TOPOLOGICAL, ALGEBRAIC AND GEOMETRIC LEARNING WORKSHOPS 2022: PREFACE

Alexander Cloninger
University of California, San Diego

Timothy Doster
Pacific Northwest National Laboratory

Tegan Emerson
Pacific Northwest National Laboratory
Colorado State University
University of Texas, El Paso

Manohar Kaul
Indian Institute of Technology, Hyderabad

Ira Ktena
Google Deep Mind

Henry Kvinge
Pacific Northwest National Laboratory
University of Washington

Nina Miolane
University of California, Santa Barbara

Bastian Rieck
Institute of AI for Health, Helmholtz Munich & Technical University of Munich

Sarah Tymochko
University of California, Los Angeles

Guy Wolf
Université de Montréal

MAGNIFICENT MANIFOLDS AND WHERE TO FIND THEM: REFLECTIONS ON TWO WORKSHOPS BRIDGING THE GAP BETWEEN ALGEBRA, GEOMETRY, TOPOLOGY, AND MACHINE LEARNING RESEARCH

The deep learning revolution has provided us with resounding successes in different domains, such as image analysis. Despite initial claims to the contrary, however, the last years showed a dire need to understand and describe fundamental aspects of modern machine learning models. In this context, algebra, geometry, and topology offer a veritable cornucopia of different methods, ranging from the description of the boundary of neural network architectures to the development of more expressive models for graph learning, for example. There are few cross-pollination efforts between the machine learning community and the mathematical community at large. The papers in this collection represent two such efforts; all of them have been originally submitted to either the ICML Workshop on Topology, Algebra, and Geometry in Machine Learning or to the ICLR Workshop on Geometrical and Topological Representation Learning. We hope that this collection demonstrates to the reader the benefits of a more fundamental perspective on machine learning, and we hope that this will constitute the first of many such collections.

ICML WORKSHOP ON TOPOLOGY, ALGEBRA, AND GEOMETRY IN MACHINE LEARNING

The ICML Workshop on Topology, Algebra, and Geometry in Machine Learning (TAG:ML) occurred on July 20th, 2022 in Baltimore MD and was organized by Alexander Cloninger, Timothy Doster, Tegan Emerson, Henry Kvinge, and Sarah Tymochko.

In the original call the organizers stated:

> ... much of the data that is fueling current rapid advances in machine learning is: high dimensional, structurally complex, and strongly nonlinear. This poses challenges for researcher intuition when they ask (i) how and why current algorithms work and (ii) what tools will lead to the next big break-though. Mathematicians working in topology, algebra, and geometry have more than a hundred years worth of finely-developed machinery whose purpose is to give structure to, help build intuition about, and generally better understand spaces and structures beyond those that we can naturally understand. This workshop will show-case work which brings methods from topology, algebra, and geometry and uses them to help answer challenging questions in machine learning. With this workshop we will create a vehicle for disseminating machine learning techniques that utilize rich mathematics and address core challenges described in the ICML call for papers. Additionally, this workshop creates opportunity for presentation of approaches which may address critical, domain-specific ML challenges but do not necessarily demonstrate improved performance on mainstream, data-rich benchmarks. To this end our proposed workshop will open up ICML to new researchers who in the past were not able to discuss their novel but data set-dependent analysis methods. We interpret topology, algebra, and geometry broadly and welcome submissions ranging from manifold methods to optimal transport to topological data analysis to mathematically informed deep learning. Through intellectual cross-pollination between data-driven and mathematically-inspired communities we believe this workshop will support the continued development of both groups and enable new solutions to problems in machine learning.

The workshop attracted 44 submissions of which 33 were accepted and 23 are included in this volume. During the workshop there were 4 keynote talks covering different areas in the application of topology, algebra and geometry to machine learning:

- Bastian Rieck – *The Memory of Persistence*
- Michael Kirby – *A Brief History of Geometric Data Science*
- Soledad Villar – *Equivariant Machine Learning with Classical Invariant Theory*

- Shubhendu Trivedi – *Recent Advances in Equivariant Learning*

and 4 spotlight talks reflecting the strongest submissions:

- Masanori Koyama – *Invariance-adapted Decomposition and Lasso-type Contrastive Learning*
- Derek Lim and Joshua Robinson – *Sign and Basis Invariant Networks for Spectral Graph Representation Learning*
- Peter Xenopoulos – *GALE: Globally Assessing Local Explanations (Spotlight Presentation)*
- Aishwarya H. Balwani – *Zeroth-order Topological Insights into Iterative Magnitude Pruning*

Throughout the day the workshop was well attended with over 125 in-person participants and an unknown number of on-line viewers. After the talks had concluded a poster session afforded all accepted authors the opportunity to exhibit their work. The recorded talks can be found here `https://icml.cc/virtual/2022/workshop/13447`.

The organizers would like to thank our amazing reviewers – without their efforts we would not have been able to accept such a large number of diverse technical papers: Ankita Shukla, Bastian Rieck, Caroline Moosmueller, Charles Godfrey, Davis Brown, Dimitra Maoutsa, Eleanor Byler, Elizabeth Coda, Erik Amezquita, Felix Hensel, George Stantchev, Grayson Jorgenson, Gregory Henselman-Petrusek, Helen Jenne, Ilya Amburg, Ilya Schurov, Ismail Guzel, James Koch, James Murphy, Jonathan Tu, Jordan Trinka, Jordan Weaver, Joshua Robinson, Julien Chaput, Kaylin Hagopian, Leslie O'Bray, Luke Richards, Maria Glenski, Michael Perlmutter, Michael Rawson, Mohammad Tariqul Islam, Nathaniel Monson, Rachel Neville, Rishi Sonthalia, Sam Polk, Sarah McGuire, Sarah Percival, Scott Howland, Scott Mahan, Shane Jackson, Sofya Chepushtanova, Thomas Gebhart, Varun Khurana, Weilin Li and William Kay.

Please see the conference website `https://www.tagds.com/events/conferences/tag-in-machine-learning` for further information including links to the posters that were presented and watch `https://www.tagds.com` and `https://twitter.com/TAGinDS` for future TAG workshops.

ICLR Workshop on Geometrical and Topological Representation Learning

The ICLR Workshop on Geometrical and Topological Representation Learning (GTRL) occurred on April 29, 2022 in a virtual session, and was organized by Alexander Cloninger, Manohar Kaul, Ira Ktena, Nina Miolane, Bastian Rieck, and Guy Wolf.

The original call for papers stated:

> Over the past two decades, high-throughput data collection technologies have become commonplace in most fields of science and technology, and with them an ever-increasing amount of big high dimensional data is being generated by virtually every real-world system. While such data systems are highly diverse in nature, the underlying data analysis and exploration task give rise to common challenges at the core of modern representation learning. For example, even though modern real-world data typically have high dimensional ambient measurement spaces, they often exhibit low-dimensional intrinsic structures that can be uncovered by geometry-oriented methods, such as the ones encountered in manifold learning, graph signal processing, geometric deep learning, and topological data analysis. As a result, recent years have seen significant interest and progress in geometric and topological approaches to representation learning, which enable tractable exploratory analysis by domain experts who are often not computation-oriented.
>
> Our overarching goal in this workshop is to deepen our understanding of the challenges and opportunities in this field, while breaking the barriers between the typically disjoint computational approaches (or communities) that work in this

field, with emphasis on the domains of topological data analysis, graph representation learning, and manifold learning.

The workshop attracted 54 submissions, of which 31 were accepted and 11 are included in this volume. A particular feature of the workshop was a distinction between *foundation talks* and *invited talks*, with the former playing the role of a sweeping overview of the field, while the latter focuses more on distinct research contributions. Finally, to induce stimulating discussions within the community, the workshop also provided the opportunity for researchers to discuss *case studies*, i.e., work in progress or position pieces:

FOUNDATION TALKS

- Smita Krishnaswamy – *Diffusion Geometry and Topology in Spatial and Frequency Domains*
- Bernadette Stolz – *Topological Data Analysis and Geometric Anomaly Detection*

INVITED TALKS

- Stefanie Jegelka – *Sign and Basis Invariant Networks for Spectral Graph Representation Learning*
- Roland Kwitt – *Topologically Densified Distributions*
- Chad Topaz – *Topological Data Analysis of Collective Motion*

CASE STUDIES

- Tara Chari – *Distortion of Single-Cell Data in Two-Dimensional Embeddings*
- Dmitry Kobak – *What are 2D neighbour embeddings of scRNA-seq data actually useful for? (Dmitry Kobak)*
- Jessica Moore – *G2 stem cells orchestrate time-directed, long-range coordination of calcium signaling during skin epidermal regeneration*

The best eight submissions to the workshop also had the option to provide a brief spotlight talk about their paper:

- Zuoyu Yan et al. – *Neural Approximation of Extended Persistent Homology on Graphs*
- Thibault de Surrel et al. – *RipsNet: a general architecture for fast and robust estimation of the persistent homology of point clouds*
- Shengchao Liu et al. – *Pre-training Molecular Graph Representation with 3D Geometry*
- Bryn Elesedy – *Group Symmetry in PAC Learning*
- Tegan Emerson et al. *TopTemp: Parsing Precipitate Structure from Temper Topology*
- Vijay Lingam – *A Piece-wise Polynomial Filtering Approach for Graph Neural Networks*
- Petar Veličković – *Message passing all the way up*
- Cristian Bodnar et al. – *Neural Sheaf Diffusion: A Topological Perspective on Heterophily and Oversmoothing in GNNs*

Throughout the day the workshop was well attended with over 100 participants. After the talks had concluded a virtual poster session on Gather.Town afforded all accepted authors the opportunity to exhibit their work. The recorded talks can be found on SlidesLive (`https://slideslive.com/iclr-2021/geometric-and-topological-representation-learning`).

The organizers would like to thank our amazing reviewers; we are grateful for their support and their diligence. Without their efforts, organizing such workshops would be impossible: Adrish Dey, Adélie Garin, Aishwarya Balwani, Alexandros Dimitrios Keros, Alvin Jin, Balasubramaniam Srinivasan, Beichen Gao, Branden Stone, Bryan Bischof, Celia Hacker, Chen Cai, Christian Bock, Cristian Bodnar, Dan Shiebler, Darrick Lee, Dongkwan Kim, Donlapark Ponnoprat, Eduardo Paluzo-Hidalgo, Edward De Brouwer, Emily T. Winn, Erik J. Amezquita, Felix Hensel, Filip Cornell, Frederik Wenkel, Gavin Kerrigan, Guillaume Huguet, Guocheng Qian, Henry Kvinge, İsmail Güzel, Jacob Bamberger, Jatin Chauhan, Johan Mathe, Jónathan Heras, Ladislav Rampasek, Leslie O'Bray, Louis J. Castricato, Maghesree Chakraborty, Marco Guerra, Mathieu Carrière, Maximilian Thiessen, Michael F Adamer, Michael Moor, Muawiz Sajjad Chaudhary, Nello Blaser, Paul Samuel Ignacio,

Rayna Andreeva, Renata Turkes, Rishab Goel, Robin Vandaele, Saiteja Utpala, Salvish Goomanee, Sara Scaramuccia, Sarah Tymochko, Sebastian Zeng, Sonky Ung, Stefania Ebli, Umberto Lupo, Wei Ye, Xiaoling Hu, Yan Yan, Yuanqi Du, Yuzhou Chen

Please see the conference website `https://gt-rl.github.io/` for further information including links to the papers and posters. This website will also contain announcements for upcoming GT-RL workshops.

ADDITIONAL RESOURCES

Everyone who is interested in entering this vibrant research field is cordially invited to join AATRN, the *Applied Algebraic Topology Research Network*. Membership is free and provides you with direct access to seminar talks, interviews, poster sessions, and much more. ATTRN is commmitted to make resources on applied (algebraic) topology available to the whole world! Please find out more at `https://www.aatrn.net/` or visit the YouTube Channel at `https://www.youtube.com/c/AppliedAlgebraicTopologyNetwork`.