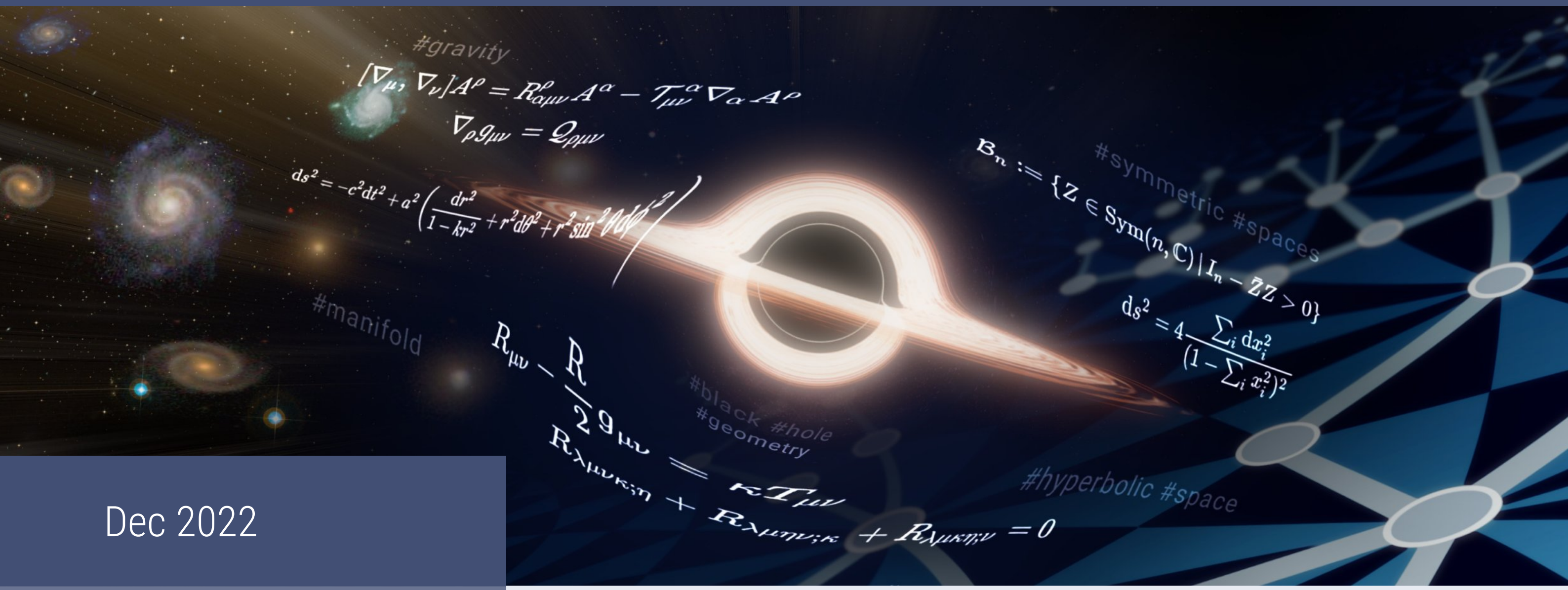
STRUCTURES | NEWS

STRUCTURES CLUSTER OF EXCELLENCE

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386



Dec 2022

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Upcoming

STRUCTURES Jour Fixe:

- Dec 16: Internal Event
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More information can be found on the **STRUCTURES website**.

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Recap 2022 and Happy Holidays

As the year comes to a close, we would like to thank you, our members and colleagues. Your excellent research, great commitment and enthusiasm form the basis of our cluster. In 2022 STRUCTURES has been happy to welcome seven new members, whose unique and complementary expertise enriches our scientific community. We are looking forward to new joint projects.

Prof Anna Marciniak-Czochra, newly elected STRUCTURES speaker.

We are most delighted to welcome Anna Marciniak-Czochra as new STRUCTURES speaker. She follows Anna Wienhard, who has accepted a prestigious position as director at MPI-MIS Leipzig. We congratulate and thank Anna Wienhard, who will remain external member, for years of dedication and outstanding contributions to the cluster.

The year 2022 has been eventful and productive for STRUCTURES, with groundbreaking research publications, prestigious research awards, new exciting exploratory projects, and the start of important initiatives like the MLAI portal for scientific machine learning in Heidelberg. Our midterm review with the International Advisory Board in June created an energetic moment of interaction among junior and senior members on a wonderful summer day at the Marsilius Kolleg. A special highlight in October was the YRC STRUCTURES Conference, which has promoted additional exchange and collaboration.

We all enjoyed being back to in-person meetings, and to continue our weekly Jour Fixe in a hybrid format, with most speakers and a large part of the audience present in the lecture hall. We are particularly proud of the IsoQuant/STRUCTURES Parent-Child Offices "KIDS" [Website], which offer child-friendly workspaces. We celebrated their opening in May.

Finally, STRUCTURES has launched various new outreach activities this year. Since August, we have been present on Twitter and Instagram with captivating visualisations of interesting structures, connected to our new science communication blog [Link].

We wish all our members and readers happy holidays and all the best for the year 2023!

The editorial board and the speakers.

PROJECT REPORT

Symmetric Spaces for Machine Learning – Representation Matters!

Invited guest article by Diaaeldin Taha (Mathematical Institute)

In this article, we report on a project which grew out of discussions during the application phase for STRUCTURES. It is concerned with leveraging geometric techniques on machine-readable representations of real-world observables, and developing novel geometrically-principled machine learning algorithms.

Representation Learning

Representation learning aims to embed data into an ambient space that can then be used for analysing and performing tasks on the data. The predominant approach has been to use Euclidean spaces, even though data in many domains, especially graphs, exhibit non-Euclidean features. For this reason, non-Euclidean ambient spaces that better match the structure of the data have caught researchers' attention. These ambient spaces include hyperbolic spaces, spherical spaces, Grassmannian manifolds, symmetric positive definite matrices, and products thereof. All these approaches are special cases of embedding data into symmetric spaces. In [1],[2] and in ongoing work, we develop a novel general computational framework for systematically implementing and optimising on these symmetric spaces.

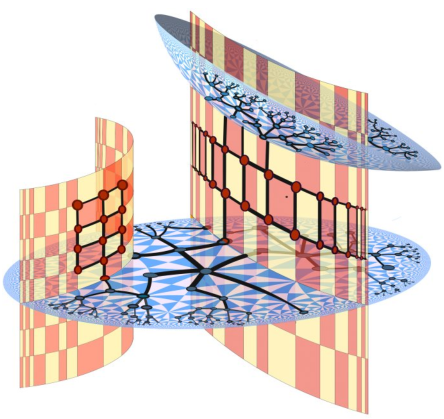


Fig. 1: Symmetric spaces have a rich structure of subspaces, including Euclidean subspaces (orange) and hyperbolic planes (blue). The graph embedded in the picture has both trees and grids as subgraphs.

Geometry

A *Riemannian symmetric space* (RSS) is a Riemannian manifold with a large symmetry group, whose geometry can be efficiently described with the theory of semisimple Lie groups. A key feature of RSSs is their rich combination of geometric features, including (in the non-compact case) many subspaces isometric to Euclidean, hyperbolic spaces, and products thereof. This makes RSSs an excellent tool for embedding complex networks without prior knowledge of the internal structure of the networks.

Methodology

In [1], [2], three important tools from the general theory of RSS were introduced to representation learning:

- **Finsler distances:** Riemannian distances are generally not well adapted to represent graphs. For instance, any embedding of a regular two-dimensional grid in the plane necessarily distorts some distances by a factor of at least $\sqrt{2}$. However, it is possible to find a perfect grid embedding in the plane with the ℓ^1 or ℓ^∞ distances, which are simple examples of *Finsler distances*. In general, RSSs support a whole family of Finsler distances more suitable for embedding complex networks.
- **Vector-valued distance:** In Euclidean, spherical, and hyperbolic geometries, a pair of points can be mapped to any other pair of points if and only if their distance is the same. In general RSSs, however, the invariant between two points is a distance *vector* in $\mathbb{R}^n$, where n is the rank of the space. This *vector-valued distance* gives a novel tool for analysing graph embeddings, as we illustrate in Fig. 2.
- **Gyrovector calculus:** *Gyrovector calculus* is a convenient mathematical language for expressing natural geometric operations on RSSs in analogy to how vector space operations are used in Euclidean geometry. Using the language of gyrovector calculus, geometrically meaningful extensions of several vector space operations that are crucial for deep learning applications can be succinctly described.

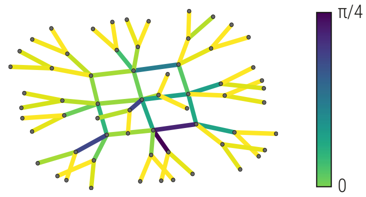


Fig. 2: Visualisation of the vector-valued distance for a rank-2 RSS embedding of a rooted product of a grid and a tree. Edge colors indicate the angle of the vector-valued distance for the embedding of each edge, separating the Euclidean (blue/green) and the hyperbolic parts (yellow).

Lastly, for optimisation, explicit formulas for employing a generalisation of stochastic gradient descent to manifolds were derived.

Applications & Ongoing Work

In [1],[2], it was demonstrated that this approach can improve the performance of different representation learning pipelines, surpassing competitive geometric machine learning baselines for several synthetic and real-world datasets. We are currently expanding on this work to provide a more complete toolbox to generalise neural network concepts from the Euclidean setting to the space of positive definite symmetric matrices, one particularly nice RSS.

Seminars & Workshops

During the summer, we organised the first *Workshop on Geometry and Machine Learning* (https://gaml.mathi.uni-heidelberg.de), and we are running a bi-weekly *Mathematics and Machine Learning Seminar* (https://hegl.mathi.uni-heidelberg.de/seminars/maml-seminar).

References

1. F. López, B. Pozzetti, S. Trettel, M. Strube, and A. Wienhard. Symmetric Spaces for Graph Embeddings: A Finsler-Riemannian Approach. *International Conference on Machine Learning,* pages 7090-7101. PMLR, 2021.
2. F. López, B. Pozzetti, S. Trettel, M. Strube, and A. Wienhard. Vector-valued Distance and Gyrocalculus on the Space of Symmetric Positive Definite Matrices. *Adv. Neural Inf. Process. Systems*, 34:18350–18366, 2021.

STRUCTURES COMMUNITY

STRUCTURES Asks: Lavinia Heisenberg

In our newsletter, we regularly interview faculty members of STRUCTURES to introduce people and their research. For this edition, we interviewed Lavinia Heisenberg, Professor at Institute for Theoretical Physics (ITP) and head of a cosmology research group. For her groundbreaking work on gravity theories, Lavinia Heisenberg has received several prestiguous awards, such as the DFG's Gustav-Hertz-Preis and the ETH Zurich Latsis Prize.

Lavinia Heisenberg, Professor at the Institute for Theoretical Physics (ITP).

Q: What are you working on and what methods do you use in your research?

A: My main area of expertise is gravity, cosmology, astrophysics and particle physics. My past research activities have both theoretical and observational aspects.

Q: What sets gravity aside from other interactions and what fascinates you about it?

A: The equivalence principle advocates to embrace the geometrical character of gravity. This is very different from other interactions. The *geometrical trinity* of gravity states that General Relativity (GR) can equivalently be represented by curvature, torsion, or non-metricity. While this trinity implies equivalent classical dynamics, differences arise in energetics, thermodynamics, and quantum theory. I also find the problem of constructing a sensible theory of quantum gravity a fascinating topic. Despite the great effort devoted to it and the existence of promising proposals, we are still far from a fully satisfactory solution. The persistence of this problem suggests that we are missing fundamental building blocks and should invest more effort into searching for them.

Q: You developed systematic approaches to generalising General Relativity (GR). How do these differ from the "gravity we know" and what makes them interesting?

A: The standard "ΛCDM" model of cosmology describes the physics on cosmological scales using two fundamental pillars: the *cosmological principle* and GR. This model is both remarkably simple and astoundingly successful, but requires the introduction of three unknown ingredients: *dark energy* or a *cosmological constant (CC)*, *dark matter*, and an *inflaton field*. We understand none of these ingredients at a fundamental level, we lack a consistent theory of quantum gravity, we have no solution to the CC problem posed by the enormous discrepancy between field theory predictions and observations, and puzzling anomalies/tensions remain in our interpretation of cosmological data. Wide classes of EFTs for gravity targetting these problems include fields in addition to the metric. EFTs underly severe restrictions. I have completed the most extensive classes of such theories, and I am studying these with respect to their theoretical consistency.

Q: You mentioned cosmological tensions. While cosmology has become a data-driven precision science, these tensions have led some to speak of a "crisis of cosmology". Is cosmology in a crisis or in a golden age?

A: Cracks have started to show in ΛCDM in form of a discrepancy between measurements of the early and late universe Hubble constant (H_0 tension). This, combined with a similar tension in measurements of the amplitude of cosmic structures (σ_8 tension), may be one of the most exciting developments in cosmology in decades. My strong tendency to confront theoretical work with observations has led me to work out model-independent and fully analytical conditions, which any late-time modification of the ΛCDM model has to satisfy in order to consistently solve both tensions. This is notoriously difficult, since models improving the H_0 tension generically tend to worsen the σ_8 tension. My work spells out precise conditions required for any model to relieve both tensions simultaneously. It can thus be used to identify unviable models and to develop resolutions that have a chance of succeeding.

Q: You have been working on Kinetic Field Theory (KFT) for cosmic structure formation. What is new about this approach and what goals are you pursuing with it?

A: So far, non-linear, late-time cosmic structure formation could only be studied with computation-extensive numerical simulations. This makes it forbiddingly time consuming to run suites of sufficiently detailed simulations for studying the effects of new cosmological models on evolved cosmic structures. A new analytic approach to non-linear cosmic structure formation was proposed by Prof. Bartelmann. Together with him, I intend to select suitable cosmological models to embed into the KFT formalism and to systematically study how these models affect non-linear structure growth.

Q: What would you recommend young researchers, and in particular young women who are looking to start their career?

A: You have to believe in yourself and not give up so easily. Self-doubt is your biggest enemy. Try different things and develop new skills. This will build your confidence. A strong will is important. It is much more important to be able to dream.

Q: Which place in the Solar System would you like to visit if you could choose?

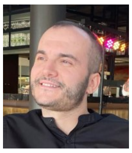
A: I would like to visit Mars. If I could, I would construct a viable physical wormhole solution and visit another galaxy far far away.

STRUCTURES COMMUNITY

We Are STRUCTURES

In each newsletter we introduce three members of the Young Researchers Convent (YRC). For this issue, we interviewed Egzon Miftari, Sara Marcos Plaza and Julian Göltz.

Interview with Egzon Miftari:



Egzon Miftari
PhD student,
AG Sadlo, IWR

What are you working on? Right now, I am working on the vector field topology of fields with discontinuities. Many new intriguing dynamics and new phenomena emerge when discontinuities can occur.

What are you an expert for? I am not an expert as of now, but working towards a better understanding of piecewise-smooth dynamics given by vector fields or maps with the use and development of new visualisation techniques.

What is your connection to STRUCTURES? I am a member of the Visual Computing Group and was up until recently funded by CP6 ("Networks and Machine Learning").

What was your greatest scientific success up to now? Becoming a member of STRUCTURES and being interviewed for this newsletter. But I expect that this changes soon, as we are moving to our first major submission, which should be sometime at the start of next year.

How does one recognise you? If you see someone quirky who is progressively getting bald, that's probably me.

Interview with Sara Marcos Plaza:

Sara Marcos Plaza
MSc student,
AG Bartelmann,
ITP

What are you working on? I apply Lagrangian Singularity Theory (LST), a generalisation of Morse Theory for Lagrangian submanifolds, to cosmic structure formation. Particularly, I apply LST to the 3d Zel'dovich Approximation to analyse the resulting "skeleton" of the cosmic web in terms of its singularity structure.

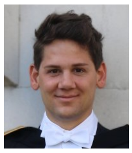
What are you an expert for? The focus of my studies lies on understanding the mathematical backbone of our physical theories. I am most familiar with manifolds, singularity theory, complex and functional analysis.

What is your connection to STRUCTURES? The concept of STRUCTURES has always attracted me, as it facilitates and promotes collaboration between researchers from different academic fields. My current project is therefore just what I was looking for.

What was your greatest scientific success up to now? One of the biggest joys during my studies was giving tutorials, as it combines scientific knowledge and teaching. If I was able to motivate just one of my students to get into mathematical physics, I would regard that as one of my biggest achievements.

How does one recognise you? If you see a short, dark-haired Spaniard at ITP, try to talk to her. If she can't stop talking, chances are you have found me ^^.

Interview with Julian Göltz:



Julian Göltz
PhD student,
AG Petrovici,
University of
Bern & KIP

What are you working on? In the NeuroTMA group we work within computational neuroscience on identifying building blocks of neural computation. Personally I am working on algorithms for deep learning in spiking ('biological') neural networks, as well as reinforcement learning in models of the brain.

What are you an expert for? This obviously depends on who you compare it to, but I guess it is fair to say that I know my way around spiking neurons and their use for Machine Learning, working with stubborn hardware, and software engineering in a somewhat professional environment.

What is your connection to STRUCTURES? My supervisor is an external member of STRUCTURES.

What was your greatest scientific success up to now? Publishing our algorithm and its implementation on the neuromorphic hardware *BrainScaleS-2* – developed by the Electronic Vision(s) group at KIP – in Nature Machine Intelligence.

How does one recognise you? (Un)fortunately, I spend some of my time in Bern. When I am around, I am at the Jour Fixe, try to boulder regularly and hang around with the Electronic Vision(s) at KIP.

STRUCTURES ON THE WEB
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