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Angelica Aviles-Rivero
Tsinghua University, China

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Frédéric Barbaresco
Thales Group, France

Symplectic Foliation-Informed Neural Network (SFINN) and Lie Groups Machine Learning Based on Jean-Marie Souriau Lie Groups Thermodynamics & Koszul Information Geometry

The symplectic model of statistical mechanics developed by Jean-Marie Souriau—termed the "Thermodynamics of Lie Groups"—extends the structures of information geometry to the realm of Lie groups. This framework enables the definition of Maximum Entropy Gibbs densities possessing the property of covariance under the action of the group operating on the system. Moreover, it generalises the Fisher-Rao-Fréchet metric to Lie groups, rendering it invariant under the group's action. Crucially, Shannon's axiomatic definition of entropy is supplanted by a purely geometric construction, wherein entropy emerges as a Casimir invariant function defined on the leaves of the foliation induced by coadjoint orbits through the moment map associated with the group action (the moment map being the geometric counterpart of Noether's theorem).

Souriau's thermodynamics of Lie groups introduces a web-like geometric structure composed of two transverse foliations: a symplectic foliation generated by coadjoint orbits (corresponding to the level sets of entropy) and a transverse Riemannian foliation (corresponding to the level sets of energy). The dynamics on each foliation make it possible to distinguish between non-dissipative phenomena (with constant entropy) and dissipative phenomena (with constant energy). This dynamic behaviour is governed by a metriplectic flow that encapsulates the first law of thermodynamics through Poisson bracket (quantitative conservation of energy) and the second law through metric flow bracket (qualitative degradation of energy and generation of entropy).

We shall explore the connections between TINNs (Thermodynamics-Informed Neural Networks), metriplectic flows, and the Lie groups thermodynamics. The overarching aim is for TINNs not merely to learn from data, but also to adhere to thermodynamic constraints, thereby enabling more accurate predictions and a deeper understanding of physical systems—particularly those characterised by dissipative phenomena.

Souriau Lie Groups Thermodynamics is studied in the framework of two european action, European CaLISTA COST action and European CaLIGOLA MSCA action.

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Tolga Birdal
Imperial College London, UK

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Cristian Bodnar
Silurian AI, UK

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Baris Coskunuzer
University of Texas Dallas, USA

Topological Compound Fingerprinting in Computer-Aided Drug Discovery

In this talk, I present a novel topology-based approach to virtual screening in computer-aided drug discovery using multiparameter persistence. Traditional methods relying on SMILES strings, molecular fingerprints, or deep learning models like VAEs and GNNs face challenges in scalability and performance saturation. Our method generates multidimensional topological fingerprints by decomposing compounds into chemically informed substructures and extracting persistent homology features at multiple resolutions. We reformulate VS as a graph ranking problem and use few-shot learning techniques to effectively rank compounds by drug-likeness. Our approach achieves substantial performance gains over state-of-the-art methods on benchmark datasets. For more details, please refer to our paper: https://arxiv.org/abs/2211.03808

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Xiaowen Dong
University of Oxford, UK

Bayesian Optimisation of Graph-based Functions

The increasing availability of graph-structured data motivates a new type of optimisation problems over graph-based functions, i.e., searching for the graph or node that maximises the value of an underlying function. Such optimisation problems are challenging due to the discrete and high-dimensional search space, as well as the underlying function that is often black-box and expensive to evaluate. In this talk, I will provide several examples on how Bayesian optimisation can be used to optimise graph-based functions, with practical applications in computational, epidemiological, and social networks. More broadly, these examples demonstrate the promise in combining probabilistic and geometric reasoning in analysing complex functions.

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Yue Gao
Tsinghua University, China

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Mustafa Hajij
University of San Francisco, USA

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Niu Huang
National Institute of Biological Sciences, China
Tsinghua Institute of Multidisciplinary Biomedical Research, China

Integrating HPC and AI: A New Paradigm for Predicting Protein-ligand Binding

In the process of small molecule drug discovery, the prediction of protein-ligand interactions urgently demands enhancements in computational accuracy and efficiency, given its crucial role in identifying novel lead compounds for new targets. However, current artificial intelligence (AI) models are constrained by the scarcity of large, high-quality protein-ligand complex structures and binding data, which consequently impairs their generalization ability, limiting their effectiveness in real-world applications. We have been actively exploring the potential of physics-based high performance computing (HPC). The remarkable computational power of HPC allows us to generate vast, top-tier datasets that are invaluable for both training and testing AI modes. When integrated with AI's proficiency in pattern recognition and predictive modelling, this combination allows for the rapid and in-depth analysis of molecular structures, more accurate prediction of drug-target interactions. Our ongoing research and practice will highlight the profound synergy between HPC and AI in facilitating more accurate and efficient calculations of molecular interactions, illuminating viable strategies to surmount existing data limitations and improve the predictive capabilities of AI models.

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Wei Huang,
RIKEN, Japan

Decoding Deep Graph Neural Networks: An Optimization and Generalization Perspective

Graph Neural Networks (GNNs) have emerged as a powerful framework for modelling graph-structured data, yet challenges such as over-smoothing, trainability degradation in deep architectures, and understanding the role of structural information remain. In this talk, we will explore two complementary research directions addressing these challenges from both optimization and generalization perspectives.

First, we will delve into the optimization dynamics of deep GNNs using a Graph Neural Tangent Kernel (GNTK) framework. This approach reveals an exponential decline in trainability as network depth increases—a phenomenon that standard residual connections can only partially mitigate. Based on these insights, we introduce the Critical DropEdge method, a connectivity-aware and graph-adaptive sampling strategy designed to fundamentally counteract this decay and enhance model performance.

In the second part of the talk, the focus shifts to the feature learning capabilities of GNNs. We will demonstrate how graph convolution, by leveraging inherent structural information, significantly amplifies signal learning while suppressing noise memorization. Comparative analyses with multilayer perceptrons (MLPs) highlight that graph convolution offers superior generalization.

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Stephen Huckemann
Georg-August-Universität Göttingen, Germany

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Stephan Klaus
Mathematisches Forschungsinstitut Oberwolfach, Germany

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Patrice Koehl
University of California, Davis, USA

A Physicist's View on Partial 3D Shape Comparison

Scientists have access to a wide range of digital sensors that allow them to report at multiple time and length scales on the subjects of their studies. Finding efficient algorithms to describe and compare the shapes included in those reports has become a central problem in data science. Those algorithms have gained from developments in computational geometry and in machine learning. In this talk I will present another source of support to further improve those algorithms. Using techniques from statistical physics, I show that we can define a possibly partial correspondence between 3D shapes, with a cost associated with this correspondence that serves as a measure of the similarity of the shapes. I will illustrate the effectiveness of this approach on synthetic data as well as on real anatomical data.

This is joint work with Dr Henri Orland, IPHT, CEA, Saclay, France.

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Ran Levi
The University of Aberdeen, UK

Foundations of Differential Calculus for Modules over Small Categories

Let k be a field and let C be a small category. A k-linear representation of C, or a kC-module, is a functor from C to the category of finite dimensional vector spaces over k. A motivating example for this work is the concept of a tame generalised persistence module, which can be reduced to the case where C is a finite poset. Unsurprisingly, it turns out that when the category C is more general than a linear order, then its representation type is generally infinite and in most cases wild. Hence the task of understanding such representations in terms of their indecomposable factors becomes difficult at best, and impossible in general. In a joint project with Jacek Brodzki and Henri Rihiimaki we proposed a new set of ideas designed to enable studying modules locally. Specifically, inspired by work in discrete calculus on graphs, we set the foundations for a calculus type analysis of kC-modules, under some restrictions on the category C. In this talk I will review the basics of the theory and describe some more recent advances.

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Zheng Ma
Shanghai Jiao Tong University, China

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Frank Nielsen
Sony Computer Science Laboratories, Japan

Computational Information Geometry on Bregman Manifolds and Submanifolds

We review the construction of a Bregman manifold from a Legendre-type convex function [1]. By further using a representation function, we show that alpha-divergences are representational Bregman divergences on the positive orthant cone and curved representational Bregman divergences on the probability simplex [2]. We describe clustering [3], nearest-neighbour query data structures [4], and Voronoi diagrams [5] on Bregman manifolds and submanifolds with several applications in statistics and data science. Finally, we present work in progress pyBregMan: A Python library for algorithms and data-structures on BREGman MANifolds [6].

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Paolo Piccione
University of Sao Paulo, Brazil

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Hans Riess
Georgia Institute of Technology, USA

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Roman Sauer
Karlsruhe Institute for Technology, Germany

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Lei Shi
Fudan University, China

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Zhiqin Xu
Shanghai Jiao Tong University, China

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Yaoyu Zhang
Shanghai Jiao Tong University, China

Towards Understanding the Condensation Phenomenon of Deep Neural Networks

Condensation (also known as quantization, weight clustering, or alignment) is a widely observed phenomenon where neurons in the same layer tend to align with one another during the nonlinear training of deep neural networks (DNNs). It is a key characteristic of the feature learning process of neural networks. However, due to the strong nonlinear nature of this phenomenon, establishing its theoretical understanding remains challenging. In this talk, I will present our systematic efforts to tackle this challenge in recent years. First, I will present results regarding the dynamical regime identification of condensation at the infinite width limit, where small initialization is crucial. Then, I will discuss the mechanism of condensation at the initial training stage and the global loss landscape structure underlying condensation in later training stages, highlighting the prevalence of condensed critical points and global minimizers. Finally, I will present results on the quantification of condensation and its generalization advantage, which includes a novel estimate of sample complexity in the best-possible scenario. These results underscore the effectiveness of the phenomenological approach to understanding DNNs, paving the way for a deeper understanding of deep learning in the near future.

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Difan Zou
University of Hong Kong, Hong Kong SAR

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