BOOK OF ABSTRACTS

The 4th International Conference
and Summer School

Numerical Computations: Theory and Algorithms NUMTA 2023

edited by
Yaroslav D. Sergeyev
Dmitri E. Kvasov
Maria Chiara Nasso

UNIVERSITÀ DELLA CALABRIA
DIPARTIMENTO DI
INGEGNERIA INFORMATICA,
MODELLISTICA, ELETTRONICA
E SISTEMISTICA
DIMES

Department of Computer Engineering, Modelling,
Electronics and Systems Science,
University of Calabria,
in cooperation with
Society for Industrial and Applied Mathematics, USA

Book of Abstracts
of the 4th International Conference and Summer School

Numerical Computations: Theory and Algorithms

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TUI Magic Life Calabria - Pizzo (VV)
Calabria, Italy
June 14-20, 2023

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NUMERICAL COMPUTATIONS: THEORY AND ALGORITHMS
Fourth International Conference and Summer School NUMTA-2023
14-20 June 2023, TUI Magic Life Calabria - Pizzo (VV), Italy

Dear Participants,

Welcome to the Fourth Triennial International Conference and Summer School NUMTA-2023 "Numerical Computations: Theory and Algorithms". The Conference is organized by the Department of Computer Engineering, Modeling, Electronics and Systems Science of the University of Calabria, Italy in cooperation with the following departments of the same university: Department of Mathematics and Computer Science; Mechanical, Energy, and Management Engineering Department; and Civil Engineering Department. We are proud to inform you that, as the previous three editions, NUMTA-2023 is organized in cooperation with the Society for Industrial and Applied Mathematics (SIAM), USA. The previous editions of NUMTA took place in several beautiful places in Calabria in 2013, 2016, and 2019. This fourth edition has been postponed from 2022 to 2023 due to the difficulties created by the COVID-19 pandemic.

The goal of all NUMTA Conferences is to create a multidisciplinary round table for an open discussion on numerical modeling nature by using traditional and emerging computational paradigms. The NUMTA-2023 Conference will discuss all aspects of numerical computations and modeling from foundations, philosophy and teaching to advanced numerical techniques. New technological challenges and fundamental ideas from theoretical computer science, machine learning, linguistic, logic, set theory, and philosophy will meet requirements and new fresh applications from engineering, physics, chemistry, biology, economy, and teaching mathematics.

Researchers from both theoretical and applied sciences have been invited to use this excellent possibility to exchange ideas with leading scientists from different research fields. Papers discussing new computational paradigms, relations with foundations of mathematics, and their impact on natural sciences have been particularly solicited. A special attention during the Conference will be dedicated to numerical optimization techniques and a variety of issues related to theory and practice of the usage of infinities and infinitesimals in numerical computations. In particular, there will be a substantial bunch of talks dedicated to a recent promising methodology allowing one to execute numerical computations with finite, infinite, and infinitesimal numbers on a new type of a supercomputer – the Infinity Computer patented in several countries.

We are happy to inform you that researchers from the following 31 countries participate at the Conference: Austria, Canada, China, Cyprus, Czech Republic, Finland, France, Germany, India, Iran, Italy, Japan, Kuwait, Latvia, Lebanon, Lithuania, Malta, Marocco, Norway, Philippines, Portugal, Romania, Russia, Serbia, Singapore, Spain, Thailand, Turkey, Ukraine, United Kingdom, and USA. Plenary lectures and tutorials will be delivered by scientists who are undiscussed leaders in their research fields.

Post conference Proceedings of NUMTA-2023 will be published by Springer as a dedicated volume of the prestigious collection "Lecture Notes in Computer Science".

Authors of selected talks will be invited to submit full papers to special issues of the premier international journals dedicated to the Conference.

The Organizing Committee expresses its gratitude to organizations that have offered their support to the international conference NUMTA-2023. This support was essential for the success of this event:

- Department of Computer Engineering, Modeling, Electronics and Systems Science, University of Calabria, Italy;
- Department of Mathematics and Computer Science, University of Calabria, Italy;
- Mechanical, Energy, and Management Engineering Department, University of Calabria, Italy;
- Civil Engineering Department, University of Calabria, Italy;
- Institute of High Performance Computing and Networking of the National Research Council, Italy;
- Springer;
- E4 Computer Engineering;
- Bonomo Editore, Italy.

We wish to all participants a very successful work and hope that the Conference will give you a lot of inspiration leading to new important results in your research fields.

Yaroslav D. Sergeyev
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Distinguished Professor
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Plenary lectures and tutorials

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Spectral solution in time of evolutionary problems

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The numerical solution of Hamiltonian and, more generally, conservative problems has led to the definition of the class of energy-conserving Runge-Kutta methods named *Hamiltonian Boundary Value Methods (HBVMs)* [1,2]. Such methods, in turn, can be regarded as a truncated expansion of the vector field along the Legendre polynomial basis.

This interpretation of the methods has naturally led to their use as *spectral methods in time*, able to obtain spectral accuracy for general ODE problems. This has been possible by virtue of an extremely efficient Newton-type procedure for solving the generated discrete problems.

In so doing, such methods can be also used for efficiently solving multi-frequency, highly-oscillatory problems, with the possibility of using relatively huge time-step in the numerical solution.

Multi-frequency, highly-oscillatory problems naturally arise when using the methods of lines for solving Hamiltonian (or in general, hyperbolic) PDEs with the method of lines. Coupling a spectral space semi-discretization with a spectral accuracy in time, then allows solving very accurately this kind of problems with a highly efficient algorithm [3].

Acknowledgements.

This work was carried out in collaboration with Felice Iavernaro, University of Bari, Italy.

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Infinite computations and Büchi automata using Grossone

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Traditional models of computation on finite strings can accept strings or produce a result of a computation (see, e. g., [2]). However, when a computation continues for an indefinite (infinite) period a different model of computation is needed. Büchi automata provide such a model of computation. Büchi automata are finite automata operating on infinite strings. A computation is successful (or accepted) by a Büchi automaton if, given a set of favorable states, a favorable state (or states) occur(s) infinitely often. However, there is no accounting for non-favorable states also occurring infinitely often. Hence, the meaning of a successful computation of Büchi automata can have lower than acceptable accuracy. In this talk, the new paradigm of the infinite unit axiom and grossone (see, e. g., [1, 3, 4]) is applied to extend the computational accuracy of Büchi automata and leads to a more accurate meaning of a successful computation on an infinite string.

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The use of Grossone in optimization, classification, and feature selection problems

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In recent years, a number of papers have demonstrated the ability of the new computational methodology proposed by Y.Sergeyev and based on Grossone in solving nonlinear single and multiobjective optimization as well as global and nonsmooth optimization problems. This new paradigm has also been successfully utilized in Machine Learning algorithms and, specifically, in solving classification problems using sparse Support Vector Machines (SVMs) and new linear and spherical separation methods. Moreover, new formulations for the L0 pseudo norm that is beneficial in inducing sparsity in the solution can be constructed thus reducing the number of input variables in a predictive model (Feature Selection). In this talk, the use of new computational methodology will be discussed in the context of novel variations of the classical SVMs methods that utilize pairs of hyperplanes that are not necessarily parallel. Also in this case, the use of Grossone will allow selecting only an important subset of the features.

Evolutionary multi-criterion optimization: An emerging computational problem-solving tool

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Most problems in science, engineering and commerce involve more than one conflicting criteria to be simultaneously optimized. Despite the vast literature on scalarizing multiple criteria into one, evolutionary optimization methods of treating them as truly multi-criterion problems in a Pareto sense produce a number of additional benefits to the users. Their ability to find and maintain multiple trade-off solutions with a flexible and customizable framework provides vital knowledge about the problem in addition to the optimal solutions themselves. In this lecture, we shall present a few popular and state-of-the-art algorithms, demonstrate their advantages on a number of real-world practical problems from engineering and society, and introduce some recent research topics. Additionally, the use of machine learning algorithms and human knowledge in enhancing their performance, and the use of multi-criterion algorithms in enhancing performance of machine learning methods will be discussed.

DC Learning: Recent advances and ongoing developments

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One of the challenges for the scientists at the present time consists of the optimal exploitation of a huge quantity of data of the information stored in various forms. The knowledge extraction from these data requires the use of sophisticated techniques and high performance algorithms based on solid theoretical foundations and statistics. Based on the powerful arsenal of convex analysis, DC (Difference on Convex functions) programming and DCA (DC Algorithms) are among the few nonconvex optimization approaches that can meet this requirement. Machine Learning represents a mine of optimization problems that are almost all DC programs for which appropriate resolutions should resort to DC programming and DCA. During the last two decades DC programming and DCA have been successfully developed for modeling and solving a lot of nonconvex programs in various areas of machine learning. They constitute the so called DC Learning (DCL) framework.

This talk presents recent developments on DCL. After a brief introduction to DC programming and DCA we give a review and analysis on the existing DCL methods. Next, we discuss recent advances and ongoing developments in DCL including DCL with sparsity and uncertainty, Online learning & Stochastic learning on Big data, etc.

Computing derivatives on the Infinity Computer

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In this lecture, algorithms for the computation of derivatives [1], Lie Derivatives [3], gradient vectors, Jacobian and Hessian matrices based on the Infinity Computer Arithmetic are presented. A preliminary Matlab class that uses a subset of the Infinity Computer Arithmetic has been implemented. The proper usage of this class enables the integration of the Infinity Computer into codes that require computation of derivatives. The potential of using this class is demonstrated by its application to the following areas:

- Computation of the Jacobian in codes for solving Boundary Value Problems. Examples of the solution of Optimal Control Problems with indirect methods will be presented [2];
- Computation of high-order dense output for super-convergent collocation Runge-Kutta methods (Gauss-Lobatto and Gauss-Legendre methods);
- Solution of Ordinary Differential equations using multi-derivative methods [3,4];
- Computation of gradients.

The discussed set of successful case-studies shows the Infinity Computer Arithmetic to be a very promising tool for scientific numerical applications.

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Computational approaches for solving general systems of nonlinear equations in the cloud

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Finding one or more solutions to a system of nonlinear equations (SNE) is a computationally hard problem with many applications in sciences and engineering. First, we will briefly discuss classical approaches for addressing (SNE). Then, we will discuss the various ways that a SNE can be transformed into an optimization problem, and we will introduce techniques that can be utilized to search for solutions to the global optimization problem that arises when the most common reformulation is performed. We will present computational results in the cloud using different state of the art heuristics.

Society-oriented developments of machine learning: Challenges and opportunities

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Over the recent years, we have been witnessing numerous achievements of Artificial Intelligence and Machine Learning (ML), in particular. We have seen highly visible accomplishments encountered in the domains of natural language processing and computer vision impacting numerous areas of human endeavours. Being driven inherently by the technologically advanced learning and architectural developments, ML constructs are highly impactful coming with far reaching consequences; just to mention autonomous vehicles, health care, imaging, decision-making processes in critical areas, among others.

We advocate that the design and analysis of ML constructs have to be carried out in a holistic manner by identifying and addressing a series of central and unavoidable societal quests. The key challenges on the list of interest concerns interpretability, energy awareness (being also lucidly identified on the agenda of green AI), efficient quantification of quality of ML constructs, and privacy. The credibility of ML models and credibility of their results are also of concern to any critical application. The above stated quests are highly intertwined and exhibit direct relationships with the computational end of ML.

The talk elaborates on the above challenges, offers definitions and identifies the linkages among them. In the pursuit of coping with such challenges, we advocate that Granular Computing can play a pivotal role offering a sound conceptual environment and realizing algorithmic development. An essential role of information granularity is identified. We advocate that the credibility (confidence) of results produced by ML constructs is inherently expressed in the form of information granules; several development scenarios are revisited including those involving constructs in statistics (confidence and prediction intervals), probability (Gaussian process models), and granular parameters (supported by fuzzy sets techniques).

As detailed studies, we discuss the ideas of federated learning (emphasizing a way in which data privacy becomes addressed) and knowledge transfer (by demonstrating on how a thoughtful and prudently arranged knowledge reuse supports energy-aware ML computing). Knowledge distillation leading to model compression is also studied in the context of transfer learning.

Smooth random functions and smooth random ODEs

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What is a random function? What is noise? The standard answers are nonsmooth, defined pointwise via the Wiener process and Brownian motion. It is equally possible, however, to define random objects via Fourier series with random coefficients, and this makes both concepts and computations simpler. In this talk we review these "smooth random functions." Integrals give smooth random walks, which approach Brownian paths as the wavelength parameter lambda shrinks to 0, and smooth random ODEs, which approach stochastic DEs of the Stratonovich variety. Numerical explorations become very easy in this framework.

Infinity computing: Foundations and practical computations with numerical infinities and infinitesimals

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In this lecture (that is self-contained, does not require any special high-level mathematical preparation and is oriented on a broad audience), a recent computational methodology is described (see [1-3]). It has been introduced with the intention to allow one to work with infinities and infinitesimals numerically in a unique computational framework and in all the situations requiring these notions (recall that traditional approaches work with infinities and infinitesimals only symbolically and different notions are used in different situations related to infinity, e.g., infinity in mathematical analysis, ordinals, cardinals, etc.). The methodology is based on the Euclid's Common Notion no. 5 "The whole is greater than the part" applied to all quantities (finite, infinite, and infinitesimal) and to all sets and processes (finite and infinite).

One of the strong advantages of this methodology consists of its computational power in practical applications (broadly discussed at these conferences by numerous colleagues, see also [1-4]). The methodology uses as a computational device a new kind of supercomputer called the Infinity Computer patented in several countries. It works numerically with a variety of infinite and infinitesimal numbers that can be written in a positional system with an infinite radix using floating-point representation. Numbers written in this system can have several infinite and infinitesimal parts. On a number of examples, it is shown that the new approach can be useful from both computational and theoretical points of view. In particular, the accuracy of computations increases drastically, and all kinds of indeterminate forms and divergences are avoided. The accuracy of the obtained results is continuously compared with results obtained by traditional tools used to work with mathematical objects involving infinity. It is argued that traditional numeral systems involved in computations limit our capabilities to compute and lead to ambiguities in certain theoretical assertions, as well. It is shown that the new methodology allows to avoid several classical paradoxes related to infinity and infinitesimals.

The Infinity Calculator working with infinities and infinitesimals numerically is shown during the lecture. Supporting materials, videos of lectures, more than 60 papers of authors from several research areas using this methodology in their applications, and a lot of additional information can be found at the page https://www.theinfinitycomputer.com The web page https://www.numericalinfinities.com developed at the University of East Anglia, UK is dedicated to teaching this methodology.

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Multidisciplinary topology optimisation: Where we are and where we aim to be

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To date, topology optimisation has been single-disciplinary, mostly structural, with a growing number of attempts to do it in other domains, e.g. in the domains of fluid mechanics and electromagnetics simulation.

This tutorial reviews the state of the art in this area as well as reports recent developments of QMUL research group in multidisciplinary topology optimisation, e.g. fluid mechanics simulation interacting with solid mechanics simulation in a topology optimisation loop.

In order to address all requirements related to the individual disciplines in an optimisation problem, the optimisation strategy has to be separated from the disciplinary simulation runs, in which the objective function(s) and constraints are evaluated. A metamodel-based optimisation strategy is used because a single-disciplinary simulation time can be several hours (can even be a day+), so coupling it directly to an optimisation routine is infeasible. Pros and cons of different parameterisation types, including level set-based, will be reviewed.

This lecture will report the current progress of the QMUL's team including problems where a structural simulation (based on the finite element analysis) is combined with computational fluid mechanics simulation in the design optimisation loop.

The presentation will conclude with a review of specific features of adding other simulation types, e.g. electromagnetic simulation and aeroacoustics. Examples will focus on of real-life aerospace-related applications including on-orbit repurposing of space structures.

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Presentations from special sessions and regular presentations

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A variational quantum soft actor-critic algorithm for continuous control tasks

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Keywords. Reinforcement Learning; Parametrized Quantum Circuits; Continuous control.

Quantum Computing promises the availability of computational resources and generalization capabilities well beyond the possibilities of classical computers. An interesting approach approach for leveraging the near-term, Noisy Intermediate-Scale Quantum Computers, is the hybrid training of Parameterized Quantum Circuits (PQCs), i.e. the optimization of a parameterized quantum algorithms as a function approximation with classical optimization techniques [1]. When PQCs are used in Machine Learning models, they may offer some advantages over classical models in terms of memory consumption and sample complexity for classical data analysis [2]. In this work we explore and assess the advantages of the application of Parametric Quantum Circuits to one of the state-of-art Reinforcement Learning algorithm for continuous control - namely Soft Actor-Critic. We investigate its performance on the control of a virtual robotic arm by means of digital simulations of quantum circuits. A quantum advantage over the classical algorithm has been found in terms of a signi

cant decrease in the amount of required parameters for satisfactory model training, paving the way for further developments and studies [3].

Acknowledgements.

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Exploratory spatio–temporal data analysis of influenza-like illness and its association with COVID-19 incidences in Baguio City

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Keywords. Influenza-like illness; spatial clustering; temporal pattern; disease mapping; SARS-CoV-2 pandemic.

Spatio-temporal data mining of small-area incidence rates derived from surveillance data portrays the distribution pattern and intensity of influenza-like illness (ILI) and its association with the spread of COVID-19. This investigation includes an exploratory analysis of the incidences of ILI surveillance from 2011 to 2022 by investigating spatial clustering, hotspots, temporal patterns, and its association with the SARS-CoV-2 pandemic from 2020 to 2022 in Baguio City. Influenza seasons and laboratory-confirmed COVID-19 epidemic curves were compared and analyzed according to granular geographic location, time distribution, and age structure. A SARIMA$(1,1,0)(1,0,0)_{52}$ model fits well for forecasting the ILI incidence in Baguio City. The mapping of hotspots of ILI and COVID-19 incidents shows that the clustering of both diseases is evident in the city center. The computed Moran's I indices for COVID-19 suggest clustering of high incidences among neighboring locals in Baguio City, Philippines. The evidence enables health-system policymakers to a proper assessment of health strategies.

Acknowledgements. This research was supported by the University of the Philippines Baguio - Research Load Credit Grant.

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Optimal control for stochastic multi-agent systems with the use of parallel hybrid genetic algorithms

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Keywords. Optimal control; multi-agent systems; hybrid genetic algorithms; particle swarm optimisation.

In modern times, stochastic large-scale multi-agent systems (MAS) aimed to supporting socio-economic planning are being developed. There is a well known problem of a high computational complexity task of an optimal control for multiple agents' behaviour in models of random interactions. In particular, agents (such as sellers and buyers, etc. [1]) should make individualised decisions on establishing interconnections to exchange products, money or information at each moment of time. Such decisions affect values of agents' utility functions that, as a rule, should be maximised. In fact, each agent forms the set of individual states that define whether or not the interaction with other agents is allowed at moments of time. As a result, the dynamic programming method should be applied at the individual level of each agent maximises own utility function, that is the extremely complexity task. To overcome appropriate difficulties and seek suboptimal individual decisions in such MAS, novel parallel hybrid real-coded genetic algorithms have been developed. The proposed hybrid methods combine the use of real-coded genetic algorithms (e.g., [2]) for an evolutionary search, particle swarm optimisation for reducing the need number of model recalculations and periodically engaging ANN-based surrogate models for the fitness-function approximation. The approach allows to improve significantly the time-efficiency of seeking optimal individualised decisions in MAS while keeping up their quality.

Acknowledgements.
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Circuit-based numerical solutions of transmission lines: application to KdV equations

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Keywords. Trasmission Lines; KdV; Soliton.

Transmission lines, devices employed for the transmission of electrical signals, can be used for the approximation of non-linear partial differential equations (PDEs) also in the nonlinear case. To this end, transmission lines are used to spatially discretize PDEs allowing the problem to be solved numerically even for intricate boundary conditions [2] - e.g. at intersection of many wires in the system. Using transmission lines to solve the Korteweg-de Vries Equation (KdV) allows for efficient and accurate numerical solutions, as it provides a method to investigate the propagation of wave-like information in nonlinear and dispersive media with multiple dimensions. In the present paper a software developed in C# is presented, the latter employs discretization by transmission lines and the Runge-Kutta 4-5 integration algorithm to numerically solve the KdV equation in the one-dimensional case. The implemented program, named "WireExplorer," is able to simulate the propagation of solitonic pulses on different types of circuits composed of one or more wires, even in the case of intersections. Such conditions are not canonically solvable by resolution of the KdV equations, while approximate numerical resolution allowed the evaluation of these intricate cases. In particular, the obtained results showed the subdivision of the wave into smaller components, at intersections between wires, which propagate in different directions showing also the formation of dispersive tails propagating in the direction opposite to that of the main wave.

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On the numerical solution of BVPs with discontinuites

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In this talk we propose a new update of the BVP-HOFiD code for the numerical solution of second order BVPs

$$f(x, y, y', y'') = 0, \qquad x \in [a, b], \quad y : [a, b] \to \mathbb{R}, \tag{1}$$

with suitable boundary conditions. This code is based on High Order Finite Differences (HOFiD), see [2]. Given a vector of mesh points $\boldsymbol{x}$ in $[a, b]$, the considered schemes allow us to approximate the derivatives as ($\boldsymbol{y} \approx y(\boldsymbol{x})$).

$$y''(\boldsymbol{x}) \approx A\boldsymbol{y} \quad \text{and} \quad y'(\boldsymbol{x}) \approx B\boldsymbol{y}$$

so that the discrete problem associated with (1) is the following nonlinear system in the unknown $\boldsymbol{y}$

$$f(\boldsymbol{x}, \boldsymbol{y}, B\boldsymbol{y}, A\boldsymbol{y}) = 0.$$

The new proposed version allows the solution or its first derivative contain discontinuites and the problem depend on a number of unknown parameters. This kind of equations often arise from physical problems and, in particular, our interest emerged from the study of a self-gravitating gas model in presence of phase changes, such as the one described in [1] concerning the van der Waals' gas model. Here we explore the solution of its isothermal fluid-static field which, through appropriate transformations, requires the solution of a single second-order differential equation with a discontinuity in an unknown point of $[a, b]$.

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On Kasner polygons defined for a sequence of complex parameters

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Keywords. keywords.

Starting with a fixed polygon $(A_0^1A_0^2\dots A_0^k)_{n\geq 0}$ and a sequence of complex numbers $(\alpha_n)_{n\geq 0}$, one defines the sequence of Kasner iterations $(A_n^1A_n^2\dots A_n^k)_{n\geq 0}$, in such a way that the point A_{n+1}^j, "divides" the segment $[A_n^jA_n^{j+1}]$, in the ratio $1-\alpha_n:\alpha_n$, for $j=1,\dots,k$ and $n\geq 0$, with the convention $A_n^{k+1}=A_n^1$.

We provide conditions ensuring that such iterations are convergent, periodic or divergent, extending some previous results.

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Dynamic geometries generated by sequences of nested triangles

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Keywords. Dynamic geometry; nested triangles; power curve of a triangle.

Starting from an initial triangle, one may wish to check whether a sequence of triangles obtained by geometric iterations is convergent, or is convergent in some shape, and to find the limit. In this paper we first prove a general result for the convergence of a sequence of nested triangles, then we study some properties of the power curve Γ of a triangle. These properties are then used to prove that the sequence of nested triangles defined by a point $Q^{(s)}$ on the power curve converges to a point for every $s \in [0, 2]$.

In particular, we obtain that the sequence of nested triangles defined by the incenter converges to a point, completing the main result in [4]. Finally, we present some numerical simulations which inspire open questions regarding the convergence of such iterations.

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Computer Analogy Method and its Application for Solving Complex Systems of Differential Equations

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Keywords. Theoretical computer model; formalization; digit shifting procedure, differential equations.

This method is based on the formalization of computer operations and new numerical and analytical representations of solutions, see [1]. This approach is actually a theoretical model of a classical computer and uses two basic operations with numbers, namely their representation in the form of segments of a power series and the digit shifting procedure. The method currently is developed for the study and solution of complex nonlinear systems of differential equations. It is possible to propose a finite-difference scheme that approximates the system. In turn, the computer analogy method approximates the solution representing by this scheme. We introduce a discrete parameter t (the time step or the iterative parameter, if we consider, for example, a stationary problem and use the iterative method for solve it). Then the algorithm (one can call it "t-computer") implies the introduction of a segment of the series in powers of t. As a result, we get the finite segment of the series, where the first term is regular, and the remaining terms are quasi-stochastic, which allows us to use probabilistic and statistical methods to obtain a solution. The computer analogy method is applied to solve systems of Lorenz, Shimizu-Morioka, Ressler and others. The given systems can create chaotic attractors. The representation of the solution is reduced to the sum of two terms for all systems of differential equations under consideration. The constraint of the highest third degree to ensure approximation is satisfied, since all of these systems have a quadratic non-linearity. An analytical representation of solutions for these systems is constructed according to the developed method.

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A nonlinear semiproximal SVM approach for Multiple Instance Learning

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Keywords. Multiple Instance Learning; semiproximal approach; instancespace.

We face binary Multiple Instance Learning (MIL) problems [3], whose objective is to discriminate between two types of point sets: positive and negative. In the MIL terminology, such sets are called bags and the points inside each bag are called instances. The main characteristic of a MIL problem is that, differently from the classical supervised classification, in the learning phase we know only the labels of the bags, whereas the label of each instance inside the bag is unknown.

Considering the case with two classes of instances (positive and negative), we start from the standard MIL assumption, very common in literature, stating that a bag is classified positive if it contains at least a positive instance and negative when all its instances are negative. In particular, for solving such problems, we propose a nonlinear version of the recent Semiproximal Support Vector Machine algorithm [1], which combines the well known Support Vector Machine (SVM) technique with the Proximal Support Vector Machine (PSVM) idea [2], the latter revealed very effective for supervised learning, especially in terms of computational time.

Numerical results are presented on some benchmark test problems drawn from the literature.

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Optimal Transport Flow Distributions on Congested Dynamic Networks

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Keywords. Network flow; Wardrop optimal flow; Wardrop optimal network; evolutionary game dynamics; replicator equation; replicator dynamics.

This paper is motivated by optimal flow allocation in networks as one of the central problems with both theoretical and practical aspects in communicaton and transportation networks. It was J. Wardrop who formulated two principles of optimality of flows in networks that describe the user (Wardrop) equilibrium and the system optimum. The Wardrop equilibrium is an optimal flow distribution across alternative parallel links in the network that minimizes the effective costs of the links defined as the sum of the latency at the given flow and the price of the link, while the system optimum is the optimal flow distribution for which the average effective cost for all used links is minimal.

We study the *Wardrop optimal flows* that satisfy both principles, the Wardrop equlibrium and the system optimum. A network that has a Wardrop optimal flow is called a *Wardrop optimal network*. We investigate dynamic properties of the Wardrop optimal networks and examine the Wardrop optimal flows on networks of parallel links. We present a characterization of Wardrop optimal flows and provide a geometric description of the set of all Wardrop optimal networks with common Wardrop optimal flow. We propose a new dynamical model of optimal flow distribution using the ideas of evolutionary game theory by presenting a discrete-time replicator equation on Wardrop optimal network. We describe the dynamics, equilibrium and stability conditions of the replicator equation. The obtained results can shed a new light on optimal transport problems related to optimal flow allocation in transportation and communication networks.

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Dimensionality Reduction with Proper Symplectic Decomposition for Learning Hamiltonian Dynamics

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Keywords. Hamiltonian dynamics; structure-preserving neural networks; symplectic dimensionality reduction; learning wave solutions.

Structure-preserving deep learning has recently received high attention, e.g., the development of symplecticity-preserving neural networks SympNets [1] for learning Hamiltonian dynamics. It is still a great challenge to obtain computationally efficient learning algorithms for high-dimensional problems. In this work, we propose dimensionality reduction with the *proper symplectic decomposition* (PSD) of the sequential training data in conjunction with SympNets. PSD was originally proposed in [2] to obtain symplectic reduced-order models of Hamiltonian systems. We demonstrate the proposed approach by learning the nonlinear localized discrete breather solutions in a one-dimensional crystal lattice model [3]. We find that learning the SPD-reduced Hamiltonian dynamics is not only more computationally efficient, but we also recover accurate spectral results from the neural network predictions in contrast to predictions by learned non-symplectic *proper orthogonal decomposition* (POD) dimensionality-reduced dynamics.

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Plastic litter sorting using hyperspectral sensing and Linear Discriminant Analysis

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Keywords. hyperspectral sensors; plastics waste; Linear Discriminant Analysis.

Plastic litter causes damage to the environment. Thus, it is mandatory to provide mechanical recycling plants with fast, accurate, and reliable tools and equipment specifically addressed to separate and recover single polymer streams, eliminating polluting elements (i.e., other polymers or other materials) present in the feed. Technologies for plastic waste separation are expected to be cost-effective and suitable to guarantee high quality of the products, mainly in terms of purity. This should guarantee the production of competitive secondary. The adoption of hyperspectral sensors working in the wavelength range 1000-1700 nm to perform sorting requires the utilization and the implementation of online analytical tools and robotic units to perform the separation. Materials in fact, have to be first detected, then identified and topologically assessed in the stream; after these steps automated devices realize the sorting. Many different polymers can be separated by near infrared sensors as they are characterized by different spectral signature in such wavelength range (i.e., PP, PE, PVC, PET, PS, etc.). This paper will describe the experimental campaign carried out to characterize plastic samples belonging to the most diffuse polymer typologies both in controlled light conditions and with natural light. Our detection methodology is based on linear classifiers, obtained by Linear Discriminant Analysis applied on a subset of spectral bands selected by minimum-redundancy-maximum-relevance criterion or by Principal Component Analysis. The classifier is obtained by optimization on a wide set of manually labeled examples. Results confirm how sorting with hyperspectral sensors may guarantee the achievement of the required standard for recycled plastics reuse.

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Deep learning methods for fMRI classification

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Keywords. fMRI; deep learning; medical imaging.

This paper aims to review some deep learning based methods for classification of functional Magnetic Resonance Imaging (fMRI) images of the brain. fMRI [1] is one of the MRI modalities which provides information about the activity of the neurons in the brain. In particular, fMRI signal is sensitive to blood dynamic changes which drive the neuron firing. This relationship is known as the Blood Oxygenation Level Dependent (BOLD) effect. Two main applications are possible: a task specific activity and a resting state one. The main difference is that in the first case a patient is asked to perform a specific task and the fMRI shows the brain response, while in the resting state no particular action is required.

The study of brain activity and response represents one of the major research challenges in order to better understand diseases and potential damages. The use of automated techniques based on artificial intelligence, such as machine learning [3] or deep learning [2] allow to analyse large datasets of fMRIs. The classification task is one of the most important since it enables the possibility to support the decision making process by healthcare experts by identify, e.g., from an image a particular disease.

This paper surveys the main deep learning methods and strategies for fMRI classification which are the most promising in terms of accuracy and computa- tional resource management.

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Application of Machine Learning to Increase the Efficiency of the Global Search Algorithm for Solving Multicriterial Problems

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Keywords. Multicriterial problems; global optimization; logistic regression.

Decision making models described as problems of multicriterial optimization are very complicated for investigation because the property of criteria contradictoriness leads to the notion of the solution as the set of non-dominated parameters (Pareto set). The complexity of these problems increases significantly in the case where criteria are multiextremal.

In the paper a novel algorithm for multicriterial black-box optimization with multiextremal criteria is considered. This algorithm applies ideas of complexity reduction when the initial multicriterial problem are reduced to a set of univariate scalar subproblems on the base of Peano mapping and maximum convolution [1]. For solving univariate problems a global optimization algorithm with guaranteed convergence to global optimum is used [2]. As a core novel feature, this algorithm includes in its computational scheme a machine learning procedure with combination of accumulating the information of solved subproblems that allows one to significantly accelerate building the Pareto set.

For verification of workability and estimation of efficiency, the representative computational experiment on test sets of multicriterial problems with multiextremal criteria constructed on the base of the test class GKLS has been conducted for different dimensions and number of criteria.

Along with the proposed algorithm, in the experiment some known methods belonging to the class of genetic algorithms have been tested and compared where the hypervolume index HV was used for assessment of algorithms' quality. According to the results of the experiment, the proposed algorithm has demonstrated its essential advantage over other methods.

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Aspects of optimization in domestic drinking water purification systems

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Keywords. Adsorption and ion exchange processes, membranes, tap water treatment.

While the European Commission encourages the use of tap water in our diets as an environmental and economic priority in the logic of plastic-free strategy, the tap water does not always meet several quality requirements compromising the confidence of the consumers. The contamination of drinking water is linked to organic, inorganic and biological pollutants from various sources, which can have serious effects on human health [1]. The unbalanced level of solutes (i.e., chlorine), the presence of persistent organic and inorganic pollutants, the residual amount of disinfection by-products drastically impact on the organoleptic properties of tap water. These aspects have stimulated the development of Point of Entry (POE), installed at the entrance to individual buildings, or Point of Use (POU), installed in the home, filtration systems to improve the tap water quality. The commercially available systems are often based on activated carbon and Reverse Osmosis [2]. The serious drawback of these systems is the lack in terms of ion selectivity leading to a drastic abatement of the concentration of solutes without considering their key role for the mineral balance in our diets and the organoleptic properties of drinking water. In this paper the main aspects and parameters to be optimized in the design of tap water treatment solutions with well-established and innovative approaches are analyzed.

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Sequential Decision Modeling for Dynamic Pricing and Revenue Management in Hotels

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Keywords. Machine learning and Intelligent optimization; Hotel revenue management; Sequential Decision Problems; Optimization Heuristics.

Determining dynamic prices of rooms in hotels is a challenging problem, known as Revenue Management (RM). Prices leading to maximized profits can be based on the pickup of reservations in time for a future window, on the evolution of the previous year, on the competition, on weather prediction, etc. Because the numbers of rooms and daily reservations in most hotels are small, the noise in the statistical estimates is large. E.g., estimating the response of customers to price changes (a.k.a. elasticity of demand), requires a careful and long experimentation to avoid hidden variables (like seasonal effects) and to produce precise estimates.

The RM task belongs to sequential decision problems. The utility of agent's actions does not depend on single decisions, but on the entire sequence. Decisions are made with uncertainty and information which is progressively revealed in time. Every price change for future days will actively influence the arrival of future reservations through the customer elasticity. Therefore, the initial forecasts and the optimal prices for the future need to be continuosly revised.

We demonstrate that a price-control system formulated as a sequantial decision problem can produce superior results w.r.t. competing techniques even in the (very frequent) situation of grossly inaccurate fortecasts and estimates of elasticity. The expected yearly profit is robust with respect to estimation errors, provided that one starts selling in advance and that prices are revised frequently before the checkin date. The optimization methods incorporate "learning" ("reactive") schemes that update strategies based on the past history of the process [1] and combine heuristics with the most effective global optimization schemes [2]. The approach is flexible and can be used in a variety of hotel settings but also in similar contexts of selling a perishable inventory over a time window.

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Gradient Fractional Physics Informed Neural Network for Solving Fractional Partial Differential Equation

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Keywords. Artificial Neural Network; Physics Informed Neural Network; Fractional Differential Equations.

Physics informed neural network(PINN) is the most effective tool in deep learning for solving differential equations. PINN is also useful in solving forward as well as inverse problems, fractional as well as stochastic differential equations. Here, in this paper PINN is used to solve fractional order partial differential equation. Further, gradient physics informed neural network(gPINN) is applied on fractional equation to improve the accuracy of the PINN. To solve this problem tanh and sigmoid activation functions are used to optimize the loss function. Since the common chain rule in integer calculus does not apply to fractional calculus, automated differentiation is not applicable to operators that employ fractions. In order to discretize the fractional operators in Poisson fractional Grünwald-Letnikov (GL) formula is used.

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New probabilistic methods for generating risk maps

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Keywords. Smooth Kernel Distribution; Fire; Risk map.

The year 2022 in Italy registered an increase of 170 percent in forested and non-forested areas devastated by fire (in 2021, fires affected 159,437 hectares). In detail, the highest number of calls to the fire fighters was recorded in Sicily and Calabria, with 301 and 223 requests respectively. The Calabria Region, with 35,480 hectares of forest area destroyed in the year 2021, is a strategic study area for conducting an in-depth analysis of how fires are spread and distributed. In light of this, the present work proposes to estimate the fire risk in the region using a non-parametric statistical technique called Smooth Kernel Distribution (SKD) [1]. This technique allows us to estimate the probability density function of a continuous random variable based on a sample dataset of the temporal sequence and geospatial location of fires in the region over the last decade. The main potential of the adopted method is that the SKD allows the creation of risk maps based on historical data, identifying high-risk areas and ensuring the development of targeted preventive actions [2]. The preliminary results obtained in the study area show that the SKD is a powerful tool for analysing fire risk. The identified risk maps show the areas in the region with the highest fire risk, enabling the competent authorities to take preventive measures to avoid further damage. Furthermore, the research conducted has shown that the use of the SKD in combination with other statistical techniques, such as multivariate analysis, can provide a more comprehensive understanding of fire risk in the region (intensity of the fire, vegetation maps, terrain orography).

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Parallel Cyclic Reduction of Bordered Almost Block Diagonal Matrices

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Keywords. Cyclic reduction; Almost Block Diagonal Matrix; Bordered Matrix; Parallel Algorithm.

In the discretization of BVPs (Boundary Value Problems) arising from OCPs (Optimal Control Problems) there is the necessity to factorize BABD (Bordered Almost Block Diagonal) matrices [1]. The factorization of such matrices, which emerge from the indirect formulation of the OCPs, is a serious obstacle to the efficient resolution process of the associated BVPs. For this reason, this work is aimed at extending the algorithm presented in [1], which limits the pattern of the border of the BABD matrix to the form of matrix A. In this work, a new BABD matrix of the form of matrix B is considered.

$$\mathbf{A} = \begin{pmatrix} A & B & & \\ & \ddots & \ddots & \\ & & A & B \\ C & & & D \end{pmatrix} \qquad \mathbf{B} = \left(\begin{array}{cccc|c} A & B & & & G \\ & \ddots & \ddots & & G \\ & & A & B & G \\ C & & & D & G \\ \hline E & E & E & E & F \end{array}\right)$$

The novel algorithm applies the cyclic reduction to the edge blocks and the bi-diagonal of part at the same time. In such a way, it is not necessary that block A in matrix B is non-singular. Cyclic reduction is achieved using LU or QR as inner factorization, so that the factorization can be used also for minimization problems. The resulting algorithm is very prone to be parallelization, and a C++ implementation is used to assess its performance.

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A Direct/Indirect Approach to Optimal Control Problems

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Keywords. Optimal Control; Direct Methods; Indirect Methods; Numerical Optimization.

Many practical numerical methods are available to approximate the solution of OCPs (Optimal Control Problems). The two most used are the direct approach [2] and the indirect approach. While the direct variant produces a constrained minimization problem, the indirect method is based on the calculus of Variations and it transforms OCPs into BVPs (Boundary Value Problems that must be discretized in order to be solved.

The direct method is usually more numerically robust and is used due to the availability of NLP (Non-Linear Programming) solvers, e.g. IPOPT. On the other hand, the indirect method has significantly faster convergence speed [4] with a smaller region of convergence. Although these approaches are very dissimilar in structure and formulation, it has been noticed that sometimes they are equivalent [3, 1]. This equivalence means the approaches get to the same solution with a discretization of the BVP that can be transformed into the minimization problem of the direct method [3]. This happens if, for example, discretization satisfies the co-vector mapping principle [1].

If we have a discretization that can be interpreted either as a minimization problem or a discretization of the BVP, we can build a robust solver that exploits the advantages of both direct and indirect approaches. In this work we present a systematic way to produce equivalent numerical methods that can be obtained both from direct and indirect approaches. Some numerical experiments show the advantage of this novel approach.

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Multiplicity results for discrete fractional boundary value problems involving p-Laplacian operator

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Keywords. Discrete fractional; p-Laplacian; Variational methods.

In this talk, we shall discuss the existence of at least one weak solution and infinitely many weak solutions for a discrete fractional boundary value problems driven by p-Laplacian operator. Our technical approach is based on variational methods. Some recent results are extended and improved. Moreover, some examples are presented to demonstrate the application of our main results. For the applications and recent studies on subject we refer to [1, 2, 3, 4].

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Deep learning for scoliosis diagnosis: methods and databases

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Keywords. Scoliosis; Machine Learning; Deep Learning; Diagnosis.

The advent of data-driven science and artificial intelligence (AI) has provided a deeper knowledge about data that has driven the clinical research to unprece- dented change. AI has shown great potential in the scoliosis diagnosis for which the current widely adopted standard of evaluation is the manual measurement on the X-ray radiographs of the Cobb angles to quantify the magnitude of spinal deformities in scoliosis. The reliability of the Cobb angle measurement mainly depends on the subjective experience of the operators and it is time-consuming. Machine learning (ML) and Deep Learning (DL) methods, at the basis of AI, can help surgeons to avoid misjudgment about scoliosis screening, diagnosis and classification by providing a powerful solution for saving time and effort in the Cobb angle measurement [1, 2]. The contribution of this work is to provide a overview of the main ML approaches, with special focus on DL approaches, at the state of art for the scoliosis diagnosis and to compare them with the tra- ditional methods in the same field. Moreover, because the reliability of the all ML approaches depends strongly on the training data [3] and often it is difficult to obtain a large amount of representative data, we survey the main databases containing spinal X-ray images with the purposes of providing the researchers with a knowledge that can substantially help them to choose the best dataset for training their ML models for the scoliosis diagnosis.

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Maximal entropy weighted least squares approximation

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Keywords. Weighted least-squares approximation; maximal entropy.

We consider using a maximal entropy argument to determine the function coefficients and squared errors weights simultaneously as output of a least-square approximation problem. Interpreting the weights as a probability distribution, we choose them by maximizing the "amount of uncertainty" or entropy, subject to the constraint that the mean squared error is prescribed to a desired (small) value. By acting on this error, we get a robust method for linear and nonlinear regression that automatically detects and removes outliers from the model during the fitting procedure, by assigning them a very small weight. We consider the use of both polynomial and spline functions, as well as of nonlinear models. A number of numerical illustrations have been included to better show the the performance and potentialities of the maximal-entropy approach in least squares approximation of data.

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Optimizing the reuse of building demolition materials for coastal dunes reestablishment

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Keywords. End of Waste; coastal dunes; numerical modelling.

Effective strategies for designing and managing coastal defenses against erosion require a multidisciplinary approach [1]. From a regulatory perspective, the Italian Dm 152/2022 "End of Waste" governs the reuse of construction and demolition waste (C&D waste) and other inert mineral waste, provided they are adequately treated to meet the minimum compliance standards set forth in the regulations [2]. A noteworthy aspect of this Dm is that it allows such waste to be used for the morphological restoration of eroded coastlines, which can be achieved through beach replenishment and the reestablishment of coastal dunes. In the latter case, the use of such waste represents an opportunity to incorporate porous materials with predetermined granulometric characteristics and values of the main hydraulic parameters, such as porosity and hydraulic conductivity. This approach could significantly optimize the process of seawater infiltration into the dune, ultimately limiting run-up. In an attempt to improve the current understanding, we utilized the Hydrus-2D software to optimize the morphology and granulometry of the dunes, with the goal of maximizing the infiltration process in the unsaturated zone. Results indicate that materials with higher hydraulic conductivity values generally exhibit superior infiltration capacity, and that soil heterogeneity can be used to optimize the process [3].

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Snoring sound processing for OSAS screening

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Keywords. OSAS; snoring analysis; long-term monitoring.

Obstructive sleep apnea syndrome (OSAS) commonly affects children and adults. It is defined as a complete cessation of airflow for more than 10 seconds, requiring a significant respiratory effort to restart normal respiration. OSAS can cause daytime sleepiness, tiredness, cardiovascular problems, and death. The 'gold' standard method for diagnosing OSAS is polysomnography (PSG) [1]. However, this diagnostic exam requires that the patients spend an entire night in the hospital. Thus it is time-consuming and requires high costs. Furthermore, it is labour-intensive because the clinicians need to collect and analyze a large number of data (e.g. different and large signals, such as EEG, ECG, oximetry, EMG, thoracic-abdominal movements).

In recent years, some simple wearable devices have been developed and launched on the market [2, 3]. These devices exploit the acquisition and pro- cessing of a few or one physiological signal, such as ECG, SpO2 and snoring [4]. This work aims to explore various technologies and methodologies for non-invasive and long-term screening of OSAS, by acquiring and automatically analyzing snoring sounds that are the most common symptoms associated with this disease. Specifically, after the preprocessing stage, time and frequency features are extracted and analysed.

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Mathematical modeling of water networks, local indices and invariance problems

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Keywords. Physical-mathematical modeling; water distribution networks; performance indices.

In the last four years a change of approach has been proposed in the study of water distribution networks from multiple points of view. Initially, in [1] the incipit of a new mathematical framework for WDNs was proposed, together with a local type analysis on the network, instead of global, as is common. The most used mathematical tools in [1] and in the framework introduced therein, come from linear algebra and vector analysis. In the talk we will then show some numerical-computational results obtained from this setting (see for example [2]). Continuing the development of the mathematical framework started in [1], the need arises for a mathematically precise determination of the reference system in the physical-energy treatment of WDNs. In fact, [3] demonstrates the existence of serious invariance problems in some of the most widespread and commonly used energy indices in design. Finally, if time permits, we will mention the open study of possible connections between the law of demand for urban WDNs and the approximations of fractal curves (see also [4]).

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Infinite computing and unimaginable numbers at school: some class experimentations in Italy

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Keywords. Mathematical education; unimaginable numbers; infinite computing.

In the literature, it is possible to find several projects that concern the development of new learning approaches in the context of high schools. These, in particular, have different purposes, such as promoting greater motivation for learning, developing skills and propensities for critical and creative thinking, and creating and transmitting knowledge, culture and values.

This context includes some studies carried out in 2019 in parallel in three different schools, chosen one in northern Italy (Treviso), one in central Italy (Pontedera, Pisa) and one in the south (Crotone). In particular, the aim was to investigate the students' response to some zero-knowledge tests on infinity and grossone (see [1] and [2]), taking into account geographical differences as well as the type of school. As of 2020, other experimental studies involve high schools (in Treviso, San Giovanni in Fiore and others) and different universities. These experimentations deal not only with infinity and grossone, but also with almost infinite numbers, the so-called unimaginable numbers.

In this talk, we report and discuss the results obtained in this first phase of involving schools, recording and interpreting students' observations. The main objective was to support and promote creating a school culture based on the construction of thought and deep understanding. A second phase will follow, characterized by differentiated lessons on the new proposed topics, final tests and comparison of results.

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Infinite computing, fractals and space-filling curves

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Keywords. Infinite computing; fractals; space-filling curves.

The Sierpinski, Peano and the Hilbert curves, are historically the first and some of the best known space-filling curves. They have a fractal structure, many variants and huge number of applications in the most diverse fields of mathematics and experimental sciences. In this talk we first present a recently proposed computational methodology based on the infinite quantity called grossone, which allows numerical calculations with infinite and infinitesimal numbers. Then we investigate the behavior of such curves and we highlight the differences with the classical treatment. Of particular interest are some power series expansions in the new infinitesimal quantities emerging from the study of the considered curves. If time allows we also use infinite computing to investigate some fractal constructions in 3 or more dimensions like the Sierpiǹski tetrahedron and the d-dimensional Sierpiǹski tetrahedron. In particular we will show some recent and beautiful results on classical Diophantine systems inspired by this setting.

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A μ-mode BLAS approach for tensor-structured problems, with an application to ODEs

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Keywords. μ-mode product; Tucker operator; exponential integrators for tensor-structured problems.

Many d-dimensional tasks in numerical analysis can be solved by applying repeatedly one-dimensional rules to all the directions, leading to the so called tensor product formulas. This is the case, for example, in the context of multidimensional pseudospectral expansions, multivariate interpolation, and solution of differential equations with tensor-structured domains.

In this talk, we present a common tensor framework from which it is possible to extract an *efficient-to-implement* solution, i.e., a BLAS-oriented formulation, of the d-dimensional task. The key point consists in the suitable usage of the μ-mode product and related operations (the Tucker operator, in particular). The MATLAB implementation of the needed tensor operations, collected in the freely-available package KronPACK[1], will be discussed as well.

We will conclude the talk with some numerical experiments showing the effectiveness of the approach in the solution of stiff evolutionary partial differential equations in three space dimensions.

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Resource Allocation via Bayesian Optimization: an efficient alternative to Semi-Bandit Feedback

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Keywords. resource allocation; semi-bandit feedback; Bayesian optimization.

Although optimal resource allocation is a well-known and studied problem, the recent technological innovations are bringing to light new specificities and issues. Some relevant real-life applications are the optimal management of cloud/high-performance computing resources, and the optimal budget allocation for multi-channel marketing. Recent formulations have led to the definition of the Semi-Bandit Feedback approach [1-3], that is the reference resource allocation method in these emerging real-life settings. In this paper we propose a novel approach, extending the Bayesian Optimization [4] framework to specifically deal with the resource allocation problem, and finally resulting more efficient than Semi-Bandit Feedback. Moreover, the proposed approach can also deal with specific (real-life) settings that cannot be covered by the Semi-Bandit Feedback method. Specifically, we have evaluated our approach on both (i) the case study reported in the original paper in which Semi-Bandit Feedback has been proposed, and (ii) a multi-channel marketing application. The paper also explains the main specificities/differences with respect to stochastic programming methods, with both Semi-Bandit Feedback and Bayesian Optimization being two learning-and-optimization frameworks.

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Multi-objective and multiple information source optimization for Fair and Green Machine Learning

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Keywords. Green AutoML; FairML; Bayesian optimization.

Democratizing Machine Learning (ML) requires endowing ML algorithms with fairness and low environmental impact. Training ML models on real-life data might lead to inherently biased predictions, a critical issue when the bias translates into discrimination of certain social groups. This unfairness is exacerbated by searching for the best predictive model only depending on accuracy [1]. FairML was initially addressed as a constrained optimization problem, but recently multi-objective methods proved to be more effective [2]. The second issue, considered here, is the carbon footprint of ML: the massive usage of computational resources for training ML models, and searching for the best one, implies a significant environment impact, leading to Green AutoML methods [3]. Recent approaches estimate the carbon footprint as a proxy of the energy consumption and reduce it by using multiple information sources (i.e., small portions of the data), each with a different fidelity and cost. We propose a method combining multi-objective and multiple information source into a single Bayesian optimization framework. It was evaluated on fairness benchmark datasets [4] and three ML algorithms (i.e., XGBoost, Multilayer Perceptron, Random Forest). Results in terms of accuracy, fairness, and "greenness", have been compared against those from state-of-the-art methods, empirically proving the better performances of the proposed approach.

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Systems by Iterations of Two Commuting Operators: a Frame Characterization

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Keywords. Frames; operator orbits; Hardy spaces with multiplicity; dynamical sampling.

The aim of dynamical sampling is to study the trade-off between spatial and temporal samples of an evolution process: assuming that a signal evolves through the action of a known bounded operator, is it possible to attain reconstruction by subsampling in space but sampling at different instances in time instead? The question can be reformulated as the study of frame properties of systems formed by orbits of vectors through the iterations of a bounded operator (the evolution operator) on a separable Hilbert space. This connection has led to extensive research on frames of operator orbits in recent years.

In this presentation, we will discuss a recent contribution in this direction. Specifically, we will present a characterization of the frames resulting from the iteration of two different operators that commute with each other. The prototype example driving this study is the dynamical sampling problem in shift-invariant spaces formulated in [1]. The achieved characterization, as established in [2], is done in terms of model subspaces of the space of square integrable functions defined on the torus and having values in some Hardy space with multiplicity.

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Variational approaches for discrete partial mean curvature problems

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Keywords. Multiple solutions; ϕ_c-Laplacian boundary value problem; variational methods.

An optimization problem consists of maximizing or minimizing a real function. Optimization problems are ubiquitous in the mathematical modeling of real-world systems and cover a very broad range of applications arising in all branches of economics, finance,materials science, astronomy, physics, engineering and computer science. Global optimization concentrates on finding the maximum or minimum over all input values. In our work, we shall look for local minima for the Euler functional corresponding to a nonlinear discrete Dirichlet boundary value problem driven by mean curvature operators. In fact, employing a consequence of the local minimum theorem due Bonanno [2] and mountain pass theorem, we obtain a new multiplicity results of the solutions for the problem, under algebraic conditions with the classical Ambrosetti-Rabinowitz (AR) condition [1] on the nonlinear term. Also, we find the existence of third solution for our problem, by mountain pass theorem given by Pucci and Serrin [3].

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Scalability of Saharan Dust Outbreak modelling with the Advanced Weather Research and Forecasting model coupled with Chemistry (WRF-Chem)

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Keywords. WRF-Chem; Scalability; Saharan Dust.

A fully coupled meteorology and chemistry model, for example, the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) [1], analyzes air pollution diffusion, including the dust aerosol, and its radiative and microphysical effects. The Mediterranean area is frequently influenced by the Saharan Dust coming from North Africa, which is a relevant source of Particulate Matter (PM) impacting climate, air quality and human health [2]. Moreover, the climate changes ongoing in the Mediterranean region suggest an enhancing frequency and intensity of the Saharan Dust events. In this study, we evaluated the forecasting skills of WRF-Chem simulations describing a Saharan Dust Outbreak (SDO) applied to a large domain, including both the Northern Africa region and central Europe. In particular, we analyzed the performances obtained using two different compilers, i.e., GNU (gfortran/gcc) and INTEL (ifort/icc). The results showed an improvement in time of the computation of Saharan Dust forecasting of approximately 7% using INTEL instead of GNU compiler. Moreover, the scalability was assessed by analyzing the speedup at different spatial resolutions.

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Neural architecture search in Deep Image Prior for image denoising

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Keywords. Image Denoising; Deep Image Prior; Neural Architecture Search.

Deep Image Prior (DIP) [1] is currently among the most effective unsupervised deep learning based methods for several imaging tasks. The DIP framework relies on the fact that the architecture itself of convolutional neural networks (CNNs) serves as an intrinsic prior inducing implicit regularization on the solutions. However the effectiveness of DIP strongly depends on proper values of the hyperparameters related to both the CNN architecture (such as the number of filters and the kernel size at each convolutional layer) and the optimization algorithm employed to train the CNN itself (such as the learning rate and the number of iterations). In general, finding the optimal hyperparameters configuration of a deep neural network is demanding, because it typically implies an expensive numerical investigation in terms of time and computational costs. In order to automate the hyperparameters tuning, Neural Architecture Search (NAS) techniques have been introduced. NAS has found applications in a broad range of computer vision tasks, including image restoration ones. In this work we adapt the NAS strategy suggested in [2] to the DIP approach for image denoising. In particular we develop a low-cost strategy able to predict the performance of a DIP-like CNN given its hyperparameters setting and its behavior after only few steps of the training process. We validate the efficacy of the suggested approach on image denoising applications whose data are real astronomical images corrupted by different levels of Poisson noise.

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Miniaturisation of binary classifiers through Sparse Neural Networks

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Keywords. Embedded Machine Learning; Sparse Neural Network Compression; Residual Networks; Binary Classification.

The continuous advances of artificial intelligence techniques have created new application domains for smaller and more efficient machine learning models. In the context of embedded machine learning, network sparsification strategies became crucial steps to fit models with severe space constraints. Hence, the aim of this research is to evaluate neural network sparsification and compression on embedded systems. To do so, we investigate the problem of miniaturised binary classifiers (*i.e.*, disease detection) in the computer vision domain. We applied a constant pruning technique [1, 2] during the training process of three architectures: a standard convolutional neural network and two residual networks (*i.e.*, DenseNet and ResNet). We varied: (i) network sparsity (up to 95%), (ii) image resolution (from 8×8 up to 32×32), and (iii) quantisation. The results indicate that the use of sparse networks has a significant impact on the accuracy of miniaturised binary classifiers. With a 70% of sparsity, it has been reached an accuracy improvement of 4% compared to the standard approach. Another relevant outcome is that sparsity outperform also by using low resolution images (*i.e.*, 8×8). Our findings suggest that sparse neural networks can significantly reduce both size and computational demands of the models, while increasing their accuracy on these edge cases.

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Choosing Kernel Shape Parameters in Partition of Unity Methods by Univariate Global Optimization Techniques

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Keywords. kernel interpolation, shape parameter, global optimization.

In [1] we considered the problem of finding an optimal value of the shape parameter in kernel-based interpolation. In particular, we proposed the use of a leave-one-out cross validation technique combined with efficient strategies of global optimization with pessimistic improvement and global optimization with optimistic improvement [3]. While the work [1] was focused on global kernel-based interpolation, here we want to extend our numerical method by employing a radial kernel-based partition of unity scheme [2]. In such a way, we can thus decompose a big problem into several (smaller) sub-problems, first computing locally local radial kernel interpolants and then gathering all partial contributions in the global fit. Numerical experiments show a promising performance and a good efficacy of the new algorithms in comparison with their direct competitors.

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How to deal with different densities of urban spatial data? A comparison of clustering approaches to detect city hotspots

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Keywords. Smart city; density-based clustering; multi-density city hotspots detection; urban data analysis.

The wide-scale diffusion of sensing networks and scanning devices over urban areas, huge volumes of geo-referenced urban data are gathered daily in modern cities. Such a large amount of data must be studied in order to find data-driven models that may be used to address the primary problems that cities deal with, i.e. human mobility, air pollution, crime predictions, virus spread, traffic flows, etc. While traditional density-based clustering methods have demonstrated their suitability for locating hotspots characterized by homogenous densities, their use with multi-density data can result in unreliable results. In fact, when clusters in different locations have densities that are significantly different from one another, or when clusters with various densities are layered, choosing an appropriate threshold can be exceedingly challenging. For this reason, multi-density clustering techniques appear to be more suitable for identifying city hotspots because metropolitan cities are largely characterized by varying densities. This study examines the research problems and difficulties involved in analyzing urban data. In particular, the paper presents an experimental evaluation of DBSCAN and CHD algorithms, showing a comparative analysis on state-of-art datasets.

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The Impact of Vectorization on The Efficiency of a Parallel PIC Code for Numerical Simulation of Plasma Dynamics in Open Trap

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Keywords. Parallel computing; Numerical Simulation; Particle-in-cell method.

Particle-in-Cell (PIC) simulation of high-beta plasmas in an axisymmetric mirror machine is of interest because of a new proposal for a plasma confinement regime with extremely high pressure, equal to the pressure of the magnetic field, so-called diamagnetic confinement. The results of simulations can be used for the development of aneutronic fusion.

In this work, we are using our own PIC algorithm and parallel implementation [1]. This parallel implementation is optimized for using CPUs with advanced vectorization instructions such as AVX2/AVX512. The high performance of modern server CPUs depends on the utilization of their vector computational blocks. In our work, we will show some optimization techniques for maximizing the performance of parallel PIC code. Some server CPUs can reduce the frequency during the usage of vector blocks because of the thermal packet. We will show the comparison of the performance with and without vectorization on different Intel and AMD server CPUs.

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Understanding spreading dynamics of COVID-19 by mining human mobility patterns

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Keywords. keywords.

Worldwide, online social media platforms like Twitter and Facebook are considerably used for information spreading. Social media data, in particular, may be a valuable support for a widely range of medical applications, including personalized medicine and disease surveillance. The possibility of using such realtime data, to provide early public health warnings and rapid alerts to hospitals has generated ever-increasing research lines [1].

The combination of health social data analytics and machine learning led to the so called big geo-social data. However, analyzing such data brings significant challenges. Therefore, new methods and high computing tools are required to effectively analyze the big data from social media platforms. In this direction, we propose an approach for gathering health-related information from social networks and combine such data with geographical, social and temporal data normally embedded in social media. Our research may offer insights into diseases, uncover social dynamics that lead to broad phenomena and forecast disease outbreaks.

Social media played also a key role in the management of COVID-19 especially in tracking disease spreading as users self-report their health-related issues. In this paper we present a case study of the proposed methodology to monitor COVID-19 spreading characteristics. Our aim is to understand spreading dynamics of the virus in US, through the analysis of people movements between US states by exploiting official surveillance data and geo-tagged tweets related to COVID-19. In the analysis we investigated human mobility patterns by considering COVID-19 related tweets posted in regions exhibiting high correlation with the official number of COVID-19 cases. As first step of the methodology, we mine users trajectories from the collected geo-tagged posts and build a mobility map including the most frequent movements. After that we extracted a set of daily snapshots of different spatial-temporal features characterizing the trajectories, including the frequency of posts in a specific locations, the distance and direction of movements among locations, the frequency of movements. The approach gives us the possibility of monitoring the spread of the epidemics and detecting outbreak locations.

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Variational Quantum Algorithms for Gibbs State Preparation

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Keywords. Quantum Computing; Quantum Thermodynamics; Quantum Algorithms.

The preparation of a quantum many-body Gibbs state on noisy intermediate-scale quantum (NISQ) devices is a highly important task to investigate quantum thermodynamical properties of different quantum many-body systems. Understanding protocols such as thermalization and out-of-equilibrium thermodynamics, as well as sampling from faithfully prepared Gibbs states, could pave the way to providing useful resources for quantum algorithms. variational quantum algorithms (VQAs) show the most promise in being able to prepare Gibbs states efficiently, however, there are many different approaches that could be applied to effectively determine and prepare the Gibbs state on a NISQ computer. In this paper, we will go through a brief review of the algorithms capable of preparing Gibbs states on a quantum computer, such as joint Hamiltonian evolution of a system–environment coupling [1], quantum imaginary time evolution [2], to modern VQAs utilizing the Helmholtz free energy as a cost function [3]. Finally, we benchmark one of the latest variational Gibbs state preparation algorithm, developed by Consiglio et al. [4], by applying it to the XY model.

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From regression models to Machine Learning approaches for long term crypto-assets price forecast

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Keywords. Bitcoin price forecast; Least Squares Problems; Regression; Support Vector Machines; Bootstrap.

We intend to comparatively study the performance of some digital assets which are currently under the spotlight of both retailers and institutional investors. More specifically, recalling that the crypto-assets market encompasses more than 22000 tokens, we shortly experience how the most renowned and dominating token, namely Bitcoin, can affect the price of the others (namely altcoins), with specific reference to the second most capitalized token (i.e. Ether). Then, we focus on the measurement of Bitcoin and Ether performance through Machine Learning (ML) techniques, proposing a long term forecast analysis for the price, based on an iterative semi-supervised ML approach. Our idea combines a multiobjective optimization method with a ML framework, and can be equivalently recast into a sequence of convex quadratic programs or through a unique more complex Mixed Integer Programming formulation. Finally, each quadratic program implies the solution of a Support Vector Machine (SVM) sub–problem, where we show that the proper initial sub-problem setting may be crucial. We remark that the contents in this paper propose a procedure which is inherently data-driven, so that it does not require any of the essential assumptions typically sought by classic regression.

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Metaplectic Gabor frames of Wigner-decomposable distributions

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Keywords. Time-frequency analysis; frames; time-frequency representations; modulation spaces; Wiener amalgam spaces; metaplectic group.

Metaplectic Wigner distributions generalize the most popular time-frequency representations, such as the short-time Fourier transform (STFT) and τ-Wigner distributions, using metaplectic operators. However, in order for a metaplectic Wigner distribution to measure local time-frequency concentration of signals, the additional property of shift-invertibility is fundamental. In addition, metaplectic atoms provide different ways to model signals. Namely, signals can be written as discrete superpositions of these operators, providing original ways to represent signals, with applications to machine learning, signal analysis, theory of pseudodifferential operators, to mention a few. Among all shift-invertible distributions, Wigner-decomposable metaplectic Wigner distributions provide the most straightforward generalization of the STFT. In this work, we focus on metaplectic atoms of Wigner-decomposable metaplectic distributions and characterize the associated metaplectic Gabor frames.

Legal systems and fractals

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Keywords. Legal systems; fractals; Hausdorff dimension.

In 1967, B. Mandelbrot, with the publication of the article *"How long is the coast of Britain?"* [1] opened up a new way of interpreting many physical objects and structures found in nature. In 2000 two eminent researchers, D. Post and M. Eisen, the first a legal scholar, the second a computational biologist with about 110 000 citations (source: Google Scholar), published an article similar to [1], entitled *"How long is the coastline of the law? Thoughts on the fractal nature of legal systems"* [2]. But the first to apply a geometric view to jurisprudence was J. Balkin in 1986 in an article entitled "The crystalline structure of legal thought". The author speaks of "the crystalline structure" because in 1986 he was not yet aware of the fractals and the results that Mandelbrot and others had achieved in the previous two decades, as he himself specifies in a subsequent article of over 120 pages in 1991 *"The promise of legal semiotics"*. Other than another article in 2013 by A. Stumpff, there are no works to our knowledge until [3] in 2022.

In this talk we will discuss the mentioned works and the possibility of investigating legal systems with metric and geometric tools. Furthermore, the idea of being able to measure sections of fractal curves not only of coastlines but also connected to legal constructions appears very interesting. For this purpose, one could probably use the Hausdorff dimension and infinite computing which allows to discern different sizes of infinite numerical values (see, e.g., [4]).

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Bilevel learning for model parameters estimation in imaging problems

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Keywords. Imaging inverse problems; bilevel learning; parameter identification.

In computational inverse problems, the forward model operator $\mathbf{A}$ encodes the information related to the geometry and the physical properties of the acquisition process. In many applications, $\mathbf{A}$ may be poorly known. This problem is particularly relevant in microscopy or astronomical imaging, where the data can be subject to the action of an unknown point spread function [2, 3], or in computed tomography, where the view angles used in the acquisition phase may be known with a certain degree of uncertainty [4]. Such scenarios can be mathematically modelled by making explicit the dependence of $\mathbf{A}$ on a number of unknown parameters $\boldsymbol{\theta}$, i.e. $\mathbf{A} = \mathbf{A}(\boldsymbol{\theta})$. In this talk, we propose a general framework for the calibration of model parameters in imaging inverse problems. Our approach is based on the solution of a bilevel learning problem, which computes optimal parameter values by solving a nested optimization problem where a variational model acts as a constraint. Here, the considered variational model presents a non-smooth regularization term, so as to make the overall machinery applicable to a wide class of real-world problems where one seeks sparse images or images characterized by sparse features. We thus outline a suitable numerical scheme based on a piggyback-type algorithm [1], and test it on different imaging problems.

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ChronoCode cloud programming

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Keywords. recursive task-parallel algorithms; distributed data-flow; dataparallel tasks.

Recent distributed computing frameworks like MapReduce, Hadoop, and Dryad have made it easier to use multiple computers in a cloud computing environment. These frameworks use coordination languages that aren't good enough for many kinds of algorithms, like iterative and recursive ones.We present ChronoCode, a Turing-powered, purely functional script language for describing distributed computations, in order to address this issue and generalize previous approaches. In this paper, we introduce ChronoCode and describe our innovative cooperative task farming execution engine. ChronoCode is designed to support iterative and recursive algorithms, making it more expressive than existing coordination languages. The cooperative task farming execution engine of ChronoCode enables efficient execution of distributed computations on a large scale.

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Influence of Bacterial Growth Rate on Pattern Formation in Aqueous Suspensions

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Keywords. Reaction-diffusion-chemotaxis; pattern formation.

Populations of bacteria such as *Escherichia coli* form patterns of millimeter-scale [1]. Mathematical models for bacterial pattern formation have been studied since the 1970s. One of the most widely used is the Keller-Segel approach [2].

E. coli exhibit attraction to self-excreted chemoattractant. Additionally, it has been shown that the activity of *E. coli* depends on available oxygen. Therefore, oxygen dynamics have an effect on pattern formation [2, 3].

The bacterial pattern formation is modeled mathematically using a system of reaction-diffusion-chemotaxis equations, representing the dynamics of bacteria, chemoattractant, and oxygen:

$$\begin{aligned}
\frac{\partial n}{\partial t} &= D_n \Delta n - \chi \nabla \left(n \nabla c\right) + \alpha n f_n(n, o), \\
\frac{\partial c}{\partial t} &= D_c \Delta c + n\, f_c(n, o) - c, \\
\frac{\partial o}{\partial t} &= D_o \Delta o - \lambda n\, f_o(n, o), \qquad (x, y) \in (0, l) \times (0, h),
\end{aligned}$$

here functions f_n, f_c, and f_o modulate growth rate, which influences pattern formation. The model is used to simulate the 2D patterns of the bacteria population near the inner lateral surface of a cylindrical micro-container.

The aim of this work is to investigate the effects of different growth rate functions on bacterial pattern formations. Four methods of growth rate modulation are considered: oxygen-dependent carrying capacity, saturating cell growth, cut-off approach, and oxygen-dependent Allee effect. The numerical simulation was conducted using the finite difference technique.

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Towards a parallel code for cellular behavior in vitro prediction

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Keywords. Cellular Pott Model; parallel strategies; GPGPU computing.

In recent years, there has been an increasing interest in developing in vitro models that predict the behavior of cells in living organisms. Mathematical models based on differential equations, and related numerical algorithms, have been developed to this aim. In this work, we present first experiences in designing parallel strategies for accelerating an algorithm for behavior prediction involved in the Cellular Potts Model (CPM) [1, 2]. In particular, we exploit the computational power of Graphic Process Units (GPUs), in CUDA environment, to address main low-level kernels involved [3]. Tests and experiments complete the paper.

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Application of Deep Learning for wildfire risk management: Preliminary results

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Keywords. Deep Learning; Wildfire susceptibility map; Machine Learning.

Due to ongoing climate change and the related increased risk of drought, wildfires in the Mediterranean are expected to become more frequent and intense. This note introduces the use of Deep Learning to produce susceptibility maps for wildfire risk assessment to tackle this scenario. Indeed, thanks to the improved computational capabilities of modern GPUs, recent literature has pointed out that it is possible to train Deep Learning models on big datasets by outperform- ing standard approaches in several application domains, including the one object of this study (see, e.g., [1]). An Artificial Neural Network (ANN) model has been developed and applied to the Calabria region (southern Italy) study area. The network has been trained and validated over ten years of data by considering both meteorological and geomorphological data, and human factors. Preliminary results are promising, evidencing a higher network's accuracy to the operational state-of-the-art Fire Weather Index (FWI) method, currently applied for forecasting and mitigation purposes in the study area [2].

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Algorithms for design with CNC machines: the case study of wood furniture

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Keywords. Parmaetric Design; CNC; Industry 4.0.

Thanks to the application of the Industry 4.0 paradigm, contemporary factories consist of flexible production lines that can generate countless product variations without substantial increases in production costs. This study highlighted a scientific and technological gap between the flexible manufacturing system and the design system adopted to make products. In fact, commonly used CAD design technologies are static and do not allow the generation of dynamic and variable designs, causing the need to redesign models in whole or in part in order to realize variations in the generated shapes. In this paper, an algorithm-based generative design methodology oriented to the flexible manufacturing paradigm is proposed. This design approach, based on parametric modeling in Grasshopper, allows countless geometric variations of a product to be automatically generated while returning input CAD files for CNC machines. Specifically, the proposed design approach was tested by making two applications for the wood furniture industry; the output obtained in the case studies consists of a generative and parametric algorithm. The generative system provides a file for advanced manufacturing systems; in the case study, a numerically controlled laser cutter, one of the most popular machines for making flat panels from wood and metal, was chosen. The results obtained showed how the algorithmic design approach is of great importance in order to ensure customized production without substantial cost increases. This is made possible through algorithmic design automation and contemporary manufacturing technologies.

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Crowd-shipping with uncertain travel times

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Keywords. Vehicle routing; Occasional drivers; Uncertain travel times; Benders decomposition; Column-and-row generation; Simheuristic.

We address the vehicle routing problem with time windows and occasional drivers (VRPODTW) in which ordinary people may perform deliveries supporting company drivers to serve a set of customers [2, 3]. We consider a VRPODTW variant with uncertain travel times and a penalty for each missed delivery, i.e., when either company drivers or occasional drivers arrive after the ending of the time window and the delivery does not take place. We consider the formulation proposed in [1] where a chance-constrained stochastic model is defined, and a probability on the maximum number of missing deliveries is imposed. We present two optimal solution approaches based on Benders' decomposition and column-and-row generation that solve an equivalent adjustable robust formulation. The optimal strategies allow to solve small size instances with up to 15 customers. We define a simheuristic to solve bigger instances. We collect numerical results on benchmarks for the VRPODTW, properly modified to take into account the uncertainty. We present the behavior of both the proposed optimal strategies and the simheuristic, and we discuss the benefit of addressing the uncertain problem showing better resource allocation with the robust solutions compared with the nominal ones, via a sampling analysis.

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Multinode Shepard method for the numerical solution of some elliptic PDEs with Neumann boundary conditions

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Keywords. Multinode Shepard operator; Collocation method; Elliptic PDEs.

In this talk, the multinode Shepard method [2] is proposed to solve elliptic partial differential equations with Neumann boundary conditions. The method has been opportunely handled to solve different equations with various boundary conditions dealing with scattered distribution of points [3,4]. The particular feature of the method, based on local polynomial interpolants on opportunely choosen nearby nodes [1], is a collocation matrix which is reduced in size with many zero entrances and a small condition number. Experiments in 2d domains have been performed with Neumann boundary conditions. Comparisons with the analytic solutions and the results generated with the RBF method proposed by Kansa are presented referring to different distribution of points.

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Extended Optimal Control Problem for Practical Application

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Keywords. optimal control; synthesis of control; machine learning; symbolic regression.

Application of the solution of the optimal control problem directly to the control object for whose model this problem was solved, it is necessary to build a system of motion stabilization along the obtained optimal trajectory. However, the construction of such a stabilization system is not provided for in the classical formulation of the optimal control problem. Therefore, additional requirements for the properties of the optimal solution have been introduced into the optimal control problem. One way to meet these requirements is to build a stabilization motion system of an object along a program trajectory.

A formulation of the extended optimal control problem and description of approaches to its numerical solving by symbolic regression are presented. The approach consists in application of machine learning by symbolic regression to the control synthesis problem. Symbolic regression allows to find a mathematical expression for control function as a function of the state space vector.

Computational example of solving the extended optimal control problem for a robot group is presented. Experimentally it is shown, that the solution of the extended optimal control problem is much less sensitive to disturbances, than a direct solution of the classical optimal control problem.

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Geometric MDS: New Insights

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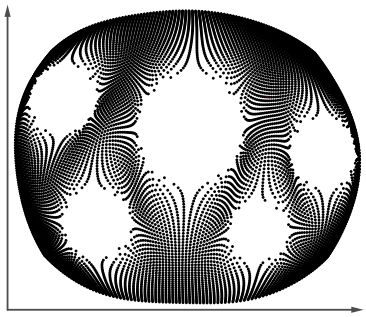
Keywords. Visualization; multidimensional scaling; Geometric MDS

Data visualization and dimensionality reduction are important in machine learning. Multidimensional scaling (MDS) [1] is a classical non-linear approach that maps a high-dimensional data set X onto a lower-dimensional data set Y. It attempts to preserve the proximities between the corresponding data points of X during the mapping. Geometric MDS proposed in [2] and [3] is an alternative/generalization of Smacof replacing the Guttman transform by a form with an explicit geometric interpretation. Sequential and parallel implementations of Geometric MDS are suggested in [4]. They are optimized for computational speed and can therefore be used to solve large data problems. Further research has focused on new coordinates for a single lower-dimensional point in the MDS stress function domain when Geometric MDS strategy is applied to this particular point. In the MDS stress function domain, empty subspaces are observed that cannot be accessed. The existence of such subspaces has been proven theoretically. The figure shows an experiment based on six data points. Denote the coordinates of two-dimensional points by $Y_1, ..., Y_6$. Let the coordinates of the first five points be fixed, and let the sixth point be moved from Y_6 to a new position Y_6^* by one step of Geometric MDS. The point Y_6 has been chosen uniformly 10000 times. The obtained positions of Y_6^* are given in the figure. Another discovery: all the resulting Y_6^* are within a circle-like area. Such discoveries can help in the search for the global minimum of MDS stress that depends on X.



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A fast algorithm for numerical differentiation from scattered data

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Keywords. scattered data; numerical differentiation; Fredholm integral operator.

Numerical differentiation from scattered data is a problem often encountered in many fields such as image processing and numerical solution of differential equations. We propose a fast algorithm for numerical differentiation starting from scattered data that could be affected by noise. The proposed algorithm uses nonuniform Fast Fourier Transform (FFT) and the explicit expression of the eigensystem of a Fredholm integral operator associated to the differentiation problem, see [1-3] for details. Error bounds for the approximation are provided as well as its computational cost.

Several numerical experiments are presented to validate the behaviour of the proposed algorithm with exact data and with noise-contaminated data.

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Numerical solution of stiff ODEs and DAEs with Adaptive Physics-Informed Random Projection Neural Networks

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Keywords. Random Projection Neural Networks (RPNN), RanDiffNet, Stiff ODEs, DAEs, Continuation methods.

In this talk, we address a novel adaptive physics-informed machine learning approach based on Random Projections Neural Networks (RPNN) for the numerical solution of nonlinear stiff ODEs and index-1 DAEs. The method is a numerical assisted one, involving an efficient computation of the unknown weights between the hidden and output layer, with Gauss-Newton and sparse QR decomposition with L^2 regularization for medium to large-scale systems, and a parsimonious selection, based on a bias-variance trade-off decomposition, of the a priori fixed internal weights and biases. Furthermore, to handle stiffness and sharp gradients, we address an adaptive step-size scheme and a continuation method for providing good initial guesses for the Newton iterations. The performance of the scheme that we call RanDiffNet, was assessed via eight benchmark problems, including three index-1 DAEs problems and five stiff ODEs problems, such as the Prothero-Robinson stiff ODE, The Robertson index-1 DAEs, the Hindmarsh-Rose neuronal model of chaotic dynamics and a finite difference discretization of a Allen-Cahn phase-field PDE. For the first time, we demonstrate that a machine learning approach can compete with, and even outperform, traditional stiff solvers like ode23t and ode15s from the Matlab ODE suite. Additionally, we compare it against the DeepXDE physics informed deep learning library, showing that our numerical-assisted machine learning scheme is much faster for the same numerical approximation accuracy.

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pyICL: A Python library for the Infinity Computer

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Keywords. Infinity Computer; Scientific Computing; Software Library.

The format of representation and storage of numbers along with the set of operations that can be performed on them are crucial aspects of traditional computer architecture that influence the accuracy of calculations. Today, almost all traditional computers use the IEEE 754-1985 binary floating point standard to represent and operate on numbers. However, the architectural restrictions of traditional computers make it difficult to perform operations involving finite, infinite, and infinitesimal numbers. To overcome these restrictions, the Infinity Computer has been conceived as a new kind of supercomputer that allows one to work numerically with such numbers [2, 3]. The existent simulator of the Infinity Computer available for the Matlab/Simulink environment is already used in several research domains to solve real-world problems, where accuracy is a crucial aspect [1]. To promote wider adoption of the Infinity Computer without requiring the use of a commercial and proprietary platform, a domain-independent Python library, named *pyICL (Python - Infinity Computer Library)*, has been developed. The *pyICL* Library allows one to work with finite, infinite, and infinitesimal numbers, expressed in the positional numeral system with the infinite radix grossone ①, by offering a set of arithmetic, elementary, and differentiation modules to perform computations with precision up to the machine one. The availability of a Python-based implementation of the Infinity Computer enables its exploitation in other research fields where Python is currently the reference programming language, such as Artificial Intelligence and Machine Learning.

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Matrix Factorization algorithms and Error Functions for the task of Change Detection in HyperSpectral Images

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Keywords. Hyperspectral images; QLP decomposition; Change detection.

When hyperspectral images are analyzed, a big amount of data, representing the reflectance at hundreds of wavelengths, needs to be processed and therefore, specific matrix factorization algorithms [1,2] are used to express the original problem in suitable subspaces. In the present talk, we show some recent results obtained by an approximated truncated SVD algorithm based on the iterative Stewart's QLP decomposition. Moreover, suitable spatial and spectral error functions are also introduced [3] to measure the reconstruction error between the input image and the approximate one, with applications to the task of change-detection.

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Exploiting the Bunch and Kaufman factorization for the efficient computation of Negative Curvature Directions

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Keywords. Large scale optimization; Convergence to second order stationary points; Negative curvature directions.

We consider the task of computing negative curvature directions, for nonconvex functions, in large scale optimization frameworks. This issue has widely been investigated in the literature, due to its relevant impact in applications. Hence, a number of different approaches have attracted the attention of the scientific community, both in small-medium and large scale settings.We specifically focus on a by-product computation of negative curvature directions exploiting the well known SYMMBK method (and the Bunch and Kaufman decomposition therein) for solving large scale symmetric linear systems. We show how to yield an effective negative curvature direction which allows the computation of promising local minima, corresponding to lower values of the objective function. A distinguishing peculiarity of our proposal is given by the fact that, under reasonable assumptions, the computation of our negative curvature direction can be iteratively carried out, without storing no more than a couple of additional vectors. The last results are accomplished through combining the Lanczos process and the Bunch and Kaufman decomposition, after a proper modification of the pivoting strategy adopted for the decomposition.

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An Alternative Nonlinear Diffusion Algorithm for Image Denoising and Deblurring

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Keywords. image processing; nonlinear diffusion; denoising; deblurring.

We discuss some applications in image restoration and enhancement, such as denoising and deblurring. The treatment involves the image processing algorithm recently introduced in [1, 2], and based on the use of Partial Differential Equations (PDEs). In this context, an image u is represented in a continuous framework and is manipulated through appropriate nonlinear time-dependent PDEs. For this purpose, a high-order space discretization scheme for a special nonlinear operator is implemented. As in the classical methods (see, for example, [3]) the idea is to level the regions of nearly uniform color, emphasizing the discontinuities. The proposed methodology is extremely efficient as excellent results are obtained after only a single step, which can provide interesting information on the image under examination. We present some numerical results regarding the deblurring and denoising of some real images. These results are obtained using the methodology introduced in [1] with appropriate filtering or adaptation when necessary. In particular, we focus on average blur and salt-and-pepper noise, which is a typical impulsive noise that may contaminate an image by randomly converting some pixel values to the maximum or minimum of the pixel variation range.

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An Application of Frequency Formulation for Nonlinear Oscillators

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Keywords. He's frequency formulation; strongly nonlinear oscillator; approximate solutions.

The paper is about nonlinear differential equations modeled for nonlinear oscillator systems, which is one of the active areas of applied mathematics. Mathematical models of real world problems are expressed in various types of equations. It is very important to develop methods for solving such equations encountered in physics, engineering and many applied sciences. For this reason, many approximate methods are suggested in the literature, especially for problems that cannot be solved analytically. In this paper, He's frequency formulation, which is an efficient method, is applied to find the frequency of the nonlinear oscillation problem. It has also been shown to be a powerful mathematical tool for different nonlinear oscillators without requirement of linearization or perturbation.

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Multi Criteria Decision Analysis, Hesitant Fuzzy Methodology and Expert Systems: some potential applications to financial markets dynamics

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Keywords. Decisions Support Systems; Machine Learning Techniques; Fuzzy Analytic Hierarchy Process.

Decisions Support Systems are a mixture of different methods and tools combined by machine learning approach. This study uses the most important machine learning techniques (logistic regression, artificial neural networks, and support vector machines) and the expert-based method (fuzzy analytic hierarchy process and hesitant fuzzy numbers) to study some financial markets dynamics. The objective of the study is to examine the main approaches developed by theory and operational practice for the purposes of conceptual representation, management and quality assessment. Different tools are applied to support decisions makers, such as AHPSort II to model the hierarchical structure, FAHP to determine weights in the construction of the matrix of the pairwise comparison and Hesitant Fuzzy Sets (HFS) to better represent the preferences of the decisions makers.

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Towards Reproducible Research in AI via Blockchain

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Keywords. Artificial Intelligence, Machine Learning, Operational Research, Reproducibility, Data Provenance, Blockchain, DLT.

Currently, Artificial Intelligence (AI), especially in the Machine Learning domain and related research fields, such as Operational Research (OR), faces a reproducibility crisis [1]. Researchers have difficulties reproducing key results due to the disconnection between publications and used codes, underlying data, parameter settings, etc., as they lack critical details. Moreover, the execution of computational experiments when solving engineering problems often requires large computing resources. Solutions that improve code accessibility, data provenance tracking, experiments transparency, auditing of obtained results, and trust can significantly accelerate algorithm and model development, validation, and transition into real-world applications. Thanks to such features as decentralization, data immutability, cryptographic hash functions, and consensus algorithm [2] provided by blockchain technology [3], such solutions could be developed. We aim to create a blockchain-based solution to ensure full research reproducibility and provide data control, improve transparency and auditing in experiments and avoid their costly re-execution, and ensure secure interchange of the obtained results that could be adapted for AI, OR, and other domains.

This work provides an overview of this field's state-of-the-art and our recent advances in this line.

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Dossier classification to support workflow management optimization

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Keywords. Natural Language Processing; Optimization; Justice sector.

One of the main challenges in optimizing services in various fields, including the legal sector, is the lack of an automatic system that can efficiently assign tasks based on predefined rules. In many cases, documents are still processed manually by qualified staff, which can be time-consuming and prone to errors. To address this issue, there is a need to develop a system that can automate the classification process, thereby simplifying the allocation of tasks to the most competent professionals in a specific field. This can be achieved by using Natural Language Processing (NLP) algorithms. In our Case Study the problem is to classify legal documents and suggest the most suitable judiciary branch for each dossier. By implementing such a system, it is possible to reduce processing times and enhance the overall efficiency of judicial offices. The proposed method can be supported by using a legal distributed system , which can facilitate seamless communication and collaboration among different actors.

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Data-Efficient Deep Learning Approach for Explainable Process Deviance Discovery

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Keywords. Process Deviance Mining; Deep Multi-Task Learning; Green AI.

Detecting deviant execution instances (e.g., related to security attacks, frauds, and faults [3]) of a business process is relevant for modern enterprises and organizations. Recent works [2] demonstrated that learning deep Deviance Detection Models (DDMs) out of process traces via (semi-)supervised methods outperforms traditional approaches based on standard Machine Learning solutions. However, deep models require to be trained with a large number of examples, which may not be available in real-life settings, especially in Green-AI applications where restrictions to data access and processing operations could be enforced [1].

To better suit such challenging applications, we propose a novel approach to discovering a deep DDM that deals with the scarcity of training data by leveraging a complementary self-supervised learning task. Specifically, the DDM discovery problem is formalized as a Multi-Task Learning one that simultaneously minimizes the classification loss and the reconstruction error of an auxiliary auto-encoder sub-net. This articulated learning scheme allows us to grasp an additional source of supervision complementary to data labels.

For the sake of interpretability and faithful explanation of predictions, our DDM is trained with a tabular representation of process traces [3], on top of which two parallel stacks of feature-representation layers are learned efficiently (and robustly to overfitting) by leveraging residual-like skip connections. The approach effectively deals with the challenging combination of data efficiency and explainability requirements in a case study concerning the execution traces of a real-life process. Future research will investigate alternative multi-objective optimization strategies and scalable uncertainty quantification methods to identify out-of-distribution instances.

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Self-sovereign identification of IoT Devices by using Physically Unclonable Functions and Blockchain

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Keywords. Digital Sovereignty; Blockchain; Cybersecurity.

In the last few years, digital sovereignty and particularly Self Sovereign Identity (SSI) paradigm, indicated that users must have control of their own digital data, allowing them to choose which ones they want to share and to whom. However, in the case of IoT devices, typically, no trusted third-party authority is recognized to have the power to verify the identity of the device's owner. Therefore, a secure mechanism to verify the identity associated with an IoT device is essential for the aims of digital sovereignty. In addition, information on data, such as data provenance, processing, etc., should be efficiently stored and accessed in real-time to associate the identity with the data usage conveniently, and also privacy and security should be guaranteed. This aspect is particularly critical when a large number of IoT devices and parallel access to data must be handled. Physically Unclonable Functions (PUFs) could be helpful in these tasks, as they can generate secure keys or fingerprints inherently and uniquely identify and authenticate physical items or physical objects in which they are embedded.

To better overcome the above-cited issues, a framework for handling the identities associated with IoT devices, based on the PUF technology to assess their identity and a blockchain network to verify the associated transactions, is proposed in this work. More into detail, our system permits the registration and verification in real-time of the identity associated with an IoT device in a self-sovereign fashion and the traceability of the accesses and processing of the data. Indeed, the identity is checked by using the PUF associated with an IoT device, and the blockchain layer ensures the security and privacy of access to the data in a decentralized way. Future works want to verify to provide the security authentication schema using PUFs hardware security elements boasting unclonability, uniqueness, and anti-tampering qualities provided by the random irregularities created during the manufacturing process as in [1].

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Efficient Solution of a Pitting Corrosion Model

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Keywords. Pitting corrosion; Reaction Diffusion PDEs; Stiff problems.

Phase field models are widely used for simulating moving boundary problems. Although on one hand these models allow for a simple treatment of the moving interface by introducing an auxiliary variable, on the other hand the nature of the equations is highly stiff and their efficient solution is challenging.

In this talk we consider a model for the pitting corrosion of a 304 stainless steel metal immersed in a sodium chloride solution [3].

We present a numerical approach for its solution based on a finite difference approximation in space and a time integrator that efficiently solves the stiff system of ODEs obtained. We consider some benchmark problems to compare the efficiency and accuracy of the new approach with other techniques from the literature based on the use of exponential methods [1, 2].

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The effects of different mesh size on a Cellular Automata based Hydrological Model

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Keywords. HydroCAL; ISSHM; Cellular Automata.

The application and development of Integrated Surface Subsurface Hydrological Models (ISHHMs) have grown in the last few decades thanks to the advent of High-Performance Computing (HPC) infrastructures, the Big Data availability and the increasing capacity to represent several hydrological processes at the same time.

Here we investigate how the mesh size affects the results of a new ISSHM based on the Cellular Automata (CA) paradigm, named HydroCAL, implemented through the OpenCAL scientific software library [1], which is able to exploit multi/many-core systems. The model is based on a coupling between a 3D variably saturated subsurface flow module [2] and a 2D surface routing module. The model was applied on a small headwater catchment (7 km^2). Two meshes have been used, with 20 m and 5 m horizontal resolutions, respectively. HydroCAL has been calibrated on the 20 m grid on a single multi-peaks flow event and subsequently validated with other events. The parameters obtained on the 20 m calibration were used on the 5 m grid.

The results highlight the capability of HydroCAL to reproduce streamflow correctly in a reasonable computing time. Moreover, adopting a high-performance parallel environment reduces the computational efforts required by a more fined grid.

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Combinators as Observable Presheaves: a Characterization in the *Grossone* Framework

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Keywords. Grossone; Combinatory Logic; Category Theory.

Combinators, as defined originally by Moses Schönfinkel give rise to a Turing-complete model of computation. In this paper we present a diagrammatic representation of combinators as presheaves defined over a category of *generic figures*. With the standard characterization of presheaves some of the resulting combinators fail the Turing observability condition. We address this question by adopting Sergeyev's *grossone* formalism, which allows to ensure the observability of the entire *topos* of combinators. The goal of this contribution is to provide a more natural representation of combinatory terms in which reductions and other operations can be applied in an elegant and homogeneous way. For that purpose, we define a category $\mathcal{CB}$ such that each combinatory term is a contravariant functor $F : \mathcal{CB}^{op} \to \mathbf{Set}$ and the morphisms are natural transformations between those functors. It is a standard result in category theory that any category of presheaves constitutes an *elementary topos* and thus provides a rich environment for modeling practically all ordinary mathematical structures and operations. In our case, a presheaf like F could be of infinite length, making its logical interpretation completely opaque. This sort of issue can be tackled by using the notion of *grossone* – first defined by Yaroslav Sergeyev [1]. We can then define a grossone category of presheaves over $\mathcal{CB}$ to give a sound and treatable version of combinatory logic, ensuring the interpretability of the combinators corresponding to the presheaves.

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Inside the Box: 0–1 Linear Programming under Interval Uncertainty

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Keywords. Integer programming; interval data; uncertainty.

Many practical optimization problems require models that are able to reflect uncertainty or inexactness inherently present in the data. Interval linear programming [4] provides a model for handling uncertain optimization problems, in which one assumes that only lower and upper bounds on the input data are available and the data can be independently perturbed within the intervals determined by the given bounds. Apart from the linear programming models with continuous variables, which have been explored by various authors, intervals also often arise in discrete optimization problems [2].

We adopt the model of integer linear programming with binary variables, in which the constraint matrix, objective vector and right-hand-side vector are affected by interval uncertainty. For this model, only a few works investigating its properties can be found in the literature (see [3] and references therein). In this talk, we characterize different concepts of feasibility and optimality in the model and discuss their properties from a theoretical and an algorithmic point of view. Moreover, building on the previous results for interval linear programs [1], we identify problems regarding the interval model that can be reduced to a single integer program and thus handled by modern integer programming solvers.

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Optimization for Machine Learning: the role of DC (Difference of Convex) algorithms

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Keywords. Supervised and Unsupervised Classification; Feature Selection; DC (Difference of Convex) algorithms.

Recent developments in Machine Learning, in particular in areas such as Supervised Classification, Clustering, Semi-supervised classification, Multiple Instance Learning, Feature Selection etc., have stimulated substantial advances in numerical optimization, as the problems involved require, in general, minimization of nonsmooth and, sometimes, even non-convex functions of several variables. The objective of the talk is to survey a number of such applications, focussing on the role of DC (Difference of Convex) optimization and presenting some effective novel approaches in the area.

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A mathematics-driven approach to detect the optimal tuning parameter for LASSO problem

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Keywords. Compressed Sensing; Inverse problems; MRI.

Compressed Sensing (CS) consists of recovering signals sampled below their Nyquist frequency (*undersampled*). Magnetic Resonance Imaging (MRI) exploits the electromagnetic properties of the protons in hydrogen atoms to produce 3D images of organs. MRI allows for the measurement of the Fourier transform of proton density: the latter is undersampled, to reduce acquisition time with benefits for patients and economy. CS has therefore the potential to retrieve missing information from sparse MRI acquisition: numerical procedures are required to recover the lost information. MRI signals are (approximately) sparse with respect to several frames and transforms, such as wavelets or total variation, cf. [2], they can be restored by solving *LASSO*: $\arg\min_x \|F_u x - b\|_2^2 + \lambda\|\Phi x\|_1$, where F_u is the undersampled Fourier transform, b is the noisy measurement, Φ is a *sparsifying transform*, and λ is a *tuning parameter*. Namely, $\|F_u x - b\|_2$ measures the fidelity of reconstruction and $\|\Phi x\|_1$ measures the sparsity of Φx. The parameter λ balances these two contributions, affecting the quality of reconstructions, but it is still chosen empirically. The origin of LASSO suggests that the parameter λ yielding to the optimal reconstruction can be computed numerically exploiting the theory of Lagrange optimization, cf. [1]. Following this idea, we effectively approximate the optimal tuning parameter of LASSO and apply our numerical results to MRI reconstruction framework.

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Preconditioning strategies for RBF interpolation

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Keywords. Interpolation; inverse multiquadric; preconditioning.

Radial basis functions (RBFs) are efficient tools for the approximation of functions [1], for scattered data interpolation problems [2, 3] and for solving real-world problems formulated by differential equations [4]. Concerning interpolation problems for scattered data, their solution leads to a linear system with a dense coefficient matrix. The ease of use of RBFs is contrasted by some difficulties in solving such linear systems, due to the properties of the interpolation matrix. First of all, a high computational cost is yielded when a large number of interpolation points is considered, in fact, the interpolation matrix is dense with order equal to the number of interpolation points. Then, numerical instability is a big issue, because the interpolation matrix usually has a high condition number.

We deal with the numerical instability issue and we propose a preconditioning strategy for interpolation problems formulated through the inverse multiquadric RBFs. Such preconditioning techniques are based on algebraic and analytical properties of the interpolation matrix, for which suitable decompositions can be devised. This preconditioning strategy and some preliminary numerical results are shown, together with some future perspectives.

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Models and Algorithms for Multiple Instance Regression

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Keywords. Multiple Instance Learning; Regression; Support Vector.

Unlike single-instance learning, where each data-sample is represented as a vector of features, in multiple-instance learning (MIL) data-sample are complex objects (bags) described by sets of instances. In this framework, each instance-vector is only characterized by its feature components and its membership in a bag, while a label is only available for the entire bag. In the multi-instance classification (MIC) version of the supervised problem each training bag is associated to a categorical label. Thus, the aim is to learn a prediction model, based on the training set, that allows to determine the class-label of new bags. The relevant difference of multi-instance regression (MIR), as an extension of the traditional regression paradigm, is that each bag is associated with a real-valued label rather than a class. Although there are significant motivation for developing MIR application, as testified by some recent interesting study regarding remote sensing, age estimation, landmark recognition, and drug activity prediction, still MIR is less widespread than MIC. This is mainly due to the intrinsic more challenging nature of the MIR where, instead of learning a classification surface based on the relative positioning of instances of categorical bags, one has to learn a function that associates real numbers to sets of points. This introduces an obvious difficulty as soon as one recognizes that there exist multiple possible mathematical descriptions of the same bag. After briefly surveying existing approaches to MIR, in this work we focus on models that adopt the support vector regression paradigm, discussing about the training algorithms, and addressing the issues posed by the validation phase.

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A Classical-Quantum Approach to Speed-up Reinforcement Learning

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Keywords. Reinfocement learning; Quantum computing.

Within the realm of machine learning, the reinforcement learning paradigm has gained huge attention in the last two decades due to the possibility of addressing complex tasks by allowing some software entities, named agents, to learn an optimal behavior through rewards and penalties received from a non-completely known environment. Agents must take advantage of the experience gained with the environment but also explore the domain of possible solutions. As a consequence, a good compromise between exploitation and exploration is to let the agents sample their next action from a probability distribution that mirrors these expected outcomes. In this work, we present a new approach that combines classical and quantum computing to achieve a significant performance improvement in the decision-making process of a learning agent. In particular, we introduce a routine that runs on a quantum computer that encodes a probability distribution. This quantum routine is then employed, in the context of reinforcement learning, to encode distributions that drive action choices. Our routine is well-suited in the case of a large number of actions and can be employed in any scenario, where a probability distribution with large support is needed.

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Quantum associative memory with a single driven-dissipative non-linear oscillator

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Keywords. Quantum associative memory; metastability.

Associative memory algorithms are typically built using a network of many connected units. The prototypical example of such systems is the so-called Hopfield model [1]. All the existing attempts to generalize it to the quantum domain are based on dissipative quantum Ising models. Here, we propose an associative memory scheme based on a single-driven-dissipative nonlinear quantum oscillator. The idea here is to exploit the infinite number of degrees of freedom in phase space [2]. The model is able to outperform the memory capability of two-level neuron-based systems in a large parameter regime and can successfully state discrimination between n coherent states, which are the stored patterns. These can be continuously tuned by changing the driving strength, constituting a modified learning rule. Moreover, by changing the system's nonlinearities, one can generate squeezed states with sub-Poissonian statistics, which constitute the first example of purely quantum-stored patterns. We show that the associative memory capability is intrinsically related to the existence of a spectral gap in the Liouvillian superoperator, which leads to a long timescale separation in the dynamics corresponding to a metastable phase. We believe that our model lays the groundwork for future research in quantum machine learning algorithms using bosonic systems.

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DC Optimization in Adversarial Support Vector Machine (SVM)

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Keywords. Adversarial Machine Learning, SVM, Sparse optimization, DC Optimization.

In supervised classification models, such as Support Vector Machine, the main purpose is that of predicting the class membership of the incoming samples. In some real applications malicious inputs are inserted to cheat a vulnerable classifier, leading to a wrong prediction. In our work we focus the analysis on the search of:

i) the smallest perturbations of samples which produces a failure of the classification process and

ii) the worse classifier after adding the malicious inputs.

The novelty of the proposed approach is in the use of Difference of Convex functions (DC) to model the formulations. We present the results of some preliminary experiments.

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Applying Variational Quantum Classifier on Acceptability Judgements: a QNLP experiment

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Keywords. Quantum Machine Learning; Quantum Natural Language Processing; Variational Quantum Classifier.

The newborn Quantum Natural Language Processing (QNLP) field has experienced tremendous growth in recent years. The possibility of applying quantum mechanics to critical aspects of language processing has dramatically impacted many tasks, ranging from theoretical approaches to algorithms implemented on real quantum hardware. From a methodological point of view, the possibility offered by new Distributional-Compositional models of language [1] is well suited to classification tasks [2]. This work aims to test the potential computational advantages offered by a hybrid algorithm, namely the Variational Quantum Classifier (VQC) [3] to perform classification on a classical Linguistics task: acceptability judgments. VQC is a quantum machine learning algorithm able to infer the relations between input features and the associated belonging class using a parametrized quantum circuit, together with an encoding layer that embeds classical data into quantum states. An acceptability judgment is defined as the ability to determine whether a sentence is considered as natural and well-formed by a native speaker. The approach has been tested on sentences extracted from ItaCoLa [4], a corpus that collects sentences in Italian language binary labeled with their acceptability judgment. The evaluation phase has considered both quantitative metrics and a qualitative analysis, to further investigate the behavior of the algorithm on specific linguistic phenomena included in the corpus.

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Multiple solutions for the fractional p-LAPLACIAN elliptic Dirichlet problems

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Keywords. Fractional p-Laplacian; Critical points; Variational method.

In this talk, we study a fractional p-Laplacian elliptic Dirichlet problem. The multiplicity of the weak solutions is proved by means of the variational method and critical point theory. We investigate the existence of at least three solutions to the fractional p-Laplacian. For recent studies on subject we refer to [1, 2]. For the applications of fractional differential equations in economics and finance we refer the reader to the paper [3, 4].

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High Performance Local Search for Global Optimization on Large Nonlinear Systems of Equations

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Keywords. Nonlinear Systems of Equations; Global Optimization; Cloud Computing.

Systems of nonlinear equations show up as a result of numerous theoretical and applied mathematical problems. Approaches to solve these systems, making use of *a priori* knowledge of the system and resultant special properties of the systems, has been studied extensively. Recent research has resulted in transforming these systems into global optimization problems in order to find solutions, without taking into account any special properties of the systems. This approach can be seen as black-box optimization. However, problem size, problem complexity, and computational power still limit the ability to find solutions to these systems.

In this research, we will begin by giving an overview of global optimization techniques to solve systems of nonlinear equations. We will then discuss a software architecture to solve these black-box global optimization problems in the cloud. We conclude by presenting numerous examples of large nonlinear systems of equations solved in the cloud utilizing a parallel implementation of the Hookes-Jeeves algorithm.

Solvability Issues of the Absolute Value Equations in Case of Interval Data

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Keywords. Absolute value equations; interval analysis; linear complementarity problem.

The absolute value equations is a feasibility problem in the form $Ax + |x| = b$, and its generalized version reads as $Ax + B|x| = b$. It caught the attention of the optimization community due to its equivalence with the linear complemen- tarity problem [3, 4]. The absolute value equation problem is NP-hard, so many questions related to this problem are hard to handle, e.g., to find a solution, to check for unique solvability etc.

Since practical problems often suffer from various types of uncertainties, the input data can hardly be considered to be exact. That is why we focus on the problem with uncertain coefficients. We model uncertainty by the interval range of possible values, so that the input matrix A and vector b become interval-valued [1, 2]. For this interval problem, we investigate the basic problems regarding solvability and the solution set. In particular, we state conditions for unique solvability for every realization of interval values, describe the solution set and present outer bounds for the solutions set. In view of the intractability of the problems, we consider also certain polynomially solvable subclasses of the interval problems.

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Unimaginable numbers. A case of study in Italian High School

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Keywords. Unimaginable numbers; grossone; Knuth's up-arrow notation.

How big is a large number? How far can our imagination go to think or to imagine a large number? The work is part of the study of didactic approaches aimed at the knowledge of unimaginable numbers in secondary school. The topic is very interesting because this numbers very large, but finite numbers can be transitioned in the passage of the concrete transition from the concept of finite to that of infinity. This work is placed in continuity with the previous case studies carried out on the computational arithmetic of infinity (the Grossone based model). Specifically, a further case study is shown here: the planning phase (research questions, additional aspects including choice of case study method and discovering strengths or limitations). In addition, it is showed the method by which these numbers together with their characteristics will be exhibiting order to give an idea of their estimated size, even with regard to the physical universe. Finally, the effects and results in terms of educational implications will be evaluated through the analysis of the results that emerged from the administration of a questionnaire proposed to the students of the classes involved.

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A new class of octagons. Differences and similarities between "Carboncettus octagons" succession and "Carboncettus-like octagons" class.

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Keywords. Carboncettus octagons, continous octagons, Fibonacci numbers.

The term 'Carboncettus octagons' refers to octagons found on one of the two facades of one of the side doors of the cathedral of Prato. The chronicles attribute their creation to a certain Carboncettus Marmorarius. This is mentioned in the scientific literature succession of octagons as one of the elements in support of a history thesis of mathematics. According to this thesis the knowledge of the so-called Fibonacci numbers dates back to a period, before the life of Fibonacci himself. In this labor, a new class of octagons will be built, in part, built similarly according to the same construction procedure used for Carboncettus octagons. For this reason, this approach would then be called Carboncettus-Like (CL). In this labour, we present the results of the properties of this new class of octagons built according to the CL approach and compare them with the original version of Carboncettus octagons. After having briefly referred to the geometric and algebraic characteristics of Carboncettus' octagons and to have specified the modalities of construction of CL-type octagons, their main characteristics will be presented and a comparison between the two classes will be carried out.

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State reconstruction with quantum extreme learning machines

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Keywords. Quantum machine learning; quantum extreme learning machines.

Quantum reservoir computing and quantum extreme learning machines (QELMs) are computational paradigms that have recently attracted considerable interest thanks to their ease of implementation in many practical scenarios, and their potential for processing data encoded into input quantum states. We present an in-depth analysis of the potential of QELMs to estimate the properties of input states. In particular, we show that a full characterisation of the target properties achievable in this way is possible, and provide explicit conditions telling us when an observable is achievable in terms of the effective measurement corresponding to the dynamic of a given reservoir. We also prove a close analogy between the training process of QELMs and the reconstruction of the effective measurement characterising the given device. Finally, we show that the estimation framework of quantum shadow tomography fits naturally to analyse the performances of QELMs in the general case. Our analysis provides the theoretical foundations to understand better the potential and limitations of QELMs and reservoir computing, as well as providing explicit methods to apply these methods for practical experimental applications.

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The combined Global-local method for Box Constraint Optimization

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Keywords. Nonlinear optimization; Global optimization; Deterministic optimization.

Global optimization seeks to identify to identify the best solution and prove its global optimality, which is crucial in many fields as in engineering, finance and logistics. Global optimization problems can be challenging due to the complexity of the objective function, the presence of multiple local solutions and the structure of the problem constraints. Here, we are interested in box constraint optimization problems, which can be described by

$$\min_{x \in X} f(x)$$

where $f \in C^2(X)$, and $X \subset \mathbb{R}^n$ is a hyperbox.

The cluster problem is well-known in global optimization field, there are many proposed methods to tackle this problem like backboxing, Interval-Newton method, Kantorovich theorem, etc. Most of these methods provide a relatively small inclusion around the solution to prevent the cluster problem. In this talk, we overcome the cluster problem by introducing our new algorithm named the combined Global-local method. The algorithm starts by computing a solution by the means of a local method, then it constructs a uniqueness inclusion around the solution by the means of the regularity of the hessian matrix, then this inclusion is excluded from the search space. Afterwards, the global part discards all other areas with no solution.

We provide theoretical analysis for an algorithm with and without the combinations, by bounding the number of bisections, boxes and iterations both algorithms need till termination.

Finally, we illustrate the numerical benefit of our approach by couple of global optimization test examples.

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Multi-Objective Support Vector Machine Classification Algorithm for Estimation of the Potential Atmospheric Water Harvesting

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Keywords. SVMs; Classification; Multi-Objective Optimization; Machine Learning; AWH.

Different studies show the advantages of atmospheric water harvesting (AWH) in different climates for irrigation, especially in dry periods [1]. Moreover, we used the advantages of multi-objective optimization to reformulation of support vector machines (SVMs) classification [2]. Therefore, the main purpose of this study is to develop a multi-objective SVM classification algorithm for the estimation of the potential AWH using major geographic and topographic indicators. In this regard, in this study, the dataset of AWH in different climates and regions has been used for training the classification learning algorithm. The results of the developed model could estimate the potential of AWH, and the verification of the results confirmed the effectiveness of the proposed method.

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Optimal subset selection using the L0-pseudonorm with an application to prognostic modelling of prostate cancer

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Keywords. L0-pseudonorm; Optimal subset selection; Prostate cancer.

In many biomedical applications, we have a large number of available predictors. Thus, we need to utilize feature subset selection to spot the most important ones for the model building. At the moment, regularized regression methods using L1-norm (LASSO), L2-norm (Ridge Regression) and their hybrid (Elastic Net) are the most popular approaches for this. I will present a new L0-pseudonorm approach OSCAR [1] designed for multivariable regression. In the method, sparse solutions are obtained with a cardinality constraint. Due to this, the optimization problem is NP-hard but OSCAR utilizes its continuous transformation making it possible to use efficient solvers in our user friendly R software package of OSCAR. Finally, OSCAR is shortly demonstrated in the prognostic modelling of prostate cancer.

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A first-order optimality condition in nonsmooth generalized semi-infinite optimization

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Keywords. Generalized SIP; Optimality Condition; Qualification Conditions.

In the present paper we consider the generalized semi-infinite programming problem (GSIP in brief).

Extensive references to optimality conditions and constraint qualifications (CQ) for smooth GSIPs, and their historical notes, can be found in the book by Stein[1]. In order to establish optimality conditions for nonsmooth GSIP, several kinds of lower-level CQs are studied in [2, 3].

This paper focuses mainly on some upper-level CQs, in Mangasarian-Fromovitz and Abadie and Guignard types, and some first-order optimality conditions, in Karush-Kuhn-Tucker type, for nonsmooth GSIPs. For this purpose, we will have to introduce a new concept, named well structured assumption. The results of the presented paper are stated by Clarke subdifferential.

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Some remarks on second-order necessary optimality conditions in optimal control problems with state constraints

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Keywords. Optimal control; Maximum principle; State constraints; Regu- larity conditions.

In this work, a smooth optimal control problem with endpoint, mixed and state constraints is considered. The second-order necessary optimality conditions are derived based on the normality condition which is presented as the condition of full rank for the controllability Gramian (controllability matrix). In this regard, the earlier result from [2] is revisited and a certain connection is established between different results in this field. The investigation method is essentially based on the maximum principle proposed in [1], which employs the second-order derivative of the mapping associated with the state constraints.

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Designing an Optimal Offshore Wind Farm Location System with De Novo Programming and Simon's Satisficing Theory: Techniques and Practical Implementation

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Keywords. De novo programming; goal programming; penalty functions; aspiration levels; offshore wind farm location.

The paper discusses the use of De novo programming (DNP) for designing systems that are satisfactory rather than optimal. The approach involves using an aspiration-level vector instead of an ideal vector and minimizing the Lp-distance metric between the aspiration level and the feasible objective region. The paper proposes two models based on goal programming techniques to generate a satisficing solution, and an extended model to achieve equilibrium between the solutions obtained from these models. The paper also introduces the concept of penalty function (PF) with DNP to deal with uncertainty and give decision-makers more flexibility to incorporate their preferences. The proposed approach is illustrated with an example and a hypothetical application to Italian offshore wind farm locations. A weight-space analysis is conducted to check the stability of the results, which confirms the usefulness of the proposed methodologies in assisting decision-makers in determining optimal locations under uncertain aspiration levels.

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SLiSeS: Subsampled Line Search Spectral Gradient Method for Finite Sums

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Keywords. Unconstrained optimization; stochastic approximation; sampling; spectral gradient methods; line search.

Spectral method is known to be a powerful tool for solving classical opti- mization problems. In this paper, we aim to exploit its advantages in stochastic optimization framework, especially in mini-batch subsampling case which is often used in Big Data setup. In order to let the spectral coefficient explore the spectrum of the approximate Hessian, we keep the same sample for several iterations before we subsample again. We analyze conditions for almost sure convergence and present initial numerical results that show the advantages of the proposed method.

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On the Use of Local Information to Accelerate Global Optimization Methods

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Keywords. Global optimization, black-box functions, Lipschitz condition, local information, acceleration of the convergence.

In this talk, numerical methods for solving black-box global optimization problems are considered (see, e .g., [1-4]). These problems are characterized by expensive evaluations of the objective function and constraints (if any) and are frequently encountered in applications (see [3]). The Lipschitz condition is used to model them, and the unknown Lipschitz constant is estimated during the execution of numerical methods (see [1]). Adaptive diagonal curves are constructed over the multidimensional search domain to extend efficient Lipschitz global optimization algorithms to the multidimensional case (see [2]). Due to high computational costs involved, acceleration techniques are required to obtain acceptable solutions to the considered problems in less function evaluations. In particular, some advanced diagonal global optimization methods will be discussed in which the local information about the behavior of the objective function is taken into account. For example, this information can include improved estimates of local Lipschitz constants, also by using function derivatives where available. In this way, a local refinement of the solution obtained during the global search can efficiently be performed (see [2, 4]). Thus, more accurate solutions of complex multi-extremal problems will be achieved while saving time-consuming evaluations of the objective function. Theoretical and experimental aspects of these techniques will be briefly presented.

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Introducing *Nondum*, a mathematical notation for computation with approximations

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Keywords. Approximation; grossone; unimaginable numbers.

In mathematics, an approximation is often used when an exact numerical form is unknown or difficult to obtain. The mainly notations used to represent numerical approximation add the margin of error to the value of the approximated number. This, although formally impeccable, is a difficult model to apply in the computation. On the other hand, the paradigm of Approximate computing is rapidly emerging. In this case, a greater obtainable precision is sacrificed in order to obtain better computational performances. This approach is useful for many application fields in which approximate results are still tolerated and valid, such as scientific computing, machine learning, or multimedia processing.

In this paper, we are introducing a symbol representing a not-yet-known value, used to represent one or more unknown digits within a number. This makes it easier to store numerical approximations and allows you to perform computations between approximate values or to perform partial or approximate computations. We called this symbol *Nondum*, the Latin word meaning not yet (known, measured, or calculated). Furthermore, on the level of symbolic computing, we will show some analogies with infinite computing, *grossone* and the so-called unimaginable numbers.

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Node-Binded Communities for Interpolation on Graphs

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Keywords. Partition of unity method, graph basis functions, kernel-based interpolation, graph signal processing, data-driven computing.

Partition of unity methods (PUMs) on graphs [1] are simple and highly adaptive auxiliary tools for graph signal processing [3]. Based only on the underlying structure of the graph, we show how a partition of unity can be generated using centrality measures and modularity. Then we integrate PUMs with a local graph basis function (GBF) approximation method [2] in order to obtain low-cost global interpolation schemes.

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Analysis and Visualization of Multilayer Networks

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Keywords. Network Visualization; Multilayer Networks; Network Metrics.

Network theory, in particular complex networks, has undergone considerable development finding its way into many real-world applications. However, they have several different types of relationships that cannot be represented by a monolayer network [3].

In fact, multilayer networks explicitly incorporate multiple channels, creating the right context to describe interconnected systems through different related layers, where nodes are the entities of the system and the edges represent the interactions between them. The application fields that may be modelled by multilayer networks range from human and social systems [2], to technological and transport systems, including biology and medicine [1]. Although various approaches for the visualisation and analysis of multilayer networks have been suggested in recent years, this is an evolving field.

In this work we first present an overview of the tools exploited for the analysis and visualization of multilayer networks. Then, we present a comparison among different tools through a case study represented by a real multilayer network. The network under investigation is a multilayer network composed of 8, 392 nodes and 128, 199 edges distributed over two levels that relate disease and gene. We propose methods for visualisation of the network that provide a topological analysis, attempting to derive the main measurement metrics.

Through the visualisation and analysis carried out on the data set, we will attempt to demonstrate the different configurations of a network depending on the tool being used, the properties that characterise it, and the parameters that can be attributed to the network in order to derive real scientific information.

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DCA-Like for solving Gaussian mixture model combined with dimension reduction via t-SNE

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Keywords. GMM; dimension reduction; t-SNE; non-convex optimization; DC Programming; DCA; DCA-Like.

In this work, we study Gaussian mixture model (GMM) clustering, the most popular model-based clustering model in the literature. GMM has been largely developed and successfully applied to several applications thanks to its interesting properties on both theoretical and computational aspect. However, the main drawback of GMM is scalability. GMM suffers from high-dimensional data, which is common these days due to the fast pace of technological advancement. To overcome this drawback, we combine GMM with a dimension reduction technique, namely t-distributed stochastic neighbor embedding (t-SNE). The resulting optimization is non-convex for which we investigate novel and efficient method based on DC (Difference of Convex functions) programming and DCA (DC Algorithm) to solve. DCA is well-known as an efficient approach in the nonconvex programming framework thanks to its versatility, flexibility, robustness, inexpensiveness and ability to adapt to the specific structure of considered problems. It turns out that DCA standard for solving the GMM combined with t-SNE can be computationally expensive for high dimensional datasets. We then develop a variant of DCA, namely DCA-Like. DCA-Like is based on a new and efficient way to approximate the DC program without knowing a DC decomposition. Numerical experiments on several benchmark datasets illustrate the efficiency of our algorithm.

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Nonlinear Inequalities, Space-filling Curves and Robots

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Keywords. Nonlinear inequalities, space-filling curves, robot workspaces.

In this talk, the problem of approximating the solution set of systems of nonlinear inequalities is considered. This kind of problems can be met in many practical applications and global optimization methods can be used to deal with them (see e.g. [1–5]).

New methods which use a dimensionality reduction through two different approximations of the Peano-Hilbert curves are proposed. Their convergence conditions are established.

Proposed algorithms are compared numerically on test functions and real problems regarding finding the workspaces of planar robots.

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Global minimization in N dimensions using Peano space-filling curves

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Keywords. Deterministic global optimization; space-filling curves approximations; Lipschitz and Hölder conditions.

In this talk, the global minimization problem of a function $F(y)$ in an N-dimensional domain D is considered. The function $F(y)$ is supposed to be: Lipschitzian with an unknown finite Lipschitz constant, multiextremal, non-differentiable, and given as a "black-box" (see [1, 2, 4] for a detailed discussion on the importance of this kind of problems). To solve this global minimization problem we propose a series of methods that use the Peano-Hilbert space-filling curves to reduce the dimensionality N of the problem in order to work with an equivalent one-dimensional problem satisfying the Hölder condition. In particular, two different approximations of Peano-Hilbert curve are discussed: the most used and known Piecewise-Linear Approximation and the less known Non-Univalent Approximation (see [1, 2, 3]). We also propose some techniques to adaptively estimate the Hölder constant during the minimization phase and thus speed up the search for the global optimum (see [1, 4]) using approximations of the Hölder objective functions obtained after the dimensionality reduction. Broad numerical experiments show a very promising performance of the methods under scrutiny.

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Benchmarking the Role of Particle Statistics in Quantum Reservoir Computing

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Keywords. Quantum machine learning; unconventional computing; information processing; reservoir computing; quantum statistics.

Quantum reservoir computing is a promising machine learning approach that uses the complex behaviour of quantum systems to store and process information. In this study, we focused on comparing the memory capacity of three types of quantum systems, namely bosons, fermions, and qubits, in the context of quantum reservoir computing.

Our analysis showed that the performance of the system improved with the size of the Hilbert space. However, we also found that the information-spreading capability of the system is also an important factor in determining its performance.

Using numerical simulations, we found that fermions provided the best memory capacity due to their intrinsic non-local properties. However, we also discovered that with a tailored input injection strategy, bosons could outperform fermions in terms of memory capacity. This is because bosons can take advantage of the abundance of degrees of freedom in the Hilbert space and enhance the computational power compared to fermions and qubits.

Our findings provide valuable insights into the best type of quantum systems to use for reservoir computing and how to optimize their performance. These insights can help guide the development of more efficient and effective quantum machine learning algorithms and contribute to the advancement of quantum computing.

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Liver Machine Perfusion Policy Iteration Using Monte Carlo Optimization

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Keywords. Monte Carlo optimization, Nash equilibrium, liver machine perfusion

Liver transplantation is the only current solution to liver failure. While the gold standard for organ preservation is static cold storage (SCS), machine perfusion (MP) is gaining acceptance as a better means of increasing (1) the number of livers available for transplantation and (2) transplantation success which has been correlated to the cellular energy state – adenosine triphosphate (ATP) synthesis and energy charge.

In this work, a first principles Nash Equilibrium approach is used to simulate a mathematical metabolic network model of the liver. Machine perfusion performance is formulated as a multi-objective function using two objective functions – a reward function that measures glucose consumption, ATP and bile synthesis, and energy charge and a network efficiency function that measures the ratio of ATP synthesis to glucose consumption. Inequality constraints for lactate concentration, pH, oxidative stress, antioxidant depletion, and malonyl coenzyme A synthesis are also used to ensure that solutions are physiologically relevant.

The novel contribution of this work is the optimization of the temperature protocol and perfusate composition using Monte Carlo policy iteration, which should also bring the temperature of the liver to body temperature during the final stages of MP and yield a medium composition that improves the energy state of the liver prior to transplantation. Monte Carlo optimization results show that there are multiple optima and a discrete Pareto optimal front. More specifically, the best temperature protocols demonstrate that gradual warming of the organ is superior to the traditional fixed temperature protocol, and this agrees with clinical research reported in the open literature [1,2]. Also, the best medium compositions along the Pareto optimal front are quite different and result in a better energy state than a pre-formulated perfusate composition. Several examples will be presented to elucidate key features of the model, the Monte Carlo policy iteration algorithm, and the physiological improvements that result.

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Local structures in time-series

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Keywords. effective dimensionality; Berezin-Lieb inequalities; quantum entropies.

The goal of this paper is to develop novel tools for understanding the local structure of systems of functions, e.g. time-series data points, such as the total correlation function, the Cohen class of the data set, the data operator and the average lack of concentration. The Cohen class of the data operator gives a time-frequency representation of the data set. Furthermore, we show that the von Neumann entropy of the data operator captures local features of the data set and that it is related to the notion of effective dimensionality. The accumulated Cohen class of the data operator gives us a low-dimensional representation of the data set and we quantify this in terms of the average lack of concentration and the von Neumann entropy of the data operator and an improvement of the Berezin-Lieb inequality using the projection functional of the data augmentation operator. The framework for our approach is provided by quantum harmonic analysis and time-frequency analysis. This is based on joint work with Monika Dörfler and Eirik Skrettingland.

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Robust and Distributionally Robust Optimization Models for Support Vector Machine

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Keywords. Support Vector Machine; Robust optimization; Distributionally robust optimization.

In this talk we present novel data-driven optimization models for Support Vector Machines (SVM). To handle uncertainty in data measurements, robust optimization models are proposed both in the linear and non linear cases. Besides, a moment-based distributionally robust optimization model enforcing limits on first-order deviations along principal directions in the linear case is presented. All the formulations reduce to convex programs. The new classifiers are evaluated on real-world databases and compared with the corresponding deterministic ones.

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A machine learning approach to speed up the solution of distributor's loading problems

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Keywords. Combinatorial Optimization; Distributor's Loading Pallet Problem; Random Forest; Support Vector Regression; Real Constraints.

We consider the distributor's pallet loading problem, whose aim is to pack on the lowest number of pallets a set of different boxes, satisfying a given set of constraints. We focus on a real-world scenario where a stability restriction and a compression limit must be respected. Each pallet is loaded with a set of layers of boxes that must not overhang beyond the maximum dimensions of the pallet.

We study a proposal to solve the problem which, firstly, builds layers heuristically, secondly, through machine learning algorithms, classifies them by "importance" and, finally, uses the classification to resolve a MILP. With "importance" we are meaning how much high is the "probability" that each layer will be used to resolve the instance. The MILP formulation seeks the best in terms of minimizing the pallets used to resolve an instance, satisfying stackability constraints, non-overhang constraints and not exceeding the weight limit between the layers loaded on the same pallet. More precisely, we describe the 4 phases for finding the solution:

1. Given an instance, we group the boxes that are not too dissimilar in height, i.e. such that $|h_i - h_j| < \Delta h$ for i, j indexes of different boxes b_i, b_j, where Δh is a real parameter.

2. To create layers, we use heuristic algorithms that resolve the 2D Bin Packing problem, including skyline and maximal rectangle algorithms.

3. We assign to each layer a score that represents its importance, through ML algorithms such as Random Forest (RF) and Support Vector Machines for Regression (SVR), which have been trained on already resolved instances.

4. We resolve a MILP through Gurobi, taking as input data the layers that have predicted scores greater than a certain threshold. In this manner we reduced the number of layers and speed up the search for the optimum.

Finally, we validate our proposed method, comparing results obtained with the machine learning approach with results obtained without machine learning techniques (without predicted scores). In general, we found that using scores helps, in many cases, to speed up the search for solutions with Gurobi, making problems of medium difficulty comparable to simpler ones in terms of resolution time.

Distributed Inexact Newton Method With Adaptive Step Size

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Keywords. distributed optimization; consensus optimization; Newton method

We consider two formulations for distributed optimization wherein N agents in a generic connected network solve a problem of common interest: distributed personalized optimization and consensus optimization.

A new method termed DINAS (Distributed Inexact Newton method with Adaptive Stepsize) is proposed. DINAS employs large adaptively computed step-sizes, requires a reduced global parameters knowledge with respect to existing alternatives, and can operate without any local Hessian inverse calculations nor Hessian communications. When solving personalized distributed learning formulations, DINAS achieves quadratic convergence with respect to computational cost and linear convergence with respect to communication cost, the latter rate being independent of the local functions condition numbers or of the network topology. When solving consensus optimization problems, DINAS is shown to converge to the global solution.

Extensive numerical experiments demonstrate significant improvements of DINAS over existing alternatives.

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A heuristic solution approach for bulk port routing optimization

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Keywords. Routing problem; bulk ports; belt-conveyor transportation; heuristics.

In today's world, the links between suppliers and customers are neither simple nor direct due to the expanded infrastructure of real supply chains, such as bulk port supply chains. In the latter, delivering the right product in good quality, to the right customer, in the right place, and at the right time by choosing the best belt-conveyor transportation routes among a complex real-world routes network is more and more challenging, making thereby the bulk port routing problem a strongly demanded optimization issue to solve. To solve the routing problem, we proposed, in a former work, a mixed integer linear program whose findings were interesting, but some means should be proposed to address difficult instances. Some closely related problems also failed to solve large instances with exact methods. In this paper, we propose a suitable solution encoding and develop a heuristic solution to handle large scale data sets. The heuristic can help the port planner to test different scenarios and provide better routing plan. The proposed method can be further refined and improved by employing a local search metaheuristic.

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Exploit Innovative Computer Architecture With Molecular Dynamics

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Keywords. Gromacs; High Performance Computing; Molecular Dynamics.

We have recently seen a rapid evolution of platforms for high-performance computing (HPC) systems, both in terms of architectures and accelerators. These new devices are intended to improve metrics such as time-to-solution and energy-to-solution. Although the benchmark test of the top500 [1] ranking is Linpack [2], each individual workload has different needs in terms of resource utilization and can completely overturn synthetic test rankings, so verification with a real-life use case becomes critical to understand which configurations to target when designing a dedicated HPC system. In this comparative study, we focused to cases of molecular dynamics.

Atomistic simulations are a powerful tool to analyse the structure and the behavior of various biological molecules and are widely use in biochemistry studies. Currently, there are several software packages available which provide the algorithms for the numerical resolution of the physical equation necessary for the simulations. Those softwares are demanding and need to handle a large amounts of resources, therefore the hardware in use has to be efficient in terms of performance and costs. Here we tested the Molecular Dynamics toolkit Gromacs [3] on different platforms: Intel, AMD and ARM clusters are considered, also with the support of NVIDIA GPUs. The highest performance is obtained with the use of NVIDIA GPU and from the comparison between the different CPU platform the best performances are obtained with Intel. During the tests energy consumption is measured in both idle and working case obtaining the energy to solution for every machine. We found that AMD and ARM servers are valid option if energy savings is considered alongside performance, the use of GPU gives a remarkable contribution to reduce consumption.

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Identifying Dengue Hotspots in Baguio City, Philippines through Spatiotemporal Analysis

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Keywords. Dengue hotspots; Temporal Means; Spatial Means; Geographic Information System.

This study analyzes the dengue incidence and potential hotspots in the 129 administrative units or "barangays" of Baguio City from 2010 to 2022 by investigating the yearly empirical spatial means, empirical temporal means, and incidence rates per morbidity week. The spatial mean was computed using the daily average incidence rates per 1000 individuals in each barangay. The temporal mean was calculated using the daily average of the cumulative cases of all barangays.

As a result, the barangays in the center of Baguio City were detected as dengue hotspots with the highest temporal means of 0.2558 and 0.1705 during September 2022 and August 2016, respectively. These barangays were mapped utilizing the Geographic Information System. Identification of these hotspots can assist the local government in designing control strategies to minimize the spread of disease.

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Game theory presented to Italian high school students in connection with infinite computing

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Keywords. Game theory; mathematical education; grossone.

Game Theory is a rather vast discipline, the purpose of which is to analyze the strategic behaviors of decision-makers (players), or to study the situations in which different players interact pursuing common, different or conflicting objectives. The first purpose of this talk is to provide a possible way of approaching elementary game theory in high schools. The second objective is to analyze the students' response in terms of learning, but also of liking. Is it possible *"giocare con la teoria dei giochi"* (Engl. transl: play with game theory) in the classroom? The third objective is to highlight the possible links between elementary game theory and the *grossone*-based system introduced by Prof. Y.D. Sergeyev. Once again with the didactic aspect of providing high school students with an "easy" and stimulating approach to modern research fields in mathematics. If time allows, we will then briefly describe the possible role of the so-called unimaginable numbers in relation to the combination of grossone and game theory.

Acknowledgements.
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Evaluation of healthcare structures in Italy through Sentiment Analysis

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Keywords. NLP; Text mining; Sentiment analysis; VADER-IT.

In health care, feedback and patients' needs are useful in highlighting the quality of the service required or not. Therefore, understanding what makes patients satisfied or dissatisfied is crucial for planning further company improvement strategies or approaches that are more useful for the required purpose. To be able to enhance and identify this, an ML technique such as Sentiment Analysis comes into play. Its objective is the automatic extraction of opinions, mainly from highlighted texts, by associating a positive and negative score of the review with this [1]. These applications are based on the assumption that users can speak publicly about their pathology or associated symptoms [2]. This article aims to analyze the correlation between the user sentiment reported on the QSalute online review platform, and the sentiment score extracted by the reviews through the use VADER-IT, a lexicon-based sentiment analysis algorithm [3]. In particular, VADER-IT will be tested on a specific dataset of health reviews of a specific pathology such as 'Diseases in Haematology', concerning hospitals in Italy. These reviews will be extracted from a public portal called QSalute https://www.qsalute.it/.

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Variational Quantum Algorithms for Energy Optimization in Prosumer Communities

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Keywords. energy optimization; quantum computing.

Variational quantum algorithms are hybrid quantum/classical where quantum computation is driven by a set of tunable parameters, and the parameter values are iteratively optimized by a classical algorithm [1]. These algorithms are today adopted to tackle optimization problems, the hope being that the parallel nature of quantum operations can lead to a significant speedup and better results with respect to classical optimization algorithms. In particular, linear problems can be reformulated as Ising problems, which can be solved with the Quantum Approximate Optimization Algorithm (QAOA), one of the most renowned hybrid algorithms. We show the formalism and the mathematical steps needed to solve the so-called "prosumer problem", i.e., the MILP (Mixed Integer Linear) problem that aims to optimize the energy exchanges in a prosumer community [2], in which some users own renewable energy plants and can share energy with other users, thus reducing the overall costs and improving the adoption of green energy. We report on preliminary experiments executed with simulators and real quantum computers. The results are encouraging, as the computation time grows slowly with the problem size, while classical algorithms show an exponential trend, due to the NP-hard nature of the problem.

Acknowledgements.

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A genetic algorithm to optimize the dispatch of firefighting resources

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Keywords. Forest Fires; Dispatching Problem; Genetic Algorithm.

Wildfires have become an important research topic among the operations research community [1]. Recently, efforts have been made to develop and implement decision support systems for forest fire management [2]. The characterization of the impacts of wildfire and fire suppression is critical information for decision-making in fire management [3].

Currently, optimization has been widely applied in the management of firefighting activities, allowing improvements in the effectiveness and speed of action of firefighters [4]. This work aims to define resource allocation strategies, through the solution of a resource dispatch problem, in order to minimize the water required to combat several ignitions. Thus, a genetic algorithm (GA) was applied, where several operators were tested to obtain the optimal solution of the problem. Finally, a statistical analysis was performed in order to show the most suitable GA operators to solve the problem.

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A framework for shape-parameterized neural networks: an overview from surrogate modeling to shape optimization

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Keywords. Physics-informed neural networks; NURBS parameterization; shape optimization.

In this talk, we discuss the formulation of neural networks that can learn and predict the solution of PDEs defined on freeform domains. In order to achieve this, non-uniform rational B-Splines (NURBS) are employed to represent the domains. In this way, each shape can be characterized by the coordinates of a set of control points, which are included among the variables of the neural network.

First, we show how our shape-parameterized networks are formulated. We discuss both purely data-driven and physics-informed neural networks (hereafter named NNs and PINNs, respectively). We consider the linear elasticity equation and show that the shape-parameterized networks can be successfully trained on IGA data generated for a set of training shapes. Furthermore, we discuss the ability of the trained network to predict the PDE solution on domains that were not included in the training dataset. We especially focus on comparing the accuracy of NNs and PINNs, with the aim to define a setting where the physics can complement incomplete data.

Our analysis finally affords us to make some considerations on the prospect of the use of our shape-parameterized neural networks to solve shape optimization problems. Results on this are presented to show the applicability of the procedure. In this context, transfer learning from one shape to another is discussed as well.

The talk is based on joint work with Xiaoping Qian and with Joshua Gasick at the University of Wisconsin-Madison (U.S.A.).

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A Galerkin-type method for 2-nd kind FIEs over equally spaced nodes

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Keywords. Fredholm Integral Equations; Mock Chebyshev Interpolation.

In this talk, we present a Galerkin-type method based on equally spaced points of $[-1,1]$, for Fredholm integral equations (FIEs) of the second kind

$$f(y) - \mu \int_{-1}^{1} f(x)k(x,y)w(x)dx = g(y), \quad y \in [-1,1], \tag{1}$$

where f is the unknown function, k is a bivariate function defined in the unit square $[-1,1]^2$ that can also contain some peculiar drawbacks, g is the right-hand side term, μ is a real parameter, and $w(x) = v^{\alpha,\beta}(x) := (1-x)^\alpha(1+x)^\beta$, $\alpha, \beta > -1$ is a Jacobi weight.

The use of equidistant points is crucial in many engineering and mathematical physics problems which are modeled by integral equations, and when k and g are available only in a discrete set of equispaced nodes as results of experiments on the field. In all these cases, the classical methods based on piecewise polynomial approximation offer a lower degree of approximation, while the efficient procedures based on the zeros of orthogonal polynomials cannot be used.

Here, we present a Galerkin method based on quadrature formulae (see, e.g. [2,2]) obtained by means of the constrained mock-Chebyshev least squares operator $\hat{P}_{r,n}$. This operator was recently introduced in order to defeat the Runge phenomenon that occurs when using polynomial interpolation on large sets of equally spaced points [1].

Stability and convergence of the method are proved in suitable spaces and some numerical tests are shown to confirm the theoretical estimates.

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Stochastic zeroth order optimization via finite differences

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Keywords. Stochastic optimization; zeroth order methods; gradient-free algorithms.

In this talk, we introduce and analyze the S-SZD algorithm (Structured Stochastic Zeroth order Descent), a finite difference scheme to approximate a stochastic gradient on a subset of directions that changes with each iteration. These directions are structured but randomly chosen. Our main contribution is to prove, for smooth convex functions, the almost sure convergence of the iterates and a convergence rate for the functional values which resembles the one for SGD algorithm. Moreover, for non-convex functions satisfying the Polyak- Lojasiewicz inequality, we establish the first convergence rate for stochastic zeroth order algorithms under such an assumption. We corroborate our theoretical findings with numerical simulations where our assumptions are satisfied and on the real-world problem of hyper-parameter optimization.

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Meta Discussion Pedagogical Model to foster Mathematics Teacher's professional development

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Keywords. Mathematical discussion, prospective teachers, mathematics teachers professional development.

In this contribution we present an experimental research undertaken with Pre-Service primary Teachers (PSTs). The aim of this study is to foster the Mathematical Discussion (MD) theoretical framework's learning (Bartolini Bussi, 1989), in order to give PSTs the opportunity to learn in and from their practice. The Mathematical Discussion combined with the Meta Discussion on a Pedagogical model, a new theoretical construct that we identified, allow prospective teachers, on the one hand to be introduced to the pedagogical model itself and, on the other hand, to develop in and from practice both theoretical knowledge and practical experience of this model. This means that the MD becomes at the same time the subject of the lecture and the methodology used during the lecture. This new theoretical approach combines Shulman's (1986) research about the Pedagogical Content Knowledge (PCK), Ball's Mathematical Knowledge for Teaching (MKT) (2009) and further research on what is relevant to learn in and from practice and how this practice can be used for teachers' learning (Ball & Even, 2009). The aim of the path has two different goals: the construction of the MD's characteristics from a theoretical point of view and the way to manage MD in the future professional practice. The possibility for the students to play two different roles at a time enables them to think and learn in a metacognitive perspective.The analysis of results highlight that the PSTs became aware of how MD works and of its value. In and from their own practice they learned how to manage MD in class.

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DG schemes for transformed master equations modeling open quantum systems

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Keywords. Open quantum systems; Master Equations; Discontinuous Galerkin

We present in this work a mathematical and numerical analysis of a master equation modeling the interaction of a system with a noisy environment in the particular context of open quantum systems. We show that a transformed equation can have a simpler structure by expressing it in convenient coordinates, making it easy to interpretation, and having a reduced computational cost in comparison to the computation of a Wigner-Fokker-Planck model of the same system. We then present specifics of a DG numerical scheme adequate for the convection-diffusion equation obtained, which lets us solve computationally the transformed system. We present as a benchmark problem the case where the potential is harmonic, for which we can compare our numerical results against the analytical steady state solution of this problem.

Acknowledgements.
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Increasing noise robustness of deep learning-based image processing with model-based approaches

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Keywords. Non-convex optimization; Neural Network; Inverse Problems.

An efficient and robust framework, based on recent works in deep learning-based image processing and non-convex iterative optimization, is here proposed for tomographic image reconstruction.
Forcing sparsity in the image gradient magnitude has proven to be an effective means for reducing the artifacts in biological and medical imaging. Most of the image reconstruction algorithms make use of the L1 norm of gradient magnitude images to solve a convex optimization problem, but employing nonconvex Lp quasinorms (with p smaller than 1) can be potentially more effective. Deep learning approaches have already been widely proposed to enhance tomographic images, but they typically disregard the mathematical problem statement and the ill-posedness of the underlying model.

In this talk, we consider the nonconvex total p-variation (TpV) and the Chambolle-Pock solver where a convolutional neural network is used to speed up the iterative reconstruction while preserving converging features. The resulting hybrid method is robust and accurate, even in case of unknown noise. Verifications and comparisons performed using different approaches illustrate that the proposed method is effective and promising.

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Optimization of EfficientNetV2 Models for Predicting Sadness Emotion

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Keywords. Optimization; overfitting; image analysis; EfficientNetV2.

Images become an attractive area for analysing emotions. The recognition of emotions in common images is attracting increasing attention from researchers. Such emotion recognition is more complex and different from conventional computer tasks. Due to human subjectivity, ambiguous judgments, cultural and personal differences, there is no single model for such emotion assessment. Current models cannot directly learn visual emotion features for a given emotion. We decided to analyze emotions using a categorical model, as this is the natural way of human expression in psychological research. We have chosen sadness as the main emotion, which is almost the most important emotion after happiness. The deep neural network was trained to recognise sadness. The problem is to find the optimal values for the parameters of the network model by determining the least number of training steps. We analyse different realizations (architectural variants) of EfficientNetV2 model [1]: EfficientNetV2S, EfficientNetV2B0 and EfficientNetV2B2. Two our objectives are to compare these realizations and to evaluate the overfitting situations during training, depending on the number of training iterations. We chose different batch sizes and applied regularization by different dropout rates. We analysed the changes in the accuracy on the test set during each training iteration. The experiments were carried out several times and the averaged accuracy of the models was collected. Our findings show that there is over 2% average optimized improvement using EfficientNetV2S with dropout rate of 0.8, following a fully connected dense layer and using a batch size equal to 128. This improvement is also useful for better generalisation in predicting the emotion class of visual sadness. An example is given in the figure. On the left we see a painting by Van Gogh, and on the right we see a picture by eight year old child. In the Van Gogh painting, the emotion of sadness has been identified.

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Using Infinity Computer in Global Optimization

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Keywords. Lipschitz global optimization, black-box functions, Infinity computing.

Global optimization is important in many fields of applications: engineering, electronics, machine learning, optimal decision making, etc.

In many of these applications, the objective functions and derivatives satisfy the Lipschitz condition, even though their analytical representation is unknown and even one of their evaluation can be really time consuming, (see e.g. [1,2]).

In this talk it is shown how the novel Infinity Computer framework (see e.g. [3]), able to work numerically with different infinities and infinitesimals, can be efficiently applied in Lipschitz global optimization (see also [4]).

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A Numerical Approach to Basic Calculus

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Keywords. infinity; grossone methodology; calculus; mathematics education.

A big body of research has been devoted to the complications faced by undergraduate students with basic calculus and means of overcoming them (for example see [3]). This situation imposes the urge to try educational approaches that are different from the traditional ones used in most curriculums worldwide. In this paper, we deal with a non-traditional method in teaching basic calculus for undergraduate students. In particular, this study explores the efficiency of a numerical method for dealing with infinity and infinitesimals introduced by Yaroslav Sergeyev in the early 2000's. The grossone methodology proposed by Sergeyev is a non-classical one yet it doesn't contradict the classical mathematics. Instead, it provides simple and easy computational way for dealing with infinite quantities [2]. It is noted that this methodology has been widely used in mathematics and applied sciences. Moreover, it has proved to be fruitful for educational purposes according to the results of several studies done recently. The experimentation involves grade 11 and 12 students in two secondary public schools in Lebanon (age 16-18). The aim of this study is to check students' intuitive reactions with the grossone methodology and compare it to their performance after being subject to a teaching unit highlighting this methodology. In the first phase of the study, students were subject to a zero-knowledge test. The second phase involved several sessions introducing grossone methodology. In the last phase, a very similar test to that held before the teaching sessions was administrated to the students to check their performance after the lectures. It is noted that this study is a replication of a study done in Italy recently (see [1]) for the purpose of comparing the results.

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Constrained Global Optimization by Smoothing

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Keywords. Constrained global optimization; discontinuous penalty; smoothing; finite-difference stochastic gradient.

A stochastic successive smoothing method for local and global optimization of nonsmooth and discontinuous functions under constraints is developed. First, a constrained problem is reduced to an unconstrained one by the exact nonsmooth penalty function method [1,2], which does not require the selection of the penalty coefficient. Then the resulting objective function is sequentially smoothed by the kernel method starting from relatively strong smoothing and with a gradually vanishing degree of smoothing. Each smoothed function is locally minimized by the finite-difference stochastic gradient descent with trajectory averaging. The stochastic gradients of the smoothed functions are estimated by finite differences over stochastic directions sampled from the kernel. As to the whole successive smoothing algorithm, the results of previous optimization runs are used for the selection of the starting point for the optimization of a successive less smoothed function. Smoothing provides the successive smoothing method with some global properties [1]. The performance of the stochastic successive smoothing method is illustrated on a variety of constrained optimization problems [1,3].

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A DCA-Like approach for solving the problem of constructing Merkle tree in Blockchain transaction system

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Keywords. Merkle tree; blockchain transaction; DC Programming; DCA; DCA-Like; binary quadratic programming.

The State Merkle tree is used in Ethereum cryptocurrency system to store and verify the current account's state in a safe and efficient manner. A particular state consists of account balances, the number of transactions, contract codes, and storage values. In this paper, we address the problem of constructing a tree structure with the minimum number of hash values required for account information modification based on the transaction distribution in order to enhance the performance of blockchain transaction system. The proposed optimization model is a combinatorial problem with quadratic functions and binary variables. We propose a conventional DC (Difference of Convex functions) program that can be effectively solved by the DCA (DC Algorithm) using the binary character of variables and penalty techniques. To get better convex approximation of the objective function without knowing a DC decomposition, DCA-Like, a novel extension of DCA, is applied. Additionally, we suggest a combined DCA-Like algorithm and divide-and-conquer algorithm, termed the recursive DCA-Like approach, for building a Merkle tree for a large number of blockchain accounts. The effectiveness of our approach and its superiority to well-known methods are demonstrated by numerical experiments on several datasets.

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A general strategy for enriching simplicial linear finite elements

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Keywords. Simplicial finite element; nonconforming finite element; enriched finite element.

Low-order elements are widely used and preferred for finite element analysis, specifically the three-node triangular and four-node tetrahedral elements, both based on linear polynomials in barycentric coordinates. They are known, however, to under-perform when nearly incompressible materials are involved. The problem may be circumvented by the use of higher degree polynomial elements, but their application become both more complex and computationally expensive. For this reason, non-polynomial enriched finite element methods have been proposed for solving engineering problems. In line with previous researches [1,2], the main contribution of this work is to present a general strategy for enriching the standard simplicial finite element by non-polynomial functions. A key role is played by a characterization result, given in terms of the non-vanishing of a certain determinant, which provides necessary and sufficient conditions, on the enrichment functions and functionals, that guarantee the existence of families of such enriched elements. We show that the enriched basis functions admit a closed form representation in terms of enrichment functions and functionals. Finally, we provide concrete examples of admissible enrichment functions and perform some numerical tests.

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Numerical Approximation of Invariant Manifolds for Singularly Perturbed Systems with Machine Learning

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Keywords. Singularly Perturbed Systems; Slow Invariant Manifolds; Physics-Informed Machine learning

Multi-scale dynamical systems exhibiting fast/slow timescale separation are frequently expressed as Singularly Perturbed Systems. The long term dynamics of such systems evolves along Slow Invariant Manifolds (SIMs) that are hypersurfaces embedded in the ambient phase-space thus attracting all neighboring trajectories [1]. In this work, based on the concept of Geometric Singular Perturbation Theory (GSPT), we introduce a Physics-Informed Machine-Learning (PIML) approach for the numerical approximation of SIMs. The proposed approach exploits the underlying physical invariance of the SIM to provide approximations of increased numerical accuracy. The proposed PIML approach is able to identify the "birth" of SIMs, in contrast to other machine learning approaches, such as simple regression, which are based on time-series data produced by the numerical solution of ODEs. Furthermore, the PIML scheme provides SIM approximations of similar or even higher numerical accuracy than that provided by well established analytic or algorithmic methods such as the CSP [2] in the context of GSPT [3].

To demonstrate the efficiency of our method, we employ the PIML scheme to two benchmark problems, namely the Michaelis-Menten reaction mechanism and the 3D Sel'kov model of glycolytic oscillations. Our approach offers a promising solution for accurately approximating SIMs of singular perturbed systems in a computationally efficient manner.

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The scaling behavior of high-order structure functions for a turbulent jet induced by a rotating propeller

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Keywords. propeller jet; high-order structure functions; Hurst coefficient.

The traditional marine propulsion system used to move a ship is constituted by an electric motor turning a propeller. The device produces a turbulent jet that impacts the seabed and banks of harbour basins or navigation channels up to a distance of several propeller diameters from them. This causes the formation of a scour hole and a deposition mound.

The present work aims at investigating, for the first time, the scaling behavior of the high-order structure functions for this turbulent jet, by discussing the experimental results in light of monofractal or multifractal models. This latter would explain the possible existence of intermittency.

To this end, an experimental campaign was performed in the "Laboratorio Grandi Modelli Idraulici" (GMI) of the University of Calabria, in an 18 m long, 0.985 m wide and 0.7 m deep horizontal flume with rectangular cross-section. The test was performed in still water condition with a fixed water depth, using a propulsion system constituted of an electric motor turning a propeller with four blades. The propeller diameter was equal to 8.2 cm. The flow field was measured with an Acoustic Doppler Velocimeter (ADV). Specifically, the longitudinal structure functions were studied in this work using Taylor's hypothesis.

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Unsupervised learning of a variational model via a quality measure score predictor

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Keywords. Unsupervised Learning, Unrolling Methods, Performance Predictor, Bilevel Optimization.

Variational models are a classical tool for many imaging problems, but they do have known limitations. One of them is the absence of general guidelines for selecting the hyperparameters they depend on. Bilevel optimization schemes have been proposed in order to overcome this issue and learn a satisfying set of hyperparameters ([1]). In particular, they offer a high level of interpretability while keeping the amount of data required low. We propose an unrolling of a FISTA-like algorithm to approximate the solution of an energy functional and use that in a training scheme to set the hyperparameters ([2],[3]). The key aspect of this framework is the loss function, where we employed a performance predictor that is built to infer the score an image would receive, with respect to some quality measure, without feeding it with the corresponding ground truth ([4]). This allows us to perform the training for the energy in an unsupervised fashion, as true images are only used in the tuning of the score predictor, which is done once and for all. Finally, we test the scheme on a standard imaging problem.

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Cost-sensitive weighted bagging DCA based method for imbalanced financial data

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Keywords. Bagging; DCA; DC programming; Financial problems; Imbalanced data.

Highly imbalanced data is a major issue in financial problems (i.e., fraudulent transactions, credit/loan approval) where the skew across categories may range from tens to hundreds of times. The problem of imbalanced data poses a challenge for machine learning algorithms, as the minority class is frequently underrepresented, resulting in poor classification performance. Misclassification caused by imbalanced data can have severe consequences for financial institutions, including significant financial losses, legal consequences, and damage to reputation. In this research, we propose a new bagging approach called cost-sensitive weighted bagging, which is based on DCA and LS-DC algorithm. The weighted bagging method combines multiple base classifiers trained on different subsets of the training data with different weights, which helps to improve the overall performance of the classification model. In addition, the cost-sensitive approach takes into account the cost of misclassifying instances of the minority class, which is typically higher than that of the majority class. In order to evaluate the effectiveness of the proposed algorithm for the imbalanced problem, we perform thorough numerical experiments using some financial datasets from UCI machine learning repository, Kaggle competitions and our financial dataset.

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IoT and Artificial Intelligence integration for a stormwater Monitoring and Management System

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Keywords. Urban flooding, Internet of Things, AI, early detection.

Stormwater management is a crucial environmental and public health issue, particularly in urban areas, where impervious surfaces limit rainwater infiltration into the soil. Traditional stormwater management systems have limitations in detecting and predicting the behavior of runoff, which can lead to flooding. This study focuses on the use of the Internet of Things (IoT) and Artificial Intelligence (AI) technologies to optimize stormwater systems. Overall, these systems employ various IoT devices to monitor critical parameters of the stormwater network in real time. The data collected by these devices are processed and analyzed using AI algorithms such as machine learning and deep learning, which enable the system to detect anomalies, predict potential flooding events [1, 2], and provide decision-makers with valuable insights into the behavior of surface runoff. Integrating IoT and AI technologies in stormwater management improves efficiency, early issues detection, real-time decision-making, and reduced environmental damage. Thus, this study demonstrates this approach's effectiveness, providing a more comprehensive and accurate monitoring and management system and network architecture compared to traditional stormwater management systems.

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Analysis of Computational Fluid Dynamics Approaches for the Development of Microfluidic Devices

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Keywords. microTAS; LOC; CFD; microsensors; microfluidics.

Nowadays, there are plenty of microfluidic-based devices, from microfabrication to micro total analysis systems (microTAS) and lab-on-a-chip (LOC). The application of these devices is very vast such as inkjet printers, biomedical, environmental, and food [1], smart textiles [2], and the detection of diseases [3]. Microdevices mainly contain microchannels, micropumps, chambers, and membranes, and the processes are based on fluid dynamic principles. At the molecular level, lattice Boltzmann methods (LBM) numerical simulation and computational fluid dynamics (CFD) are the prominent simulation techniques. However, there are many challenges in the acceleration of these techniques. Therefore, this research aims to analyze techniques for modeling micro-devices/sensors and applying CFD tools in optimal design, manufacturing, operation, and control. The main advantages of CFD would be the optimization of micro-sensor design, device innovation, cost reduction, a decrease of failure risk, shortened production and regulatory approval process time, improvement of design based on safety standards, and providing more insights for sensor development.

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Optimization Method Development for Water Management of Green Roof Systems

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Keywords. NBS; AWH; greywater; multidisciplinary; optimization.

Green roofs present several advantages at multiple scales [1]. However, the applications are still not spread enough, which could be mainly due to the uncertainty about some factors such as water consumption in the dry season, the usage of the roof for other purposes like solar panels, and the construction issues such as initial and maintenance cost [2]. Thus, this study aims to develop an optimization method for an independent multidisciplinary green roof system disconnected from the urban water network. It means the optimized size of a green roof, in which the precipitation, runoff, atmospheric water harvesting (AWH), and greywater could be enough for the green roof's water requirements without further irrigation. In this regard, a mathematical model is developed and verified based on experimental data of a green roof in a Mediterranean climate. The developed model is optimized considering different scenarios, and the results show the maximum area of the independent green roof in each scenario.

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The unreasonable effectiveness of optimal transport distance in the design of multi-objective evolutionary optimization algorithms

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Keywords. Wasserstein distance; multi-objective optimization; evolutionary algorithm.

Randomness is a critical component in genetic operators of evolutionary algorithms. Individuals are selected by mechanisms which drives exploration of the search space to improve diversity in the generated population to achieve a satisfactory global performance of the algorithm. This exploration might become less effective as the number of dimensions and objectives grow. In this paper a strategy for exploiting the randomness in evolutionary algorithms is proposed. The key idea is to embed in the design of the multi-objective evolutionary algorithm probability distributions. In particular, the selection of the individuals to mate takes place in a space of probability distributions endowed with the Wasserstein distance. This distance has been applied both to NSGA-II to sample from the approximation of the Pareto set and a scalarization approach as MOEA/D to sample the scalarizing vector. Computational experiments on standard test functions and real-world applications shows a significant improvement in terms of performance which becomes relevant as the number of objectives increases.

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Variable metric proximal stochastic gradient algorithms for deep learning optimization

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Keywords. Stochastic optimization; variable metric proximal algorithms; deep learning.

Many machine learning applications involves the minimization of an objective function accounting for both the so called empirical risk, i.e. the sum of several loss functions, whose number depends on the cardinality of a given training set and a regularization term, possibly non differentiable. Due to the high dimension of the dataset, the evaluation of the objective function and its derivatives may be prohibitively expensive, making deterministic proximal gradient methods computationally not feasible. For this reason, the research focus has shifted toward stochastic gradient approaches in the last decade. However, it is well known that proximal stochastic gradient algorithms can exhibit poor practical performance due to a bad choice of the learning rate parameter and a large variance of the stochastic directions. In this talk we present a proximal stochastic gradient method whose aim is to overcome these two drawbacks [1]. We indeed introduce a proximal stochastic gradient algorithm which fixes the learning rate by means of a non-monotone line search and controls the variance of gradients by combining a variable metric to precondition the stochastic gradient directions with an automatic sample size selection. Converge results can be proved for both convex and non-convex objective functions. Several numerical experiments show the effectiveness of the suggested approach in training both statistical models for binary classification and artificial neural networks for multi-class image classification.

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Numerical Optimization in Hyperbolic Space - Applications to Systems Biology

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Keywords. Numerical Optimization; hyperbolic space; network embedding.

State-of-the-art machine learning methods for predicting associations between biological objects rely on representing those objects as points in a classical Euclidean space. While the assumption of Euclidean geometry has been convenient due to availability of advanced analytic, numerical, and statistical tools in the Euclidean spaces, recent theoretical studies demonstrate that all complex networks exhibit hierarchical, tree-like organization, characterized by heterogeneous degree distribution and a high degree of clustering. Hence, embedding those systems in a flat Euclidean space distorts the proximity of individual objects. Recent years have seen development of methods that use non-Euclidean geometries to model proximities between network objects [1]. One space that can accommodate exponential growth in the number of such objects is a hyperbolic space of negative Gaussian curvature [2]. Unfortunately, minimizing objective functions used in hyperbolic network embedding is a notoriously hard problem due to rough and rugged surfaces of those functions [3]. We present a technique for addressing numerical instability of the hyperbolic gradient descent in vicinity of steep cliffs and deep valleys. Controlling erratic behavior of the hyperbolic gradient on the error surfaces enables us to design an accurate method for bipartite network embedding into a hyperbolic space. We demonstrate that the accuracy of our method compares favorably to the accuracy of the existing state-of-the-art techniques, while lowering the embedding dimension by more than an order of magnitude.

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On the worst-case RSS in linear regression with interval outputs

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Keywords. RSS in interval regression; QP; hyperplane arrangement.

Many problems in robust statistics lead to NP-hard optimization problems. One of the well studied ones is the problem of maximizing sample variance (a convex quadratic function) over interval-valued dataset [1]. Despite its NP-hardness, it was shown that the problem can be solved efficiently on average under a fairly general probabilistic setup [2] using a simple pruning of the feasible set that exploits the special structure of the underlying quadratic form [3].

The maximization of sample variance over interval data is a special case of maximization of residual sum of squares (RSS) for OLS-estimator in linear regression with interval outputs (crisp values of input observations and interval-valued observations of outputs are given, more on this setup e.g. in [4]).

We firstly generalize the pruning approach from [3] to handle maximization of RSS in its full generality. Then we show that the good average behavior (shown for the maximization of sample variance in [2]) is likely for the RSS case, too. We also show that the pruning framework is usable for a more general class of quadratic problems.

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Exploring Quantum kernel methods for breast cancer subtyping: a real-world experiment

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Keywords. Quantum Enhanced Machine Learning; Omics data; Quantum Kernel methods; Cancer subtyping.

Quantum Machine Learning (QML) has been proposed as one of the most promising applications of quantum computing for currently accessible Noisy Intermediate Scale Quantum (NISQ) devices. Quantum kernel estimators, specifically, hold great versatility and can be applied to any classical ML model, both unsupervised and supervised [1]. However, whether these quantum models can outperform classical ML in solving real-world problems still needs to be explored and demostrated [2] as they have so far only been tested on ad hoc simulated data [3] or simplified artificial datasets. We aimed to evaluate the performance and usability of Quantum Support Vector Machine (QSVM) for the classification task of a real complex tumor dataset. The dataset encompasses multi-omics breast cancer sample data and the subtypes are not separable by classical SVM. We therefore tested a QSVM based on ZZ-feature map [3] and compared it to a classical SVM with the same task and optimization procedure. Our results showed that complex quantum decision boundaries suffer from generalization capabilities, in contrast with the ideal simulated dataset for which the used encoding map was formulated. To overcome this limitation, we have explored better-suited feature map configurations, tailored to the data. Our work is one of the first attempts to show how QML can be effectively exploited in a realworld clinical-translational context.

Acknowledgements.

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The Arithmetic of Infinity and Reflective Enquiry

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Keywords. Arithmetic of Infinity; mathematics education; pragmatism.

Our goal in this paper is to use J. Dewey's conception of reflective enquiry (see in particular [1]) to exhibit an important correspondence between a pragmatist interpretation of these classroom activities and the original motivation put forward by Sergeyev for the introduction of the Arithemtic of Infinity (AoI, see e.g. [4]). Sergeyev's motivation was to show that the rough mathematical experience of infinite collections can be resolved into finer numerical distinctions with the aid of a more effective symbolic instrument, namely a richer numeral system.

On Dewey's account of enquiry rough, primary experience acquires focus and sharpness when object of reflections are introduced to interact with it for the sake of resolving primary experience into a richer picture under the pressure of specific problems that already arise in the rough, primary setup. Recent work in mathematics education based on AoI ([2, 3]) and reliant on the author's teaching materials shows that, under the pressure of problems posed by paradoxes of infinity, students naturally take up AoI as an object of reflection enabling them to find resolutions and reconstruct the landscape of their engagements with the concept of infinity.

This parallel shows AoI to provide a very useful instrument for the practice of mathematics education and has an even broader cultural significance, insofar as it contributes to the active acquisition of the habit of reflective, intelligent enquiry. We conclude our discussion by pointing to the relationship between this acquisition and student emancipation from so called 'math anxiety', outlining plans for further experimental work.

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A Bayesian Approach for Simultaneously Radial Kernel Parameter Tuning in the Partition of Unity Method

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Keywords. Kernel-based interpolation; hyper-parameter optimization; partition of unity methods.

In this contribution, *Bayesian Optimisation* (BO) is used to simultaneously search the optimal values of the shape parameter and the radius in Radial Basis Function interpolation together with the *Partition of Unity Methods* (PUMs) [2, 3]. BO is a probabilistic iterative approach that models the error function with a step-by-step self-updated Gaussian Process [4], whereas PUMs are meshfree interpolation techniques that allow us to reduce cost-intensive computations when the number of scattered data is very large, as the entire domain is decomposed into several smaller sub-domains of variable radius [1]. Numerical experiments show that the combination of these two tools sharply reduces the search time with respect to other techniques such as the Leave One Out Cross Validation.

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Weighted finite element method and body of optimal parameters for one problem of the fracture mechanics

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Keywords. Boundary value problems with a singularity; R_ν-generalized soluiton; weighted finite element method.

Mathematical models with a singularity play a decisive role in predicting the development of processes in fracture mechanics and physics. In the engineering literature, computational methods are widely studied for problems of electromagnetism, hydrodynamics and the theory of elasticity with a singularity caused by the presence of re-entrant corners on the boundary of a domain. We have constructed a weighted finite element method (WFEM) based on the introduction of the definition of an R_ν-generalized solution for the listed problems (see [1]-[4]). This method allows finding a solution with high accuracy compared to the classical finite element method. At the same time, it retains the simplicity of the stiffness matrix structure, unlike other numerical methods of increased accuracy. To use WFEM effectively, it is necessary to correctly set the control parameters of the approach. In this report, the weighted finite element method and an algorithm for determining the optimal parameters for finding an approximate solution to the Lamé system in domains with a boundary containing re-entrant corners α in the range from π to 2π are presented.

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Computation of the confluent hypergeometric function $M(a, b, x)$

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Keywords. Confluent hypergeometric functions; Approximation methods; Numerical algorithms.

Confluent hypergeometric functions play a relevant role in numerous problems in science and engineering. For few examples of applications in Physics, see for example [1]. Recently [2], we have considered the computation of one of the solutions of the confluent hypergeometric equation, the Kummer $U(a, b, x)$ function and its derivative [2]. In this contribution, a computational algorithm for the other standard solution of the confluent hypergeometric equation (the function $M(a, b, x)$) is presented. As we will see, series and asymptotic expansions will play a key role in the resulting algorithm. Examples of the performance of a double precision implementation of the algorithm will illustrate the accuracy and efficiency of the computational scheme.

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Numerical Bifurcation Analysis of Symmetry Breaking Turing Instabilities

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Keywords. Numerical Bifurcation Analysis; Partial Differential Equations; Turing Instabilities; Symmetry Breaking.

We perform the numerical bifurcation analysis of the pattern formation dynamics of a system of PDEs modelling the vegetation dynamics in water-limited regions. We perform a linear stability analysis, thus deriving analytically the conditions for the appearance of Turing instabilities marking the onset of spatio-temporal patterns from the homogeneous patterns. Furthermore, we provide their dependence on the size of the domain. Importantly, exploiting the arsenal of numerical bifurcation analysis toolkit, we trace the branches of the pattern formation of the inhomogeneous solutions, which form due to the onset of secondary bifurcations from the primary Turing instabilities, marking the onset of multistability of asymmetric patterns [1].

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Heuristics with Local Improvements for Two-processor Scheduling Problem with Energy Constraint and Parallelization

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Keywords. Parallelizable job, speed scaling, energy, scheduling, approximation algorithm, computational complexity.

Modern computer systems offer some type of parallelism and use restricted resources. Parallel jobs require more than one processor at the same moment of time [1]. Processors may operate at variable speeds. Running a job at a slower speed is more energy-efficient. However, it takes a longer time and affects the performance. We investigate the speed scaling scheduling problem [2] with the total completion time criterion for two processors.

We show the problem is polynomially solvable where all jobs are sequential (require only one processor) or fully-parallelizable (require both processors). Also we prove that the problems is NP-hard when we have both sequential and parallelizable jobs. For the last case we suggest heuristic methods based on greedy rules and list scheduling. The generated schedules have the block structure [3]. We also propose procedures of local improvements inside and between blocks.

For the testing purpose we generate series of instances of various structure. Firstly, we compare the record values of our initial heuristic (HE) and its modification with local improvements (HE_{LI}) to lower bound. HE_{LI} demonstrates statistically significant better results than HE or each test series. Also we compare the record values generated by HE_{LI} with optimal objective of the same problems, but where all the jobs are single-processor ones. We can conclude that parallel execution of a part of the jobs can improve the sequential case even in approximate solution in most of the considered instances.

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The advantages of hyperentanglement in quantum telecommunications processes

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Keywords. Entanglement; hyperentanglement; quantum cryptography; Jaynes-Cummings model.

Entanglement is a very useful phenomenon for quantum information processes. It can be considered as a special case of hyperentanglement, i.e., hyperentanglement with one degree of freedom (DOF). Two particles are hyperentangled if they are entangled in more than one DOF. The main advantage of hyperentanglement is that of being able to encode a greater amount of information by exploiting the DOF of the system. This advantage is due to the fact that it is possible to extract information for each DOF.

We propose a modelling of a hyperentangled state through copies of a Bell state and evaluate its functionality in a quantum communication protocol. The goal is to simulate the transport of a hyperentangled state through a classical channel in the presence of a system-environment interaction. In particular, we study the trend of the quantum bit error rate (QBER) as a function of the parameters of the Jaynes-Cummings model which simulate the interaction with the environment. By virtue of an increased Hilbert space following the increase in the DOF, the entanglement quantifier, as well as the concurrence, decays slower with the distance compared to the case of one DOF and shows a peculiar behavior, which will be discussed in detail.

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Variational Inequality Problems Beyond Convex Settings

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Keywords. Convex optimization; fixed points; iterative algorithms; variational inequality.

In practice, nonlinear problems often manifest as optimization problems with certain constraints. However, these problems or constraints may lack interesting properties such as convexity, linearity, or smoothness of the objective functions. This lack of properties results in tediousness when trying to find solutions to these problems. This work provides notions of distances in $\mathbb{R}^n$ that offer great flexibility regarding convexity, linearity, and smoothness. As a result, non-convex (or constrained) problems can be transformed, to some extent, into convex (unconstrained) problems. The work illustrates the approximation of solutions to variational inequality problems through a fixed-point scheme, with examples. A particular case of Korpelevich approaches to a solution of a variational inequality problem of monotone type mapping is analyzed.

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Machine learning techniques for Branch-and-Cut methods: the selection of cutting planes

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Keywords. Branch-and-Cut; machine learning; scoring function.

Branch-and-cut is an exact algorithm for solving Integer Linear Programming problems (ILPs). It integrates polyhedral methods, such as Cutting Plane Algorithms, and the divide-et-conquer strategy provided by Branch-and-Bound. During the cutting phase valid inequalities violated by the optimal solution of the current LP relaxation (cuts), are added to the problem at hand, in view of strengthening its formulation and obtaining tighter dual bounds. Modern ILP solvers (CPLEX, GUROBI, XPRESS) are able to generate several general-purpose cuts; moreover, end-users are allowed to define problem-specific cuts. They form the so called cut *pool*. The second step is to choose a subset of cuts to add to the current LP relaxation. This is a critical task. In fact, a trade-off between the number of added cuts and the overall computing time must be pursued, given that adding many cuts could reduce the Branch-and-Bound tree, but the time needed to solve the LP relaxations possibly increases. The management of the pool is generally carried out by heuristic rules and easy-to-compute cut efficacy metrics. Recently, machine learning algorithms have become popular to define effective cut selection strategies. In this talk we explore the possibility of ranking sets of cuts using Multiple Instance Learning (MIL) techniques. In MIL, training instances are arranged in sets, called bags. Instance labels are not available, while supervision is provided at the bag level. The goal of MIL is to learn a function f over the bag space that can predict the label of new bags as accurately as possible. In our setting any instance is a cut, described by a real valued feature vector, and a bag is a subset of cuts. The label returned by the function f represents some performance metric, used to perform the cut selection in a Branch-and-Cut framework.

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Shallow water 1D vs. 2D models: Analytical and numerical study for simulating coastline evolution over time

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Keywords. Shallow water equations; Coastline time evolution; COMSOL Multiphysics.

The aim of this work is to analyze and improve existing analytical models able to predict and simulate the time evolution of the coastline, taking into account the variation of seabed topography (and morphology), as well as resistance conditions, time intervals between storm surges, seasonal variations and viscosity, all factors that greatly influence coastal dynamics. Relying on a numerical approach, we will start implementing our investigation considering waves analytically modeled through the Saint–Venant equations [1], [2].

We will rely on the COMSOL Multiphysics simulation platform, which allows to handle engineering problems governed by PDEs, highlighting first how the seabed topography influences the elevation of the water surface which, in turn, has an impact on the coastal erosion. To this end, particular topographies will be considered, designed to simulate seabeds and stretches of coast actually existing in a territory of interest; subsequently, attention will be devoted to the 2D shallow water (or depth-averaged [1]) model.

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Named Entity Recognition to extract knowledge from clinical texts

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Keywords. Named Entity Recognition; Natural Language Processing; Clinical Reports.

Clinical texts encompass a wide range of information such as patient's history, disease diagnosis and prescribed drugs, reflecting details and nuances that are valuable in providing knowledge [2]. In the present study, a Natural Language Processing approach, specifically Named Entity Recognition (NER), is applied to extract important concepts from gastroenterology clinical texts.

NER is a task of text analytics to identify, in written documents, named entities ranging from general concepts to information in specific fields [1].

The application is performed through freely available Python packages for spaCy adapted to the English language. Although the spaCy's NER is generic, models trained in the clinical domain are used to identify categories belonging to the medical sector of interest. In particular, the main goal is to find as much entities as possible by paying attention to major bowel diseases, such as Ulcerative Colitis and Crohn's disease. The first battery involves the use of the ScispaCy package for scientific text processing [4]. The second step is to apply Med7 for identification of 7 medication-related concepts, dosage, drug names, duration, form, frequency, route of administration, and strength [3].

The results obtained will allow to evaluate the efficiency of the proposed methodology and to analyze, through the extracted entities, the profile and aspects of the diseases considered and the associated drugs.

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Applied mathematical modelling in the Physics problem-solving classroom

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Keywords. Mathematical modelling; Problem-solving; Maths education.

Applied mathematical problem-solving processes constitute an important part of the "basic skills" required for mathematical literacy among average citizens; yet, in the Italian high schools in secondary education, they are not emphasized enough in teaching practice. Mathematical modelling is a special type of problem-solving concerning problems related to science or everyday life situations. Kaiser et al.(2010) emphasized mathematical modelling integration in the classroom to enable students to solve real-life problems by using mathematical knowledge. The relevance of promoting applications and mathematical modelling in schools currently has consensus all over the world (Borromeo Ferri, 2018). Teachers play an important role in implementing mathematical modelling successfully into mathematics lessons and in fostering students modelling competencies. For example, modelling activities in an interdisciplinary context between physics and mathematics have a twofold educational benefit: physics provides mathematics with interesting problems to investigate, and mathematics provides physics with powerful tools for analyzing data and theorizing. This article contributes to the literature regarding the planning and implementation of mathematical modelling tasks in the higher education curriculum. Specifically, it presents an example of didactic activity carried out in the course of Mathematical Education II - Master's Degree in Mathematics - which prepares future teachers of physics and mathematics not only for interdisciplinary teaching; but also for teaching mathematical modelling to solve real-world problems, identifying mathematical reasoning as a core aspect of being mathematically literate.

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Adaptive Synthesized Optimal Control for Quadrocopter

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Keywords. Stabilization; symbolic regression; particle swarm optimization.

The development of artificial intelligence systems assumes that a machine can independently generate an action algorithm or a control system for solving assigned tasks. To do this, the machine must have a formal description of the problem and have computational methods for solving it.

The paper considers the problem of optimal control in an extended formulation, taking into account its practical implementation. To solve it, an adaptive synthesized optimal control approach based on the use of numerical methods of machine learning is presented. The method move a control object changing location of stable equilibrium point and takes into account some uncertainties of initial position. As a result, it chooses from all possible optimal synthesized controls such that is less sensitive to changes of initial states.

As an example, the optimal control problem of quadrocopter with complex phase constraints is considered. To solve this problem firstly the control synthesis problem is solved for obtaining stable equilibrium point in the state space by numerical symbolic regression approach. After that positions of the stable equilibrium points are searched according to source functional from the optimal control problem by particle swarm optimization algorithm.

It is shown that such approach allows generating the control system automatically by computer basing on the formal statement of the problem and then directly being implemented onboard.

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Equation-free, Variable Free Numerical Bifurcation Analysis and Control of Complex Systems via Manifold Learning

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Keywords. Complex Systems; Manifold Learning; Numerical Bifurcation Analysis, Control, Equation-Free, Variable-Free, Machine Learning.

We present a three-tier machine learning framework for the numerical bifurcation analysis and control of the emergent dynamics of complex systems, that bypasses the construction of surrogate models [1]. In particular, the proposed methodology (i) finds via nonlinear manifold learning from high-dimensional agent-based simulations a set of variables that parametrize the low-dimensional manifold on which the emergent/collective dynamics evolve, and based on these variables, and the solution of the pre-image problem, it enables in the ambient/high-dimensional space the Equation-free (ii) numerical bifurcation analysis of the emergent dynamics, and (iii) the design of controllers that stabilize the emergent dynamics of the imprecisely known, open-loop unstable steady-states. Furthermore, we demonstrate the robustness of the scheme against numerical approximation errors and modelling uncertainty. The proposed data-driven numerical analysis/machine learning-based framework is illustrated via an agent-based model of traffic dynamics.

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Applications of tensor network methods to quantum emulators and optimization problems

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Keywords. tensor network methods; quantum emulator; digital quantum computing.

Tensor networks (TNs) have emerged as a powerful approach for efficiently representing the quantum many-body wave function and have been successfully applied in various field ranging from quantum many-body systems to lattice gauge theories and machine learning. TNs methods have also played a vital role in supporting the development of quantum technologies as they lie at the core of classical emulators. In this work, we present our emulators for digital quantum computing and quantum simulators, which offer a classical path to simulate quantum hardware. We focus on the Hubbard model on a two-dimensional square lattice as a physically relevant setting and investigate both equilibrium and out-of-equilibrium properties. We identify the transition between liquid and insulating phases at equilibrium and attempt to provide signatures of spin-charge separation in real-time dynamics via digital quantum simulation. Furthermore, we apply TNs algorithms to solve hard optimization problems. We are specifically interested in the mission planning problem for earth observation, which involves optimal scheduling of satellite observations for a given set of user requests. We map the classical cost function into an Ising-like Hamiltonian, where the optimization variables are represented as a set of interacting spins and solve the optimization problem by finding the ground-state using TNs.

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GPU Acceleration of the Enhanced Jaya Optimization Algorithm for Solving Large Systems of Nonlinear Equations

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Keywords. metaheuristic optimization; enhanced Jaya algorithm; parallel GPU algorithms; nonlinear equation systems.

This paper presents a GPU-based parallel implementation of the Enhanced Jaya (EJAYA) optimization algorithm for solving high-dimensional systems of nonlinear equations. EJAYA is a gradient-free metaheuristic optimization scheme based on the population-based parameter-less Jaya algorithm that has recently been shown to be quite effective in solving nonlinear equation systems, a class of challenging numerical problems that are difficult to solve by traditional approaches, particularly as systems become larger. EJAYA uses the parameters from the original Jaya algorithm, like the current best and worst solutions, while manipulating new parameters such as the mean solution and the historical solutions to balance its local exploitation and global explorations strategies. The proposed parallel version of EJAYA was implemented using the Julia programming language on a high-performance GeForce RTX 3090 GPU with 10,496 CUDA cores and 24 GB GDDR6X VRAM, and was tested using a set of difficult scalable nonlinear equation system problems. The obtained results demonstrated the effectiveness and the efficiency of the proposed GPU-based massively parallel implementation of EJAYA for solving large-scale systems of nonlinear equations in terms of speed-up.

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An Improved Modified Jaya Optimization Algorithm: Application to the Solution of Nonlinear Equation Systems

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Keywords.metaheuristic optimization; modified Jaya algorithm; hybrid metaheuristic algorithms; systems of nonlinear equations.

Nonlinear equation systems appear in the vast majority of simulations of physical processes and are extremely important in many fields of knowledge, including chemistry, physics, economics, and various engineering specialties. However, there is no sufficiently efficient and robust general numerical method for solving systems of nonlinear equations, which is likely the most difficult problem in numerical mathematics and whose solution difficulty grows as the system dimension increases. On the other hand, the original problem of solving a nonlinear equation system can be transformed into an equivalent nonlinear optimization problem, which can be solved by using a metaheuristic algorithm or a hybrid metaheuristic-based strategy capable of numerically approximating the solutions of the considered problem. These metaheuristic approaches and other computational intelligence algorithms are characterized by their robustness and their ability to escape from local optima, which, despite being fundamental to any search algorithm, it is not found in traditional iterative optimization methods. One of these metaheuristic approaches is that of the Modified Jaya (MJAYA) algorithm, which uses information about the best and worst candidate solutions to determine the population's search direction. This drives the algorithm's search in a quite narrow and focused direction. In view of this, in this paper we propose a new population-based optimization algorithm called Improved Modified Jaya (IM-Jaya) for solving nonlinear equation systems. The proposed hybrid algorithm achieves a better balance between global exploration and local exploitation, permitting a broader and more comprehensive exploration of the search space and a more efficient local search in its most promising regions.

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Effective Resistance based Community Detection in Complex Networks

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Keywords. Community detection; effective resistance; genetic algorithms;graph sparsification.

Many real-world systems in nature can be modeled as complex networks with interacting nodes, where nodes correspond to the objects of the system and the interactions are modeled with edges representing the relationship between the objects. Many researchers have devoted the study of complex networks focusing on their community structure. For grouping nodes, distance measures are fundamental for assessing the similarity between them and organize them in communities accordingly. In this paper, we start exploring and exploiting the effective resistance for the problem of community detection in networks, a measure derived from the field of electric circuits whose square root has been shown to be a Euclidean metric. Specifically, we propose a new community detection method for complex networks based on genetic algorithms (GAs) which considers the equivalent electric network of the input graph for weighting its edges with the similarity computed through the effective resistance between two nodes.

Since most of the real networks are characterized by very high edge densities, the method also introduces a preprocessing technique aiming at reducing the graph density through a sparsification strategy. Sparse graphs are easier to handle than dense ones. Most graph algorithms run faster, sometimes by orders of magnitude, when there are fewer edges, and the graph itself can be stored more compactly. Specifically, our method approximates the input dense graph of interest with a suitable sparse one without significantly altering the underlying community structure. Through several experiments over both real-world and synthetically generated networks, we demonstrate that our approach is effective when compared to other benchmark methods.

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Transparent Execution of Cellular Automata Models on a Multi-GPU Architecture

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Keywords. GPU Computing; Multi-GPU; Cellular Automata.

In this work, we propose a method for transparently executing cellular automata models on a multi-GPU architecture. Although cellular automata models can be easily parallelized on a single GPU, the domain size and transition function complexity may require the use of multiple GPUs. Our method allows the modeller to write code that is independent of the parallel execution context, whether it is on a CPU, GPU, or multi-GPU system. This is achieved through a transparent layer that abstracts the parallelization details and allows the modeller to focus on the model's implementation. The typical bottleneck of a multi-GPU execution mainly resides in inter-card communications, requiring device-to-host and host-to-device data exchanges as well as network inter-node communications. In order to mitigate such a burden, an optimized procedure is also introduced in this paper that forces the mentioned communication operations to be executed concurrently with the transition function computation. A subsurface flow Cellular Automata (CA) model, namely the XCA-Flow model, has been adopted as testbed for proving the achievable performance speed-up. The experiments have been executed on the cluster CTE-POWER available at the Barcelona Supercomputing center (BSC). Our experimental results show that our method can effectively parallelize cellular automata models on a multi-GPU architecture, achieving significant speedups without requiring any modifications to the model code and reaching a further 68% improvement when the aforementioned optimization is applied. Our proposed approach can enable modellers to simulate larger and more complex cellular automata models, with the flexibility of running on different parallel execution contexts.

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A comparison of formulations for aircraft deconfliction

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Keywords. Mathematical optimization; mixed integer nonlinear programming; air traffic management.

In this work, we aim to compare different methods and formulations to solve a problem in air traffic management to global optimality. In particular, we focus on the aircraft deconfliction problem, where we are given n aircraft, their position at time 0, and their (straight) trajectories. We wish to identify and solve potential pairwise conflict within the time horizon $[0, T]$ by temporarily modifying the aircraft's trajectory. A pair of aircraft are in conflict when, at any time $t \in [0, T]$ they are too close, i.e., they do not respect a minimum, predefined safety distance.

The problem has been formulated as a mixed integer nonlinear program (MINLP), see, for example, [1]. We compare this formulation, solved by opensource MINLP solvers for global optimization, against a formulation that shows a larger number of variables and constraints but only separable nonconvexities. We solve such a separable formulation with the same MINLP solvers or the Sequential Convex Mixed Integer Nonlinear Programming method (see [3, 4, 2]). The separable formulation, despite being larger, shows to be easier to handle.

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Data-driven numerical bifurcation analysis of complex systems using sparse identification of dynamical systems

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Keywords. numerical bifurcation analysis; sparse identification of dynamical systems (SINDY); equation-free methods.

We develop a data-driven numerical method for the computation and continuation of equilibria and periodic orbits of dynamical systems. Using the sparse identification of dynamical systems (SINDY) [2] as a regression problem, fitting model basis functions onto data, we approximate the right-hand side of the dynamical system numerically from time series. The method is combined with traditional numerical analysis tools to perform bifurcation analysis. The method is presented by using miscellaneous examples [3, 1, 4] from computational neuroscience and mechanics.

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A Mixed Symbolic/Numeric Approach to DAEs Index Reduction

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Keywords. Symbolic Computations; Index Reduction; Matrix Factorization; Large Expressions.

We present a hybrid symbolic/numerical approach to reduce the index of generic DAEs systems. Specifically, we compute a kernel basis using symbolic matrix factorization. In our work we exploit state-of-the-art symbolic matrix factorization algorithms, which include techniques to limit the output expression swell [2, 3, 4]. As it is shown in [1], applying factorization with a purely symbolic approach is unsuitable in terms of numerical stability of the output. On the other hand, a purely numerical approach does not offer the flexibility of leaving some or all parameters unspecified. A robust solution is to merge these two techniques in order to take advantage of their strengths.

In our work we present novel techniques for matrix factorization and for reducing output expression swell. By using tailor-made symbolic LU and QR factorization algorithms, the DAEs system index is conveniently reduced. Expression complexity growth is limited by introducing veiled symbolic expressions that can be interpreted as the introduction of additional index-1 equations to the system. To perform effective expression veiling and simplification, a mixed symbolic/numerical approach is adopted. This hybrid technique is used speed up symbolic calculations and to find a numerically stable solution. The quality of the reduced-index system is verified by appropriate tests on multi-body models of various kinds. In addition, other interesting engineering applications of these factorization and veiling techniques are reported.

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An improved QPSO based Algorithm for USV Path Planning

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Keywords. QPSO; Path Planning; USV.

Quantum behaved Particle Swarm Optimization (QPSO) is a stochastic optimization technique that uses a population of particles to explore the search space and find the best solution, and it combines the advantages of particle swarm optimization (PSO) with the power of quantum computing to provide a powerful and efficient optimization algorithm. Generally, it is used to find the optimal solution to a given problem by searching through a large search space. This approach has been used in a variety of applications, including machine learning, robotics, and engineering design. In this paper, we developed an improved QPSO based Algorithm for the path planning of Unmanned Surface Vehicles(USVs). Simulation results are satisfactory and the addressed approach can be applied to several types of autonomous vehicles.

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A Review on Quantum-like Approach to Human Cognition and Decision Making

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Keywords. Human Cognition; Decision Making; Quantum-like Approach.

Future autonomous systems will need cognitive capabilities, including reasoning and decision making. This paper presents a survey on quantum-like approach to human cognition and decision making during the recent ten years. The study of human cognition and decision making in a quantum-like framework is still in its infancy. There have been a few studies that have explored the potential of quantum-like models to explain human behavior, but the majority of research has focused on the theoretical aspects of quantum-like models, which includes exploring the implications of quantum-like models for decision making, as well as the potential implications for cognitive processes such as memory and learning. This survey aims to attract attention to the possibilities of these quantum-like approaches that can enrich theoretical consideration and be useful for practical purposes in various sciences and applications, especially in the future autonomous systems.

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On Dividing Fractions in Binary BBP-type Formulas for Mathematical Constants

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Keywords. BBP-type formulas; fixed-point arithmetic; exact division.

In this paper, we discuss dividing fractions in binary Bailey–Borwein–Plouffe (BBP)-type formulas for mathematical constants. The BBP formula for π [1] is known to be able to compute a specific bit in π without computing all the previous bits. In order to compute a specific digit of mathematical constants using BBP-type formulas, it is necessary to compute the sum of the fractional parts of the fractions. Since the range of the absolute value of each fraction is $[0, 1)$, it is sufficient to use fixed-point arithmetic. For dividing each fraction in BBP-type formulas, it is known that the exact division algorithm [2] is more efficient than integer division based on Newton's method [3].

However, when computing an exact division in binary, the denominator of the fraction must be an odd number. Thus, if the denominator of the fraction in a binary BBP-type formula (excluding the power of the base) is an even number, exact division cannot be used directly. In this paper, we show that even in such cases, exact division can be performed using a method that applies Montgomery multiplication to modular exponentiation in binary BBP-type formulas [4].

The quotient of the result of dividing a fraction using fixed-point arithmetic with integer operations is a truncated value. If binary BBP-type formulas are alternating series, errors are unlikely to accumulate because the errors cancel out. However, when binary BBP-type formulas are not alternating series, error accumulation is a problem. We show that error accumulation can be reduced by rounding the quotient.

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An efficient implementation of a multireference perturbation method for NISQ devices

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Keywords. VQE; ADAPT-VQE; NEVPT2; POVM.

In recent years, quantum computers have successfully simulated small chemical compounds such as H_3^+, HHe^+, H_2O, and hydrogen chains containing up to 12 atoms. However, scaling quantum algorithms to treat larger systems of real chemical relevance, such as for drug design, remains a major challenge due to the limited availability of quantum hardware. Moreover, most of the variational quantum algorithms available today are restricted to valence spaces description that often led to incorrectly prediction of the stability of the molecular species being investigated. Here we present a scheme for the inclusion of dynamical electron correlations from non-valence orbitals that combines a self-consistent field adaptive variational quantum eigensolver (ADAPT-VQE-SCF) [1–3] together with the workflow of strongly contracted n-electron valence state perturbation theory (SC-NEVPT) [4]. Traditional implementations of NEVPT2 require calculating and storing the three- and sometimes four-body reduced density matrices (RDMs) within the active space, which require $\mathcal{O}(n_a^6)$ and $\mathcal{O}(n_a^8)$ storage respectively, introducing a considerable measurement overhead. Both its generation and storage become quickly problematic in particular for near-term quantum devices with limited capabilities. In this work, we attempt to mitigate this measurement overhead by exploiting a recently introduced method for energy evaluation relying on Adaptive Informationally complete generalised Measurements (AIM) [5, 6]. Besides offering an efficient way to measure the energy itself, Informationally Complete (IC) measurement data can be reused to estimate all the matrix elements of the 4RDM for the SC-NEVPT2 scheme, using only classically post-processing [7].

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Clustering based on Copulas Families and empirical density estimation with Spline Quasi-Interpolation.

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Keywords. Copula; Unsupervised Learning; Spline.

Clustering data remains a challenge in the scientific community due to the heterogeneous nature and size of the data. It is difficult to determine "a priori" how the data can be grouped together, especially when their joint distribution does not fit the classical Gaussian distribution and the data size is too large for visual inspection. In recent years, Copulas have become increasingly popular for overcoming these issues [1, 4]. Copulas allow for capturing the dependence between data features independently of the choice of marginal distributions [2]. In this work, we propose a flexible Copula mixture model with a non-parametric estimation of the marginals using spline quasi-interpolation [3]. Some numerical experiments show how using this strategy for non-parametric estimation of the marginals results in better computational cost and component identification, and allows for the treatment of larger datasets. The proposed method is tested on artificial and real dataset.

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The Theory of Grossone and the Continuum Problem

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Keywords. Continuum Problem; Grossone; Infinity.

The Continuum Problem is the problem of whether there exists one intermediate cardinality between $\aleph_0$ and $\mathfrak{c}$. As is known, the problem is unsolvable by the axioms of set theory, ZFC. In recent years, new axioms have been investigated but there is no broad consensus on the justifiability of such axioms (cf. [2], and [1]). Hence, one likely scenario is that the Continuum Problem will keep being seen as unsolved by most set-theorists. The question of why it should be so is also a very old question, and it would seem that no univocal answer may be provided. Cantor himself seems to have already had, at some point, a glimpse of what the troubles with solving the problem might be, insofar as he realised that one could potentially adopt a richer notion of continuum, in the context of which the Continuum Problem has a completely different meaning. The purpose of the present paper is to approach the problem from an equally radical, and a lot less explored, point of view, according to which *different* continua are *observable* according to which *representation* of the real numbers is chosen. This is the point of view of the theory of grossone (①), a novel approach to the infinite formulated by Y. Sergeyev in recent years ([3]).

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Line search techniques within stochastic methods for deep learning applications

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Keywords. Stochastic gradient methods; dynamic hyperparameters selection; deep learning.

In stochastic minimization problems, such as machine learning applications with large-scale data sets, the objective function is approximated by the sample average, i.e., as a finite sum of functions. A very popular approach to address these problems is provided by stochastic gradient methods. To ensure convergence properties and good practical performance, stochastic schemes need proper selection rules for the hyperparameters adopted in their implementation. In this talk we discuss a possible technique to avoid a pre-selection of the learning rate, recently proposed in [1, 2]. In particular, a learning rate updating rule based on a line search like procedure can be introduced. Convergence results can be obtained by combining this approach with an adaptive reduction of the variance of the stochastic gradients along the iterations. For general objective functions, the a.s. convergence of the limit points of the sequence generated by the proposed scheme to stationary points can be proved. For convex functionals, both the a.s. convergence of the entire sequence of the iterates to a minimum point and a convergence rate $\mathcal{O}(1/\mathrm{k})$ for the objective function values can be obtained. The dynamic reduction of the variance of the stochastic gradients is obtained by increasing the size of the mini-batch, similarly to that has been proposed in [3]. Variants of this approach can be discussed under suitable assumptions or for special objective functions [4]. Numerical experiments are carried out to evaluate the effectiveness of the discussed strategies, also on artificial neural networks.

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Global Optimality Condition for the Convex Maximization Problem by Dimensionality Reduction

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Keywords. convex maximization; optimality conditions; global optimization.

In this talk we consider the convex maximization problem (CM) :

$$\begin{cases} \text{maximize} & f(x) \\ \text{subject to} & x \in D \end{cases}$$

where $f : \mathcal{R}^n \to \mathcal{R}$ is a strictly convex quadratic function and the set of feasible vectors $D \subset \mathcal{R}^n_+$ is a polyhedron defined by m linear equality constraints.

It will be shown that such problem of dimension n can be reduced into another optimization problem in $\mathcal{R}^{n-m}$ of smaller dimension $n - m$:

$$\begin{cases} \text{maximize} & \varphi(y) \\ \text{subject to} & y \in \tilde{D} \end{cases} \qquad (\mathcal{HT})$$

with a convex quadratic function $\varphi : \mathcal{R}^{n-m} \to \mathcal{R}$ and a feasible set $\tilde{D} \subset \mathcal{R}^{n-m}_+$.

We provide a global optimality condition which is based on solving the reduced problem $(\mathcal{HT})$. We illustrate the efficiency of the optimality condition on a numerical example.

$$\begin{cases} \text{maximize} & f(x) = x_1^2 + x_2^2 + x_3^2 + x_4^2 \\ \text{subject to} & x_1 + 2x_2 + 3x_3 + 18x_4 = 78 \\ & 3x_1 + 4x_2 + 11x_3 + 48x_4 = 216 \\ & x_i \geq 0, i = 1, 2, 3, 4 \end{cases}$$

The search for pairs of arithmetic triangles. Computational aspects

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Keywords. Hyperelliptic curves, Rational triangles, elliptic Chabauty.

In this work, we will explain how pairs consisting of specific arithmetic triangles (taken up to similitude) are parameterized by rational points on hyperelliptic curves. We discuss computational aspects regarding the computation of rational points on these curves. The search for some pairs of triangles can be settled using classical algorithms for determining the rational points on a fixed elliptic curve. Searching for other pairs leads to more difficult computational tasks. We show how some of the latter can be settled using the methods of Chabauty and (elliptic) Chabauty.

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Numerical Analysis of Sedimentation Tanks Efficiency Using CFD Simulation

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Keywords. Computational fluid dynamics (CFD); Sedimentation tank (ST); Numerical analysis; stormwater runoff; residence time.

Sedimentation tanks (ST) are commonly used in stormwater treatment to remove solid particles. This study aims to investigate the efficiency of a rectangular ST for stormwater treatment by analyzing the effects of temperature, inlet flow rate, short circuit, and residence time on particle removal. Computational fluid dynamics (CFD) is a valuable tool for the evaluation of sedimentation tank efficiency. CFD software can provide detailed insights into fluid flow patterns, which can help identify areas of high turbulence, dead zones, and short-circuiting. The main objective of this study is to investigate the considerable effect of temperature and inlet flow rate variation on the overall efficiency of ST. CFD commercial software was performed to create a 3D model of the ST, and the simulations were calibrated using data from previous case studies conducted in the Vermicelli catchment located at the University of Calabria (Cosenza, southern Italy). By varying the inlet flow rate, it is concluded that a plug flow pattern and longer residence time in the tank resulted in better ST efficiency and temperature variation of the inlet may have an effect on the hydrodynamic of the ST. Our study demonstrates the importance of considering temperature, flow pattern, and residence time when evaluating the efficiency of rectangular sedimentation tanks for treating stormwater runoff. The numerical simulations also provided insight into optimizing the design and operation of rectangular sedimentation tanks for the effective removal of solid particles from stormwater runoff in urban areas.

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An Innovative Sentiment Analysis Model for COVID-19 Tweets

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Keywords. Sentiment Analysis; COVID-19; BERT.

COVID-19, declared as pandemic by WHO (world health organization), is one of the most severe pandemic faced by whole world. It has not only caused health issues all over the globe but it has created the feelings of fear, anxiety among the people. With the rapid spread of the virus and the resulting changes to our daily lives, there has been a significant shift in people's emotions and attitudes towards various aspects of life. Sentiment analysis during COVID-19 has been a crucial tool in understanding how people are feeling and reacting to the pandemic. In this research, we have proposed a novel sentiment analysis model for COVID-19 tweets. CT-BERT is used a base model, then we applied the MAX Pooling function on the last four layers of the CT-BERT model individually. It means that for each layer, the maximum value of each embedding dimension is selected. This results in a reduced dimensionality of the output, as the maximum value for each embedding dimension is selected, rather than the entire embedding. This can help to identify the most relevant and informative features of the embeddings, which can improve the performance of downstream tasks such as sentiment analysis. The resulting embeddings are then summed using the PyTorch sum function to obtain a single embedding vector. The obtained embeddings are then concatenated with the classification (CLS) token, which is a special token added at the beginning of the input text sequence when using BERT models. The concatenated embeddings and the CLS token are forwarded to a classifier. The classifier takes the concatenated embeddings as input and outputs a probability distribution over the possible classes. The class with the highest probability is typically selected as the predicted class for the input text. Hence, sentiment analysis during COVID-19 has been a valuable tool for gaining insights into public opinion and emotions during this unprecedented time, which can inform decision-making and communication strategies moving forward.

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Accelerated Mann-type algorithm via two-step inertial points for solving a fixed point problem of a nonexpansive mapping and application to image restoration problems

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Keywords. Mann-type algorithm; fixed point problem; two-step inertial points; monotone inclusion problem; image restoration problem.

The fixed point problem of a nonexpansive mapping is solved by using an accelerated Mann-type technique via two-step inertial points in the framework of Hilbert spaces. We can obtain strong convergence of an accelerated Mann-type algorithm via two-step inertial points under some appropriate assumptions on step-size scalars and certain useful properties and nice inequalities that are available on Hilbert spaces. We apply an accelerated Mann-type algorithm via two-step inertial points to solve the zero-point problem of some monotone operators. Furthermore, we utilize an accelerated Mann-type algorithm via two-step inertial points to solve some image restoration problems. To demonstrate the advantage of the new algorithm, some numerical experiments are established to compare and illustrate the behavior of the new algorithm with some previous existing algorithms.

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Numerical simulation of crack propagation in oil shale ash concrete

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Keywords. concrete; crack propagation; FEM; oil shale ash; softening.

Concrete has a wide range of applications as a construction material, while at the same time it has a huge carbon footprint around the world, mainly related to the production of cement. Therefore, there is a trend to conduct research aimed at making cement production more environmentally friendly. One way to ensure this is to use industrial waste materials or reuse some other materials as components of the concrete mixture. In this study, numerical modelling of crack propagation in concrete, one of the components of which is oil shale ash, is performed.

Using the finite element method, a linear elastic 2D problem is solved for basalt fibre concrete samples with and without oil shale ash in its mixture. The in-house software used is based on cohesive crack model. The propagation of a crack in the prism beam is numerically modelled using the principles of force balance and energy minimization. Four softening functions were implemented in the finite element software and the obtained results were compared with laboratory bending tests. The best fit is shown by bilinear [1] and non-linear functions [2].

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Exploring hierarchical MPI reduction collective algorithms targeted to multicore node clusters

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Keywords. MPI; HPC; multicore cluster; collective algorithms.

High-performance computing applications to be run on clusters make intensive use of message-passing mechanisms in order to share the data, where the MPI library is the de facto communication library for parallel applications. In this sense, there has been much effort towards optimizing how the data is distributed and buffered depending on its size to improve communication performance and avoid errors like running out of memory on the target node. Furthermore, the emergence of multicore clusters with larger node sizes has stimulated the investigation of hierarchical collective algorithms that take into consideration the placement of processes within the cluster and the memory hierarchy.

This paper studies and compares the performance of several collective algorithms from the literature that do not form part of the current MPI standard, which tackle this issue. We implement the algorithms on top of Intel MPI library using the MPI profiling interface, and test them on platforms with different characteristics such as node size, processor architecture, and interconnection network.

Experimental results on the Intel MPI Benchmarks, OpenCAL++ library, Parallel K-Means Data Clustering application and miniMD from Mantevo suite, show that there is much room for improvement in the performance of collectives depending on the target platform and applications.

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Feedback Linearization of Discrete Nonlinear Systems with Machine Learning

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Keywords. Physics-Informed Machine Learning; Feedback nonlinear control; Nonlinear Discrete-time systems.

We present a novel a machine learning approach to perform feedback linearization and control of nonlinear discrete-time systems [1]. In particular, we address a physics-informed machine learning (PIML) scheme that constructs analytically a nonlinear transformation function, which both linearizes and stabilizes the system by placing in one step. The feedback linearization in one step has been introduced in [2] using a power series expansion for the transformation law and its Equation-free approach in [3]. The training of the PIML is performed via a greedy approach, facilitating convergence in the presence of steep gradients in the transformation law. The performance of the proposed greedy PIML was assessed via a benchmark nonlinear discrete map for which the nonlinear transformation law is known [2], thus characterized by steep gradients due to the presence of singularities. For its implementation, we developed a "home-made" MATLAB code using the Levenberg-Marquard optimization algorithm for training and the Keras API of TensorFlow library in Python. We show that the proposed greedy PIML succeeds to approximate accurately enough the feedback linearization law, thus outperforming the traditional power series expansion scheme.

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AIR SAFE: leveraging IoT sensors and AI models to foster optimal indoor conditions

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Keywords. Air quality, Neural Networks, Internet of Things, Artificial Intelligence.

The need of safe and livable indoor environments has intensified recently, given that the majority of people spend most of their time indoor. In addition, the recent COVID-19 pandemic has pushed global authorities to focus more heavily on new human health risks pertaining no longer to outdoor spaces but also to indoor ones. In order to guarantee an optimal indoor environmental quality, monitoring and regulating many variables (such as indoor and outdoor temperature, pollutants concentration, noise, and brightness) is necessary. The high number of variables and the complexity of the system makes it advisable to employ high performance models to predict and control the state of the room environment.

In this context, we have developed AIR SAFE, an IoT and AI based infrastructure to monitor and control environmental quality in closed spaces where people stay for long periods of time, such as offices or schoolrooms. AIR SAFE uses Machine Learning models to make predictions of temperature, relative humidity, and CO2 concentration. These predictions, together with data from a network of IoT sensors, are used to take actions on windows and air condition-ing system with the aim of modifying for the better the room environment.

With this contribution we show the results of the AI model we have developed for predicting indoor concentration of CO2, relative humidity, and temperature. Our Long Short Term Memory (LSTM) model has been tested against literature models. For the prediction of CO2 concentration and indoor temperature we compared LSTM with Random Forest (RF), Convolutional Neural Network (CNN) and Multi-layer Perceptron (MLP). For relative humidity forecast we compared with RF, support vector regression (SVR) and multi-linear regression (MLR). At first, the performances of the sets of models are examined on simulated data; then, we test the results of the best models on real data. With simulated data RF is the best model for predicting CO2 concentration and temperature, while LSTM is better at predicting relative humidity. Using real data, the LSTM network performs best at forecasting temperature and relative humidity, while RF remains the best CO2 concentration predictor.

Improving Feasibility of Optimal Control via Obtaining High-precision Models

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Keywords. Identification; artificial neural network; optimal control.

The problem of practical implementation of the solution of the optimal control problem is considered. When solving the classical optimal control problem, the control is obtained as a function of time, the implementation of which in a real object leads to an open-loop control. Such a system is sensitive to small perturbations. The main generic way to solve it is to build feedback control systems. To create such systems with feedback, it is necessary to have an observation block that provides a complete state vector. In the absence of any observation system or low veracity of the data, it is possible to provide control over a limited time interval basing on a high-precision control object model used.

The paper proposes to use a multilayer artificial neural network to obtain a high-accuracy model. In this case, instead of the ODE system in the Cauchy form, we get an ANN mathematical model, the parameters of which are tuned to the dynamics of a particular control object. The paper describes the process of identification of the control object model including obtaining a sufficient volume of the training sample. General data properties are formulated to obtain a good model from the point of view of use in control problems.

The problems of optimal control and control synthesis for a high-precision model based on ANN are formulated. In this case, due to the lack of a familiar description of the model with differential equations, analytical solutions to these problems are impossible. Numerical methods for solving these problems are proposed. An example of solving the optimal control problem for a mobile robot based on the identified ANN model is given.

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Dimension reduction in quantum sampling

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Keywords. Quantum Stochastic modelling; Tensor Networks; Dimensional Reduction; Quantum Sampling; Quantum Machine Learning.

The quantum advantage relies on preparing a quantum sample that superposes all possible outcomes of stochastic processes [1, 2]. This necessitates a specific memory capacity to maintain correlations between the past and future of these processes. Consequently, a natural question arises: how can one find the least distorted quantum model given a particular memory resource?

In this study, we explore the trade-off between memory resources and the distortion of quantum models. First, we establish an upper bound on the distortion of optimal quantum models with a given memory resource. Next, we develop a systematic algorithm to identify quantum models that utilize a specified memory resource. To demonstrate the effectiveness of our approach, we apply our algorithm to both Markovian and non-Markovian processes, where future behaviors depend on events near and far in the past. We show that accurate quantum samples can be obtained using limited memory resources, while the exact preparation of quantum samples scales with the system size.

Despite dimensional advantages for exact simulation exist for specific processes, our research reveals that the accuracy advantage of quantum models is universally applicable to stochastic processes simulation.

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Applying Machine Learning to improve weather forecasting in a Mediterranean area: Preliminary experiments

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Keywords. Artificial Neural Networks; Random Forest; Weather Forecasting.

The development of Machine Learning (ML) [1] opens up new opportunities, representing an alternative or a complementary tool to classical applications in many fields.

Here we investigate the effectiveness of ML as a complementary tool in enhancing the accuracy of rainfall weather forecasting in the Calabria region (south of Italy), a Mediterranean area frequently affected by extreme rainfall events, with significant material damage and potential loss of human lives. In particular, the operational forecasting system based on the Weather Research and Forecasting (WRF) model developed at the University of Calabria is considered [2].

In this work, we test two ML models, namely an artificial neural network and a random forest, to improve the accuracy of WRF forecasting. We provide several WRF output variables to the ML models. After a proper calibration (learning and test phases) over a two-year-long extended dataset, we assess the results to the original WRF outcomes (validation phase). Preliminary experiments result in a significant improvement by the WRF-ML coupled systems.

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A Stochastic Algorithm with Combined Search Directions in Deep Neural Network Training

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Keywords. 1^{st}- and 2^{nd}-order Directions Combination; DNNs Training; Stochastic Optimization

Deep Neural Networks (DNNs) are leading techniques finding a wide range of applications for solving large-scale problems such as image recognition. Efforts have been made to train a DNN by solving a nonlinear and nonconvex optimization problem through gradient information. Since neither computing the true gradient nor Hessian is practical, the problem is usually solved by means of the stochastic 1^{st}-order optimizers e.g. SGD or Adam [1], mainly because of their proven practical efficiency. Moreover, in the last few years, stochastic 2^{nd}-order methods such as Quasi-Newton variants whether in line-search or trust-region (see e.g. [2] and references therein) strategies have been analyzed, with the aim of including partial curvature information in the search direction. Inspired by recent developments in the case of deterministic optimization problems e.g. [3], we investigate a strategy to combine Quasi-Newton trust-region directions and specialized 1^{st}-order directions, aiming at exploiting the pros of both two classes mentioned above. Our numerical experiments, including comparisons with 1^{st}- and 2^{nd}-order stochastic optimization methods, show the performance of the proposed approach.

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Optimal Recombination Problem in Genetic Programming for Boolean Functions

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Keywords. genetic programming; evolutionary algorithm; local search; optimal recombination.

We consider a problem of boolean function approximation by some set of basic functions $F = \{f_1, \ldots, f_k\}$. The solution is constructed by boolean functional tree $T = (V, E)$, where V is the set of vertices and E is the set of edges. Leaves are assigned by variables $x_1, \ldots, x_n \in \{0, 1\}$, nodes are corresponded by basic functions. The value of the basic function in the root of the tree T on the variables $x = (x_1, \ldots, x_n)$ we denote as $T(x)$. Input data of approximation problem (training set) are defined by pairs $\{(x^{(i)}, y^{(i)})\}$, $i = 1, \ldots, m$, $x^{(i)} = (x_1^{(i)}, \ldots, x_n^{(i)})$, $y^{(i)}$ is value of approximated function on the value of variables $x^{(i)}$. We consider the objective function as sum of squared deviations between training set and the solution of genetic programming $g(T) = \sum_{j=1}^{m} (y^{(j)} - T(x^{(j)}))^2$.

We construct genetic programming [1] algorithms with steady state replacement scheme and generational model. Initial population is constructed by crow method and its modification. In evolutionary process we use randomized local search and optimized crossover constructed in accordance with gene transmitting properties and the given objective [2]. Local search is based on neighborhood with respect to subtree updating.

Experimental evaluations are carried out on instances with even-5-parity and 6-mux functions. The experiment shows that algorithm demonstrates competitive results.

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Population Local Search for Single Processor Energy Efficient Scheduling Problem

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Keywords. Speed scaling; energy; scheduling; local search.

Energy consumption of computing devices is an important question at this day [1, 2]. One effective method for reducing energy consumption is dynamic speed scaling. The purpose is to dynamically set the speeds of processors so as to minimize energy consumption while still providing a desired quality of service. We consider the NP-hard offline energy-efficient scheduling of jobs on single speed-scalable processor [1]. A job set $J = \{1, 2, \ldots, n\}$ is given, where each job j is characterized by release date r_j, deadline d_j and volume (work) W_j. A schedule is feasible if the processor performs at most one job at a time, and each job j is executed in the required work between its release date and deadline. We assume that the homogeneous model in speed scaling is considered. When the processor runs at a speed s, then the power is s^α, where α is a constant [2]. The objective is to find a feasible schedule that minimizes the total energy consumption.

Previous researches provide various constructive approximation algorithms with approximation guarantees (see, e.g. [2]). In this paper we propose a population local search algorithm [3] with two types of neighborhoods. The first one is constructed on the bases of one solution and uses swap and insert strategies with problem-specific adaptation. The second one is defined for pairs of solutions and based on inheritance of values in positions of solution permutations. Experimental evaluation on instances of various structure shows that the algorithm demonstrates competitive results.

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Chronostamp, a general-purpose runtime for data-flow computing in a distributed environment

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Keywords. Parallel programming; distributed execution engine; distributed data-flow.

This article presents Chronostamp, a universal data-flow program execution engine. Chronostamp, like previous execution engines, conceals the complexity of distributed programming. A Chronostamp job, unlike those systems, can make data-dependent control-flow decisions, allowing it to compute iterative and recursive algorithms. We have also developed ChronoCode, a scripting language that is Turing-complete and runs directly on Chronostamp. The execution engine provides ChronoCode scripts and high-performance code written in other programming languages with transparent fault tolerance and distribution. Chronostamp has been deployed on a cloud computing platform, and its performance is scalable for both iterative and non-iterative algorithms. This makes Chronostamp a powerful tool for complex data processing tasks, especially those that require iterative or recursive computations.

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A New Blockchain-Based Meritocratic Marketplace for Distributed Machine Learning Model Training

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Keywords. Blockchain; Artificial intelligence; Distributed systems.

Decentralized AI model network Learningchain supports peer collaboration to improve machine learning precision. Peers can submit accurate models in this peer-to-peer network. The system keeps a decentralized, append-only ledger to track who trained and improved the model, when and by how much, and where to find the latest model. Learningchain gives donors cryptographic tokens. This research develops a simple wallet API that isolates low-level node communication across a temporal cluster of compute nodes and allows finegrained parameter-sharing behavior modification. We created a low-overhead, blockchain-based communication layer for compute cluster developers. This API connects model training and parameter pooling. Stateless, machine-learningindependent Learningchain operations are required. Dispersed learning benefits medical, reconnaissance, and resource-limited situations. Decentralization lets nodes learn without sharing data. Decentralized learning methods may modify cluster connectivity and node sharing to take advantage of this emerging technology. Advanced learning frameworks improve codebase homogeneity and readability.

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Discrete Facility Location with Ranking of Location Candidates Using High-Performance Computing Systems

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Keywords. Competitive Facility Location; Discrete Optimization; Random Search Algorithms; High-Performance Computing.

Facility location problems are aimed at finding optimal locations for facilities that provide goods or services to customers in a specific geographic area. Different models of facility location problems exist, varying in their characteristics, such as customer behavior rules, location space, and constraints for the locations of facilities. Solving a real-world facility location problems is usually complex and computationally expensive due to reasons such as complex objective function(s) or need of complex analysis of a large amount of data, e.g. population of prospective customers, their current and expected behavior when choosing the facility for a service, etc. Due to these and similar reasons it can be impossible to find the optimal solution(s) within a reasonable time and, therefore, heuristic methods, which can be applied to approximate the optimal solution(s) of a specific optimization problem, are often used to tackle a real-world facility location problems.

Our research focuses on the discrete competitive facility location problem for an entering firm, where the firm must choose locations for the new facilities from a given set of location candidates while considering the competition for the market share with other facilities already in the market. The heuristic algorithm with ranking of location candidates is proposed and experimentally investigated by solving different instances of the facility location problem. The new algorithm is based on previously proposed single-agent random search with ranking of candidate locations, but includes strategies for handling population of solutions and ranking candidate locations on the basis of solutions in the population. The proposed modifications made the algorithm much more suitable for distributing computational work among computing nodes thus utilizing high-performance computing systems for solution of complex facility location problems. The results of the experimental investigation demonstrate that the new algorithm outperforms its predecessor by efficiency in approximating the optimal solution of the problem. Experimental computations in the high-performance computing system showed the ability of distributing the computational workload among over one hundred computing nodes with almost linear speed-up.

Numerical Analysis of Optimal Control of Assets and Liabilities by a Bank

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Keywords. optimal control, phase constraints, banking system.

In the majority of national banking systems in the world, there are several large influential banks. In order to study the behavior of such banks, we consider a general mathematical model of a bank that manages assets and liabilities using interest rates on loans and deposits. While planning, the bank faces regulatory constraints that are in fact, phase constraints in the mathematical model of optimal control. We base the banking model on works [1]-[2], but make the interest a control variable. The bank maximizes the utility of the dividend income of its owners (the wealth of the owners) over some time horizon. The mathematical model of the bank has the form of an optimal control problem with constraints due to capital adequacy ratio and bank's liquidity constraints. In view of the complexity of this class of problems, we try to numerically calculate the optimal plan by the bank. The fundamental problem that arises when applying indirect methods in the presence of state constraints is related to the fact that the Lagrange multiplier is a Borel measure whose support is embedded in the set of times at which the state trajectory crosses the state constraint boundary. The singular component of this measure, more precisely, its atomic component, causes difficulties for the direct application of the Maximum Principle. Numerical analysis is based on the approach in [3]-[4].

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Concentration inequalities and martingale inequalities for rounding error analysis

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Keywords. Hoeffding inequality; Azuma inequality; Householder QR; Gram–Schmidt; backward error

Since numerical algorithms are often built upon inner products, the γ_n-based bounds in [1] are widely employed in modern error analysis. However, the worst-case bound can be pessimistic, and the condition $nu < 1$ may be violated when either n or u is large, where n denotes dimension and u denotes unit roundoff. Recently, Higham and Mary [2] suggest a new probabilistic model for analyzing rounding errors, which also contains a literature review of earlier work. The mean independence assumption used in [3] is weaker and more realistic than the assumption of unconditional independence used in [2]. It is proved in [3] that stochastic rounding, which can prevent stagnation and give more accurate results in certain numerical contexts, does enforce mean independence of rounding errors. These assumptions are directly related to concentration inequalities and martingale inequalities. In this talk, we give some historical remarks about these inequalities and their applications in numerical linear algebra. In particular, Connolly and Higham [4] derive probabilistic bounds for the standard Householder QR algorithm. Under some technical assumptions, they prove that for an $m \times n$ matrix the column-wise backward error in terms of the upper triangular factor is of order $\sqrt{mn}u$. We also introduce some new probabilistic results about modified Gram–Schmidt.

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