algorithm for optimal recommendation of radio stations for new users.
  - o Created personal recommendations of podcasts and promotions.
 July 2017 - **Summer Intern, Intel**, *Nizhny Novgorod, Russia*.  
 Aug 2017
  - o Implemented and integrated additional split criteria in Decision Tree algorithm for Intel DAAL.

## Teaching & Mentorship

- Feb 2021 - **Academic course "My first scientific paper" at MIPT**, *Mentor*.  
 May 2021
  - o 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
  - o Supervised a MIPT student in research project on spherical convolutions for molecular graphs.
 July 2019 - **Sberbank Machine Learning Course, Moscow**, *Lecturer*.  
 Aug 2019
  - o Taught introductory Python and Machine Learning courses for Sberbank employees.

## Projects & Activities

- Jul 2021 **ICML 2021 Workshop on Computational Biology**, *Speaker*.  
  - o 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*.  
  - o Report "Graph Convolutional Networks for Protein Model Quality Assessment".
 Dec 2020 **Critical Assessment of protein Structure Prediction: CASP14 Conference**, *Poster session*.  
  - o Posters with VoroCNN and S-GCN.
 May 2020 - **Critical Assessment of protein Structure Prediction: CASP14 Challenge**, *Participant*.  
 Aug 2020
  - o S-GCN is in the top-1 by MCC(40) on CAD-score and in the top-5 by AUC on CAD-score.
  - o 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
  - o 2 variations of VoroCNN participated in CASP\_Commons, COVID-19.
 Dec 2019 **Tsukuba University - UGA Computer Science Workshop, Grenoble**, *Speaker*.  
  - o Report "Graph convolutional networks in Structural Biology".
 Oct 2018 **Vk Hackathon, Saint Petersburg**, *Participant*.  
  - o Created an Android application for recognition composers on wall posters (Moscow Philharmonia project).
 Feb 2018 - **DeepPavlov**, *Contributor*.  
 May 2018
  - o Took part in building an active-learning process for training a model for NER in Russian language.

## References

### Sergei Grudin

CR1 CNRS, group leader  
 Nano-D, Inria Rhône-Alpes  
 Minatec Campus 17 rue des Martyrs  
 38054 Grenoble, France  
 ✉ sergei.grudin@inria.fr  
 ☎ +33 4 38 78 16 91

### Vadim Strijov

DSc, Professor  
 Moscow Institute of Physics and  
 Technology  
 9 Institutskiy per.  
 141701 Dolgoprudny, Russia  
 ✉ strijov@phystech.edu  
 ☎ +7 499 135 41 63

### Daniil Burlakov

Yandex.Music  
 Leader of the Recommender Team  
 Sadovnicheskaya Ulitsa 82-2  
 115035 Moscow, Russia  
 ✉ burlada@yandex-team.ru  
 ☎ +7 916 218 52 74