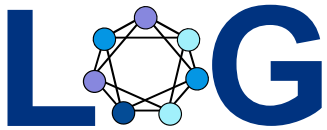

LoG 2023

Proceedings of the Second Learning on Graphs Conference

November 27–30, 2023

Virtual Event

Program Chairs:

Soledad Villar & Benjamin Chamberlain

Advisory Board:

Regina Barzilay, Xavier Bresson, Michael Bronstein, Stephan Günnemann, Stefanie Jegelka, Shuiwang Ji, Thomas Kipf, Jure Leskovec, Pietro Liò, Razvan Pascanu, Bastian Rieck, Jian Tang, Jie Tang, Petar Veličković, Soledad Villar, Marinka Zitnik, Wei Wang, & Smita Krishnaswamy

Organizers:

Yuanqi Du, Hannes Stärk, Chaitanya K. Joshi, Andreea Deac, Iulia Duta, Joshua Robinson, Yanqiao Zhu, Kexin Huang, Michelle Li, Sofia Bourhim, Ilia Igashov, Alexandre Duval, Mathieu Alain, Dominique Beaini, & Xinyu Yuan

Foreword

Welcome to the second Learning on Graphs (LoG) conference, held virtually from November 27 to 30, 2023. Building upon the success of our inaugural event, we are thrilled to present an expanded and enriched program that showcases the latest advancements in machine learning on graphs and geometry.

This year we received 122 full paper submissions. After a rigorous reviewing process, we accepted 38 papers, which corresponds to an acceptance rate of 31.14%. Additionally, we received 70 extended abstract submissions, among which we accepted 32 extended abstracts. These extended abstracts are not included in the proceedings. Among these, 6 papers and 6 extended abstracts were selected for oral presentations, highlighting their exceptional quality and potential impact.

We continued to emphasize and encourage high-quality review by a rigorous double-blind review process, a careful selection and vetting process of reviewers, and high monetary awards for excellent reviews. The initial review assignments were made using the bidding and matching system on OpenReview and were manually adjusted as needed. The final decisions were made by the program chairs, considering the discussions among authors, reviewers, and meta-reviews from area chairs.

Our four-day conference features an exciting lineup of programs, including 2 tutorials, 5 keynote talks, 12 oral presentations, 2 poster sessions, and 1 social hour. To foster a sense of community and encourage global participation, we have also organized 13 featured local meetups around the world.

Putting together the LoG 2023 conference was the collective effort of the entire organizing committee and the invaluable contributions of numerous volunteers who have dedicated their time and expertise to making this conference a reality. We extend our heartfelt gratitude to the Program Chairs, Soledad Villar and Benjamin Chamberlain, for their commitment to the review process. We also express our sincerest thanks to all of the advisors who have provided invaluable guidance and continued support throughout the planning and execution of the conference. Furthermore, we are delighted to welcome two new advisors, Wei Wang and Smita Krishnaswamy, whose insights and expertise will undoubtedly enrich our community.

We are grateful for the generous sponsorship provided by Pfizer, Genentech, Noeon Research, neo4j, Genesis Therapeutics, Charm Therapeutics, ELLIS Munich Unit, and Kumo. Their support has been instrumental in ensuring the success of the conference and facilitating the recognition of outstanding reviewers through monetary awards.

As we embark on this second iteration of the LoG conference, we remain committed to providing a platform for the dissemination and discussion of cutting-edge research and best practices in the fields of machine learning on graphs and geometry. We hope that this virtual gathering will foster meaningful collaborations, inspire new ideas, and contribute to the advancement of our field. Looking ahead, we hope to bring the LoG conference to an in-person global event in the future, further strengthening the bonds within our community and facilitating even more dynamic exchanges of knowledge.

LoG 2023 Organizing Committee

Yuanqi Du, Hannes Stärk, Chaitanya K. Joshi, Andreea Deac, Iulia Duta,
Joshua Robinson, Yanqiao Zhu, Kexin Huang, Michelle Li, Sofia Bourhim,
Ilia Igashov, Alexandre Duval, Mathieu Alain, Dominique Beaini, and Xinyu Yuan

Review Process

Most reviewers engaged with the paper bidding process, typically making in excess of 50 bids. Whenever available, OpenReview profiles, including publication track records and relevant keywords, were used to improve assignments. Four reviewers were assigned to each paper. A very small number of reviewer reassignments were requested and these were handled on a case-by-case basis, ensuring that no conflicts of interest appeared. Reviewing was double-blind, but program chairs had visibility of the identities of the reviewers and the area chairs, with the excepion for their own submissions. Reviewers were asked to "Review the papers of others as you would wish your own to be reviewed" and shown the following short review text to help guide their writing:

> Be sure to: (1) summarize the contributions of this work, (2) list strong and weak points of the paper, (3) clearly state your recommendation (accept or reject) with key reasons, (4) provide supporting arguments for your recommendation, (5) ask questions to authors to help you clarify your understanding of the paper, (6) provide additional feedback with the aim to improve the paper. Please refer to the reviewer guidelines: `https://logconference.org/reviews`

Program chairs monitored the review process in collaboration with the area chairs, reminding reviewers about the review guidelines and pointing out reviews that could be improved. In several cases, area chairs raised issues with papers having less than three complete reviews at the end of the review process. When missing reviewers could not be contacted in time, best efforts were made to find emergency reviewers and in a small number of cases, program chairs provided additional reviews.

Area chairs moderated the discussion period, asking reviewers for additional clarifications and potential updates during the rebuttal phase. Area chairs were then asked to provide a meta-review listing the main strengths and weaknesses of the submission and exactly how the respective weighting of those strengths and weaknesses led to their recommendation to reject, borderline, accept or commend. During the discussion period authors were also given the opportunity to comment on and rate their reviews on a five point scale. Generally reviewer scoring was handled in good faith with the score representing the depth of insight and effort shown by the reviewer rather than reciprocating the score they had awarded the paper.

Towards the end of the discussion period, a technical issue was discovered whereby some author replies not being set as visible to reviewers or area chairs. The program chairs were made aware of the problem and notified reviewers and area chairs about responses they may have missed during the discussion period. For two submissions, this led to changes in decision from reject to accept. This issue has been flagged and will be addressed in subsequent LoG conferences.

The final decision making process involved the program chairs first flagging borderline papers and those papers where the AC recommendations were significantly different from the opinions of reviewers. The discussion for such borderline cases was used to calibrate decisions and agree on criteria for acceptance.

LoG 2023 Program Chairs

Benjamin Chamberlain, Staff Researcher, Isomorphic Labs
Soledad Villar, Assistant Professor, Johns Hopkins University

Invited Talks

Designing Antibodies to Target Disease with Generative AI: Reporting from the Trenches

Presenter: Andreas Loukas (Senior Principal Scientist, Prescient Design, Genentech, Roche)

Bio: Andreas Loukas is a Senior Principal Scientist and Machine Learning Lead at Prescient Design within Genentech Research & Early Development (gRED). His work focuses on the foundations and applications of machine learning to structured problems. He aims to find ways to exploit (graph, constraint, group) information, with the ultimate goal of designing algorithms that can learn from fewer data. He is also focusing on the theoretical analysis of neural networks and in using them to solve hard bioengineering problems (especially protein design). Andreas obtained his Ph.D. in computer science from TU Delft in 2015 and pursued postdoctoral studies at TU Berlin and EPFL . He became an SNSF Ambizione fellow at EPFL in 2018 and an Assistant Professor at the Computer Science department of the University of Luxembourg in 2021. He joined Genentech/Roche in 2022.

Relational Deep Learning: Where Do Graphs Come From?

Presenter: Jure Leskovec (Professor, Stanford University)

Bio: Jure Leskovec is a Professor of Computer Science at Stanford University. His general research area is applied machine learning for large interconnected systems focusing on modeling complex, richly-labeled relational structures, graphs, and networks for systems at all scales, from interactions of proteins in a cell to interactions between humans in a society. Applications include commonsense reasoning, recommender systems, computational social science, and computational biology with an emphasis on drug discovery.

Learning ∩ Physics ∩ Graphs

Presenter: Kyle Cranmer (Professor, University of Wisconsin-Madison)

Bio: Kyle Cranmer is a professor in the Physics Department with affiliate appointments in Computer Sciences and Statistics. He is also the David R. Anderson Director of the American Family Insurance Data Science Institute (DSI) at the University of Wisconsin-Madison. Prior to joining UW-Madison in 2022, Cranmer spent 15 years at New York University.

On Learning with Symmetries — Models and Theory

Presenter: Stefanie Jegelka (Associate Professor, Massachusetts Institute of Technology (MIT))

Bio: Stefanie Jegelka is a Humboldt Professor at TU Munich and an Associate Professor in the Department of EECS at MIT (on leave). She is a member of the Computer Science and AI Lab (CSAIL), the Center for Statistics and an affiliate of IDSS and ORC. Before joining MIT, she was a postdoctoral researcher at UC Berkeley, and obtained her PhD

from ETH Zurich and the Max Planck Institute for Intelligent Systems. Stefanie has received a Sloan Research Fellowship, an NSF CAREER Award, a DARPA Young Faculty Award, an Alexander von Humboldt Professorship, Google research awards, a Two Sigma faculty research award, the German Pattern Recognition Award and a Best Paper Award at the International Conference for Machine Learning (ICML). She has also been invited as a sectional lecturer at the ICM 2022. She has served as an Area Chair for NeurIPS and ICML, as Action Editor for JMLR and as Program Chair for ICML 2022. Her research interests span the theory and practice of algorithmic machine learning, including learning with graphs, learning with symmetries, robustness to distribution shifts, and learning with limited supervision.

Graph Learning for Chemical Discovery (Sponsor Talk)

Presenter: Kristof Schütt (Senior Machine Learning Research Scientist, Pfizer)

Bio: Kristof Schütt is a Senior Machine Learning Research Scientist at Pfizer. He completed his PhD in Computer Science on the topic of Deep Learning for Quantum Chemistry from the Technical University of Berlin. He was a group leader at the Berlin Institute for the Foundation of Learning and Data until 2022. His current research focuses on Machine Learning for Drug Discovery.

Tutorials

Scalable GNN Training using HPC & Supercomputing

Organizers: Massimiliano (Max) Lupo Pasini, Jong Youl Choi, Pei Zhang, Kshitij Mehta, Jonghyun Bae, and Khaled Ibrahim

Date: November 28, 2023

Abstract: Graph Neural Networks (GNNs) are gaining traction across various scientific fields, demonstrating significant success. Leveraging High-Performance Computing (HPC) is becoming increasingly vital for Department of Energy (DoE) scientists as they handle extensive large number of graph datasets. Yet, the task of managing and processing millions, if not billions, of graphs remains a considerable challenge. Maximizing throughputs for multi-CPUs/GPUs and efficiently utilizing multi-level memory structure poses several computational challenges that need to be addressed. To this effect, a myriad of methods and tools have emerged, capitalizing on the parallel capabilities of expansive computing infrastructures. Familiarity with these available algorithms and tools is essential, and understanding their respective strengths and weaknesses is crucial. Our tutorial aims to provide an introduction of GNN training and parallel techniques and tools using distributed training to harness the power of parallel computing resources. This will enable users to gain insights into GNNs and parallel processing and equip them with necessary knowledge for their scientific challenges. The tutorial will focus on three main topics: i) GNNs, ii) parallelism, and iii) HPC infrastructures.

Website: `https://github.com/ORNL/HydraGNN/tree/LoG2023_tutorial`

GNNs for Recommendation: Reproducibility, Graph Topology, & Node Representation

Organizers: Daniele Malitesta, Claudio Pomo, and Tommaso Di Noia

Date: November 30, 2023

Abstract: Graph neural networks (GNNs) have gained prominence in recommendation systems in recent years. By representing the user-item matrix as a bipartite and undirected graph, GNNs have demonstrated their potential to capture short- and long-distance user-item interactions, thereby learning more accurate preference patterns than traditional recommendation approaches. In contrast to previous tutorials on the same topic, this tutorial aims to present and examine three key aspects that characterize GNNs for recommendation: (i) the reproducibility of state-of-the-art approaches, (ii) the potential impact of graph topological characteristics on the performance of these models, and (iii) strategies for learning node representations when training features from scratch or utilizing pre-trained embeddings as additional item information (e.g., multimodal features). The goal is to provide three novel theoretical and practical perspectives on the field, currently subject to debate in graph learning but long been overlooked in the context of recommendation systems.

Website: `https://sisinflab.github.io/tutorial-gnns-recsys-log2023/`

Organizing Committee

Advisory Board

- Regina Barzilay, Professor, Massachusetts Institute of Technology (MIT)
- Xavier Bresson, Associate Professor, National University of Singapore (NUS)
- Michael Bronstein, Professor, University of Oxford
- Stephan Günnemann, Professor, Technische Universität München (TUM)
- Stefanie Jegelka, Associate Professor, Massachusetts Institute of Technology (MIT)
- Shuiwang Ji, Professor, Texas A&M University
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- Jian Tang, Associate Professor, HEC Montréal, Mila
- Jie Tang, Professor, Tsinghua University
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- Marinka Zitnik, Assistant Professor, Harvard University
- Wei Wang, Professor, University of California, Los Angeles (UCLA)
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- Michelle Li, PhD Student, Harvard University
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- Ilia Igashov, PhD Student, École Polytechnique Fédérale de Lausanne (EPFL)
- Alexandre Duval, PhD Student, CentraleSupelec, Université Paris-Saclay
- Mathieu Alain, PhD Student, University College London (UCL)
- Dominique Beaini, Head of Graph Research, Valence & Adjunct Professor, Université de Montréal
- Xinyu Yuan, PhD Student, Université de Montréal, Mila

Local Meetups

- Stanford, USA
- Munich, Germany
- Amsterdam, Netherlands
- Shanghai, China
- Lausanne, Switzerland
- Paris, France
- Tromso, Norway
- Madrid, Spain
- Beijing, China
- Trento, Italy
- New York, US
- Oxford, UK
- Montreal, Canada

Awards

Best Paper Awards

- *Representing Edge Flows on Graphs via Sparse Cell Complexes*
  By Josef Hoppe and Michael T. Schaub

Best Area Chair Awards

- Minjie Wang
- Petar Veličković
- Xiaowen Dong

Best Reviewer Awards

- Francesco Di Giovanni
- Dobrik Georgiev
- Rishi Sonthalia
- Gecia Bravo-Hermsdorff
- Giorgos Bouritsas
- Alex Morehead
- Yunan Luo
- James Nastos
- Arjun Subramonian
- Ralph Abboud

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Wengong Jin
Smita Krishnaswamy
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Shurui Gui, Texas A&M University
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Thien Le, Massachusetts Institute of Technology

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Lingwei Chen, Wright State University

Runxue Bao, NEC Labs America

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Peiyuan Liao, rabbit

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Defu Cao, University of Southern California

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Ziwei Zhang, Tsinghua University, Tsinghua University

Haoyu Geng, Shanghai Jiao Tong University

Ingo Scholtes, University of Würzburg

Ziwei Fan, Amazon

Sheng Zhou, Zhejiang University

Ruixiang ZHANG, Mila, UdeM

Zuoyu Yan, Peking University

Joshua Southern, Imperial College London, Imperial College London

Liudmila Prokhorenkova, Yandex

Santiago Velasco-Forero, Mines ParisTech

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Shanda Li, Carnegie Mellon University

Namkyeong Lee, Korea Advanced Institute of Science & Technology

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Adeesh Kolluru, Carnegie Mellon University

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Yu Wang, Vanderbilt University

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Michail Chatzianastasis, École Polytechnique

Qiaoyu Tan, New York University Shanghai

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Jintang Li, SUN YAT-SEN UNIVERSITY

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Fan Feng, City University of Hong Kong

Zhimeng Jiang, Texas A&M University

Joydeep Chandra, Indian Institute of Technology, Patna

Prasanna Balaprakash, Oak Ridge National Laboratory

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Cheng Wan, Georgia Institute of Technology

Rishi Sonthalia, University of California, Los Angeles

Siwei Wang, Intelligent Game and Decision Lab (IGDL)

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of Science and Technology

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Mikhail Galkin, Intel

Suman Kalyan Bera, Katana Graph Inc

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Hua Wei, Arizona State University

Eda Bayram, Accenture

Shuai Zheng, Beijing Jiaotong University

Yue Yu, Georgia Institute of Technology

Zhichun Guo, University of Notre Dame

Jindong Wang, Microsoft Research

Yu Liu, Tsinghua University, Tsinghua University

Derek Lim, Massachusetts Institute of Technology

Vignesh Ram Somnath, Swiss Federal Institute of Technology, Zurich

George Dasoulas, Harvard University

Yifei Wang, Peking University

Hongyi Ling, Texas A&M University

Harlin Lee, University of North Carolina at Chapel Hill

Dingsu Wang, University of Illinois at Urbana-Champaign

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