STRUCTURES | NEWS

STRUCTURES CLUSTER OF EXCELLENCE

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

Oct 2023

Networks & Artificial Intelligence

Contents

Upcoming

STRUCTURES Jour Fixe:

- Oct 27: Informal Meeting at EINC.
- Nov 3: Holger Fröning (ZITI, pretalk by Guido Kanschat), Phil 12 & online

Oct 21: Hengstberger Award Ceremony Anja Randecker

Connect with Us

@structures_hd
@structures_heidelberg
@STRUCTURES_HD

STRUCTURES BLOG:
www.structures.uni-heidelberg.de/blog

STRUCTURES + FIELD OF FOCUS IV WORKSHOP

Human Intelligence Meets Artificial Intelligence

How can cognitive science inform artificial neural network research and vice versa? This question was the focus of the interdisciplinary workshop *Human Intelligence meets Artificial Intelligence*, jointly organized by STRUCTURES and Field of Focus IV: "Self-Regulation & Regulation: Individuals & Societies" at Heidelberg University.
Over the course of two days, nearly one hundred participants with diverse academic backgrounds convened at Marsilius Kolleg to engage in a vibrant exchange of ideas with invited experts spanning the fields from cognitive and neuroscience to scientific machine learning, biomedicine and brain-inspired computing. Through instructive keynote talks and stimulating discussions, the workshop provided a unique multidisciplinary perspective on the phenomenon of intelligence and its emergence from neural structure and cognitive processes. The event generated novel insights about common principles, ideas and promising pathways for collaboration to advance our understanding of both human intelligence and modern AI tools.

MEMBER NEWS

Maria Beatrice Pozzetti Promoted to W3 Professor

We are thrilled to announce that STRUCTURES member Maria Beatrice Pozzetti has been promoted to W3 professor in Pure Mathematics. Prof Pozzetti is a principal investigator for STRUCTURES and a coordinator for Comprehensive Project *CP 7: Quantum Geometry & Topological Methods in Physics*. She leads the Emmy-Noether group on *Discrete subgroups of semisimple Lie groups* and is a driving force of the Mathematics & Data research line, the Research Station Geometry + Dynamics and Heidelberg's Experimental Geometry Lab HEGL. Congratulations, Beatrice, on this well-deserved promotion! We appreciate your outstanding work and leadership, and look forward to your ongoing contributions to STRUCTURES and the broader academic community.

RESEARCH SPOTLIGHT

Assignment Flows: New Insights for Deep Learning & Data Analysis

Data labeling is the task of partitioning data, such as an image, into meaningful parts by assigning pre-defined or learned labels. This is crucial for algorithms spanning from computer vision (e.g. for self-driving cars) to medical image analysis. Assignment flows are models that formulate the assignment of labels to data as a smooth dynamical process, using methods from information geometry. Their geometric interpretation makes it easier to analyze and understand how labels are assigned to data points. Apart from providing a better understanding of learned parameters, assignment flows are well adapted to realistic datasets and can be connected to deep learning models.

Geometric Mechanics of Assignment Flows

Quite remarkably, the dynamical equations describing the labeling process display analogies to classical mechanical systems of interacting particles studied in theoretical physics. In exploratory project (EP) 2.1, STRUCTURES scientists found that such systems obey a set of *Euler-Lagrange equations* [1], allowing to apply methods from mechanics to find optimal paths for assigning labels.

Self-Certifying Classification

Deep assignment flows offer improvements also in the field of risk certification for image classification. In recent work [2], scientists from STRUCTURES were able to develop a new approach to self-certified learning. Self-certified learning refers to methods that do not just learn from data, but simultaneously certify their own performance on the same data. The use of assignment flows allows making a specific class of self-certifying models computationally tractable.

Literature:

1. Savarino, F., Albers, P., and Schnörr, C. (2021), Information Geometry, in press.
2. Boll, B., Zeilmann, A., Petra, S., & Schnörr, C. (2023). PAMM, 23(1), e202200169. doi:10.1002/pamm.202200169.

RESEARCH SPOTLIGHT

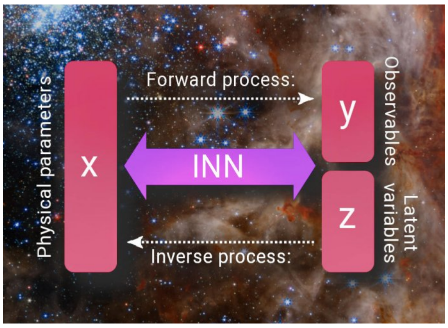
Invertible Neural Networks: Deep Learning Sheds Light on Cosmic Structures

When studying structures and their formation in diverse contexts, a recurring challenge is solving inverse problems. These involve the task of reconstructing unknown values ("X") of physical parameters of a system from actual observations ("Y"). For instance, this could involve inferring physical properties of stars, such as age, mass or composition, from their spectra.

Whereas the "forward" process, mapping physical properties X to observations Y, is often fairly well understood through simulations, the reverse task (predicting X from Y) is ambiguous. This is because, in general, the mapping of X to Y is not invertible. Observations can often constrain models only up to certain degeneracies, as different parameter sets may give rise to the same observations.

The Power of Invertible Neural Networks

The same problem arises in many areas of science and engineering, from biomedicine to cosmology. STRUCTURES groups (Klessen, Rother, Köthe) are addressing the challenges posed by inverse problems by developing and applying advanced deep learning approaches, known as *Invertible Neural Networks (INNs)* [1], which belong to the larger group of nor-



malizing flow methods [2]. In contrast to conventional neural networks, INNs learn the forward mapping from physical parameters X to observations Y – while simultaneously storing information about X that is not explained by the observations Y into an additional set of "latent" output variables Z. As a result, potentially relevant information is preserved, and the mapping becomes invertible. A variation of this approach, so-called *conditional INNs (cINNs)* uses the observables Y as a conditioning input for the mapping X→Z [3]. Both types of networks implicitly learn the inverse mapping too. This allows to recover the full posterior distribution of physical parameters X and to characterize possible degeneracies.

Unique Multidisciplinary Teamwork

The combined expertise and close collaboration of astrophysicists and computational scientists in STRUCTURES are crucial for developing, training and applying these methods. The INNs provide precise and reliable tools for astrophysics, while in turn, the physical inputs from simulations and observations inform the research on INNs.

Recently, international research teams led by scientists from STRUCTURES have used cINNs to characterize exoplanets [4], infer properties of star clusters and star-forming clouds [5], classify stars spectrally [6] and reconstruct 3D interstellar dust distributions [7]. They showed that INNs are a feasible and promising approach to gain new, unprecedented physical insights.

Literature

1. Ardizzone, L., Kruse, J., Wirkert S., Rahner, D., Pellegrini, E.W., Klessen, R.S., Maier-Hein, L., Rother, C., Köthe, U. (2018). Int. Conf. on Learning Representations.
2. Kobyzev et al. arXiv:1908.09257 29 (2019).
3. Ardizzone, L., Lüth, C., Kruse, J., Rother, C., Köthe, U. (2019). arXiv e-print.
4. Haldemann, J., Ksoll, V., Walter, D., Alibert, Y., Klessen, R. S., Benz, W., Koethe, U., Ardizzone, L., Rother, C. (2023). A&A, 672, A180.
5. Kang, D.E., Ksoll, V.F., Itrich, D., Testi, L., Klessen, R.S., Hennebelle, P., Molinari, S. (2023), A&A, 674, A175.
6. Kang, D.E., Pellegrini, E.W., Ardizzone, L., Klessen, R.S., Köthe, U., Glover, S.C.O., Ksoll, V.F. (2022), MNRAS, 512(1), 617.
7. Ksoll, V.F., Reissl, S., Klessen, R.S., Stephens, I.W., Smith, R.J., Soler, J.D., Traficante, A., Testi, L., Hennebelle, P., Molinari,S. (2023), in prep.

PROJECT REPORT

From CP6: Visualization of Discontinuous Vector Field Topology

Invited article by Egzon Miftari and Filip Sadlo (IWR)

Dynamical systems that include abrupt changes, known as piecewise-smooth systems, are encountered in various research and engineering domains, including *recurrent neural networks*.

To comprehend such systems, which can be formulated as *ordinary differential equations (ODEs)* with discontinuous right-hand sides, certain relaxing assumptions are required. In our research, we focus on *Filippov systems*, which extend differential equations to differential inclusion problems for which the right-hand side is set-valued. These Filippov systems exhibit crossing and sliding flow at discontinuities, i.e., trajectories can either cross or slide on them. We refer to such flow on the discontinuities as *discontinuity flow*.

Due to the nature of differential inclusion problems, solutions to Filippov systems are generally non-unique, which leads to time-irreversibility. That is, the preimage of the flow map becomes set-valued. To address this issue, we establish equivalence classes from these preimages, resulting in time-reversible flow on equivalence classes. As a consequence, streamlines generalize to "streamsets", on which we base our approach.

Vector field topology provides a qualitative understanding of vector fields by analyzing distinguished invariant sets, like critical points and their separatrices. At a critical point, the vector field is zero, i.e., its action has no effect. A *separatrix*, on the other hand, is a manifold consisting of streamlines that separates regions with qualitatively different flow behaviour. When applied to the lower-dimensional discontinuity flow in terms of streamsets, the streamsets of emerging critical structures within the discontinuity induce novel separating manifolds in the smooth regions, separating streamsets with qualitatively similar behaviour.

Moreover, so-called boundary switch curves, which mark the transition between sliding and crossing flow, significantly impact the nearby flow properties. This leads to the introduction of novel types of separatrices, so-called "equitrices", which play a pivotal role regarding the impact of discontinuities on the vector field topology of the smooth regions. Furthermore, traditional separatrices can be bypassed by streamsets, resulting in loss of their separating property. The regions of initial conditions capable of bypassing a separatrix are exactly bounded by equitrices.

In summary, our research introduces novel topological structures induced by discontinuity flow. This, along with the separatrices and equitrices arising from the boundary switch curves on discontinuities, extends traditional vector field topology to discontinuous flow, and accommodates its non-unique nature.

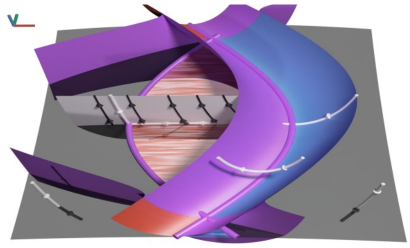


Fig 1: Topological analysis of a vector field with discontinuity (transparent gray) exhibiting sliding flow (red, line integral convolution). Qualitatively different equivalence streamsets (white) are separated by stable (blue) and unstable (red) manifolds. Equitrices (violet) separate streamsets of different dimensionality.

ABOUT CP6: NETWORKS & MACHINE LEARNING

Machine learning has become a spectacularly successful tool. The "learned machine" is an emergent structure that is not completely understood. CP6 addresses questions both of fundamental and practical importance: how can the structure of natural data be characterized? How can we improve training & representation? CP6 brings together expertise in network theory, image recognition, topology, and input from statistical mechanics.

STRUCTURES COMMUNITY

STEPS Mentoring Winter Semester 2023/24

The STEPS mentoring programme is set to kick off a new round of mentor-mentee pairing in winter 2023/24. Whether you are a first-time participant or have previously been involved, we eagerly anticipate your participation!

The STEPS Mentoring Programme

The *STRUCTURES Training & Education Programme for Success (STEPS)* is a step-by-step career programme for young researchers, designed to counsel and support them in particular at the transitional points of their scientific career, and to improve diversity and work-family balance in STRUCTURES. The mentoring programme is one of several measures, tailored to encourage meaningful interactions and networking among individuals from diverse professional backgrounds, fostering a culture of openness and mutual learning.

Application is open until November 06, 2023 Please feel free to contact us anytime in case of questions at office@structures.uni-heidelberg.de. The STRUCTURES Project

APPLY NOW

Simply fill out the matching form and send it via mail to office@structures.uni-heidelberg.de. **The call is open until Nov 06, 2023!**

Management Office is glad to help!

For this newsletter, we interviewed two YRC members on their experience with the programme: Sara Konrad (theoretical physics) and Denis Brazke (applied analysis):

Interview with Sara Konrad (Postdoc):

Sara Konrad (ITP)
AG Bartelmann, EP 6.3

Q: How was your experience with the mentoring programme? A: For me, it was a great experience! I was not only happy to help coordinating the programme for several semesters, but also took part as both a mentee and a mentor for PhD students.

Q: How well did you feel supported in your career? A: My mentor shared numerous enlightening tips that helped me on multiple levels, ranging from paper recommendations to career opportunities in academia that suit me and my family. In turn, my own interactions with mentees offered me many helpful insights and reflections.

Q: What advice would you give someone considering becoming a mentee or mentor? A: First, do it! Second, as a mentee, be open to what your mentor has to offer. Even if they have busy schedules, they genuinely enjoy being helpful. This leads to the third point: becoming a mentor is a truly rewarding and fulfilling endeavour, because you can give someone else so much by simply sharing your experience.

Interview with Denis Brazke (PhD student):

Denis Brazke (IMa)
AG Knüpfer and AG Marciniak-Czochra, CP 3

Q: How was your experience with the mentoring programme? A: I took part as a mentee, and it proved to be a enriching experience for me. Having regular appointments and a great mentor allowed me to track my progress effectively. My mentor's different field provided a diverse perspective on my issues, helping me understand the dynamic nature of the scientific environment and that there are multiple ways to work with people around you.

Q: How well did you feel supported in your career? A: It was reassuring to realize I wasn't alone in facing challenges. The programme went far beyond traditional support, offering insights into navigating my professional environment. Receiving a mentor's feedback and evaluation let's YOU make the changes.

Q: What advice would you give someone considering becoming a mentee or mentor? A: Take the opportunity seriously. Dedication and honesty are important for its effectiveness. I am immensely grateful that my mentor exemplified both, as I believe this is crucial for a successful mentorship.

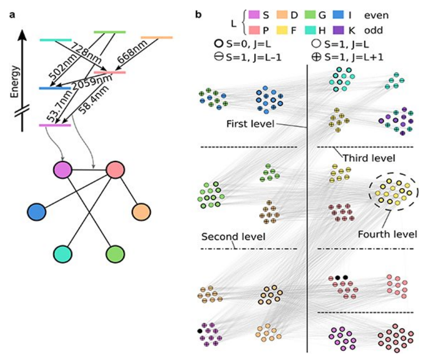
RESEARCH SPOTLIGHT

A Network Approach to Atomic Spectra

Network science is the analysis and modeling of complex systems as networks. As such, it provides a universal framework for understanding the structure and dynamics of a wide range of systems, with applications ranging from biological to social and computer networks. Its underlying holistic approach of analyzing connectivity and "community" patterns contrasts the reductionist viewpoint usually adopted in physics, where complex systems are modeled starting from fundamental sets of equations.

As system size increases, however, solving these equations becomes intractable. For instance, while the hydrogen spectrum can be derived analytically by solving the *Schrödinger equation* with a Coulomb potential, already the helium atom with just two electrons needs to be treated numerically. This is where network science becomes useful.

In a new interdisciplinary study, STRUCTURES scientists in collaboration with researchers from Strasbourg and Konstanz have applied network models to spectroscopic data of atoms to predict properties of their spectra. They found that *communities* reveal the emergence of quantum numbers and symmetries. A tool known as *link prediction* may furthermore allow to discover yet unknown atomic transitions. The work promotes a bidirectional exchange of methodology between network science and physics.



Credit: Wellnitz et al.

Original Publication:

Wellnitz, D., Kekić, A., Heiss, J., Gertz, M., Weidemüller, M., and Spitz, A. (2023), Journal of Physics: Complexity, vol. 4, no. 3, 2023. doi:10.1088/2632-072X/ace1c3.

STRUCTURES ON THE WEB

https://structures.uni-heidelberg.de

@structures_hd
@structures_heidelberg
@STRUCTURES_HD

The production of this newsletter is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy EXC 2181/1 - 390900948 (the Heidelberg STRUCTURES Excellence Cluster).

IMPRESSUM & CONTACT

Exzellenzcluster STRUCTURES
Universität Heidelberg
Philosophenweg 12 & Berliner Straße 47
D-69120 Heidelberg
office@structures.uni-heidelberg.de

Text & Editing: STRUCTURES Office: Sebastian Stapelberg, Guest Authors and Speakers