Approximation, AI and inverse problems: A physics-driven perspective

Session at the *6th Dolomites Workshop on Constructive Approximation and Applications*

Organizers: S. Guastavino, E. Perracchione

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Short description

In the last few years physics-driven methods, and/or more in general data-driven models, have gained popularity in various fields, such as in approximation theory, inverse problems and machine learning. Indeed, in approximation theory new target-driven bases are currently under investigation and could be successfully used for inverse issues. Moreover, as far as AI is concerned, many studies are devoted to penalizing the loss function with some physics constraints. This session welcomes contributions both theoretically and computationally-oriented related to these research topics, and eventually, with a particular focus on solar physics applications such as space weather, image reconstruction and signal processing.

This session is co-organized by the Politecnico di Torino and Università di Genova thanks to the funded project: Physics-based AI for predicting extreme weather and space weather events (AIxtreme) funded by La Compagnia di San Paolo and Fondazione CDP.

List of participants

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- Salvatore Cuomo, University of Naples Federico II, Napoli, Italy,
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- Mattia Rossi, Dipartimento di Matematica DIMA, Università di Genova, Genova, Italia,
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- Anna Volpara, Dipartimento di Matematica DIMA, Università di Genova, Genova, Italia

Schedule

	Mon. 9th	Tue. 10th	Wed. 11th	Thu. 12th	Fri. 13th
9:00 – 10:00					RoundTable
10:30 – 12:30		Volpara Cuomo Filbir Pintore		Legnaro Nicolini Mohammadami Pezzi	Final Remarks
16:00 – 18:00	Camattari Della Santa Audone Rossi	Round Table Free Discussion			

List of contributions

Time Series Decomposition: A Numerical Linear Algebra approach

Gianluca Audone
Politecnico Di Torino

Abstract: Non-stationary time-series are ubiquitous in real-world phenomena, and their complex nature poses challenges for traditional analysis methods like Fourier Transforms and wavelets. Understanding their components like trends, seasonality, and residuals provides valuable insights. This has led to the development of data-adaptive decomposition techniques, with Empirical Mode Decomposition (EMD) [4] being a prominent example. While EMD and other data-driven methods offer advantages, their performance can be sub-optimal in terms of accuracy, robustness to noise, and computational efficiency. To improve upon existing methods, hybrid techniques combining classical decomposition and deep learning approaches have emerged [1,2].

In this talk, we begin by reviewing state-of-the-art classical decomposition methods, including Seasonal and Trend Decomposition using Loess (STL) [3], Empirical Mode Decomposition (EMD), and Fast Iterative Filtering (FIF) [5]. We will then explore these methods through the lens of numerical linear algebra, revealing their underlying computational mechanisms. This perspective offers insights into how these methods might be further developed or integrated into hybrid approaches for improved analysis.

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Joint work with: Matt Nunes (University of Bath), Philippe Blondel (University of Bath) and Chris Budd (University of Bath)

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AI for feature selection in the context of geo-effective solar events prediction.

Fabiana Camattari
Università degli Studi di Genova

Abstract: In statistical learning and, specifically, in supervised learning enhancing sparsity is a crucial issue. In the machine learning (ML) framework, feature reduction techniques allow to identity which dimensions of a given dataset are more relevant to a specific task, then supervised learning models are trained with that reduced number of significant features. The first step is usually performed by means of linear models such as Lasso regression (or variations of it), Recursive Feature Elimination (RFE) and linear Support Vector Machines (SVMs), and once the features are identified non-linear models are exploited to predict the given task. Here we introduce a new approach, called in what follows greedy feature selection, which allows to perform an iterative selection depending on the classifier that has been chosen for the prediction phase. This technique is specifically applied in the realm of solar physics for the prediction of geo-effective manifestations of the active Sun, to understand which physical parameters are decisive for classifying an event. The models that have been considered include non-linear SVM and a Feed-forward Neural Network (FNN). Regarding the prediction phase, the selection of features with non-linear greedy method is then compared with state-of-art ML algorithms. Numerical results show that, usually, when only the few greedily selected relevant features are considered, classification performances are improved.

References

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Joint work with: Sabrina Guastavino (Università degli Studi di Genova), Francesco Marchetti (Università degli Studi di Padova), Michele Piana (Università degli Studi di Genova), Emma Perracchione (Politecnico di Torino)

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The Scientific Machine Learning Paradigms to Enhance Explainability in AI:

Salvatore Cuomo
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Abstract: Scientific Machine Learning (SciML) has emerged as a powerful tool for a wide spectrum of real-world challenges. This novel methodology has led to a reassessment and rethinking of traditional numerical methods, highlighting the need for more efficient and reliable approaches that integrate both model-driven and data-driven methodologies [1]. In this presentation, we will explore novel theoretical and applied challenges in SciML and their potential for practical applications in explainable Artificial Intelligence (XAI). By examining how these integrated methodologies enhance interpretability, we aim to discuss how SciML is a brach of XAI, fostering trust and reliability in AI systems across various scientific domains [2].

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Discontinuous Neural Networks for Learning Scaling Functions of Variably Scaled Kernels

Francesco Della Santa
Dipartimento di Scienze Matematiche, Politecnico di Torino

Abstract: This presentation introduces a novel approach for improving the accuracy of interpolation methods based on Variably Scaled Kernels (VSKs), learning the scaling function from data. The efficiency of using a proper scaling function in VSK methods is known to be critical and works in the literature suggest that such a function should mimic the key features of the target one (e.g., have the same discontinuity interfaces) [1]. Despite these empirical suggestions, there is a lack of practical methodologies for constructing such scaling functions; moreover, there is also a lack of theoretical justification behind these observations. The work illustrated in this presentation addresses these tasks by providing a theoretical foundation and a practical, user-independent tool for learning scaling functions using *Discontinuous Neural Networks*. The theoretical contribution of the work proves that a scaling function reflecting the target function can significantly enhance the approximation accuracy, providing solid foundations for the empirical observations reported in earlier studies. On the other hand, to fill the gap between theory and practice, we introduce a method for automatically learning the scaling function from data via a Discontinuous Neural Network (δNN) model [2]; indeed, δNNs are a class of neural networks capable of learning both continuous and discontinuous functions. Therefore, our approach leverages the learning abilities of δNNs to construct scaling functions that closely resemble the target function, both in the case of continuous and discontinuous target functions. We will present numerical examples that validate our theoretical claims and illustrate the practical benefits of our approach. These examples involve classic interpolation problems where the target function can be either continuous or discontinuous. In particular, we observe that the results demonstrate that the scaling functions learned by δNNs guarantee very good accuracy of VSK methods, outperforming standard kernel interpolation methods, particularly in scenarios with discontinuous target functions.

References

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Joint work with: Gianluca Audone, Emma Perracchione, Sandra Pieraccini (Dipartimento di Scienze Matematiche, Politecnico di Torino).

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Phase Retrieval from Spectrogram Measurements

Frank Filbir
Helmholtz Munich & Technische Universität München

Abstract: Phase retrieval (PR) in its general form refers to the problem of recovering a signal f from the magnitude of its frame coefficients $|\langle f, \phi_m \rangle|$. In the classical setting the analysing frame ϕ_m is given by the Fourier basis. The PR problem is of great interest in various fields of applied science like crystallography, diffraction imaging and many more. Recently a new diffraction imaging technique, now known as ptychographical imaging, was developed in order to image materials and biological tissue. Ptychography is a purely computational imaging technique. A detector (CCD camera) measures the intensity of many diffraction patterns each obtained by illuminating a small part of the object at a time. The measurements are produced by using light (X- rays) of one specific very short wavelength λ or an electron beam. The detector placed in the far-field distance (Fraunhofer diffraction). Mathematically this experimental set-up leads to the problem of phase retrieval from spectrogram measurements. That means we are given samples of

$$\mathfrak{I}(x,\xi) := \left| \int_{\mathbb{R}^2} f(t) g(t-x) e^{-2\pi i, \xi \cdot t}, \mathrm{d}t \right|^2$$

for a known window function g. The aim is to reconstruct the object f. However, often experimental set-ups do not allow to work with one specific wavelength λ but we have to deal with polychromatic measurements, i.e. we are given

$$\mathfrak{I}_\lambda(x,\xi) = \left| \int_{\mathbb{R}^2} f(t) g_\lambda(t-x)\, e^{-2\pi i, \xi \cdot t/\lambda}\, \mathrm{d}t \right|^2$$

for $\lambda \in \{\lambda_1, ..., \lambda_L\}$. Moreover, in many cases even the g_λ is unknown. This then leads to what is called *Blind Polychromatic Ptychographic Imaging* (BPPI). In this talk we will provide an overview of BPPI and we present some reconstruction methods and results.

Joint work with: The talk is based on joint work with Oleh Melnyk (TU Berlin), and our project partners Jan Rothardt (GSI Jena) and Nico Hoffmann (HZDR, Dresden) and the grup of Christian Schroer (DESY, Hamburg).

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Deep Learning Techniques for Sunspot Classification

Edoardo Legnaro
MIDA, Department of Mathematics, University of Genova

Abstract: A solar active region can significantly disrupt the Sun–Earth space environment, often leading to severe space weather events. Sunspots serve as the primary markers of these active regions, and specific sunspot types are closely associated with extreme space weather events such as coronal mass ejections and solar flares. Consequently, the automatic classification of sunspot groups is crucial for accurately and promptly predicting solar activity. In this talk, we will present our results in applying deep learning techniques to the classification of sunspot magnetograms based on the Mount Wilson classification scheme. We will explore the latest advancements in image classification architectures, from Convolutional Neural Networks to Vision Transformers, and determine the most effective network architectures for the sunspot classification task.

Joint work with: Sabrina Guastavino, Anna Maria Massone, Michele Piana (MIDA, Department of Mathematics, University of Genova).

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AIXtreme: the physics behind the space weather prediction tools

Gianalfredo Nicolini
INAF - OATo

Abstract: The Coronal Mass Ejections (CMEs) are the most violent manifestations of solar activity. They are huge eruptions of magnetized plasma that are expelled from the solar corona (the upper layer of the Sun's atmosphere) into interplanetary space. When directed towards the Earth, they interact with the Earth's magnetic field causing severe disturbances in the terrestrial magnetosphere, known as geomagnetic storms. The energy released by CMEs in geospace can induce major effects on human activities, either on ground or in space. Predicting CMEs, their time of arrival on Earth, and their geo-effectiveness, namely the intensity of induced geomagnetic storms, is therefore vital. This activity falls within the branch of heliophysics known as "Space Weather", which deals precisely with the study of solar-terrestrial relations. The different forecasting methods proposed so far can be classified into three major categories, namely empirical, drag-based and physics-based models. Recently, new approaches using Artificial intelligence (AI) are gaining increasing popularity in the prediction of geo-effective solar events. In fact, Machine/Deep Learning (ML/DL) techniques are increasingly being employed in Space Weather studies, often performing far better than previous models. This talk explores the physics of solar and magnetospheric processes behind the Space Weather prediction tools developed within the AIxtreme project.

An Unsupervised Quality Measure Predictor Loss for Algorithm Unfolding

Danilo Pezzi
Università degli studi di Modena e Reggio Emilia

Abstract: in the computational imaging domain, one classical tool is represented by variational models. With their established theoretical background, they have been, and still are, widely used in a variety of inverse problems. However, a persistent challenge lies in the selection of parameters, lacking definitive guidelines, which ends up limiting their potential. Bilevel optimization and algorithm unfolding, drawing inspiration from machine learning principles, present a promising road to address this issue by enabling the training of task-specific variational models with minimal data and computational resources. In this presentation, we delve into an approach aimed at constructing an unsupervised loss function tailored for bilevel optimization problems [1]. Unlike supervised methods reliant on ground truth data, our approach aims to directly assess image quality perceptually, aligning with human visual perception. To achieve this, we introduce and analyze a Mean Structural Similarity Index (MSSIM) predictor, whose performance is enhanced by taking advantage of the basic principles of no-reference image quality measures such as BRISQUE [2]. This model is tested on standard imaging problems, and while certain components exhibit task-specific characteristics, the overarching framework remains highly versatile, readily applicable across a spectrum of imaging applications.

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Joint work with: Silvia Bonettini, Giorgia Franchini, Elena Govi and Marco Prato from Università degli studi di Modena e Reggio Emilia.

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Joint work with: Roberto Susino, Daniele Telloni (INAF - OATo).

Computable and sharp upper bounds for the Lipschitz constant of neural networks

Moreno Pintore
Inria, Sorbonne University

Abstract: Precisely evaluating the Lipschitz constant of deep neural networks is computationally impractical even for neural networks with few layers. Indeed, the computational cost of such a computation scales exponentially with the number of neurons. On the other hand, the Lipschitz constant of a neural network is strictly related to its robustness and stability, and it is therefore important to efficiently estimate it. In this presentation [2], we discuss two novel upper bounds for fully-connected feed-forward neural networks and we prove that they are cheaper or sharper (in the ℓ^1 norm or in the ℓ^∞ norm) than similar alternatives available in literature [1,3]. A direct extension to convolutional neural networks including convolutional layers, average pooling layers and dense layers is possible, since such layers represent linear operators. Two generalizations to convolutional neural networks including max pooling layers are proposed. Numerical results in strong agreement with the theory are presented to test the novel bounds and compare their accuracy on different architectures.

References

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Joint work with: Bruno Després

Analyzing the application of the Physics-Informed Neural Network in financial calibration tasks.

Mohammadamin Raeisi Makiani
Allameh Tabatabai University, Teheran, Iran,

Abstract: In the calibration of a financial model, the process is an optimization task that can be viewed as an inverse problem. Solving this problem typically necessitates having an appropriate pricing function. With recent breakthroughs in machine learning, i.e., physics-informed neural network (PINN) a cutting-edge approach that combines artificial neural networks with fundamental physical principles, the task can be efficiently accomplished by constructing a proper map that acts like the pricing function. This paper centers on solving an inverse problem for a financial PDE model by means of PINN. Firstly, we will begin by modeling the bond price dynamics of catastrophe bonds (CAT bonds) and derive a partial integro-differential equation (PIDE) through a no-arbitrage strategy within the framework of an incomplete market. After that, we employ the PINN to estimate the model parameters by simulating the solution that pertains to the price of a particular CAT bond. We set the parameters as learnable ones, and then the network approximates the value of the parameters in a such way that the loss function can be minimized.The outcomes demonstrate that PINNs have the capability to solve the inverse problem effectively.

Joint work with: Abdolsadeh Neisy and Salvatore Cuomo

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Modeling the Dynamics of Interplanetary Coronal Mass Ejections: A Physics-Informed Machine Learning Approach

Mattia Rossi
MIDA, Department of Mathematics, University of Genova

Abstract: Interplanetary Coronal Mass Ejections (ICMEs) are large explosions resulting from solar activity that propagate through the interplanetary medium. ICMEs impacting the Earth may be correlated with geomagnetic storms, which, in turn, may significantly affect the near-Earth space environment. Consequently, for space weather monitoring, it is essential to estimate ICMEs' travel time.

To this end, unlike purely data-driven Machine Learning (ML) techniques, we will present a physics-informed ML approach, where physics enters a) the loss functions, designed on the basis of various extensions of the drag-based deterministic model (DBM; see, e.g., [1]), and b) the data, both real and synthetically DBM-generated. Validations of the models presented, as well as sensitivity analyses on the propagation of the uncertainty affecting the data, will be examined.

References

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Joint work with: Sabrina Guastavino, Anna Maria Massone, Michele Piana (MIDA, Department of Mathematics, University of Genova), Daniele Telloni, Roberto Susino (INAF–OATo, Osservatorio Astrofisico di Torino).

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A new approach for regularized imaging-spectroscopy in high-energy solar astronomy

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Abstract: Fourier-based imaging is a key methodological approach in several astronomical frameworks. The Spectrometer/Telescope for Imaging X-rays (STIX, [1, 2, 3]) on-board ESA Solar Orbiter is an indirect imaging telescope designed to observe a wide range of solar flares in the energy range from 4 up to 150 keV. In this case, very few samples of the spatial Fourier transform of the incoming radiation flux, named visibilities, are measured by few sub-collimators providing information about flaring X-ray sources. Hence, the imaging problem for STIX consists in reconstructing the X-ray photon flux from a sparse sampling of its Fourier transform. This problem is particularly challenging due to the limited number of visibilities measured by the instrument, which makes image reconstruction ill-posed in the sense of Hadamard. Several image reconstruction methods have been developed and are available to the STIX community, including constrained maximum entropy [4], multi-scale CLEAN, feature augmentation [5], and Particle Swarm Optimization for parametric imaging [6].
In this presentation, we introduce a new approach to image reconstruction across many different energy channels. Our method is designed to generate smoothed reconstructed maps along the energy direction, enabling effective regularization in imaging-spectroscopy. Applications concerned with both synthetic visibilities and experimental data are eventually showed to demonstrate the efficacy and efficiency of this approach.

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Joint work with: Michele Piana (Università di Genova), Anna Maria Massone (Università di Genova), Fabiana Camattari (Università di Genova), Emma Perracchione (Politecnico di Torino), Frank Filbir (Helmholtz Center Munich German Research Center for Environmental Health), Alessandro Lupoli (Technical University of Munich and Munich Center for Machine Learning)