4th AMMODIT Conference

Book of Abstracts

Malekhiv (Lviv region), Ukraine
March 19 – 23,   2018

Information on the project:

The goal of the AMMODIT project is joint research in six research tasks concerning the study of mathematical methods for Magnetic Particle Imaging; entropy-like measures and quantification of system complexity; coarse-grain modelling for (bio)polymers; diagnostic tools for cardiac surgery; regularization methods for causality detection; meta-learning approach to Nocturnal Hypoglycemia prediction. This project brings together research teams from the EU (Germany, Italy, and Austria) and the Ukraine (Kyiv, Donezk) in the area of applied mathematics with emphasis on medical and life science applications.

Information on the conference: This is the fourth meeting in the series of events to be organized in the framework of the Marie Curie RISE project "Approximation Methods for Molecular Modelling and Diagnosis Tools"(AMMODIT). The previous conferences were in Rivne (September 2015), Hasenwinkel (March 2016) and Kyiv (January 2017).

The conference is devoted to recent research in life sciences based on applications of mathematics to biological and medical studies. It is a multidisciplinary meeting forum for researchers who develop and apply mathematical and computational tools to the study of phenomena in the broad fields of biology, ecology, medicine, bioengineering, environmental science, etc.

Organizers and Partners:

- Institute of Mathematics of the National Academy of Sciences of Ukraine

- Humboldt Club Ukraine

- Universität zu Lübeck, Institute of Mathematics

- Politecnico di Milano, Biomechanics Research Group

- Österreichische Akademie der Wissenschaften, Johann Radon Institute for Computational and Applied Mathematics

- Institute of Applied Mathematics and Mechanics of the National Academy of Sciences of Ukraine

- National Technical University of Ukraine "Kyiv Polytechnic Institute", Faculty of Applied Mathematics

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Dates: March 19 – 23, 2018.

Location: Malekhiv (Lviv region), Ukraine.

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ABSTRACTS[1]

Application of the p-adic analysis to the modelling of the capillary flow in porous medium

ALEXANDRA V. ANTONIOUK

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This talk is dedicated to the the p-adic model of propagation of fluids (e.g., oil or water) in capillary networks in a porous random medium. Theoretical studies of the capillary motion of fluids and gases runs back to the paper by Washburn who proposed a mathematical model for this. Typical application of the capillary phenomena explored in geophysics, such as leakage in the oil pollution of soil, the capillaries form a tree. The hierarchic structure of a system of capillaries is mathematically modeled by endowing trees of capillaries with the structure of an ultrametric space.

We introduce and study an inhomogeneous Markov process describing the penetration of fluid into a porous random medium. Mathematically such trees can be represented as ultrametric (non-Archimedean) spaces. This ultrametric representation will be explored, where we study the idealized model based on regular p-trees, for which p branches come forward from each vertex. By the purely mathematical reason it is convenient to restrict considerations to the case of prime $p > 1$. The crucial point is that such trees can be endowed with the natural algebraic structure of the number field: addition, subtraction, multiplication and division (in the case of the prime p) are well defined on the set of branches of a p-tree.

The presented talk is based on the joint work with Klaudia Oleschko, Anatoly Kochubei and Andrei Khrennikov.

Application of data grid and graphics processing units for distributed cloud-based high-performance computing

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[1]The abstracts are published in the author's version without making any significant changes by the editors.

Simulation of biological and physical systems, namely large systems of coupled non-linear oscillators, are computationally demanding due to the large scale networks of units, variativity of system parameters state space and sophisticated inter-element coupling. In our study, software for simulation of biological model given by system of differential equations in clusters, data grids and clouds using graphical processing units (GPU) was designed, developed, tested and applied for scientific simulations.

The software provides easy integration of new oscillators' models support, dynamic load distribution between hosts' central processing units (CPU) and several GPU devices. Different GPU devices provide speed-up of $12 - 50$ compared to single core Intel Xeon, 2.4 GHz depending on GPU and job types. The software was efficiently applied for modelling of 3D networks with $10^7 - 10^8$ oscillators described by Kuramoto-Sakaguchi model and new phenomena related to phase transitions, synchronization, and network effects were observed in such simulations.

In the talk, we mostly focus on computing system architecture design and setup, and discuss optimizations made to achieve scalable parallel performance.

Finding patterns of glycemia behavior for prediction of nocturnal hypoglycemia

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The problem of nocturnal hypoglycemia is important due to its connection to human's health. In some cases it can lead to fatal consequences because people sometimes can not feel nocturnal hypoglycemia event in time they are asleep.

The aim is to predict nights when there is a risk of it. We have the data from DirecNet about the level of glucose of different patients during some period with the interval of 10 minutes.

These data have been already filtered, smoothed out, sampled and the most important peaks were identified. It was decided to solve the task of prediction using the classification approach, not the regression one. This task was reduced to the problem of finding patterns of glycemia behavior during days when nocturnal hypoglycemia event was noticed. Some of patterns that have been found include parabolic behavior, reaching the

critical maximum value of glucose level and fluctuations within a slight deviation from the minimum allowable value of it during the day.

Flexible protein-ligand docking: preliminary results

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We are working on development of new software for the protein-ligand docking. The scoring function is defined by using Lennard-Jones and Coulombic potentials. We consider two approaches: classical approach when protein is treated as rigit and ligand as flexible molecules and other approach when both protein and ligand are treated as flexible molecules. In addition, in both cases ligand has flexible torsion bonds. Preliminary results will be presented.

Nikolskii-type estimate for nearly copositive approximation of continuous on an interval functions

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If a continuous on a closed interval function f changes its sign at s points $y_i : -1 < y_s < y_{s-1} < ... < y_1 < 1$, then for each $n \in \mathbb{N}$, greater then some constant $N(k, y_i)$ depending only on $k \in \mathbb{N}$ and $\min_{i=1,...,s-1}\{y_i - y_{i+1}\}$, we construct an algebraic polynomial P_n of degree $\leq n$ such that: P_n has the same sign as f, everywhere except, perhaps, small neighborhoods of the y_i :

$$(y_i - \rho_n(y_i), y_i + \rho_n(y_i)), \quad \rho_n(x) := 1/n^2 + \sqrt{1-x^2}/n,$$

$P_n(y_i) = 0$ and

$$|f(x) - P_n(x)| \leq c(k,s)\,\omega_k(f, \rho_n(x)), \quad x \in [-1,1],$$

where $c(k, s)$ is a constant depending only on k and s, and $\omega_k(f, \cdot)$ is the modulus of continuity of the k-th order of the function f.

Relationship between permutation entropy and Kolmogorov-Sinai entropy for ergodic interval maps with positive entropy

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Permutation entropy is a measure for the complexity of dynamical systems. It is a question of interest for what classes of dynamical systems the permutation entropy is equal to the Kolmogorov-Sinai entropy, a classical measure for complexity.

It was shown in [1] by Unakofova, Unakafov and Keller that for one-dimensional systems the difference between the permutation and the Kolmogorov-Sinai entropy, which was considered using ordinal partitions, is related to the measure of specific sets V_d, $d = 2, 3, ...$, which depend on specific ordinal patterns.

It was proved in [1] that for mixing interval maps the measure of V_d converges to zero for increasing d and that equality of permutation and K-S entropy depends on the rate of this convergence.

Here we show that for interval maps with strictly positive Kolmogorov-Sinai entropy, the weaker condition of ergodicity is sufficient for the measure of V_d to converge to zero. Proving this we used tools from [1] together with the fact that ergodic maps exhibit Bernoulli-Factors with the same entropy to create upper bounds for the measure of V_d.

[1] V.A. Unakofova, A.M. Unakafov and K. Keller, *An approach to comparing Kolmogorov-Sinai and permutation entropy.* The European Physical Journal Special Topics, Vol. 222, No. 2, June 2013

Convolutional neural network for recognition of the problem zones on ultrasound images of blood vessels with atherosclerotic lesion

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Today the problem of cardiovascular disease is one of the leading causes of death in the world. Therefore, new methods of treatment and detection of diseases are necessary for the successful struggle against such ailments. There are a lot of techniques, based on the using information

technology, which can help to identify cardiovascular diseases. Most of them are associated with articial neural networks.

In this paper a method for the recognition of problem zones on ultrasound images is considered. The image classifier is built on an ensemble of convolutional neural networks (CNN). This technology allows to determine the features for each individual class of images automatically at the training stage. This function makes CNN a powerful tool for solving problems associated with the classification of images, including medical ones. The proposed method allows to identify problem zones on an ultrasound image and also to identify zones with a risk of spreading the disease.

The main contributions of this paper are:

1) prepare dataset for training model,

2) build classier for fragments of medical images,

3) propose effective classier for the recognition of the problem zones on medical images.

Computational study of electrical restitution in cardiomyocytes

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The relationship between cardiac electrical instability and the slope of restitution curve has been established by many scientists by means of experimental methods and mathematical models.

This study is devoted to investigate the electrical restitution dynamics in cardiomyocytes electrically stimulated with use of different pacing protocols. The new approach to stimulate cardiomyocytes for modeling action potential (AP) alternans due to the heart rate variability is proposed.

Computational simulation of AP and currents for K^+, Na^+, Ca^{2+} ions in cardiomyocytes has been performed by using an improved parallel conductance model in Matlab environment. Areas with the maximum slope in electrical restitution curves for ventricular and atrial cardiomyocytes have been determined. The occurrence of action potential duration (APD) alternans in areas of the electrical restitution curve

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with a maximum slope has been received. Obtained results suggest that the new approach to investigate cardiomyocytes electrical activity unmasks mechanisms for appearance of alternans, which cannot be seen with current experimental stimulation protocols. The calculated restitution curves allow for identifying the maximum slopes, which determine the arrhythmogenic properties of heart cells.

Computational results are useful to interpret experimental results with human-induced pluripotent stem cells differentiated into cardiomyocytes (hiPSC-CMs) on the lab-on-chip platform and to propose the new design of the experiments for studies of heart disease, drug screening and tissue regeneration in cell-replacement therapies.

Ordinal spaces as a generalization of metric spaces

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Ordinal data analysis is an interesting direction in machine learning. It often deals with data for which only the relationships '$<$','$=$','$>$' between pairs of points are known. We do an attempt of formalizing structures behind ordinal data analysis by introducing the notion of ordinal spaces on the base of a strict axiomatic approach. For these spaces we study general properties as isomorphism conditions, connections with metric spaces, embeddability into Euclidean spaces, topological properties etc.

A general symbolic approach to nonlinear data analysis

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Using symbolizations to study observed data plays an important role in nonlinear time series analysis. Particularly, the Kolmogorov-Sinai entropy as a measure quantifying complexity of dynamical systems and data coming from it is based on the idea of symbolization. Here the problem is to find symbolizations which contain enough information on the system, as in the ideal case symbolizations associated to generating

partitions do. Such partitions are usually not a priori given or not practicable. In this talk we describe a general symbolic approach providing a direct route to Kolmogorov-Sinai entropy and discuss it in relation to known symbolization strategies.

On the shadow problem

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Further, under m-dimensional planes we mean m-dimensional affine subspaces of the Euclidean space $\mathbb{R}^n$.

Definition. We say that the set $E \subset \mathbb{R}^n$ is *m-convex* with respect to the point $x \in \mathbb{R}^n \backslash E$ if there exists an m-dimensional plane L such that $x \in L$ and $L \cap E = \varnothing$.

For every set $E \subset \mathbb{R}^n$ we can consider the minimal m-convex set containing E and call it *m-convex hull* of a set E.

The shadow problem. What is the minimum number of mutually disjoint closed or open balls in the space $\mathbb{R}^n$ with centers on the sphere S^{n-1} and of radii smaller than the radius of the sphere with condition that the center of the sphere belongs to an 1-convex hull of the family of these balls?

Theorem. *Any set consisting of three balls of the same radius which do not intersect pairwise forms an 1-convex set in the three-dimensional Euclidean space $\mathbb{R}^3$.*

[1] Yu. B. Zelinskii, H. K. Dakhil, B. A. Klishchuk On weakly m-convex sets, *Reports of the NAS of Ukraine*, no. 4, (2017), P. 3–6 (in Ukrainian).

A generalized implicit function theorem with applications to hyperbolic PDEs

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Our first result is a generalized implicit function theorem for abstract equations of the type $F(\lambda, u) = 0$. We suppose that $F(\lambda, \cdot)$ is smooth for all λ. It should be stressed that we do not suppose that $F(\cdot, u)$ is smooth for all u. Let $F(0, u_0) = 0$. We state conditions under which for all $\lambda \approx 0$ there exists exactly one solution $u \approx u_0$, this solution u is smooth in a certain sense, and the data-to-solution map $\lambda \mapsto u$ is smooth. Then

we apply this result to time-periodic solutions of first-order hyperbolic systems

$$\partial_t u_j + a_j(x,\lambda)\partial_x u_j + b_j(t,x,\lambda,u) = 0$$

and second-order hyperbolic equations

$$\partial_t^2 u - a(x,\lambda)^2 \partial_x^2 u + b(t,x,\lambda,u,\partial_t u,\partial_x u) = 0.$$

This is a joint work with Lutz Recke.

Parameters estimation of active contour models for the problem of automatic cellular filaments tracking

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Active contour models or snakes [1] are widely used and have large application area in computer vision, image analysis and especially in the analysis of biomedical and microscopic images. In this work we apply gradient vector flow-based [2] active contour models for segmentation and tracking of cellular intermediate filaments. As a part of the cells cytoskeleton, these filaments have notable diversity between different cell-types and play a crucial role in the mechanical behaviour and properties of living cells [3].

The best fitting position of the active contour (snake) to an observed filament on the selected image can be obtained by minimizing a parametrized energy functional of the snake, which incorporates elastic properties of the contour as well as the image data term. The latter can be replaced, according to [2], by a vector field called gradient vector flow, which provides better convergence [2] of the method in case of concavities compared to [1].

In this work we focus on the problem of automatic estimation of the model free parameters [4] based on an image data driven approach.

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The resulting method is incorporated into our image analysis framework comprising automatic filaments detection and tracking.

[1] Kass, M., Witkin, A., & Terzopoulos, D. (2002). Snakes: Active contour models. International Journal of Computer Vision, 1(4), 321-331.

[2] Xu, C., & Prince, J. L. (1997). Gradient vector flow: a new external force for snakes. In Proceedings of IEEE Computer Society Conference on Computer Vision and Pattern Recognition. IEEE Comput. Soc.

[3] Leube, R.E., Moch, M., and Windoffer, R. (2017). Intracellular Motility of Intermediate Filaments. Cold Spring Harb Perspect Biol June 2017.

[4] Chen, J., Pereverzyev Jr, S., & Xu, Y. (2015). Aggregation of regularized solutions from multiple observation models. Inverse Problems, 31(7).

Embedding Hidden Markov Models into Reproducing Kernel Hilbert Spaces

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Hidden Markov models (HMMs) are a widely used probabilistic graphical model for time series of discrete, partially observable stochastic processes. In this paper, we discuss an approach to extend the application of HMMs to non-Gaussian continuous distributions by embedding the belief about the state into a reproducing kernel Hilbert space (RKHS). This method may be applied to various statistical inference and learning problems, including Kalman Filters, belief propagation in probabilistic graphical models, planning Markov decision processes and partially observed Markov decision processes. This implies a necessity to consider a new regularization for the posterior embedding estimator. We investigate, theoretically and empirically, the effectiveness of kernel samples as landmarks in the Nyström method for low-rank approximations of kernel matrices, namely estimate the approximation error of the Nystr om method as a regularization of kernel embedding.

Furthermore, we discuss applications of the method to real-world problems, comparing the approach to several state-of-the-art algorithms.

Statistical analysis of the relationship between the velocity and body mass in human sport activities (running, swimming, skiing, skating, cycling and rowing)

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A significant amount of data on the velocity and body mass of both female and male athletes professionals in Olympic sports (running, swimming, skiing, skating, cycling and rowing) was collected. The average values for different distances were calculated and the linear regression analysis was applied to find the relationships between the body mass and the velocity for every distance. For longer distances, results show that the most performing athletes are characterized by a lower body mass, except for skating.

Mathematical aspects within the epistemology of modeling

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Since the last decades, mathematical modeling plays an increasing role in e. g. life-science applications. Oftentimes, the mechanisms are not well-distinguished from each other, not really quantified and not given in a hierarchical order. Thus, the questions occur what we do, when we construct a mathematical model, and what we expect.

We present a conceptual framework which allows us to differentiate between mathematical and epistemological questions. For this purpose, we use a general evolution equation representing the system to be modeled, and formulate the question of model selection as an approximation of the system equations by model equations.

This approach enables us to determine the causation structure in systems, to formalize and evaluate the model selection process, to discuss the hierarchical order in model families and to describe the robustness of model components and the respective reproduction of observations against model refinements.

Generalized modeling in the neuro-interstitial and neuromuscular interaction research problem

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The research of the features of intercellular and interstitial interactions is an actual direction of modern scientific research. The modeling of even individual metabolic, physiological or pathophysiological changes in a living cell requires the consideration of a large number of parameters of biological processes, many of which have not been fully studied. Therefore, the development of models that adequately describe biological processes in the cells and tissues of living organisms is a complex task. The solution of this problem requires an integrated approach that allows describing the features of chemical and physical changes taking into account their probabilistic nature.

In this paper we consider the problem of modeling the interactions of visceral neurons, Cajal cells and smooth muscle cells in the intestinal wall. The complexity and ambiguity of regulatory influences within the intestinal wall creates a variety of effector reactions, and the lability of the contribution of each of the regulatory components is the uncertainty of the expected results in the development of individual pathological changes in the digestive system. Therefore, the modeling of these processes is clinically justified and important for practical medicine.

Convergence of solutions of TV-regularized linear inverse problems

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RICAM, Austrian Academy of Sciences

In a recent paper by A. Chambolle et al. [Geometric properties of solutions to the total variation denoising problem. Inverse Problems 33,

2017] it was proven that if the subgradient of the total variation at the true data is not empty, the level-sets of the total-variation denoised solutions converge to the level-sets of the true solution with respect to the Hausdorff distance. This talk explores a new aspect of total variation regularization theory based on the source condition introduced by Burger and Osher [Convergence rates of convex variational regularization. Inverse Problems 20, 2004] to prove convergence rates results with respect to the Bregman distance. We generalize the results of Chambolle et al. to total variation regularization of general linear inverse problems and show that the source condition implies Hausdorff convergence of level-sets of the total variation regularized solutions.

This is a collaboration with José A. Iglesias and Otmar Scherzer.

Regularized Nyström subsampling in regression and ranking problems

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In the supervised learning, the Nystrom type subsampling is considered as a tool for reducing the computational complexity of regularized kernel methods in the big data setting. Up to now, the theoretical analysis of this approach has been done almost exclusively in the context of the regression learning and in the case where the smoothness of the target functions is restricted to the Holder type source conditions. Such conditions do not cover the case of target functions with high and low smoothness, which are also of practical interest. Moreover, in the case of the Holder source conditions, there is no need to consider a regularization with high enough qualification because order-optimal learning rates are achieved by the simple Tikhonov regularization known also as the kernel ridge regression. At the same time, this learning method does not improve its performance for any smoothness higher than Holder ones. Therefore, in this presentation, our goal is to extend previous analysis of the Nystrom type subsampling to the case of the general source conditions, and to the regularization schemes with high enough qualification. We also show that under rather natural assumption, our results can be easily reformulated in the ranking learning setting.

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Mathematical modeling of vortex processes in the left ventricle and aorta

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A detailed analysis of the approaches to the description of swirling fluid flows in the left ventricle of the heart (LV) is performed. The formulation of the problem of the study of vortex processes in the LV with mobile walls of the LV is formulated as a system of differential equations in a moving system of ellipsoidal coordinates with respect to the flow velocity, vorticity and movement of the LV wall. For the solution of the problem in the form of a system of nonlinear differential equations in partial derivatives, an iterative numerical-analytic method based on the use of integral transformations on spatial variables and time is proposed. The obtained simulation results indicated the presence of vortex rings at the entrance to the aorta and their distribution on the aorta during fluid movement.

Blood flow characteristics in the ventricles and large vessels: calculations based on 4D MRI data and user-friendly software

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Magnetic resonance imaging (MRI) gives the opportunity to quantify time-resolved 3D flow patterns in vivo. However, its space and time resolution is limited thus compromising the accuracy of flow-based measurements and can cause significant discrepancies, especially when a flow derivative calculation is required. In previous investigations it was shown that the relative error of the shear stresses, calculated at a fixed moment of time with the use the space derivatives of the velocity components, can exceed 100 %. In turn, the time-averaged characteristics can be calculated with higher accuracy. In this project, we present original methods to estimate shear stresses and pressure gradients without

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using flow derivatives. The new algorithms are implemented in a new software tool, which is user-friendly and provides information along the whole vessel, between two selected cross-sections or in the proximity of selected points.

Analyzing the video data of cell oscillations in microchips: algorithm and preliminary results

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An algorithm of the video data analysis is proposed, which allows for estimating both the micrometer absolute magnitude of cell contraction and the rate of oscillations in m/s. Moreover, it allows for decomposing the mechanical oscillations of cells into components. The algorithm has been used to evaluate the change in the contraction rate of cardiomyocyte cells cultured in a lab-on-chip, as a function of voltage intensity and excitation frequency under different experimental conditions. Examples of changes in the shape of the pulses at different frequencies and in the spatial heterogeneity of the mechanical activity of cells in microchip as a function of the excitation frequency and the voltage intensity are presented.

The influence of left ventricle's torsion motion on the helical flow in the aorta

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The left ventricular torsion motion plays an important role for LV ejection and forming the complex structure of flow in the aorta.

The pressure in a rotating body i.e. left ventricle decreases from rotating walls to a center of rotation. The pressure gradient imparts the necessary centripetal acceleration. The fluids admit a motion on a curved path. The torsional motion influences to the pattern of flow in the left ventricle. It creates the condition for more quick filling of the left ventricle because the gradient of the pressure significantly greater.

The helical flow appears in the aorta in the second part of the systole. The intensity of primary and secondary (Dean-like) flows is more high then intensity oh the helical flow and, consequently, the pattern of flow doesn't have the clear evidence of existing this flow. In conclusion, this study shows that the of helical blood flow is feasible, and essentially depends from features of blood flow in the LV.

Legendre polynomials as a recommended basis for numerical differentiation in the presence of square summable or stochastic white noise

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We consider one of the classical ill-posed problems: estimating the derivative of a function from its observable version contaminated by additive square summable or stochastic white noise. In the talk we are going to present and analyze an efficient method for the reconstruction of the derivative by the derivatives of the partial sums of Fourier-Legendre series of noisy function. We argue that in certain relevant cases this method has advantage over the standard approach, when the derivative is reconstructed as the solution of the corresponding ill-posed Volterra equation. Another interesting observation is that in a Hilbert scale generated by the system of Legendre polynomials the stochastic white noise does not increase, as it might be expected, the loss of accuracy compared to the deterministic noise of the same intensity. Moreover, we discuss the relation of the considered numerical differentiation scheme with the well-known Savitzky-Golay derivative filters, as well as possible applications in diabetes technology.

Application of graph Laplacian in semi-supervised learning

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In this contribution we investigate the problem of learning from labeled and unlabeled data (semi-supervised learning) by Tikhonov regularization method in Reproducing Kernel Hilbert Spaces. We propose

new technique for constructing a reproducing kernel directly from data that based on technology of spectral graph theory. Namely, the eigenvectors of the graph Laplacian associated to the unlabel data are used for estimation of underlying manifold that is usually unknown.

Note that the concept of the graph Laplacian has been already employed in the context of semi- supervised learning in [1], [2], where the graph Laplacian associated to the data has been used to form additional penalty terms for Tikhonov regularization. In contrast to [1], [2] we use the approach to construct a data-dependent kernel that generates directly RKHS, where a regularization is performed.

We successfully verified proposed scheme on two- and tree-moons data sets as well as problem of automatic gender identification.

[1] M. Belkin, P. Niyogi, and V. Sindhwani. *Journal* J. Mach. Learn. Res., **7**, (2006), p. 2399.

[2] A. L. Bertozzi, X. Luo, A. M. Stuart, and K. C. Zygalakis. *arXiv:1703.08816*

Entropy numbers for the classes $B_{p,\theta}^{\Omega}$ of periodic multivariate functions

K. V. Pozharska

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We obtain order estimates for entropy numbers [1] of the classes $B_{p,\theta}^{\Omega}$ [2] of periodic multivariate functions in the metric of the space L_q, $1 \leq q \leq \infty$. These classes with a certain choice of the function Ω coincide with the Nikol'skii–Besov classes $B_{p,\theta}^{r}$.

In certain cases, in particular, in two-dimensional case, for $2 \leq p \leq \infty$, $1 \leq \theta \leq \infty$ and $q = \infty$, the exact-order estimates of the entropy numbers of the corresponding classes are established.

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A parameter estimation of multivariate exponential sums

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The reconstruction of sparse exponential sums out of sampling values is an essential problem in signal processing. Namely, let us consider N-sparse d-variate exponential sum, $s_{\mathbf{k}} = \sum_{j=1}^{N} a_j \exp\left(-\mathrm{i}\langle \mathbf{w}_j, \mathbf{k}\rangle\right)$, where $\mathbf{w}_j \in (0, \pi]^d$, $\mathbf{k} \in \mathbb{Z}_+^d$, $\langle \mathbf{w}_j, \mathbf{k}\rangle$ denotes the inner product of $\mathbf{w}_j$ and $\mathbf{k}$, $a_1, a_2, \ldots, a_N \in \mathbb{C}\backslash\{0\}$. The aim is to determine the parameters $\mathbf{w}_j$, $j = 1, \ldots, N$, given finitely many samples of $s_{\mathbf{k}}$. In one-dimensional case, a solution of such a problem can be easily found by the well-known Prony method. In recent years, a lot of research has been carried out in order to obtain such a method in higher dimensions (see, e.g., [2]).

Based on the one-dimensional approach developed in [1], we propose to find the parameters $\mathbf{w}_j$, $j = 1, \ldots, N$, as common zeros of some special kind of d-variable polynomials. Using Cantor tuple functions allows to give the lower number of samples needed for recovery of parameters, in comparison with the other existing methods. As well combining the new approach with an autocorrelation sequence can give stable solunions in the case of noisy data.

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Cardiovascular Imaging: advanced computational techniques for 4D data representation, quantification and surgical planning

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4D imaging represents a huge source of information that is clearly underexploited in the clinical setting. Computational techniques derived from standard fluid dynamics and structural simulation software can be

usefully implemented for an intuitive representation of the imaging data. Moreover, they can condense the information and provide synthetic and quantitative data to be used for risk stratification analysis in an unprecedented way.

All these data can then be used in combination with advanced visualization tools, such as augmented or mixed reality glasses, or with numerical simulation tools, such as finite element, spring mass or finite volume models, to obtain patient specific models to be used for surgical planning, teaching and training purposes

Rational design of a thermostable FAOX enzyme

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Fructosyl Amino Acid Oxidases (FAOX) are enzymes that can deglycate amino acids, cleaving the sugar unit from the amino acidic moiety. These enzymes have been used as biosensors for diabetes monitoring, by measuring the concentration of glycated haemoglobin in blood samples. However, the used FAOX enzymes show relatively low stability levels, which affect their conditions of use. In this work, we show a rational design method based on molecular dynamics simulations through which we screen a library of potentially stabilizing mutants. The most promising mutants are then experimentally produced and tested. Using this approach we obtained two thermostable FAOX I mutants showing a significantly higher T_{50} (55.3°C and 60.6°C, respectively) compared to the wild-type enzyme (52.4°C). In addition, one mutant exhibit hyper-stabilization, showing residual activity up to 95°C, while the wild-type enzyme becomes inactive at T>55°C. In conclusion, the computational method presented here represents a useful approach to expedite the design of thermostable enzymes.

Optimal recovery of Cauchy type integrals in the unit disk

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Let K be the set of holomorphic functions f in $\mathbb{D} := \{z : |z| < 1\}$ which is represented by Cauchy type integral

$$f(z) = \frac{1}{2\pi i} \int_{\mathbb{T}} \frac{h(t)}{t - z} dt, \quad z \in \mathbb{D},$$

where $h : \mathbb{T} \to \mathbb{C}$ is essentially bounded function on $\mathbb{T} := \{t : |t| = 1\}$ and ess $\sup_{t \in \mathbb{T}} |f(t)| \leq 1$.

For distinct points $\mathbf{a} := \{a_0, a_1, \ldots, a_{n-1}\}$, $n \in \mathbb{N}$, in $\mathbb{D}$ consider the quantity

$$\mathscr{E}_n(K; \mathbf{a}; z) := \inf_{\mu_j} \sup_{f \in K} \left| f(z) - \sum_{j=0}^{n-1} f(a_j) \mu_j(z) \right|, \quad z \in \mathbb{D},$$

where infimum is taken over all linearly independent systems of continuous functions in $\mathbb{D}$.

Theorem. *Let $n \in \mathbb{N}$, $\mathbf{a}$ be as above and*

$$B_j(t) := \prod_{k=0}^{j-1} \frac{-|a_k|}{a_k} \cdot \frac{t - a_k}{1 - t\overline{a_k}}, \quad j = 1, 2, \ldots, n, \ t \in \mathbb{D}.$$

Then for each $z \in \mathbb{D}$,

$$\mathscr{E}_n(K; \mathbf{a}; z) = \frac{|B_n(z)|(1 - |z|^2)}{1 - |zB_n(z)|^2} \int_{\mathbb{T}} \frac{\left| 1 - \overline{zB_n(z)} t B_n(t) \right|}{|1 - \overline{z}t|^2} \frac{|dt|}{2\pi}.$$

Direct and inverse approximation theorems of functions of several variables in the spaces S^p

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Let $L_1 = L_1(\mathbb{T}^d)$ be the space of all functions f, given on the d-dimensional torus $\mathbb{T}^d = \prod_{j=1}^{d}[-\pi, \pi]$ with the usual norm $\|f\|_{L_1}$.

The space S^p, $1 \leq p < \infty$, [1, Chap. XI] (see also [2]) is the space of all functions $f \in L_1$ such that $\|f\|_{S^p} := \left(\sum_{\mathbf{k} \in \mathbb{Z}^d} |\widehat{f}(\mathbf{k})|^p \right)^{1/p} < \infty$, where $\widehat{f}(\mathbf{k})$ are the Fourier coefficients of the function f. Functions $f \in L_1$ and $g \in L_1$ are equal in the space S^p if $\|f - g\|_{S^p} = 0$.

The modulus of continuity of $f \in S^p$ of index $\alpha > 0$ is defined by

$$\omega_\alpha(f, t)_{S^p} = \sup_{|h| \leq t} \|\Delta_h^\alpha f\|_{S^p} = \sup_{|h| \leq t} \left\| \sum_{j=0}^{\infty} (-1)^j \binom{\alpha}{j} f(\mathbf{x} - jh) \right\|_{S^p}, \quad t > 0,$$

where $\binom{\alpha}{j} = \alpha \cdot \ldots \cdot (\alpha - j + 1)/j!$, $(\mathbf{x} - jh) := (x_1 - jh, \ldots, x_d - jh)$.

Denote by

$$E_n^\triangle(f)_{S^p} = \inf_{a_\mathbf{k} \in \mathbb{C}} \| f - \sum_{\nu=0}^{n} \sum_{|\mathbf{k}|_1 = \nu} a_\mathbf{k} e^{i(\mathbf{k}, \mathbf{x})} \|_{S^p}, \quad |\mathbf{k}|_1 := \sum_{j=1}^{d} |k_j|$$

the best approximation of the function $f \in S^p$ by the triangular polynomials of the order $n - 1$.

Theorem. *Assume that $f \in S^p$, $1 \leq p < \infty$. Then for any $n \in \mathbb{N}$ and $\alpha > 0$ the following relation is true:*

$$\omega_\alpha\left(f, \frac{\pi}{n}\right)_{S^p} \leq \frac{\pi^\alpha}{n^\alpha} \left(\sum_{\nu=1}^{n} (\nu^{\alpha p} - (\nu - 1)^{\alpha p}) E_\nu^\triangle(f)_{S^p}^p \right)^{1/p}.$$

In the case of approximation of functions of one variable, for modulus of continuity of integer index, the corresponding result was obtained in [2].

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Multivariate directional wavelet systems on the torus

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For regular matrices $\mathbf{M} \in \mathbb{Z}^{2 \times 2}$ we consider finite dimensional spaces $V_\mathbf{M}^\xi$ containing translates of functions $\xi \in L_2(\mathbb{T}^2)$ on the pattern $\mathbf{M}^{-1} \mathbb{Z}^d \cap$

$[-\frac{1}{2}, \frac{1}{2})^2$. The factorization $\mathbf{M} = \mathbf{JN}$ with regular matrices $\mathbf{J}, \mathbf{N} \in \mathbb{Z}^{2\times 2}$ and $|\det \mathbf{J}| = 2$ leads to a decomposition of $V_{\mathbf{M}}^{\xi}$ into the direct sum $V_{\mathbf{M}}^{\xi} = V_{\mathbf{N}}^{\varphi} \oplus V_{\mathbf{N}}^{\psi}$, which was investigated in [2]. In particular, multivariate trigonometric polynomials of Dirichlet-type were used as scaling functions with corresponding wavelets.

In [1], the extension to multivariate wavelet systems with trigonometric polynomials of de la Vallée Poussin-type was developed. The construction allows for many different dilation matrices, especially shearing matrices, which can be used for anisotropic wavelet decompositions that prefer certain directions.

This talk presents a systematic way to choose the dilation matrices such that directional features of functions are revealed in certain wavelet spaces.

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Mathematical Analysis of Imaging Modalities using Electric or Magnetic Nanoparticles as Contrast Agents

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In this talk, we are concerned with the mathematical analysis of imaging modalities using electric or magnetic nanoparticles as contrast agents. An electric (resp. magnetic) nanoparticle is characterized by a large contrast of its own relative permittivity ϵ (resp. relative permeability μ) which is of the order $a^{-\alpha}$, with $\alpha > 0$, where a is its relative radius, $a << 1$ (estimated with few nanometers). Several examples of electromagnetic nanoparticles used in medical imaging having such characteristics are reported in the literature. The general idea in such imaging modalities is to collect remotely the data (i.e. the scattered fields generated by incident fields) before and after injecting (or delivering) the nanoparticles in the targeted region. The believe is that by contrasting these data we can recover the inner values of the permittivity coefficients of the tissue in that region. Our goal is to analyze mathematically such

ideas by providing quantitative estimates of these coefficients in terms of the collected data.

Sparse trigonometric approximation of classes of functions with mixed smoothness

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In the talk we are going to present results regarding to exact order bounds of the best m-term approximation of the classes of functions with mixed smoothness. These results were published in [1–6].

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The shadow problem and its generalization

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This thesis is devoted to investigation of properties of generalized convex sets in the real Euclidean n-dimensional space $\mathbb{R}^n$ and in the n-dimensional complex and hypercomplex spaces $\mathbb{C}^n$ and $\mathbb{H}^n$ respectively. The significant results in these directions were obtained by A. Martino, L. Aisenberg, G. Hudajberganov, Yu. Zelinskii, G. Mkrtchyan, M. Tkachuk, T. Osipchuk, B. Klishchuk and others.

In the thesis there was solved the classical problem of shadow (What minimal quantity of pairwise disjoint balls with centres on the sphere S^{n-1} is enough for any straight line, passing through the centre of the sphere, to cross at least one of these balls?). There was also studied some generalizations of this problem: the problem of shadow for half-convexity, the problem of shadow for arbitrary point of the interior of a sphere, the problem of shadow for the family of sets obtained from

a convex set with non-empty interior by a group of geometric transformations which consists from parallel translations and homotheties, the problem of shadow in the complex and hypercomplex spaces.

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Multi-Task Convolutional Neural Network for Image Classification

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Nowadays the most popular approaches for solving different image classification problems it is using the convolutional neural network. And very difficult to find the convolutional neural network that can solve more than one problem. Motivated by limited resources, we try to find the unifying solution for more than one problem. In the present paper, we will describe our approach how to fit one convolutional neural network model with markers which can solve more than one image classification and image recognition problems. Describe the design of convolutional neural network model and training process. Given recommendation about how should use markers for achieving better results with difficult input data. The results are precisely compared with training one multi-task convolutional neural network model with markers for solving two image classification problems and two trained separated convolutional neural network models to solve a particular problem, each.

All training experiments were conducted on one of most popular benchmark dataset.

Solvability of linear boundary value problems for the stationary fractional advection dispersion equation

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Fractional partial differential equations (FPDE) play a key role in the description of the so-called anomalous phenomena in nature and in the

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theory of complex systems. In particular, these equations provide a more faithful representation of the long-memory and nonlocal dependence of many anomalous processes. In the last two decades, FPDE have drawn an increasing attention in several research fields, including Mathematical Modeling, Electromagnetism, Polymer Science, Hydrology, Geophysics, Biophysics, Finance and Viscoelasticity.

For a fixed $\nu \in (1, 2)$, we analyze the stationary fractional advection dispersion equation for the unknown function $u = u(x, y) : \Omega\{(x, y) : x \geq 0, \ y \geq 0\} \rightarrow R^1$

$$\mathbf{D}_x^\nu u(x, y) + \mathbf{D}_y^\nu u(x, y) = f(x, y)$$

subject either to the Dirichlet boundary condition or to the Neumann boundary condition.

The symbols $\mathbf{D}_x^\nu$ and $\mathbf{D}_y^\nu$ denote the Caputo fractional derivatives of order ν with respect to space variables x and y correspondingly.

Under certain conditions on the given functions, we establish one-valued classical solvability of BVP in the fractional weighted Hölder spaces.

A non-contact Photoacoustic Tomography reconstruction procedure. Requirements for data processing algorithms

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A non-contact Photoacoustic Tomography (PAT) is relatively new imaging method with penetration depth up to few centimeters. It measures a tissue surface displacement instead of the pressure in contact PAT. According to the same physical fundamentals, all algorithms of the contact PAT may be implemented for the non-contact PAT. It is only necessary to develop the approach of recalculation the acoustic wave pressure to the surface displacement and vice versa. An approach of calculating the displacement ξ based on the acoustic pressure on the surface p is developed in [1].

The quality of the obtained result is worsened by the speckle noise [2] and model error. As result, the contrast and resolution of the reconstructed image are decreased. Requirements for a noise filter according to features of experimental data are discussed. An appropriate method of

the speckle noise elimination is proposed. The tissue parameters estimation approach is developed. The quality parameters of the reconstructed image are calculated.

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[2] K. Thangavel, R. Manavalan, Laurence Aroquiaraj, *Removal of Speckle Noise from Ultrasound Medical Image based on Special Filters: Comarative study.* ICGST-GVIP Journal, Vol. 9, Issue:3, June 2009, 25-32.

Hydro-vibroacoustic diagnostics of operation of the prosthetic bileaflet heart valve

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The results of experimental studies of sounds and noise of a mechanical beleaflet heart valve are presented in the report. Physical simulation of the heart valve was performed in the laboratory at the Polytecnico di Milano. A special experimental stand was created in the laboratory. The bileaflet mitral valve of Sorin Biomedica (Italy) was located between the model of the atrium and the left ventricle of the heart. Unique heart sensors, pressure fluctuation sensors and miniature accelerometers, which were designed and manufactured at the Institute of Hydromechanics of the National Academy of Sciences of Ukraine [1, 2], were used to study the hydrodynamic noise and sounds of the heart valve operation. A group of piezoceramic accelerometers were mounted on the surface of the experimental bench, which recorded the benchs vibration from the operation of the heart valve. Hydrodynamic noises, vibrations and sounds of the heart model were simultaneously registered in conditions of open and semi-closed valve operation. The sensors were installed in various places in the upper and down flows through the heart valve. The simulation

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was performed for stationary flow of pure water and glycerol solution through the mitral valve, as well as for pulsating flow. Differences in the hydrodynamic noise, vibration, and sounds of the heart valve operation in open and semi-closed valve conditions have been determined [3]. The hydro-vibroacoustic diagnostic features of the prosthetic bileaflet heart valve are determined and solutions for the creation of diagnostic equipment based on hydro-vibroacoustic measurements are proposed.

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Quantification of in vivo fluid dynamics in diseased left ventricles and aortas

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Space and time-resolved phase contrast magnetic resonance imaging (4Dflow) is the latest advancement in phase-contrast magnetic resonance imaging. 4D-flow data yield the quantification of the space- and timedependent velocity field of blood within heart chambers and vessels, as well as within blood-processing devices.

By developing processing tools that allow for coping with data noise and artefacts, it is possible to compute derived quantities, such as shear stresses [1] and relative pressures [2], which can be translated into clinically relevant indices.

The latest activities carried out at Politecnico di Milano in this specific field of research and within the framework of the Ammodit project will be showcased. Moreover, ongoing developments will be presented, with an emphasis on the analysis of the in vivo fluid-dynamics i) in the

left ventricle affected by post-ischemic disease and ii) in the thoracic aorta affected by coarctation. In these two specific clinical scenarios, the exploitation of 4Dflow data may be particularly challenging and require novel processing techniques. The possibility for applying adsvanced mathematical methods to cope with these issues will be discussed.

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