Preface to Geometry-grounded Representation Learning and Generative Modeling (GRaM) Workshop

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Motivation

By recognizing that nearly all data is rooted in our physical world, and thus inherently grounded in geometry and physics, it becomes evident that representation learning should preserve this grounding in order to remain meaningful.

For example, preserving group transformation laws and symmetries through equivariant layers is crucial in domains such as computational physics, chemistry, robotics, and medical imaging, and leads to effective and generalizable architectures and improved data efficiency. Similarly, in generative models applied to non-Euclidean data spaces, maintaining the manifold structure is essential in order to obtain meaningful samples. This workshop focused on the principle of *grounding in geometry*. We define this as follows:

A representation, method, or theory is grounded in geometry if it can be amenable to geometric reasoning, that is, it abides by the mathematics of geometry.

We accepted submissions that present theoretical research, methodologies, applications, insightful analysis, and even open problems, within the following topics:

1. **Structure-preserving learning** : Preservation of symmetries, e.g., through equivariant operators, dynamical systems on manifolds, representation learning and generative modeling using ordinary, stochastic and differential equations (ODEs, SDEs, PDEs) on manifolds, computing with geometric representations, such as the processing of multi-vectors using geometric algebra, steerable vectors using Clebsch-Gordan products, and hyperbolic features using Fréchet means.
2. **Structure-inducing learning**: Self-supervised learning, e.g., learning to embed data in geometric latent spaces through (geodesic) distance-based similarity metrics, geometric priors, e.g., soft constraints on model weights, physics-informed neural networks, e.g., inducing the structure of established physical and geometric laws into neural networks through dedicated losses.
3. **Generative modeling and density estimation**: Geometric latent variable models, i.e., the use of Latent variables that live in a manifold, new methods and adaptations of methods capable of generating geometric objects, e.g., generating atomic point clouds or shapes, generating fields over manifolds, e.g., generating vector fields or spherical signals.
4. **Grounding in theory**: Theoretical frameworks, unifying analyses and formulations that provide a generalizing perspective on deep learning paradigms, open problems identifying and addressing unresolved questions and challenges that lie at the intersection of geometry and learning.

GRaM Workshop at ICML

The first edition of GRaM Workshop at ICML took place on the 27th of July 2024 in Vienna Austria.

Figure 1: A jam-packed audience at GRaM workshop in Vienna, Austria

Call for Papers

The workshop accepted submissions in the following tracks

1. **Proceedings track**: 8-page paper submissions (excluding appendices and references). All submissions were peer-reviewed (double-blind via openreview). Accepted papers are published this proceedings, Volume 251 of PMLR.

2. **Extended abstract track**: 4-page paper submissions (excluding appendices and references). All submissions were peer-reviewed (double-blind via openreview). Accepted papers can be viewed on openreview as well as the workshop website.

3. **Blogpost and Tutorial track**: Blog posts and Tutorials that explain previously published papers or important topics in the field or include easy-to-use code for the same. GRaM workshop accepted submissions in markdown format for blog posts and colab files for tutorials. Selected submissions were posted on the GRaM website. All the submissions were reviewed single-blind.

4. **Topological deep learning challenge**: We teamed up with TAG and hosted an ICML Topological Deep Learning Challenge 2024: Beyond the Graph Domain challenge.

The call for papers yielded **97** submissions combined in the paper tracks, **15** in the Blogpost and Tutorial Track, and **56** submissions in the Competition Track. Each submission in the proceedings track received a minimum of three reviews, which were aggregated and assessed by the Area Chairs for final inclusion. Each submission in the rest of the tracks received a minimum of two reviews which were assessed by the program chairs of the respective tracks. This resulted in **147** accepted works: **29** proceedings papers, **52** extended abstract tracks, **14** blog posts/tutorials, and **52** in the competition track. All of the 29 papers in the proceedings track are published in this volume, by choice of the authors. Reviews of the accepted works can be found on the GRaM openreview page.

Schedule

The workshop was held on July 27th, 2024, in Vienna Austria, and attracted between 300 and 400 in-person attendees. The workshop featured five invited speakers, listed below, with talks spanning topics in geometric representations, the geometry of generative models, improving sampling using geometric-generative models, discovering symmetries, and learning representation beyond the Euclidean manifold. In addition, one discussion panel was held. All accepted works were presented as posters during the workshop, with the top five submissions selected for contributed talks. Awards were given to the best contribution in the proceedings track and extended paper track. All talks and the panel were live-streamed and recorded and can be found online on SlidesLive. GRaM attendees joining online, had their posters displayed on the main screen during afternoon breaks.

Talks

Keynote presentations

1. The Platonic Representation Hypothesis - **Phillip Isola**, MIT.
2. Automatic Symmetry Discovery from Data - **Rose Yu**, UCSD.

Invited talks

1. Simulation Free Generative Models for Protein Structures, Single-Cell RNA, DNA sequences and Beyond!, **Joey Bose**, Oxford University.
2. Generalization in diffusion models arises from geometry-adaptive harmonic representations, **Zahra Kadkhodaie**, Flatiron Institute.
3. Beyond Euclid: An Illustrated Guide to Modern Machine Learning with Geometric, Topological, and Algebraic Structures, **Nina Mialone**, UCSB.

Contributed talks

1. Adaptive Sampling for Continuous Group Equivariant Neural Networks, **Berfin Inal**, University of Amsterdam.
2. Variational Inference Failures Under Model Symmetries: Permutation Invariant Posteriors for Bayesian Neural Networks, **Yoav Gelberg**, University of Oxford.
3. Probabilistic World Modeling with Asymmetric Distance Measure, **Meng Song**, UCSD.
4. Lift Your Molecules: Molecular Graph Generation in Latent Euclidean Space, **Mohamed Amine Ketata**, Technical University of Munich.
5. Bundle Neural Networks for message diffusion on graphs, **Jacob Bamberger**, University of Oxford.

Panel Discussion

The panel topic was "Geometric deep learning and Generative modeling: Past and Future." The panelists were **Max Welling, Phillip Isola, Zahra Kadkhodaie, Joey Bose, and Rianne van der Berg**. The panel was moderated by **Erik Bekkers**.

Figure 2: Panel discussion at GRaM workshop

Program Committee

We extend our immense gratitude to our area chairs, who have diligently supervised the reviewing process and led the selection of contributed talks. Our heartfelt thanks also go out to the 87 reviewers, whose collective efforts resulted in high-quality reviews for the submissions. Their dedication and expertise have been integral to the success of this workshop.

Area Chairs

Alison Pouplin, Erik Bekkers, Hannah Lawrence, Henry Kvinge, Robin Walters, Sekou Oumar Kaba, Sharvaree Vadgama, Shubhendu Trivedi, Tegan Emerson served as Area Chairs.

Figure 3: A few members of GRaM team at GRaM workshop

Reviewers

Guillaume Huguet
Martin Uray
Serguei Barannikov
Georg Bökman
Kumar Krishna Agrawal
Nikhil Akalwadi
Maksim Zhdanov
Bálint Máté
Siba Smarak Panigrahi
Dhananjay Bhaskar
Giovanni Luca Marchetti
Georgios Arvanitidis
Benjamin Kurt Miller
Victor Livernoche
Jan E Gerken
Artur Petrov Toshev
Tycho F. A. van der Ouderaa
Emanuele Sansone
Yun Young Choi
Mathilde Papillon
Peter Potaptchik
Mary Letey
Patryk Rygiel
Kunvar Thaman
Floor Eijkelboom
Tara Akhound-Sadegh
Stefanie Jegelka
Hae Jin Song
Babak Esmaeili
David Wessels
Sharut Gupta
Yingying Wu
Sugandha Sharma
Elyssa Hofgard
Putri A Van der Linden
Noga Mudrik
Luca Ambrogioni
Gabriele Cesa
Xiusi Li
Marimuthu Kalimuthu
Jinwoo Kim
Anna Kuzina
Deepak Kumar Pokkalla
Dimitra Maoutsa
Ameya Daigavane
Ayon Borthakur
Federico Barbero
Thien Le
Vineet Jain
Thijs P. Kuipers
Leo Zhang
Max van Spengler
Sven Dummer
Jakub Tomczak
Luca Thiede
Axel Flinth
Mit Kotak
Nina Miolane
Teodora Reu
YuQing Xie
Gautam Pai
Farzaneh Heidari
Xinhe Zhang
Mingyu Kim
Santiago Velasco-Forero
Sampada Malagi
Cong Liu
Rohith Peddi
Bo Zhao
Julia Balla
Zhenjie Zhao
Puck Van Gerwen
Julian Suk
Daniel Levy
Liheng Ma
David M Knigge
Tobias Cheung
Vasco Portilheiro
David Ruhe
Yan Zhang

served as reviewers.

ELLIS Mobility Grant for GRaM workshop

ELLIS Amsterdam Unit, ELLIS Linz Unit, and Elise Network generously supported GRaM workshop. With their support, we were able to fund **18** GRaM attendees from **10** countries across **4** continents with a travel grant to attend the GRaM workshop in person in Vienna, Austria.

GRaM Social

With ICML, we were able to create a strong community in the emerging field of geometric representations.

Figure 4: A snapshot from post-workshop GRaM social

Continuing GRaM

We will review blog posts and tutorials regularly and post them on the GRaM website. We believe that continuing to accept submissions for blog posts and tutorials would be a great way to build easily accessible resources for learning geometric deep learning and generative modeling.