Sesión Especial 15

Numerical Methods and Computational Mathematics

Organizers:

- Pablo M. Berná (CUNEF Universidad)
- Antonio Falcó (Universidad CEU Cardenal Herrera)

Summary:
The scientific computing community has shown increasing interest in Tensor Numerical Methods and Deep Neural Networks. Concerning the use of these methods in engineering and industrial applications, among the family of tensor-based methods, the Proper Generalized Decomposition has been used in surgery simulations, design optimization, etc. The special session aims at gathering experts to present their recent work in this field, including rank tensor format approximation, greedy algorithms, etc.

Programa

Jueves, 25 de enero:

11:30 – 12:00	Antonio Falcó (Universidad CEU Cardenal Herrera) *The variational principle of Dirac-Frenkel*
12:00 – 12:30	Elías Cueto (Universidad de Zaragoza) *Thermodynamics of learning physical phenomena*
12:30 – 13:00	Francisco de la Hoz (Universidad del País Vasco) *A second-order fast-convolution method for the fractional Laplacian*
13:00 – 13:30	Sandeep Kumar (CUNEF Universidad) *On Pseudorandomness of the Schrödinger map*
16:00 – 16:30	Beatriz Gómez (Universidad de Valladolid) *Artificial Neural Networks with Chebyshev Polynomials in Option pricing*
16:30 – 17:00	Edgar Arribas (Universidad CEU Cardenal Herrera) *Approach to optimization problems in network engineering: The case of mmWave backhauls*
17:00 – 17:30	Alejandro Bandera (Universidad de Sevilla) *Intrinsic Proper Generalized Decomposition modes on Grassmann manifolds. Computation via Gradient Descent Algorithm*

Viernes, 26 de enero:

11:30 – 12:00	Alberto Conejero (Universidad Politécnica de Valencia) *Structure and approximation properties of Laplacian-like with applications*
12:00 – 12:30	Jorge Herrera de la Cruz (Universidad San Pablo CEU) *Successful love stories as differential games*
12:30 – 13:00	Simone Rusconi (CUNEF Universidad) *Model & Methods for Chemical Kinetics: Study of Latex Particles Formation*
13:00 – 13:30	Carlos Esteve (Cambridge University) *Visibility-based pursuit-evasion games in domains with obstacles*

The variational principle of Dirac-Frenkel

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Abstract: The main goal of this talk is to review the so-called Dirac-Frenkel Variational Principle in the framework of tensor Banach spaces. To this end we introduce the Banach manifold structure for the different tensor formats based in subspaces for which we provide a local chart system. The description of the local charts of these manifolds appears crucial for an algorithmic treatment of high-dimensional partial differential equations and minimization problems. In order to describe the relationship between these manifolds and the natural ambient space we prove under natural conditions that each can be immersed in a particular ambient Banach space. This fact allows us to finally extend the Dirac-Frenkel variational principle in the framework of topological tensor spaces.

Thermodynamics of learning physical phenomena

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Abstract: Thermodynamics could be seen as an expression of physics at a high epistemic level. As such, its potential as an inductive bias to help machine learning procedures attain accurate and credible predictions has been recently realized in many fields. We review how thermodynamics provides helpful insights in the learning process. At the same time, we study the influence of aspects such as the scale at which a given phenomenon is to be described, the choice of relevant variables for this description or the different techniques available for the learning process.

A second-order fast-convolution method for the fractional Laplacian

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Abstract: In this talk, we explain a new method for approximating numerically the fractional Laplacian of functions defined on $\mathbb{R}$. After mapping $\mathbb{R}$ into a finite interval, we use two main ideas to obtain an approximation of the resulting convolution-like operator: a second-order modified midpoint rule, and the so-called fast convolution. We first prove rigorously that the method gives a second-order approximation of the fractional Laplacian; then, we detail the implementation of the method using the fast convolution; and finally, we give some numerical examples that support its applicability.

On Pseudorandomness of the Schrödinger map

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Abstract: In this talk, we will discuss the random behaviour of the Schrödinger map, a geometric partial differential equation by considering its evolution in different geometrical settings. Its equivalent form in the Euclidean space describes the evolution of a vortex filament in a real fluid, as a result, it is also known as the vortex filament equation. The dynamics of these equations for polygonal initial data when solved numerically exhibit several interesting characteristics of real fluids, e.g., the axis switching phenomenon. On the other hand, the algebraic construction of these solutions not only supports the numerical evolution but also indicates randomness. I will present some recent results, in particular, the case of helical-shaped vortices and curves in the hyperbolic space, and show that this unusual behaviour (randomness) resulting from a differential equation is indeed a generic phenomenon for these equations. A part of the talk is a work in collaboration with Francisco de la Hoz (UPV/EHU) and Luis Vega (BCAM, UPV/EHU).

References

[1] F. de la Hoz, S. Kumar, L. Vega (2022). Vortex Filament Equation for a regular l-polygon in the hyperbolic plane. Journal of Nonlinear Science, 32(9).

[2] S. Kumar. Pseudorandomness of the Schrödinger map. In preparation.

Artificial Neural Networks with Chebyshev Polynomials in Option pricing

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Abstract: Pricing different types of options is a subject of interest in finance. Classical numerical methods such as finite difference, finite elements or spectral methods, have been successfully applied to solve pricing problems in low-dimensional cases. However, the mentioned numerical methods suffer from the curse of dimensionality. When working in high-dimensional spaces, or with several underlying stocks, they become inefficient, as the computational cost grows exponentially. Artificial Neural Networks are a good solution to overcome the limitations of the previous methods. In particular, the purpose of this work is to combine the benefits of Artificial Neural Networks with Chebyshev polynomial approximation properties. We will see that applying a Chebyshev polynomial expansion can improve convergence rates of Artificial Neural Networks, providing an interesting framework for option pricing.

Approach to optimization problems in network engineering: The case of mmWave backhauls

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Abstract: In recent decades we have observed a very quick technological development in the field of network engineering that has taken us to the fifth generation of mobile telephony (5G). This rapid development entails a large number of technological problems that require rigorous mathematical analysis. Each bit of information that travels through the network is subject to addressing decisions that must guarantee a completely secure and very fast service to the user. Every time a decision has several alternatives, wanting to choose the best one gives rise to a mathematical optimization problem. Thus, there are countless optimization problems that networks must solve in very short time scales in order to have fast and secure access to the network. In this talk, we will describe the path to follow to analyze an optimization problem in the telematic engineering field, what considerations must be taken into account, and what alternatives we can present when we demonstrate that, as is often the case, it is not possible to obtain instantaneous solutions. In particular, we will present this path followed in the scheduling optimization problem of a wireless backhaul network enabled by millimeter waves.

References

[1] E. Arribas, et al. (2019). Optimizing mmWave wireless backhaul scheduling. IEEE Transactions on Mobile Computing 19.10: 2409-2428.

[2] Michael R. Garey and David S. Johnson (2022). Computers and intractability. Vol. 29. New York: wh freeman.

[3] E. Arribas, et al. (2019). Fair cellular throughput optimization with the aid of coordinated drones. IEEE INFOCOM 2019-IEEE Conference on Computer Communications Workshops.

[4] E. Arribas, et al. (2023). Optimizing fairness in cellular networks with mobile drone relays.Computer Networks 224: 109623.

Intrinsic Proper Generalized Decomposition modes on Grassmann manifolds. Computation via Gradient Descent Algorithm

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Abstract: In this work, we introduce an iterative optimization algorithm to obtain the intrinsic Proper Generalized Decomposition modes [1] of elliptic partial differential equations. The main idea behind this procedure is to adapt the general Gradient Descent algorithm to the algebraic version of the intrinsic Proper Generalized Decomposition framework, and then to couple a one-dimensional case of the algorithm with a deflation algorithm in order to keep enriching the solution by computing further intrinsic Proper Generalized Decomposition modes. For this novel iterative optimization procedure, we present some numerical tests based on physical parametric problems, in which we obtain very promising results in comparison with the ones already presented in the literature [2]. This support the use of this procedure in order to obtain the intrinsic PGD modes of parametric symmetric problems.

References

[1] M. Azaïez, F. B. Belgacem, J. Casado-Díaz, T. C. Rebollo, F. Murat (2018). A new algorithm of proper generalized decomposition for parametric symmetric elliptic problems. SIAM Journal on Mathematical Analysis, 50, pp. 5426-5445.

[2] M. Azaïez, T. C. Rebollo, M. G. Mármol (2020). On the computation of proper generalized decomposition modes of parametric elliptic problems. SeMA Journal, 77, pp. 59-72.

Structure and approximation properties of Laplacian-like with applications

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Abstract: An accurate prediction of the formation of latex particles is vital for Many of today's problems require techniques that involve the solution of arbitrarily large systems $A\mathbf{x} = \mathbf{b}$. A popular numerical approach is the so-called Greedy Rank-One Update Algorithm, based on a particular tensor decomposition. The numerical experiments support the fact that this algorithm converges especially fast when the matrix of the linear system is Laplacian-Like. These matrices that follow the tensor structure of the Laplacian operator are formed by sums of Kronecker product of matrices following a particular pattern. Moreover, this set of matrices is not only a linear subspace it is a a Lie sub-algebra of a matrix Lie Algebra. In this talk, we characterize and give the main properties of this particular class of matrices. Moreover, the above results allow us to propose an algorithm to explicitly compute the orthogonal projection onto this subspace of a given square matrix $A \in \mathbb{R}^{N\times N}$. Some applications will be given.

Successful love stories as differential games

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Abstract: Understanding the dynamics of long-term romantic relationships is essential for individual and social well-being. This study presents a model for romantic relationships as stochastic differential games.
The state of the relationship is represented by the "feeling" variable, $x(t)$, which evolves over time and serves as a measure of marital satisfaction. The evolution of this feeling variable is described by the stochastic differential equation:

$$\mathrm{d}x(t) = [-rx(t) + a_1c_1(t) + a_2c_2(t)]\,\mathrm{d}t + \sigma(x(t))\mathrm{d}w, \tag{1}$$

This equation includes parameters such as r, a_1, and a_2, control variables $c_i(t)$ representing partner efforts, and a Wiener process $w(t)$.
Effort controls, defined by $c_i = S_i(x)$, known as feedback controls, are crucial. Both partners aim to maximize their total happiness by balancing the benefits derived from their feelings, measured by functions $U_i(x)$, and the costs of exerting effort, as given by functions $D_i(c_i)$. The expected happiness of partner i is expressed as:

$$\mathbb{E}\left[\int_0^\infty e^{-\rho_i t}\left(U_i(x(t)) - D_i(c_{i1}(t); c_i^*)\right)\mathrm{d}t | x(0) = x_0\right],$$

where ρ_i represents discount parameters and c_i^* indicates the minimum level of effort each partner is ready to exert.
An equilibrium is achieved when optimal feedback controls, $\left(S_1^\heartsuit(x), S_2^\heartsuit(x)\right)$, are found to ensure that both partners maximize their expected happiness. The optimal effort paths are determined by $c_i^\heartsuit(t) = S_i^\heartsuit(x(t))$, and the relationship's feeling trajectory is calculated by solving the stochastic differential equation. In our case, we seek for the Feedback Nash equilibria of the game.
This research aims to address the challenge of calibrating the model with real-world data, offering insights into the parameters that replicate observed marital satisfaction curves. It also investigates the model's sensitivity to small parameter perturbations and how they affect equilibrium satisfaction and effort levels.

Model & Methods for Chemical Kinetics: Study of Latex Particles Formation

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Abstract: An accurate prediction of the formation of latex particles is vital for synthesis of high quality materials, but still not feasible due to its complexity. We present a set of Population Balance Equations (PBE) to model the kinetics of interest and attempt the prediction of particles synthesis. When experimentally grounded values of physical parameters are employed, a first difficulty is given by the great difference in magnitude of the involved variables. Thus, we propose a novel approach able to scale the PBE model to dimensionless variables, assuming a computationally tractable order of magnitude, even though experimental values of parameters are used. Then, with the aim of enhancing performance of the prospective PBE model, we investigate a possibility of reducing its complexity by neglecting the aggregation terms. In particular, we derive a quantitative criterion for locating regions of "slow" and "fast" aggregation and introduce a dimensionless PBE model of reduced complexity. When compared with the original PBE model, the resulting model demonstrates several orders of magnitude improved computational efficiency.

Visibility-based pursuit-evasion games in domains with obstacles

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Abstract: In this talk I consider a two-player zero-sum game in which the pay-off involves the visibility between the players. First, I formulate the problem using the framework of differential game theory. After discussing the difficulties arising in the associated Hamilton-Jacobi-Isaacs (HJI) equation, I will present a new formulation of the problem which relies on a convenient quantification of the visibility. This formulation allows the construction of sub-optimal feedback controls which are computationally efficient, even in high-dimensional scenarios. I will discuss the performance of these controls in comparison with the optimal ones provided by the HJI equation. Finally, I will conclude the talk with some possible directions about how these computationally efficient controls could be improved to approximate optimality.