Boris Knyazev

AI Research Scientist & Adjunct Professor

Email: boris.knyazev@umontreal.ca
Website: `https://bknyaz.github.io`
Status in Canada: Citizen

Research areas

- Relational and graph-structured learning, graph neural networks (GNNs)
- Optimization, efficient training and inference of large (language) models (LLMs)
- Reasoning and scientific discovery
- Weight space learning

Team leading experience

- Mentoring and supervising of 10+ graduate students at Mila - Quebec AI Institute
- Leading internal Samsung projects on LLMs

Education

PhD, University of Guelph — Guelph (Ontario), Canada
Machine Learning Research Group — **2017 - 2022**
Thesis: Assessing and Improving Generalization in Graph Reasoning and Learning
Advisor: Graham W. Taylor
Teaching assistant: 2017-2019
Scholarships: IGTS, OGS, Dean's scholarship

MSc, Bauman Moscow State Technical University — Moscow, Russia
Diploma with Honors in Information Technology, *GPA: 4.8/5.0* — **2005 - 2011**
Scholarships: **German Academic Exchange Service (DAAD)**

Professional experience

University of Montreal — Montreal, Canada
Adjunct professor, DIRO (affiliation) — **2025 - present**

Samsung AI Lab — Montreal, Canada
Research Scientist (full time) — **2022 - present**

- Projects: LLMs, improving mixtures of experts, material discovery
- Manager: Simon Lacoste-Julien

Facebook AI Research — Montreal, Canada
Research Intern (full time) — **Summer 2020**

- Project: Parameter Prediction for Unseen Deep Architectures
- Advisors: Adriana Romero and Michal Drozdzal

Mila - Quebec AI Institute — Montreal, Canada
Research Intern (full time) — **2019 - 2020**

- Project: Compositional Generalization in Scene Graphs
- Advisors: Eugene Belilovsky and Aaron Courville

NextAI — Toronto, Canada
Scientist in Residence (part time) — **2018 - 2019**

- Consulting startup teams

SRI International Princeton, NJ, USA

Research Intern (full time) **Summer & Fall 2018**

- Project: Graph Neural Networks for Classification of Images and Other Modalities
- Advisor: Mohamed R. Amer
- Awards: Top-2 in all interns poster presentations

Institute for Neuro- and Bioinformatics, University of Luebeck Luebeck, Germany

Visiting researcher **2015 - 2016**

- Project: High-performance Image Classification with Small Training Datasets
- Advisors: Thomas Martinetz and Erhardt Barth

Invited talks & interviews

- "Neural Networks as Graphs" at ICLR 2025 Workshop on Weight Space Learning
- Interview with Yannic Kilcher about "Parameter Prediction for Unseen Deep Architectures" (YouTube, Nov 2021)

Selected publications

*equal contribution

complete list: Google Scholar link

1. Li Y, Cloutier F, Wu S, Parviz A, **Knyazev B**, Zhang Y, Berseth G, Bang L. Mol4Gen: Multi-Agent, Multi-Stage Molecular Generation under Precise Multi-Property Constraints. **Under review**, 2025.
2. Qin G, Gupta R, **Knyazev B**, Zhang Y, Berseth G, Bang L. Concept-Based Steering of LLMs for Conditional Molecular Generation. **Under review**, 2025.
3. Moudgil A, **Knyazev B**, Belilovsky E. Towards Learned Optimization Free Lunch. **Under review**, 2025.
4. Jolicoeur-Martineau A, Baratin A, Kwon K, **Knyazev B**, Zhang Y. Any-Property-Conditional Molecule Generation with Self-Criticism using Spanning Trees. **TMLR**, 2025, arXiv.
5. Singh J, Misra D, **Knyazev B**, Orvieto A. (Almost) Free Modality Stitching of Foundation Models. **EMNLP** (Main track), 2025, arXiv.
6. **Knyazev B**, Moudgil A, Lajoie G, Belilovsky E, Lacoste-Julien S. Accelerating Training with Neuron Interaction and Nowcasting Networks. **ICLR**, 2025, arXiv.
7. Joseph C-E, Thérien B, Moudgil A, **Knyazev B**, Belilovsky E. Meta-learning Optimizers for Communication-Efficient Learning. **TMLR**, 2025, arXiv.
8. Moudgil A, **Knyazev B**, Lajoie G, Belilovsky E. Learning Versatile Optimizers on a Compute Diet. **TMLR** (J2C Certification), 2025, arXiv.
9. Thérien B, Joseph C-E, **Knyazev B**, Oyallon E, Rish I, Belilovsky E. μLO: Compute-Efficient Meta-Generalization of Learned Optimizers. **NeurIPS OPT Workshop (oral)**, 2024, arXiv.
10. Kofinas M, **Knyazev B**, Zhang Y, Chen Y, Burghouts G.J., Gavves E, Snoek C.G., Zhang D.W. Graph Neural Networks for Learning Equivariant Representations of Neural Networks. **ICLR (oral)**, 2024, arXiv.
11. **Knyazev B**, Hwang D, Lacoste-Julien S. Can We Scale Transformers to Predict Parameters of Diverse ImageNet Models? **ICML**, 2023, arXiv.
12. Schürholt K, **Knyazev B**, Giró-i-Nieto X, Borth D. Hyper-Representations as Generative Models: Sampling Unseen Neural Network Weights. **NeurIPS**, 2022, arXiv.
13. Thompson R, **Knyazev B**, Ghalebi E, Kim J, Taylor G.W. On Evaluation Metrics for Graph Generative Models. **ICLR**, 2022, arXiv.
14. **Knyazev B**, Drozdzal M, Taylor G.W., Romero-Soriano A. Parameter Prediction for Unseen Deep Architectures. **NeurIPS**, 2021, arXiv.

15. Chung H, Kim J, **Knyazev B**, Taylor G.W., Lee J, Park J, Cho M. Brick-by-Brick: Sequential 3D Object Construction with Deep Reinforcement Learning. **NeurIPS**, 2021, arXiv.

16. **Knyazev B**, de Vries H, Cangea C, Taylor G.W., Courville A, Belilovsky E. Compositional Augmentations for Scene Graph Generation. **ICCV**, 2021, arXiv.

17. Lu Y, Rai H, Chang C, **Knyazev B**, Yu G, Shekhar S, Taylor G.W., Volkovs M. Context-aware Scene Graph Generation with Seq2Seq Transformers. **ICCV**, 2021, iccv.

18. **Knyazev B***, Augusta C*, Taylor G.W. Learning Temporal Attention in Dynamic Graphs with Bilinear Interactions. **PLOS One**, 2021, arXiv.

19. **Knyazev B**, de Vries H, Cangea C, Taylor G.W., Courville A, Belilovsky E. Graph Density-Aware Losses for Novel Compositions in Scene Graph Generation. **BMVC**, 2020, arXiv.

20. **Knyazev B**, Lin X, Amer M.R., Taylor G.W. Image Classification with Hierarchical Multi-graph Networks. **BMVC**, 2019, arXiv.

21. **Knyazev B**, Taylor G.W., Amer M.R. Understanding Attention and Generalization in Graph Neural Networks. **NeurIPS**, 2019 (also a *contributed talk*, 4% accept. rate, at *ICLR Workshop on Representation Learning on Graphs and Manifolds*), arXiv.