Olomoucian Days of Applied Mathematics
ODAM 2023
12 - 14 June

BOOK OF ABSTRACTS

June 12–14, 2023 | Olomouc, Czech Republic

Department of Mathematical Analysis and Applications of Mathematics
Faculty of Science, Palacký University Olomouc

Preface

Dear Friends and Colleagues,

we warmly welcome you to the international conference "Olomoucian Days of Applied Mathematics 2023" (ODAM). Our primary aim is to bring together researchers and practitioners in mathematical modelling across various scientific domains to discuss current challenges and opportunities driven by practical problems. This conference serves as a platform for introducing new developments and applications in probability theory, statistics, numerical mathematics, optimization, and other areas of applied mathematics.

ODAM originated in 1999 under the guidance of Professor Lubomír Kubáček, a prominent figure in Czech and Slovak mathematical statistics. Inspired by the seminars on applied mathematics conducted at the Department of Mathematical Analysis and Applications of Mathematics at the Faculty of Science of Palacký University in Olomouc, Professor Kubáček established a tradition of congenial gatherings among applied mathematicians. These gatherings alternated between focusing on mathematical statistics on one hand, and mathematical modelling on the other. Since 2011, ODAM has been organized biennially as a comprehensive international conference. After the COVID-19 break in 2021, we are now here to carry on the tradition of bringing researchers together and fostering fruitful interactions at ODAM, as we continue to build upon the previous rich legacy of this conference. The scientific program of ODAM 2023 including 49 presentations, 8 posters and 2 invited lectures promises to touch variety of interesting problems in applied mathematics.

During the conference, we have arranged two special events to enhance networking. On Monday, there will be a welcome drink held on the sixth floor of the Faculty of Science building. This gathering will provide an informal setting for participants to meet and engage with one another. On Tuesday, we have organized a special excursion to witness the production of Olomouc curd cheese, where you can indulge in a delightful culinary experience. The excursion is followed by the Conference Dinner at the Tvarg Restaurant in Velká Bystřice. This evening of fine dining and socializing will offer a delightful opportunity to further connect with fellow attendees.

We sincerely hope that you will find this conference both productive and stimulating, and that your time spent in Olomouc will be truly memorable.

Eva Fišerová, Karel Hron and Jitka Machalová, editors

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Olomouc 2023

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Potential of Interactive Methods in Data-Driven Multiobjective Optimization

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When we deal with data, we can use descriptive analytics to understand it or predictive analytics to make predictions, but this is not enough when we need to know what actions to take to reach desired outcomes. We need prescriptive or decision analytics to make recommendations or decisions based on the data. We can fit models in the data and derive decision problems. Typically outcomes of decisions are characterized by perspectives that may be conflicting. Thus, we must optimize several conflicting objective functions simultaneously. By applying appropriate multiobjective optimization methods, we can find the best balance among the trade-offs.

In this talk, I introduce a seamless chain from data to data-driven decision support involving multiobjective optimization. Eventually, the derived multiobjective optimization problem is solved with an appropriate interactive method. In that way, a decision maker with domain expertise can augment information contained in the data and direct the solution process with one's preferences to find the most preferred solution. At the same time, the decision maker gains insight into the interdependencies and trade-offs among the conflicting objective functions and can get convinced of the quality of the most preferred solution. I demonstrate the advantages of applying interactive methods in data-driven decision support with some example problems. In addition, I give a brief overview of the modular, open-source software framework DESDEO containing different interactive methods.

Bayes Spaces.
An Overview

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Bayes Hilbert spaces $B^2(P)$ describe a Hilbert space structure on a set of mutually continues probability measures, improper priors and likelihoods with origin P.

The talk will give an overview of Bayes Spaces and their relation to various concepts of mathematical statistics. Several deep results of statistics and information theory become obvious and geometrically intuitive corollaries, when viewed in the light of this vector space structure.

The name comes from the fact that vector addition in this space is given by Bayes theorem. A distribution family is an exponential family if and only if its a finite dimensional subspaces of a Bayes Space. In case of regular exponential families its a Bayes Hilbert Space. The geometry of the space is closely related to Fisher information. There is a canocial isometric mapping to $L_0^2(P)$ called centered log ratio transform, proving score functions. The P-a.s. constant ratio of this centered log ratio transform to the log density is Kullback Leibler Divergence. The Basis vectors of conjugated priors can be directly interpreted in terms of information and the basis of the original family. I.e. we explicitly give the conjugated prior for every exponential family.

In a multivariate setting, we can identify conditional distributions with quotient spaces, and provide a straight forward decomposition into a sum of products of marginal spaces closely related to the Hammersley Clifford Theorem, Graphical models and generalizing log-linear models to continues distributions.

References:

[1] van den Boogaart, K. G.; Egozcue, J. J.; Pawlowsky-Glahn, V.: Bayes Hilbert Spaces. *Australian & New Zealand Journal of Statistics* **56**, 2 (2014), first 171-194, http://dx.doi.org/10.1111/anzs.12074

[2] van den Boogaart, K. G., Tolosana Delgado, R.: Multivariate Bayes Spaces and Compositions, Proceedings of CoDaWork2022, 28.06.-01.07.2022, Toulouse, France

Contributed talks and posters

On an Estimation of Parameters of Discrete Distributions from the Schröter Family

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One of the common problems in actuarial mathematics is modeling the aggregate claims distribution of a collective risk model, with the claim severity and the number of claims considered as discrete random variables. The distribution of aggregate claims is, in fact, a convolution of the distributions of the number of claims and the claim severity. From a theoretical perspective, the convolution approach is unambiguous. However, when the number of claim events increases, the computation of the aggregate claim distribution using the convolution approach becomes difficult. This problem has led researchers to search for alternative methods for computing the aggregate claim distribution of collective risk models. We focus on one of them, namely, the recursive method.

A family of recursively defined discrete distributions was introduced in [1]. Due to a relatively complicated formula for the probability mass function of distributions from this family, classical parameter estimation methods (e.g. the maximum likelihood method) result in a system of equations that has no explicit solutions and must be solved numerically. Potential problems of such numerical solutions are mentioned in [2], where also a method specific for that family is presented. The method is based on a linear regression, but as it involves e.g. matrix inversion, it can also be numerically unstable in some cases. In addition, also this method leads to a system of equations without an explicit solution.

We therefore suggest a new, simple method to estimate three parameters of distributions from the Schröter family [1]. The method gives explicite estimations, which can serve as initial values in more sophisticated procedures (such as e.g. those from [2]).

References:

[1] Schröter, K.J.: On a family of counting distributions and recursions for related distributions. *Scandinavian Actuarial Journal* **1990**, 2–3 (1990), 161–175.

[2] Luong, A., Garrido, J.: Minimum quadratic distance estimation for a parametric family of discrete distributions defines recursively. *Australian Journal of Statistics* **35**, 1 (1993), 59–67.

Differentiation of Manuscripts Based on Analysis of NIR Spectra

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One of the tasks facing historians and librarians is the authentication or dating of manuscripts. It appears that non-destructive techniques such as spectroscopy and reflectography are suited not only to the study and preservation of manuscripts, but also to their differentiation.

Thus, our goal is to develop computational models and algorithms an automated differentiation of manuscripts based on data from the near-infrared (NIR) spectra measured on different parts of the books (center, margin, gutter, respectively beginning, center or end of the book, etc.) using both the classical statistical approaches as PLS and/or PCA regression and the functional data analysis.

Solving Multiple-choice Knapsack Problems by Multi-objectivization and Chebyshev Scalarization

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Multiple-choice knapsack problems appear in modeling a number data analysis problems, see e.g. [3], [4]. In [1] the method BISSA is proposed to approximate the optimal solution to the multiple-choice knapsack problem (MCKP) by problem multi-objectivization and the linear scalarization. The scalarization of the resulting bi-objective problem has two important properties: - (1), it does not lead, in general, to solutions of the bi-objective problem due to the fact that the problem is in binary variables, - (2) the special form of the scalarized problems allows to provide a closed-form expressions for its optimal solutions. To fathom the optimality gap that is left by BISSA, we present a method that starts from the approximate solution obtained by BISSA and improves the approximation, and in consequence provides a tighter optimality gap. Like BISSA, the new method is based on multi-objectivization of the multiple-choice knapsack but instead of the linear scalarization used in BISSA, it makes use of the Chebyshev scalarization, see e.g. [2]. Theoretical results are accompnied by a computational experiments using banchmark problems.

References:

[1] Bednarczuk, E.M., Miroforidis, J., Pyzel, P: A multi-criteria approach to approximate solution of multiple-choice knapsack problem. *Computational Optimization and Applications* **vol.70** (2018), 889–910.

[2]] Kaliszewski I.:*Quantitative Pareto Analysis by Cone Separation Technique.* Kluwer Academic Publishers, 1994.

[3] Lee S., Kim S., Kim Y.: Multimode Image Compression Algorithm Employing Multiple-Choice Knapsack Problem-Based Encoding Mode Selection. *J. Display Technol.* **vol.12** (2016), 549-556.

[4] Montalbano, P., de Givry, S., Katsirelos, G. (2022). Multiple-choice Knapsack Constraint in Graphical Models. In: Schaus, P. (eds) Integration of Constraint Programming, Artificial Intelligence, and Operations Research. CPAIOR 2022. Lecture Notes in Computer Science, vol 13292. Springer, Cham. https://doi.org/10.1007/978-3-031-08011-1_19

On the Use of Octree Method in Application to Cultural Heritage

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In this contribution, we present the ongoing research on the technical approach to the 3D point cloud data analysis. In our work, we use the Octree method for compressing and analysing the initial data. Based on the point cloud of a large number of vertices by using the octree method, we aim to distinguish the objects, such as tree branches, electricity cables, bridges, etc., from the surface. The proposed approach is straightforward and does not require the comparison of positions between each vertex.

References:

[1] Octree encoding: A new technique for the representation, manipulation and display of arbitrary 3-d objects by computer, *Rensselaer Polytechnic Institute. Image Processing Laboratory*, Report number: IPL-TR-80-111, 1980

[2] Almost constant-time 3d nearest-neighbor lookup using implicit octrees *Machine Vision and Applications*, **vol. 29(2)**, 2018

On Dynamic Contact Problems for Viscoelastic and Elastic Plates

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Contact problems represent an important but complex topic of applied mathematics and mechanics. Its complexity profounds if the dynamic character of the problem is respected. For the elastic problems there is only a very limited amount of results available. A problem of the vibrating elastic membrane against a rigid obstacle is still not solved. Viscosity makes possible to prove the existence of solutions for a broader set of problems. We deal here with simply supported short memory viscoelastic and elastic anisotropic plates vibrating against a rigid obstacle. We have considered similar problems for a viscoelastic von Kármán plate in [1] and for a thermoelastic plate in [2]. Initial-value problems for hyperbolic variational inequalities form mathematical models of vibrations. The penalization method is used here in order to verify existence theorems. Comparing with [1] and [2] we take the generalized penalization function $\eta^{-1}\beta$ instead of the classical $u \mapsto \eta^{-1}u^{-}$. We distinguish the cases of continuous and continuously differentiable functions β. The deriving of *a priori* estimates of accelerations plays the crucial role in proofs of existence theorems. While in the viscoelastic case the acceleration term does not appears in a weak form of the problem, in the elastic case it has a form of a vector measure. Comparing with papers [1] and [2] we assume a variable thickness of a plate and more generalized type of the obstacle in the same way as in [3].

References:

[1] Bock, I. and Jarušek, J.: Unilateral dynamic contact of viscoelastic von Kármán plates, *Adv. in Math. Sci. and Appl.* **16**, 1 (2006), 175–187.

[2] Bock, I., Jarušek, J. and Šilhavý, M. : Existence of solutions to a dynamic contact problem for a thermoelastic von Kármán plate, *Nonlin. Anal. RWA* **32** (2016) 111–136.

[3] Bock, I. and Kečkemétyová, M. : An optimal control problem for a viscoelastic plate in a dynamic contact with an obstacle, *Tatra Mt. Math. Publ.* **71** (2018), 27–37.

Okun's Law Disaggregated and Factors behind: a Case Study of V4 Countries

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The paper estimates Okun's law on a regional level and explores its determinants for the four Visegrad Group (V4) countries in Central Europe. Unlike other studies on regional Okun's law, the paper applies a mathematically valid disaggregation procedure developed by Boďa & Považanová [1] to estimate Okun's law for economies and regions, and seeks to identify the factors that determine the regional heterogeneity observed in Okun coefficients. The analysis uses data for NUTS 2 regions of Czechia, Hungary, Poland and Slovakia for a twenty-year period 2001–2020. The disaggregation framework provides formal arguments to justify why regions around the capital cities display higher unemployment-output responsiveness that is detected in the analysis. When endogeneity is handled, the level of economic prosperity and accumulated human capital are found to be drivers of differences in the unemployment-output elasticity on a regional level.

References:

[1] Boďa, M., Považanová, M.: Formal and statistical aspects of estimating Okun's law at a regional level. *Papers in Regional Science* **99**, 4 (2022), 1113–1136.

Multiobjective Optimization of Hydraulic Pump Design Problem with Computationally Expensive Simulations

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Real-world optimization problems typically consist of multiple conflicting objective functions that represent different trade-offs. The main focus of this contribution is on the hydraulic pump design optimization problem, which aims to maximize pump efficiency at three different flow rates. The objective function evaluations necessitate computationally expensive CFD simulations. Thus, the high computational cost limits the number of evaluations, and the problem is challenging to solve. The computation time can be reduced with several approaches. Firstly, surrogate models are employed to approximate the underlying objective functions. Next, information about the decision maker's preferences is utilized to guide the search to and within the region of interest. We show how interactive multiobjective optimization methods can benefit from additional information given by the decision maker during the solution process. Moreover, we discuss the presence of simulation failures that occur when a nonviable geometry is created. In such a case, a simulation does not lead to objective function evaluations and hinders the solution process. We address these challenges and solve the pump design problem using a surrogate-assisted reference-vector guided evolutionary algorithm.

References:

[1] Miettinen K.: *Nonlinear Multiobjective Optimization.* Kluwer, Boston, MA, 1999.

[2] Aghaei Pour P., Rodemann T., Hakanen J., Miettinen K.: Surrogate assisted interactive multiobjective optimization in energy system design of building. *Optimization and Engineering* **23.** (2022), 303–327.

[3] Mazumdar A., Chugh T., Hakanen J., Miettinen K.: Probabilistic selection approaches in decomposition-based evolutionary algorithms for offline data-driven multiobjective optimization. *IEEE Transactions on Evolutionary Computation* **26.** (2022), 1182–1191.

Existence of Solutions of Degenerate Semilinear Elliptic Boundary Value Problems

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We show an existence and a uniqueness of a weak solutions of a degenerate and/or singular semilinear elliptic boundary value (nonhomogeneous) problem lying between given weak sub- and supersolution. It has been applied for an existence and a uniqueness results of large solutions to a similar problem with its blow-up rate.

References:

[1] Deuel and Hess: A criterion for the existence of solutions of non-linear elliptic boundary value problems. *Proc. Roy. Soc. Edinburgh Sect. A*, **74** (1976) 49–54.

[2] Dhara R. N.: Existence of solutions of degenerate semilinear elliptic boundary value problems, arxiv:2112.06014.

[3] Keller J. B.: On solutions of $\triangle u = f(u)$. *Communications on Pure and Applied Mathematics*, **10(4)** (1957), 503–510.

[4] López-Gómez J.: The boundary blow-up rate of large solutions. *J. Differential Equations*, **195(1)** (2003), 25–45.

[5] Osserman R.: On the inequality $\triangle u \geq f(u)$. *Pacific J. Math.*, **7(4)** (1957), 1641–1647.

Classification of Cyclists and Pedestrians Data Measured by LiDAR Sensor

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The collected data about how many people are using different modes of transport can provide insights to make informed decisions about infrastructure development. A low-energy device using artificial intelligence for recognizing and counting cyclists and pedestrians can be a radar sensor that can detect the size and speed of traffic participants based on reflected waves. The sensor can be placed in a location such as a busy intersection or a popular pedestrian/cycling route and continuously capture footage of the area. The TFmini Plus LiDAR sensor module [1] is a popular object detection technology with several advantages over other sensing methods.

In our contribution, we classify the data collected by the TFmini Plus LiDAR sensor module collected during a controlled experiment with a limited number of measured signals for pedestrians and cyclists. The observations have been preprocessed at the first step. The signals were normalized to one and sampled to the length of 100 points. We analyzed data by four different algorithms using MATLAB software: machine learning logistic regression [2], scaled absolute differences algorithm, binary linear classifier to high-dimensional data, and k-nearest neighbor classifier. The normalized measured data were divided into the train and test datasets in a ratio of 4 : 1. To evaluate the performance of the analyzed classifier, we randomly selected the train and test sample 10000 times repeatedly. The highest score of correct predictions was observed for the k-nearest neighbor classifier with $k = 1$. However, the scaled absolute differences method is also suitable for low-energy systems due to its low computational power.

Acknowledgement: This work was supported by Slovak Scientific Grant Agency, project VEGA 2/0141/21, VEGA 2/0096/21 and within the projects of the Slovak Research and Development Agency Nr. APVV-21-0299.

References:

[1] Benewake (Beijing) Co., Ltd. Product Manual of TFmini Plus. [Available online: 07.10.2022] http://en.benewake.com/product/detail/5c345cd0e5b3a844c472329b.html.

[2] Rymarczyk, T., Kozlowski, E., Klosowski, G., Niderla, K.: Logistic regression for machine learning in process tomography. Sensors *19* (2019), 3400.

Effectiveness of Road Marking and Signing Assessed by Functional Interval Testing

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Around the world, excessive speed is the most critical factor in road safety, causing the most severe traffic accidents. The situation is particularly risky in urban areas with a high frequency of pedestrians or cyclists, who are considered vulnerable road users. In this context, various traffic calming devices are used, however often without knowing their impact on reducing vehicle speed. To fill this gap, we used the methodology based on the analysis of GPS data by functional data framework.

Connected vehicle data is considered a very new source in the field of transport, with more than 50% new vehicles being connected, which makes it an ideal source for speed evaluations. Functional smoothed speed profiles were used as input for the interval-wise test to assess the statistical significance of speed differences along the road, in the periods before and after the installation of road marking and signing. Following the traffic calming concepts, the study aims to assess the effectiveness of road marking in two scenarios: either applied as isolated (with longer spacing) or applied in a combination along a longer segment.

References:

[1] Pini, A., Vantini, S.: Interval-wise testing for functional data, Journal of Nonparametric Statistics, **29** (2017), 407–424, https://doi.org/10.1080/10485252.2017.1306627.

[2] Ramsay, J., Silverman, B.W.: Functional Data Analysis, Springer New York, 2005. https://doi.org/10.1007/978-1-4757-7107-7.

[3] Římalová, V., Elgner, J., Ambros, J., Fišerová, E.: Modelling the driving speed on expressway ramps based on floating car data. Measurement, **195** (2022), https://doi.org/10.1016/j.measurement.2022.110995.

Analysis of Two-way Compositions Based on the Elemental Information

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Compositional data are commonly known as multivariate observations carrying relative information. The analysis of compositional data arranged in a table, resulting from two underlying factors, has been introduced in the literature as compositional tables approach. Similarly to vector compositions, also the analysis of compositional tables is based on its coordinate representation. However, this can lead to unfavorable aggregation of information. The contribution therefore introduces the concept of backwards pivot coordinates, originally invented for vector compositional data, and its extension to the case of two-way compositions. The main idea is to focus on elementary information about the compositional structure, which is contained in pairwise logratios for vectors and in four-part log odds ratios for tables. The use of methodology will be explained in terms of regression and principal component analysis, and its performance will be demonstrated in an application to movement behavior data.

A Robust Knockoff Filter for Sparse Regression with Microbiome Compositions

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Microbiome data analysis often relies on the identification of a subset of potential biomarkers associated with a clinical outcome of interest. Robust ZeroSum regression, an elastic-net penalized compositional regression built on the least trimmed squares estimator, is a variable selection procedure capable to cope with the high dimensionality of these data, their compositional nature, and, at the same time, it guarantees robustness against the presence of outliers. The necessity of discovering "true" effects and to improve clinical research quality and reproducibility has motivated us to propose a two-step robust compositional knockoff filter procedure, which allows selecting the set of relevant biomarkers, among the many measured features having a nonzero effect on the response, controlling the expected fraction of false positives. We demonstrate the effectiveness of our proposal in a simulation study, and illustrate its usefulness in an application to intestinal microbiome analysis.

References:

[1] Barber, R.F., Candés, E.J.: Controlling the false discovery rate via knockoffs. *Annals of Statistics* **43(5)** (2015), 2055–2085.

[2] Barber, R.F., Candés, E.J.: A knockoff filter for high-dimensional selective inference. *Annals of Statistics* **47(5)** (2019), 2504–2537.

[3] Monti, G.S., Filzmoser, P.: Sparse least trimmed squares regression with compositional covariates for high-dimensional data. *Bioinformatics* **37(21)** (2021), 3805–3814.

[4] Monti, G.S., Filzmoser, P.: Robust logistic zero-sum regression for microbiome compositional data. *Advances in Data Analysis and Classification* **16(2)** (2022), 301–324.

[5] Monti, G.S., Filzmoser, P.: A robust knockoff filter for sparse regression analysis of microbiome compositional data. *Computational Statistics* (2022), 1–18.

Statistical Inference in a Spatial Functional Model in the Presence of Heteroscedasticity

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The aim of the contribution is to introduce a permutation-based test for the effect of covariates for a functional regression model with the heterogeneous spatial structure. In this context, a permutation of residuals from the functional regression model instead of the observations themselves is proposed. A weighted least squares model is fitted to the observations, resulting into approximately exchangeable, and thus permutable, residuals. A simulation study shows that the proposed testing procedure outperform the competitor approaches that neglect the spatial structure, both in terms of power and size. The methodology will be demonstrated on a real-world geochemical data set. The spatiotemporal models are used to analyse and reveal differences in the geochemical properties of the soil at the border between the forest and field.

References:

[1] Ramsay, J.O., Silverman B.W. (2013). *Functional data analysis.* New York, NY, Springer.

[2] Římalová, V., Menafoglio, A., Pini, A., Pechanec, V., Fišerová, E. (2020). A permutation approach to the analysis of spatiotemporal geochemical data in the presence of heteroscedasticity *Environmetrics*, *31*:e2611.

Inferring Vaccine Effectiveness From Observational Data

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For the past three years, there has been a debate about the effectiveness and safety of mRNA vaccines against the covid-19 disease. Efficacy estimates from registration studies that took place during 2020 ceased to be valid already at the beginning of the vaccination campaign, because new variants of the virus appeared, and convalescent population increased. Since the beginning of 2021, estimates of vaccine effectiveness have been entirely based on observational data. In this talk, we will use Czech health insurance company (VZP) data to prove that observational data are heavily biased. Next, we will present two simple mathematical models to explain how different types of bias manifest in observational data. We will show that the reported "vaccine waning efficacy" may be a pure statistical artefact caused by observational data bias. We will conclude that currently we know absolutely nothing about the true effectiveness of mRNA vaccines against various clinically relevant endpoints.

Next-generation Fluorescence Telescopes for Cosmic Rays

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The origin and nature of ultra-high-energy cosmic rays (UHECR) are one of the most important questions in astroparticle physics. The Fluorescence detector Array of Single-pixel Telescopes (FAST) [1, 2] is a prospective next-generation, ground-based UHECR observatory aiming to cover an enormous area by deploying a large array of low-cost fluorescence telescopes suitable for measuring the properties of UHECR, having energies exceeding 3×10^{19} eV.

The talk will introduce a concept of FAST project, principles of extensive-air-shower (EAS) detection, and the reconstruction process which requires a more sophisticated approach, the top-down technique [3], heavily based on EAS Monte Carlo (MC) simulations of UHECR. This technique typically requires a very large number of iterations (with a full event MC simulation in each iteration), and hence is very computationally demanding. A potential room of an advanced artificial intelligence implementation for a significant reduction of MC iterations (as demonstrated in [4]) will also be discussed.

References:

[1] T. Fujii, and et al.: Detection of ultra-high energy cosmic ray showers with a single-pixel fluorescence telescope. *Astroparticle Physics* **74**, (Feb, 2016), 64–72.

[2] M. Malacari, and et al.: The first full-scale prototypes of the fluorescence detector array of single-pixel telescopes. *Astroparticle Physics* **119**, (May, 2020), 102430.

[3] F. Schuessler: Top-Down Reconstruction of Ultrahigh Energy Air Showers. *29th International Cosmic Ray Conference* Pune (2005) **7** (99-102).

[4] J. Albury: Extending the energy range of ultra-high energy cosmic ray fluorescence detectors. *Ph.D. thesis, University of Adelaide, Faculty of Science* (2020).

Approximation and Numerical Realization of the Stokes System with Nonsmooth Slip Boundary Conditions

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This contribution is devoted to an approximation and numerical realization of the Stokes system in 3D with threshold slip boundary conditions, i.e. the conditions of the following form:

$$\|\boldsymbol{\sigma_\tau}\| \leq g,$$
$$\text{if } \mathbf{u}_{\boldsymbol{\tau}} \neq \mathbf{0} \text{ then } \mathbf{u}_{\boldsymbol{\tau}} \cdot \boldsymbol{\sigma_\tau} = -g\,\|\mathbf{u}_{\boldsymbol{\tau}}\|,$$

where $\mathbf{u}_{\boldsymbol{\tau}}$, $\boldsymbol{\sigma_\tau}$ is the tangential component of the velocity vector $\mathbf{u}$, and the shear stress, respectively, g is a slip bound and $\| \; \|$ is the Euclidean vector norm. The complexity of the problem depends on the choice of g. This contribution is focused on the local Coulomb type slip conditions in which the slip bound $g = F\,|\sigma_n|$, where F is the slip coefficient and $|\sigma_n|$ is the modulus of the normal stress. Weak formulations of the Stokes flow with threshold slip boundary conditions lead to inequality type problems which can be equivalently written as systems of nonsmooth equations involving multivalued mappings. After an appropriate discretization by mixed finite elements these systems can be solved by nonsmooth variants of the Newton method. The presentation will by completed with several numerical examples illustrating the efficiency of this approach.

Multivariate Permutation Tests and Functional m-sample Comparisons

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Permutation tests are widely used in statistical hypothesis testing, especially when the null distribution of the test statistic T_0 is not available. Assuming exchangeability, the null hypothesis is rejected if and only if the observed T_0 (computed from the original sample) fails to concur with a set of test statistics $T_1, \ldots, T_k$ obtained from permutation samples. If the test statistics are scalars, we can simply order the values T_i, $i = 0, \ldots, k$, and reject the null hypothesis if T_0 is larger than a given quantile of the set $T_0, T_1, \ldots, T_k$. However, considering several pairwise comparisons of m samples, the test statistic T_0 becomes multivariate (with dimension given by the number of comparisons) and we cannot easily determine whether it is large enough to reject the null hypothesis.

In the multivariate setup, permutation tests can be based on a suitable one-dimensional transformation. For example, it is possible to investigate the distribution of the maximum of appropriately defined contrasts [3] or, more generally, to use the so-called nonparametric combining functions on the vector of marginal permutation p-values [4]. In this contribution, we compare these previously proposed approaches to a new method based on the measure transportation [1, 2] of the points $T_0, T_1, \ldots, T_k$ (in R^d) to a conveniently chosen set of approximately uniformly distributed points, leading to an entirely natural definition of critical value even in the multivariate setup.

Apart of describing an application to the functional m-sample problem and investigating small sample properties of the proposed method in a simulation study, we arrive to a general approach to construction of multivariate permutation critical values and corresponding p-values.

References:

[1] Hallin, M.: On distribution and quantile functions, ranks, and signs in R^d. *Working Papers ECARES 2017-34*. Université Libre de Bruxelles, https://ideas.repec.org/p/eca/wpaper/2013-258262.html (2017).

[2] Hallin, M., Hlubinka, D., Hudecová, Š.: Efficient fully distribution-free center-outward rank tests for multiple-output regression and MANOVA. *Journal of the American Statistical Association*, accepted for publication, https://doi.org/10.1080/01621459.2021.2021921 (2022).

[3] Hlávka, Z., Hlubinka, D., Koňasová, K.: Functional ANOVA based on empirical characteristic functionals. *Journal of Multivariate Analysis* **189** (2022), 104878.

[4] Pesarin, F.: *Multivariate permutation tests: with applications in biostatistics.* Wiley, 2001.

Orthogonal Decomposition of Multivariate Densities in Bayes Spaces with Application to Functional Data Analysis

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Probability density functions can be embedded in the geometric framework of Bayes spaces which respect their relative nature and enable further modeling and analysis. Specifically, the Hilbert space structure of Bayes spaces has several important implications for estimation theory, Bayesian statistics as well as functional data analysis [2,3]. In this contribution, an orthogonal decomposition of multivariate densities in Bayes spaces using a distributional analog of the Hoeffding–Sobol identity is constructed [1]. The decomposition is based on reformulation of the standard (arithmetic) marginals to so-called geometric marginals which are orthogonal projections of the univariate information contained in multivariate densities, follow the Yule perturbation and coincide with the arithmetic ones in case of independence. Accordingly, the decomposition contains an independent part and all possible interaction terms. The orthogonality of the decomposition results in Pythagoras' Theorem for squared norms of the decomposed densities and margin-free property of the interaction terms. There is also a relation with copula-based representation of densities and their functional data analysis. The latter will be illustrated with empirical geochemical data.

References:

[1] Genest, C., Hron, K., Nešlehová, J.: Orthogonal decomposition of multivariate densities in Bayes spaces and relation with their copula-based representation. *arXiv*, (2022), 2206.13898.

[2] Hron, K., Machalová, J., Menafoglio, A.: Bivariate densities in Bayes spaces: orthogonal decomposition and spline representation. *Statistical Papers* (2022), DOI: 10.1007/s00362-022-01359-z.

[3] van den Boogaart, K.G., Egozcue, J.J., Pawlowsky-Glahn, V.: Bayes Hilbert Spaces. *Australian & New Zealand Journal of Statistics* **56** (2014), 171–194.

Detection of Changes in Panel Data Models

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Panel regression models with cross-sectional dimension N are considered. The aim is to test, based on T observations, whether the intercept in the model remains unchanged throughout the observation period. The test procedure involves the use of a CUSUM-type statistic derived via a quasi-likelihood argument. Limit behavior under the null distribution of the test under strong mixing and stationarity conditions on the errors and regressors are presented. Both independent panels as well as the case of mild cross-sectional dependence are considered. It is also proposed a self-normalized version of the test which is convenient from a practical perspective in that the estimation of long-run variances is avoided entirely. The theoretical results are supported by a simulation study that indicates that the test works well in the case of small to moderate sample sizes. An illustrative application of the procedure to US mutual fund data demonstrates the relevance of the proposed procedure in financial settings.

Multi-surrogate Approaches in Multi-objective Bayesian Optimisation

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Many real-world optimisation problems involve multiple conflicting objectives to be achieved. For example, maximising environmental emissions and minimising fuel consumption in the automotive industry and optimising different properties of a drug in the biochemical industry are examples of problems with conflicting objectives. Such problems with multiple objectives are known as multi-objective optimisation problems (MOPs). There is no single solution to such problems because of the conflicting nature of the objectives. The solutions to such problems are known as Pareto optimal solutions and represent the trade-off between objectives [1]. In some cases, e.g., engineering applications, the objective functions rely on computationally expensive evaluations. Such problems are usually black-box optimisation problems without any closed form for the objective functions. Bayesian optimisation (BO) has emerged as an efficient tool for solving such problems [2]. BO relies on a Bayesian model as the surrogate (or metamodel) and finds promising decision vectors by optimising the so-called acquisition function (AF). The AF balances exploitation and exploration during the search process. This work discusses two main approaches for Bayesian model building in multi-objective BO, mono-surrogate (one model after scalarising objective functions) and multi-surrogate (one model for each objective function). The previous study [3] found that the multi-surrogate approach performs better than the mono-surrogate approach as it does not build a latent space model and does not assume that the distribution of the scalarising function is Gaussian. This work extends the previous study and utilises different AFs within the multi-surrogate approach. This work shows the potential of using the multi-surrogate approach by comparing different AFs within a multi-surrogate approach with their mono-surrogate counterparts on standard benchmark MOPs.

References:

[1] Miettinen, K.: *Nonlinear multiobjective optimization.* Kluwer, Boston, MA, 1999.

[2] Shahriari, B., Swersky, K., Wang, Z., Adams, R.P., Freitas, N. de: Taking the Human Out of the Loop: A Review of Bayesian Optimization. *Proceedings of the IEEE* **104** (2016), 148-175.

[3] Chugh, T.: Mono-surrogate vs multi-surrogate in multi-objective Bayesian optimisation. In *Proceedings of the Genetic and Evolutionary Computation Conference Companion (GECCO). Association for Computing Machinery* (2022), 2143–2151.

Estimation and Significance Testing of Rényi Tranfer Entropy

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Revealing causal relationships from observed time series is one of the current challenges of a nonlinear time series analysis. It seems that the Rényi transfer entropy (RTE) with its control parameter $\alpha > 0$ can be the essential approach for analysing the causal relationships in time series with extrema. Jizba et al. (2012) derived a formula for determining RTE in the case of discrete time series. However, the transfer entropy estimates are biased for continuous data, which must be discretised for the formula's application. We analysed the Rényi information flow between two-dimensional time series generated from a vector autoregressive model (VAR) of order one with a unidirectional connection between Gaussian variables. Since RTE can be analytically quantified for a given VAR with Gaussian variables, the bias of RTE estimates was measured by the mean squared error. The data was discretised by three possible schemes: equidistant binning, equiquantal binning, and binning using two quantiles. We also investigated the equality between the estimates of RTE obtained by the proposed formula with those obtained by an alternative formula of RTE written in terms of joint Rényi entropies. The joint Rényi entropies, besides the binning method, can be estimated by the k-nearest-neighbor method suggested by Leonenko et al. (2008), which seems to be more suitable in the case of continuous data. Considering that RTE estimates are generally difficult to interpret due to their bias and no distribution of an RTE estimator is known, the statistical significance of RTE is possibly tested by using surrogate data. Two techniques for synthesising such data were considered. The confidence and power of the tests were investigated by a simulation study.

Acknowledgement: The work was supported by the Slovak Research and Development Agency, project APVV-21-0216, and by the Scientific Grant Agency of the Ministry of Education of the Slovak Republic and the Slovak Academy of Sciences, project VEGA 2/0023/22 and project VEGA 2/0096/21.

References:

[1] Jizba, P., Kleinert, H., Shefaat, M.: Renyi's information transfer between financial time series. *Physica A* **391.** (2012), 2971—2989.

[2] Leonenko, N., Pronzato, L., Savani, V.: A Class of Rényi information estimators for multidimensional densities. *The Annals of Statistics* **36.** (2008), 2153–2182.

Parameter Estimation in an SPDE Model for Cell Repolarisation

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As a concrete setting where stochastic partial differential equations (SPDEs) are able to model real phenomena, we propose a stochastic Meinhardt model for cell repolarisation and study how parameter estimation techniques developed for simple linear SPDE models apply in this situation. We pursue estimation of diffusion term based on continuous time observations which are localised in space. We show asymptotic normality for our estimator as the space resolution becomes finer. We define the time to repolarisation and study its dependence on the strength of the noise and the diffusivity. We demonstrate the performance of the model and the diffusivity estimator in numerical and real data experiments.

References:

[1] Altmeyer, R., Bretschneider T., Janák, J., Reiß, M.: Parameter estimation in an SPDE model for cell repolarisation. *Journal on Uncertainty Quantification* **10**, 1 (2022), 179–199.

[2] Altmeyer, R., Reiß, M.: Nonparametric estimation for linear SPDEs from local measurements. *Annals of Applied Probability* **31**, 1 (2021), 1–38.

[3] Altmeyer, R., Cialenco, I., Pasemann, G.: Parameter estimation for semilinear SPDEs from local measurements. *Preprint* arXiv:2004.14728.

[4] Lockley, R., Ladds G., Bretschneider T.: Image based validation of dynamical models for cell reorientation. *Cytometry Part A* **87**, 6 (2015), 471–480.

Methods of Estimating Parameters of Skewed or Truncated Normal Distribution in the Presence of Observations Outside of Measurable Range

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Every laboratory equipment has limits to what it can accurately measure. Generally, for every laboratory apparatus three types of limits should be defined – limit of blank (LoB), limit of detection (LoD) and limit of quantitation (LoQ). If an observation falls outside of the measurable range, there is an issue of estimating parameters of the distribution.

In this contribution we look at four different methods applied to samples generated from skewed and truncated normal distributions – ignoring censored observations, replacing censored observations, using a truncated version of target distribution, and using target distribution with censored observations.

To compare these methods we designed a simulation study, where generated samples were truncated from the left at selected quantiles. Parameters' estimates were then compared to the original values. Simulation study was run separately on skewed normal distribution and truncated normal distribution.

Based on the results we created recommendations for practical data analysis.

Methods were then applied to real-life laboratory data measured from human blood samples in laboratories at SK-Lab spol. s.r.o. in Lučenec and at Institute of Neuroimmunology SAS in Bratislava.

This work was supported by Masaryk University's specific research support for student projects MUNI/A/1132/2022 and long-term strategic development financing of the Institute of Computer Science (RVO:67985807).

References:

[1] Berger, T., Hilgers, R.-D., Heussen, N.: Observations below multiple lower limits of quantification: How to estimate the mean and variance. *Biom J* **vol. 61**, 5 (2019), 1258-1269.

[2] Glass, D.C., Gray, C.N.: Estimating mean exposures from censored data: exposure to benzene in the Australian petroleum industry. *Ann Occup Hyg* **vol. 45**, 4 (2001), 275-282.

Sparse Pairwise Logratio Variable Selection for High-dimensional Compositional Data

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When selecting significant features from high-dimensional data, such as in the omics sciences, the interpretability of the resulting biomarkers is of a primary importance. This interpretability can be considered from two aspects. First, biomarkers are usually obtained in the form of general logcontrasts or more specifically as balances or pivot coordinates, but for many users it is natural to consider them directly in terms of seminal information in compositional data, namely on pairwise logratios. Second, these logcontrasts should be orthogonal (or even orthonormal) in the regression context, otherwise the interpretation of the regression coefficients will not conform to common expectations. In [1], a selection algorithm for non-overlapping pairwise logratios (referred to as pile logratios in this context) was presented that corresponds to the two advances described above. However, the algorithm is too restrictive to satisfy the orthogonality requirements in a forward search. In this paper, the pile logratios are simply completed to an orthonormal coordinate system. All other possible pairwise logratios in a subcomposition defined by parts contained in the pile logratios are analysed with as little effort as possible by exploiting the orthogonal equivariance of the underlying regression model (e.g. PLS regression). Consequently, all resulting pairwise logratios are tested for significance with respect to the response. The properties of the new approach are analysed with real high-dimensional compositions.

References:

[1] Coenders, G., Greenacre, M. : Three approaches to supervised learning for compositional data with pairwise logratios. *Journal of Applied Statistics* (2022), 11–22.

Clustering of Shapes. A Study of Selected Similarity Measures for the Clustering of 2D Curves

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In this contribution, we present the results of our ongoing research on clustering with respect to the shape and size of 2D contours that are boundaries of crosssections of 3D objects of revolution. We propose several similarity measures based on combined disparate Procrustes analysis (PA), dynamic time warping (DTW), and Wasserstein distance. We investigate the properties of the proposed similarity measures through a series of computational experiments. The motivation and the main application for this study come from the field of archaeology and the classification of archaeological pottery.

References:

[1] Kaliszewska, A., Syga, M.: On representative functions method for clustering of 2d contours with application to pottery fragments typology. Control and Cybernetics 47(1), 85–108, (2018).

Combinatorial Optimization Models of RNA Structural Motifs

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Combinatorial optimization methods are widely used in planning and management, design and engineering industries, etc. However, optimization techniques can be applied in a non-traditional way to model complex biological systems and processes. The current work considers integer programming formulation of the RNA folding problem. This fundamental problem in molecular biology aims to predict the three-dimensional structure of an RNA molecule from the nucleotide sequence.

From a perspective inspired by statistical physics, RNA folds into a stable structure with the minimum free energy. The lower the free energy, the more stable an RNA structure is. The free energy of a structure depends largely on base pairs, in other words, various nucleotide interactions. In integer programming formulation, the most stable structure maximizes the total score of base pairs.

The present approach is focused on finding structures of functional subunits, structural motifs, that comprise RNA structure. Motifs are built of diverse non-canonical base pairs that are hard to predict. In the current model, the optimal motif structure has a maximum total score that does not exceed some allowed upper bound and number of base pairs. The motif model finds a set of optimal solutions that contain candidates for biologically relevant native structures.

The designed method of generating motif structures was verified on realistic RNA data. Numerical experiments were conducted in python language using the Gurobi optimization solver. For each considered RNA sequence a set of optimal solutions were produced. The results demonstrate the efficient use of integer programming modeling for predicting motif structure.

References:

[1] Ponty, Y., Reinharz, V.: *RNA Folding. From text to graphs: Discrete structures and methods for Bioinformatics.* ISTE, London, United Kingdom, 2022.

[2] Gusfield, D.: *Integer Linear Programming in Computational and Systems Biology.* Cambridge University Press, Cambridge, United Kingdom, 2019.

[3] Leontis, N.B., Westhof, E.: Geometric nomenclature and classification of RNA base pairs. *RNA* **vol.7**, 4 (2001), 499–512.

Next-generation Fluorescence Telescopes for Cosmic Rays: Data Analysis and Categorization

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Ultra-high energy cosmic rays (UHECR) are among the highest energy particles observed in the Universe. These particles are associated with extremely energetic astrophysical phenomena such as gamma-ray bursts or active galactic nuclei, but their nature and origin are still a mystery. UHECR can be detected with the fluorescence detectors. One such detector is the fluorescence detector array of single-pixel telescopes (FAST) [1, 2], developed in collaboration with Joint Laboratory of Optics. In this talk, we present the analysis and categorization of data acquired using FAST. The concept of data analysis from acoustic emission is used, so that the specific properties of all captured events are calculated. This approach helps to significantly reduce the amount of acquired data and thus subsequently determine which events are of interest for further analysis, e.g. for full event reconstruction.

References:

[1] T. Fujii, and et al.: Detection of ultra-high energy cosmic ray showers with a single-pixel fluorescence telescope. *Astroparticle Physics* **74**, (Feb, 2016), 64–72.

[2] M. Malacari, and et al.: The first full-scale prototypes of the fluorescence detector array of single-pixel telescopes. *Astroparticle Physics* **119**, (May, 2020), 102430.

Modelling of Lithium-ion Batteries' Reliability in Electric-Powered Aircraft

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A high-quality and stable source of electrical energy is an essential part and requirement in many of today's technical systems. The requirement for quality and stability of the source is crucial in systems whose operation is entirely dependent on the electrical energy source. We observe the properties and reliability indicators in Li-ion batteries that are the energy source for an electric aeroplane. These batteries have been stored for several years. We focus on creating and describing a modelling approach that will enable us to work efficiently with the discharging process in the batteries. We aim to find the probability density of the distribution of the first hitting time (FHT), which in our setting is defined as the time when the voltage on the battery cell reaches the critical value of 2.51 [V]. Then, we compare the results with the values for the same types of new Li-ion batteries that have not been stored. For modelling the Li-ion battery voltage drop, we use functional data analysis techniques since we analyse high-frequently measured data with negligible measurement error, i.e., the data evinces the functional character.

References:

[1] Kokoszka, P. and Reimherr, M.: *Introduction to functional data analysis.* CRC press, 2017.

[2] Prochazka, P., Knobloch, J., Cervinka, D., Kadlec, J., Cipin, R. and Pazdera, I.: Communication and Energy Management System of Small Electric Airplane. *Mechatronika* **2014**.

[3] Ramsay, J. O. and Silverman, B.W.: *Functional data analysis.* Springer, New York, 2. edition, 2005.

Existence and Multiplicity of Solutions of the Linear Boundary Value Problem for the Stieltjes Differential Equation

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This is a joint work with Alberto Cabada and F. Adrián F. Tojo (Departamento de Estatística, Análise Matemática e Optimización, Universidade de Santiago de Compostela, Spain).

We investigate a first order non-linear boundary value problem

$$u_g'(t) + b(t)u(t) = f(t, u(t)), \quad t \in [0, T]$$

with linear boundary conditions

$$u(0) = u(T) + k\, B(u),$$

where k is a real constant and B is a linear functional. Note that boundary conditions extend the periodic case.

We use techniques from Stieltjes calculus and fixed point index theory to show the existence and multiplicity of solutions.

Multiobjective Optimization of an Axial Pump

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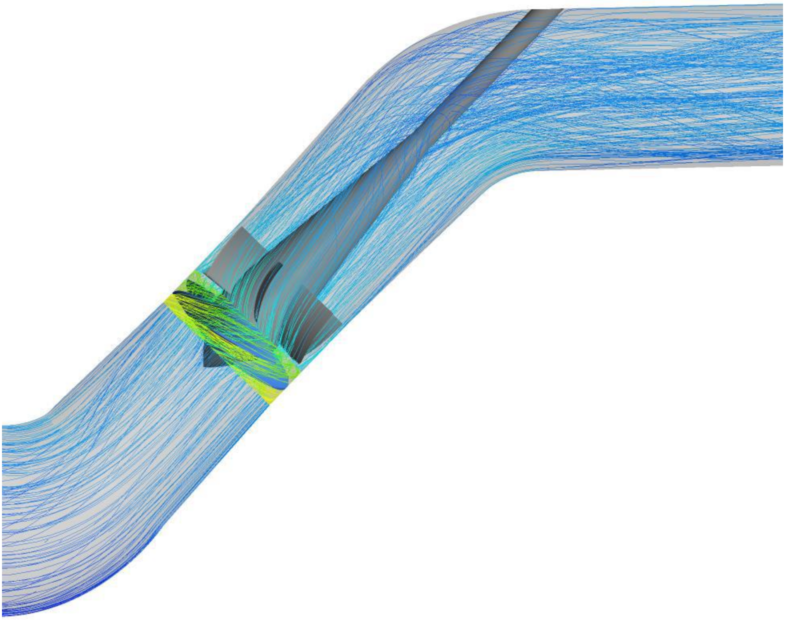
This article deals with a multiobjective optimization of an axial pump. Parametric model of the pump geometry was created using ANSYS CFX tools and Python scripts. It is a very complex and computationally expensive problem, as some of the objective functions are based on numerical simulations, and some are difficult to formulate properly. The text is focused on practical problems and discussion related to application of (multiobjective)optimization for hydraulic design.



References:

[1] Guelich, Johann. (2015). Centrifugal Pumps. 10.1007/978-3-642-40114-5.

[2] Krátký, T. 2020. "Shape optimization of hydraulic surfaces of the impeller and stator parts of hydrodynamic pumps." PhD diss., Palacký University Olomouc, 55-72

[3] Regis, R., Shoemaker. C.: Parallel Stochastic Global Optimization Using Radial Basis Functions. *INFORMS Journal on Computing* **vol. 21** (2009), 411–426.

Prediction Sets for Sparse Functional Data: How to Fail It and How to Fix It

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We revisit the classic situation in functional data analysis in which data items such as curves are observed at discrete (possibly sparse and irregular) arguments with observation noise (see [1] or [2]). We focus on the reconstruction of individual curves, especially on prediction intervals and prediction bands for them. The standard approach is to proceed in two steps: First, one estimates the mean and covariance function of curves and observation noise variance function by smoothing techniques such as penalized splines. Second, under Gaussian assumptions, one derives the conditional distribution of a curve given its noisy discrete observations and constructs prediction sets with required properties (usually employing sampling from the predictive distribution).

This approach is indeed well established, commonly used and theoretically valid but practically, it surprisingly fails in its key property: prediction sets constructed this way often do not have the required coverage. The actual coverage is lower than the nominal one. This has been little reported and studied in the literature, with the exception of [3]. We investigate the cause of this issue and propose a remedy that leads to prediction regions with the right coverage and is computationally feasible.

References:

[1] Staniswalis, JG, Lee, JJ: Nonparametric Regression Analysis of Longitudinal Data. *J. Amer. Statist. Assoc.* **93**, 444 (1998), 1403–1418.

[2] Yao, F, Müller, HG, Wang, JL: Functional Data Analysis for Sparse Longitudinal Data. *J. Amer. Statist. Assoc.* **100**, 470 (2005), 577–590.

[3] Goldsmith, J, Greven, S, Crainiceanu, C: Corrected Confidence Bands for Functional Data Using Principal Components. *Biometrics* **69** (2013), 41–51.

Matching of 3D Surfaces Using Approximations of Wasserstein Distance

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Archival survey data are essential resources for historians, archaeologists, geographers, and other researchers interested in understanding the past. These data contain valuable information about the landscape, infrastructure, and settlements of past societies, which can help researchers reconstruct historical events and processes. However, archival survey data can also be prone to errors due to the limitations of data storage methods.

One common error in archival survey data is related to the data storage method itself. In many cases, survey data is stored in the form of a graphic sign on a map. However, the accuracy of archival topographic maps is often insufficient due to factors such as map scale and human fatigue during fieldwork. This can result in errors in the location of points as compared to their coordinates given in archival documentation.

In this presentation, we aim to determine the magnitude of such errors using unique documentation that includes both point coordinates and topographical descriptions. To address this issue, we approach it mathematically by comparing surfaces. We discretize both surfaces and treat them as discrete measures, using the Wasserstein distance as our primary tool.

The Wasserstein distance, also known as Monge-Kantorovich-Rubinstein distance, earth-mover's distance, or optimal transport distance, is a natural way to compare measures. It can be useful when transporting goods between producers and consumers, where the spatial distribution of each is modeled by probability measures. By using the Wasserstein distance, we can measure the difference between the true coordinates of a point and the coordinates as read from the map.

We compare two methods for matching discrete probability measures. The first method is the 1D Gromov-Wasserstein metric, which is related to the assignment problem. The assignment problem is a combinatorial optimization problem in which we want to assign a set of objects to another set of objects, minimizing the total cost of the assignments. The 1D Gromov-Wasserstein metric allows us to compare the two measures by finding the optimal assignment between them.

For the second method, we use linear optimization methods. Linear optimization is a mathematical technique for optimizing a linear objective function subject to linear constraints. In our case, we use linear optimization to minimize the Wasserstein distance between the two measures.

Our research offers a new perspective on analyzing archival survey data, and may have implications for improving accuracy in related fields. By using mathematical methods to measure the error in archival survey data, we can gain a deeper understanding of the limitations of these data and develop new techniques for improving their accuracy

Buckling of the Gao Beam

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In this contribution we analyze static buckling problem for the nonlinear beam model which was firstly introduced in 1996 by D.Y. Gao. The vertical load is omitted here, i.e. only pure buckling problems are considered. Using mathematical methods, new results regarding the post-buckling solution are presented, particularly the existence and number of solutions. The determination of the relationship between the classical Euler critical load and the corresponding critical load of the Gao beam is also important. Some computational results are introduced for fixed axial loading. Finally, we discuss the effect of input parameters on the results, which leads to interesting observations.

References:

[1] Gao, D.Y.: Nonlinear elastic beam theory with application in contact problems and variational approaches. *Mechanics Research Communications* **23**, 1 (1996), pp. 11–17.

[2] Machalová, J., Netuka, H.: Bending of a nonlinear beam reposing on an unilateral foundation. *Applied and Computational Mechanics* **5**, 1 (2011), pp. 45–54.

[3] Machalová, J., Netuka, H.: Solution of Contact Problems for Gao Beam and Elastic Foundation. *Mathematics and Mechanics of Solids*, Special Issue on Inequality Problems In Contact Mechanics, **23**, 3 (2018), pp. 473–488.

[4] Machalová, J., Netuka, H.: Post-buckling solution for nonlinear beam developed by D.Y. Gao. *Proceedings of the conference SNA'23, Ostrava*, January 23 - 27, 2023, (editors J. Starý, S. Sysala, D. Sysalová), Institute of Geonics of the CAS, pp. 48–51.

Recent Advances in Functional Data Analysis Using Machine Learning Techniques

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Artificial intelligence and machine learning have been steadily on the rise during the past decade. These methods usually offer a number of advantages over traditional statistical approaches, such as being better equipped to handle high-dimensional data, non-linearity, and providing a way to capture complex interactions between variables to such an extent as engineering features.

Number of recent papers have delved into exploring the potential of adapting and applying machine learning algorithms for functional data. We understand functional data as essentially continuous, often represented as curves or surfaces instead of individual data points. Research in this area has so far been focused mostly on estimation of the mean function [1], covariance [2], or simple classification of dense non-problematic functional data [3].

A natural progression could be to use these highly scalable models for solving more complex tasks such as regression or classification of models based on functional inputs and outputs. Application of these methods to sparse functional data is also largely unexplored.

In this presentation we shall explore the fundamental advantages of artificial intelligence which makes it a powerful tool to be used in the analysis of functional data. Recent advances in this area will be presented and the future of this emerging research area will be debated. Last but not least we will also delve into the disadvantages and shortcomings or the machine learning approach both in general and in functional data analysis setting. We will briefly explore the topic of somewhat controversial artificial intelligence explainability, transparency and ethics.

References:

[1] Wang, S., Cao, G., Shang, Z., and Initiative, A. D. N. Estimation of the mean function of functional data via deep neural networks. *Stat*, **10(1)**. (2021):e393.

[2] Sarkar, S. and Panaretos, V. M. Covnet: Covariance networks for functional data on multidimensional domains. *Journal of the Royal Statistical Society Series B: Statistical Methodology*, **84(5)**. (2022):1785–1820.

[3] Rossi, F. and Villa, N. Support vector machine for functional data classification. *Neurocomputing*, **69(7-9)**. (2006):730–742.

Bohl-Marek Formulation of the Nonlinear System of ODEs for a Class of Mathematical Models With Conservation Laws

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Our study presents an application of one special technique, further called the Bohl-Marek formulation, related to the mathematical modeling of biochemical networks with mass conservation properties.

Nonlinear cooperative systems possessing certain conservation laws, arising frequently in biology and chemistry, were studied by Erich Bohl and Ivo Marek in different papers [1], [2]. The conservation law guarantees a lot of mathematical properties, e.g. the existence and uniqueness results, the positivity of the solutions (for positive inputs), periodicity and controllability, or proposing a stability theorem. These properties are consequence of the fact that the underlying nonlinear dynamical systems describing a class of biochemical networks are built up of linear evolutions with negative M-matrices whose entries depend on the dynamical variables of the other subsystems involved. Thus, the nonlinearity of the whole system is created via this dependence, i.e., the matrix of the complete system is blockwise diagonal.

On a case study, namely the Michaelis-Menten enzyme-catalyzed reaction with a substrate transport chain [3], we show how to transform the system of nonlinear ODEs into a set of smaller, quasi-linear subsystems of ODEs with negative M-matrices. For the two model formulations, the classical nonlinear formulation and the quasi-linear Bohl-Marek formulation, we determine and compare the results and show the computational advantages of the latter formulation.

References:

[1] Bohl, E., Marek, I.: Input-output systems in biology and chemistry and a class of mathematical models describing them. *Applications of Mathematics* **50.** (2005), 219–245.

[2] Marek, I.: On a Class of Stochastic Models of Cell Biology: Periodicity and Controllability. *In: Bru, R., Romero-Vivó, S. (eds): Positive Systems. Lecture Notes in Control and Information Sciences* **389.** (2009), 359–367.

[3] Matonoha, C., Papáček, Š., Lynnyk, V.: On an optimal setting of constant delays for the D-QSSA model reduction method applied to a class of chemical reaction networks. *Applications of Mathematics* **67.** (2022), 831–857.

Explainable Multivariate Outlier Detection Based on Shapley Values

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Multivariate outlier detection poses a topic of unabated popularity in statistics and computer science. We aim to detect outlying observations and explain which coordinates cause the outlyingness by decomposing the squared Mahalanobis distance of an observation into outlyingness contributions originating from individual variables. Those additive outlyingness scores are obtained using the Shapley value, a well-known concept from cooperative game theory that became popular in the field of Explainable AI. This concept can also be related to the cellwise contamination setting, where Shapley values can be employed to obtain variable contributions for outlying observations with respect to their "expected" position given the multivariate data structure. Shapley values for multivariate outlier explanation are based on the squared Mahalanobis distance, and it is shown that they can be calculated at a low numerical cost, making them an even more attractive tool. Simulations and real-world data examples illustrate the effectiveness of these concepts.

References:

[1] Shapley, L.S: A value for n-person game. *Contributions to the Theory of Games* **2.** (1953), 307–317.

[2] Lundberg, S.M., Lee, S.I.: A unified approach to interpreting model predictions. *Advances in Neural Information Processing Systems* **30.** (2017), 4765–4774.

[3] Mayrhofer, M. and Filzmoser, P.: Multivariate outlier explanations using Shapley values and Mahalanobis distances. *arXiv:2210.10063* (2022).

[4] Alqallaf, F., Van Aelst, S., Yohai, V.J., Zamar, R.H.: Propagation of outliers in multivariate data. *The Annals of Statistics* **37.** (2009), 311–331.

Data Mining Methods in Value Stream Mapping

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Value stream mapping is a lean manufacturing tool that tries to analyze and evaluate specific work processes in a manufacturing operation. This tool is used primarily to identify, demonstrate and decrease waste, as well as create flow in the manufacturing process. Value stream mapping can be made merely using paper and pencil, but modern mathematical models and data mining techniques might be beneficial and bring a potential advantage in practice. Although value stream mapping is often associated with manufacturing, it is also used in logistics, supply chain, service related industries, health care, software development, product development, and administrative and office processes.

This contribution introduces mathematical methods for value stream mapping and presents their advantages to standard techniques (current state and future state). We will discuss methods for time series modeling, estimation of distributions of underlying characteristics, and regression modeling. Finally, we will use multi-dimensional OLAP cubes and tools from business intelligence. All the above methods help to remove or reduce waste in value streams, thereby increasing the efficiency of a given value stream. Waste removal is intended to increase productivity by creating leaner operations which in turn make waste and quality problems easier to identify.

Identification of Important Pairwise Logratios in Compositional Data Employing Sparse Principal Component Analysis

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Compositional data are data that carry relative information as their elemental information is contained in the pairwise logratios of the parts that constitute the composition. While pairwise logratios are typically easy to interpret, the number of such possible pairs to consider quickly grows, thereby leading to a potentionally exhaustive analysis even for medium-sized compositions. Sparse principal component analysis (PCA) therefore forms an appealing tool to identify important pairwise logratios, and in turn, the important parts in the composition. To this end, we apply the sparse PCA of [1] to the possibly high-dimensional matrix of all pairwise logratios. The L1 penalty in the optimization problem serves as tradeoff bethween explained variability and sparsity in the loadings of the pairwise logratios.

The procedure is demonstrated on both simulated and empirical (geochemical) data sets. To aid practitioners in the discovery of important pairwise logratios, we introduce three practical visualization tools that (i) balance between the explained variability and sparsity of the model, (ii) show the stability of pairwise logratios, and (iii) highlight the importance of each particular parts in the composition.

References:

[1] Erichson, N. B., Zheng, P., Manohar, K., Brunton, S. L., Kutz Nathan, J. and Aravkin, A. Y.: Sparse principal component analysis via variable projection. *SIAM Journal on Applied Mathematics* **vol. 80**, 2(2020), 977–1002.

Gao Beam: Thirteen Years After

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It was 2010 when we first encountered an article describing a nonlinear beam model invented by David Yang Gao [1]. This model impressed us especially with its simplicity and the fact that it gives results comparable to the classical Euler–Bernoulli model – essentially, it represents a mildly nonlinear extension of it. The next year we published our first paper which deals with the Gao beam resting on the Winkler foundation [2]. In the following years, we gradually worked on the issue of convex problems, including the contact of the beam with a deformable foundation, e.g. [3].

Here we want to provide an overview of our research, focusing on the latest results from the critical analysis of the Gao model and taking into account our latest works relating to the buckling phenomenon [4] which represents, from the mathematical point of view, nonconvex problem. The issue of buckling itself will be presented in more detail in a special talk.

References:

[1] Gao, D.Y.: Nonlinear elastic beam theory with application in contact problems and variational approaches. *Mechanics Research Communications*, 23 (1), pp. 11–17, 1996.

[2] Machalová, J., Netuka, H.: Bending of a nonlinear beam reposing on an unilateral foundation. *Applied and Computational Mechanics*, 5(1), pp. 45–54, 2011.

[3] Machalová, J., Netuka, H.: Solution of Contact Problems for Gao Beam and Elastic Foundation. *Mathematics and Mechanics of Solids*, Special Issue on Inequality Problems In Contact Mechanics, Vol. 23, Issue 3, pp. 473–488, 2018.

[4] Machalová, J., Netuka, H.: Post-buckling solution for nonlinear beam developed by D.Y. Gao. *Proceedings of the conference SNA'17, Ostrava*, January 23 - 27, 2023, (editors J. Starý, S. Sysala, D. Sysalová), pp. 48–51, Institute of Geonics of the CAS, 2023.

Minimum Regularized Covariance Trace Estimator and Outlier Detection for Functional Data

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Outlier detection is a big part of functional data analysis as it is crucial to find atypical curves to prevent bias in subsequent analysis. In this paper we propose a new method for finding irregular functional data, the minimum regularized covariance trace estimator. It searches for a subset of the data for which the standardization results in the covariance with minimal trace. This framework includes inverting the singular covariance operator by the Tikhonov regularization. The proposed iterative algorithm consists of concentration steps in which the dissimilarity is based on a functional Mahalanobis distance defined on the reproducing kernel Hilbert space. Furthermore, the selection of the Tikhonov regularization parameter is automated. The method converges fast in practice and performs favorably when compared to other functional outlier detection methods.

References:

[1] Berrendero, J. R., Bueno-Larraz, B., and Cuevas, A.: On Mahalanobis distance in functional settings. *Journal of Machine Learning Research* **21.**, 9 (2020), 1–33.

[2] Mas, A.: Weak convergence in the functional autoregressive model. *Journal of Multivariate Analysis* **98.**, 6 (2007), 1231–1261.

[3] Rousseeuw, P. J. and Driessen, K.: A fast algorithm for the minimum covariance determinant estimator. *Technometrics* **41.**, 3 (1999), 212–223.

On the D-QSSA Method With Optimal Constant Delays Applied to a Class of Mathematical Models

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The existence of the fast/slow phenomena in (bio)chemical reaction systems represents difficulties for numerical simulation. However, it provides opportunities to reduce the system order. A well-known example of a classical model reduction method is the so-called quasi-steady-state approximation (QSSA) method, usually applied to a system of ODEs describing chemical reaction networks where one or more reactions are so fast that a quasi-steady-state for some species concentration is reached almost instantaneously.

In this contribution, we develop and test a novel model reduction method, the delayed quasi-steady-state approximation (D-QSSA) method, which was first proposed by Vejchodský [1], [2] and further developed by Matonoha and Papáček [3]. While Vejchodský *et al.* developed their method for the generally *time-dependent delays*, we newly analyzed theoretical and numerical issues related to the existence and setting of *constant delays* in some sense optimal. As a numerical case study, we took the paradigmatic example of the Michaelis-Menten kinetics with a simple transport process. The results of the comparison of the full non-reduced system behavior with nine respective variants of reduced models are discussed.

References:

[1] Vejchodský, T., Erban, R., Maini, P.K.: Reduction of chemical systems by delayed quasi-steady state assumptions. *arXiv preprint*, arXiv:1406.4424 (2014).

[2] Vejchodský, T.: Accurate reduction of a model of circadian rhythms by delayed quasi-steady state assumptions. *Math. Bohem.* **139** (2014), 577–585.

[3] Matonoha, C., Papáček, Š., Lynnyk, V.: On an optimal setting of constant delays for the D-QSSA model reduction method applied to a class of chemical reaction networks. *Applications of Mathematics* **67.** (2022), 831–857.

Phase Measuring Deflectometry – Measurement Uncertainty by Cramér – Rao Inequality

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Phase measuring deflectometry (PMD) is an accurate method to measure the shape of objects with specular (mirrorlike) surfaces. The word "deflection" means the act of changing or causing something to change direction [1]. In the case of the described measurement method, the specular surface changes the direction of incident light rays, which is used to measure the shape of the object [2]. An array of fringes with sinusoidally varying intensity is used as a light source. The measurement of the phase of the sinusoidal waveform determines the deviation of the light ray. The advantages of PMD are full-field measurement, large dynamic range, fast data acquisition, and low measurement uncertainty. An important advantage is that PMD is able to measure the shape of both small and large objects. The principle of PMD is as follows: A screen with an incoherently radiating sinusoidal fringe pattern is observed by a camera. The surface of the measured object serves as a mirror. The camera is focused on the measured object and not on the screen with fringe pattern. Because the camera is focused on the surface of the measured object, the captured sinusoidal pattern is defocused. If the surface of the measured object is curved, the image of the fringes is distorted. From the defocused and distorted image of the fringes it is possible to determine the shape of the object. The captured fringe pattern is evaluated, and the quantitative phase values are retrieved with well-developed fringe analysis algorithms. PMD (like other deflectometry methods) measures in principle the local slope of the surface. Mathematically, it is the derivative of the surface function with respect to the lateral coordinates. The shape of the object can be calculated from the measured slope values using integration. Our aim is to determine the measurement uncertainty of PMD. A suitable tool is the Cramér–Rao inequality [3]. It shows that the measurement uncertainty is expressed in the form of an uncertainty product. The factors of the product are the angular uncertainty and lateral resolution. The magnitude of the uncertainty product depends on the mean wavelength of the light used and the number of photons detected.

References:

[1] *Encyclopedia Britannica*, available at , (March 5, 2023).

[2] Knauer, M. C., Kaminski, J., Häusler, G.: Phase measuring deflectometry: a new approach to measure specular free-form sufaces. *Proc. SPIE 5457*, (2004) 366-376.

[3] Nobach, H.: Cramér-Rao lower bound (CRLB), in *Laser Doppler and Phase Doppler Measurement Techniques*, Albrecht, H. –E., Borys, M., Damaschke, N., Tropea, C. eds. (Springer, 2003), 290–300.

Distributional Principal Component Analysis With Application to Particle Size Distributions

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Particle or grain size distributions often play an important role in understanding processes in geosciences. Functional data analysis allows applying multivariate methods like principal components and discriminant analysis directly to such distributions. These are however often observed in the form of samples, and thus with a sampling error, i.e. each data point is a distribution, but one where the sampling error is present. This additional sampling error changes the properties of the multivariate variance and thus the relevance and direction of the principle components. The result of the principal component analysis becomes an artefact of the sampling error and can negatively affect the following data analysis. Our contribution presents how to compute this sampling error and how to confront it in the context of principal component analysis. We demonstrate the effect of the sampling error and the effectiveness of the correction with a simulated dataset. We show how the interpretability and reproducibility of the principal components improve and become independent of the selection of the basis. We also demonstrate how the correction improves interpretability of the results on a grain size distribution dataset from river sediments.

Stochastic Modelling Based on Diffusion and Jump Processes

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We will show some examples of stochastic modelling based on diffusion and jump processes inspired by our previous and current work.

Homogenization of Compressible Navier–Stokes–Fourier System in Domains with Tiny Holes

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We consider the compressible Navier–Stokes–Fourier system in a domain with large number of holes. Under the assumption that the holes are sufficiently small, together with certain standard assumptions on the adiabatic exponent and the behaviour of the heat conductivity, we show that if passing simultaneously with the number of holes to infinity and their size to zero, in the limit we obtain again a solution to the compressible Navier–Stokes–Fourier system in the domain without holes.

References:

[1] Oschmann, F., Pokorný, M.: Homogenization of the unsteady compressible Navier–Stokes equations for adiabatic exponent $\gamma > 3$. ArXiv:2302.13789 (2023).

[2] Pokorný, M., Skříšovský, E.: Homogenization of the evolutionary compressible Navier–Stokes–Fourier system in domains with tiny holes. *J. Elliptic Parabol. Equ.* **7** (2021), 361–391.

Detecting Local Outliers Using the Spatially Smoothed MRCD Estimator

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Many methods are available for multivariate outlier detection but until now only a hand full are developed for spatial data where there might be observations differing from their neighbors, so-called local outliers. There are methods based on a pairwise Mahalanobis distance approach, however the type of the covariance matrices used is not yet agreed upon and covers only a global covariance (Filzmoser et al. (2013)) and a very local covariance structure (Ernst and Haesbroeck (2016)), more precisely one covariance estimation per observation.

To bridge the gap between the global and local approach by providing a refined covariance structure we develop spatially smoothed robust and regular covariance matrices based on the MRCD estimator (Boudt et al. (2020)) for pre-defined neighborhoods. As well known from the MCD literature, a subset of observations, the so-called H-set, is obtained by optimizing an objective function. In our case we obtain a set of optimal H-sets from minimizing an objective function which is based on a linear spatial smoothing design of local covariance matrices.

A heuristic algorithm based on the notion of a C-step is developed to find the optimal set of H-sets which also shows stable convergence properties in general. We demonstrate the applicability of the new covariance estimators and the importance of a compromise between locality and globality for local outlier detection with simulated and real world data including measurements of Austrian weather stations and further compare the performance with other state-of-the-art methods from statistics and machine learning.

This project has received funding by the European Commission within the Horizon 2021 programme under grant agreement ID 101057741.

References:

[1] Filzmoser, P., Ruiz-Gazen, A., and Thomas-Agnan, C.: Identification of local multivariate outliers. *Statistical Papers* **55**, (2013), 29–47.

[2] Ernst, M. and Haesbroeck, G.: Comparison of local outlier detection techniques in spatial multivariate data. *Data Mining and Knowledge Discovery* **31** (2016), 371–399.

[3] Boudt, K., Rousseeuw, P. J., Vanduffel, S., and Verdonck, T.: The minimum regularized covariance determinant estimator. *Statistics and Computing* **30** (2020), 113–128.

Order Determination for Tensor-valued Observations Using Data Augmentation

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Tensor-valued data benefits greatly from dimension reduction as the reduction in size is exponential in the number of modes. To achieve maximal reduction without loss in information, our objective in this work is to give an automated procedure for the optimal selection of the reduced dimensionality. Our approach combines a recently proposed data augmentation procedure with the higher-order singular value decomposition (HOSVD) in a tensorially natural way. We give theoretical guidelines on how to choose the tuning parameters and further inspect their influence in a simulation study. As our primary result, we show that the procedure consistently estimates the true latent dimensions under a noisy tensor model, both at the population and sample levels. Additionally, we propose a bootstrap-based alternative to the augmentation estimator. Simulations are used to demonstrate the estimation accuracy of the two methods under various settings.

References:

[1] L. De Lathauwer, B. De Moor, and J. Vandewalle: A multilinear singular value decomposition. *SIAM Journal on Matrix Analysis and Applications* **21.**, 9 (2020), 1253–1278.

[2] W. Luo and B. Li: On order determination by predictor augmentation. *Biometrika* **108.**, 3 (2021), 557–574.

[3] U. Radojičić, N. Liétzen, K. Nordhausen, and J. Virta: Dimension estimation in two-dimensional PCA. *12th International Symposium on Image and Signal Processing and Analysis (ISPA)*, 6 (2021), 16–22.

Parameter Identification for Gao Beam and Foundation

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Identification problem involves the determination of unknown parameters in many practical applications. Using experimentally measured data, the goal of this problem is to identify parameters of the considered model that are not known.

This contribution deals with the identification of the coefficients representing material properties of the nonlinear Gao beam in contact problems. In the case of a deformable foundation, the foundation modulus can also be identified. For identification, an optimal control approach is used together with an appropriate least squares cost functional. The unknown material coefficients play the role of control variables. The presented theory is completed by several illustrated numerical examples.

References:

[1] Gao, D. Y.: Nonlinear elastic beam theory with application in contact problems and variational approaches. *Mechanics Research Communications* **23**, 1 (1996), 11–17.

[2] Machalová, J., Netuka, H.: Control variational method approach to bending and contact problems for Gao beam. *Applications of Mathematics* **62**, 6 (2017), 661–677.

[3] Machalová, J., Netuka, H.: Comments on the large deformation elastic beam model developed by D.Y. Gao. *Mechanics Research Communications*, **110**, (2020), 103607.

[4] Radová, J., Machalová, J., Burkotová, J.: Identification problem for nonlinear Gao Beam. *Mathematics* **8**, 11 (2020), 1916.

Lagrangian Duality for Nonconvex Optimization Problems

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We investigate Lagrangian duality for nonconvex optimization problems in spaces without linear structure. To this aim we use the Φ-convexity theory and minimax theorem for Φ-convex functions. We provide conditions for zero duality gap.

References:

[1] E. Bednarczuk, M. Syga, Lagrangian duality for optimization problems in spaces without linear structure, *preprint*

Different Approaches in the Shape Index Calculation on a Human Face

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A human face, captured by stereo-photogrammetry, is characterised by about 100,000 points. These points are triangulated by about 200,000 triangles. In order to perform further statistical analysis of the surface of the human face, based on the automatic identification of several anatomical and geodetical curves, we need to clean and smooth the raw data, and perform remeshing of a triangulated surface.

Our goal is to calculate the shape index (SI), a measure of local surface topology, which is done by using several different standard linear statistical models (LM) and ridge regression models (RM) of z coordinates on x and y coordinates. In both cases (LM, RM), the models of different order were used, i.e. quadratic, cubic and quartic, with the interaction of x and y in every case, and with and without an intercept. The estimates of regression coefficients related to the quadratic terms and their interaction are elements of the Weingarten matrix from which the principal curvatures (and subsequently SI) are calculated.

LM and RM are applied on a sufficiently large neighbourhood of all surface points in a local 3D coordinate system. The goodness of fit is measured by (adjusted) coefficients of determination. Since, in some cases, the results may not be satisfactory, the additional smoothing of SI itself is applied.

The results are compared numerically and graphically with static images of the human face in different views, i.e. frontal, lateral and vertical. All statistical analyses and visualisations are performed in R.

Acknowledgement: The work of S.K. and V. Š. was supported by the Grant Agency of the Masaryk University, Project No. MUNI/A/1132/2022. The work of S.K. was also supported by a Wellcome Trust grant (WT086901MA) to the Face3D research consortium Face3D.

References:

[1] Bowman, A., Katina, S., Smith, J., Brown, D.: Anatomical curve identification. *Computational Statistics and Data Analysis* **86(6)**, 2015, 52–64.

[2] Katina, S. et al.: The definitions of three-dimensional landmarks on the human face: an interdisciplinary view. *Journal of Anatomy* **228(3)**, 2016, 355–365.

[3] Vittert, L., Bowman, A., Katina, S.: A hierarchical curve-based approach to the analysis of manifold data. *Annals of Applied Statistics* **13(4)**, 2020, 2539–2563.

[4] Katina S, Vittert L, Bowman A.: Functional data analysis and visualisation of three-dimensional surface shape. *Journal of the Royal Statistical Society Series C: Applied Statistics.* **70(3)**, 2021, 691–713.

Bivariate Compositional Splines for Representation of Density Functions

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Multivariate densities occur naturally as result of aggregation of massive data in many applications and they are used to analyze the association structure as well as to further process them using methods of functional data analysis. Accordingly, proper spline (continuous) representation of the input discrete data (e.g. in form of histograms) is crucial for their statistical analysis.

Bayes Hilbert spaces methodology enables to capture specific properties of probability density functions and to construct so-called compositional splines which respect their decomposition into interactive and independent parts [1]. Using the centered log-ratio (clr) transformation, the original densities (as well as compositional splines) can be represented in the standard L^2 space by ZB-spline representation. The resulting spline functions fulfill zero-integral constraint, which must be taken into account already when building the basis of the ZB-spline representation. Hereby, either the standard B-spline basis with implemented zero-integral constraint by following [1, 2] can be used, or spline representation is constructed using the ZB-spline basis, which satisfies the zero-integral constraint automatically [3]. In the contribution we focus on the latter case, provide a detailed simulation study and apply the resulting spline representation for descriptive analysis of geochemical density data.

References:

[1] Hron K., Machalová J., Menafoglio A., Bivariate densities in Bayes spaces: orthogonal decomposition and spline representation. *Stat Papers.* https://doi.org/10.1007/s00362-022-01359-z

[2] Machalová J., Hron K., Monti G. S. (2016) Preprocessing of centred logratio transformed density functions using smoothing splines. *Journal of Applied Statistics* **43**, 8 (2016), 1419-1435

[3] Machalová J., Talská R., Hron K., Gába A. Compositional splines for representation of density functions. *Computational Statistics* **36**, 2 (2020), 1031-1064

Statistical Characteristics in Study of Structural Changes During Desiccation Stress of Plant Leaf by Speckle Effect

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The speckle effect occurs, for example, when laser light scatters after it is transmitted through a non-homogeneous transparent object [1]. The speckle pattern (a random distribution of dark and bright speckles) can then be observed on a screen behind the object. A temporal analysis of changes in the speckle pattern reveals the gradual structural changes of the object. Methods based on the speckle effect are commonly used in both the field of physics [2] and biology, where the dynamic processes on the surface of plant leaves exposed to various stresses may be disclosed [3]. Different indicators have been proposed for the temporal study of the speckle patterns, such as the mean, entropy, inertia moment, and generalized difference. The inertia moment estimates the global activity of the monitored plant tissue with a summary value; the rest indicators represent themselves as two-dimensional images. However, these indicators do not quantitatively analyse the local dynamic processes in the tested plant tissue. Therefore, we have proposed two statistical indicators based on standard deviation. They allow us to quantify the temporal progress of dynamic response both in the whole selected local region of the plant tissue and at different points of this region. Here we demonstrate structural changes occurring in the vascular bundle and mesophyll cells of the leaflet during its desiccation after the leaflet is detached from the maternal tomato plant. The temporal behaviour of the statistical indicators shows the opposite stress responses in the selected regions of the leaflet.

Acknowledgement: The authors gratefully acknowledge the support of the MEYS of the Czech Republic project No. CZ.02.1.01/0.0/0.0/17_049/0008422.

References:

[1] Dainty, J. C.: Laser Speckle and Related Phenomena, 2nd Edition. *Springer-Verlag*, Berlin, 1984.

[2] Smid, P., Horvath, P., Hrabovsky, M.: Speckle correlation method used to measure object's in-plane velocity. *Appl. Optics* **46**, 18 (2007), 3709–3715.

[3] Zhong, X., Wang, X., Cooley, N., Farrell, P., Moran, B.: Application of laser speckle pattern analysis for plant sensing. In: *Proc. SPIE* **8761**, 3rd International Conference on Photonics and Image in Agriculture Engineering (PIAGENG) - Image Processing and Photonics for Agricultural Engineering, Tan, H. ed., 2013, Article No. 876102.

Variable Selection in Restricted Regression Models

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The use of prior information in the linear regression is a well-known approach to provide more efficient estimators of regression coefficients. The methods of non-stochastic restricted regression estimation proposed by Theil and Goldberger (1961) are preferred when prior information is available. In this study, we aim to compare variable selection methods in a non-stochastic restricted linear regression model using popular variable selection techniques: Lasso, SCAD bridge and Elastic net. To evaluate the performance of these methods, we conduct a simulation study and present a real data example, analyzing their accuracy in variable selection, prediction, and model stability.

References:

[1] Fan, J., Li, R.: Variable selection via nonconcave penalized likelihood and its oracle properties.*Journal of the American statistical Association* **96**, 456 (2001), 1348-1360.

[2] Theil, H., Goldberger, A., S.: On pure and mixed statistical estimation in economics. *International Economic Review* **2**, 1 (1961), 65-78.

[3] Tibshirani, R:. Regression shrinkage and selection via the lasso. *Journal of the Royal Statistical Society: Series B (Methodological)* **58**, 1 (1996), 267-288.

[4] Zou, H., Trevor, H.: Regularization and variable selection via the elastic net. *Journal of the royal statistical society: series B (statistical Journal of the Royal Statistical Society: Series B (Methodological) methodology)* **67**, 2 (2005), 301-320.

Protein Intensity or Occurrence: Which of the Two Should be Used for Statistical Analyses in Animal Studies of Alzheimer's Disease?

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Alzheimer's disease (AD), the major cause of dementia, is a widespread neurodegenerative disease induced by misfolded protein tau [1]. The neurofibrillary degeneration significantly correlates with disease progression, thus a better understanding of the tau cascade represents an important target for potential therapeutic strategies in the clinical course of AD [2, 3].

In this study, we investigate and compare the protein expression in choroid plexus tissue from transgenic rodent models expressing human truncated tau with three microtubule-binding repeats (SHR24) and spontaneously hypertensive rats (SHR) used as controls. SHR24 line satisfied several key histological criteria typical for neurofibrillary degeneration in human AD, the rats developed tau pathology in the spinal cord and partially in the brainstem, and in the motor cortex.

Choroid plexus tissue was isolated from 4 to 14 months old rats (with 2 months step). Our data contain normalized abundances of 11 245 proteins in 52 animal samples [4]. Also the raw abundance, spectral count and other variables are included. 2209 proteins were identified by 3 or more peptides. On average a protein was identified by 9 peptides.

Data were analysed in R using multivariate statistical methods such as PCA for protein intensity and correspondence analysis for protein occurrence in order to find differences in protein expression between transgenic and control rats.

Acknowledgment: The work was supported (partly) by specific research of Masaryk University as support for student projects (MUNI/A/1132/2022).

References:

[1] Zilka N., Kazmerova Z., Jadhav S., et al.: Who fans the flames of Alzheimer's disease brains? Misfolded tau on the crossroad of neurodegenerative and inflammatory pathways. *Journal of Neuroinflammation 9*, **1** (2012), 1–9.

[2] Novak P., S Katina., et al. Safety and immunogenicity of the tau vaccine AADvac1 in patients with Alzheimer's disease: a randomised, double-blind, placebo-controlled, phase 1 trial. *The Lancet Neurology 16*, **2**, 123–134.

[3] Novak P., Kovacech B., Katina S., et al. ADAMANT: a placebo-controlled randomized phase 2 study of AADvac1, an active immunotherapy against pathological tau in Alzheimer's disease. *Nature Aging 1*, **6** (2021), 521–534.

[4] Levarska L., Zilka N., Jadhav S., et al.: Of rodents and men: the mysterious interneuronal pilgrimage of misfolded protein tau in Alzheimer's disease. *Journal of Alzheimer's Disease 37*, **3** (2013), 569–577.

Depth-based Detection and Classification of Outliers for Functional Data

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Functional data analysis has developed greatly in the last decade. In this contribution, we introduce a new procedure for detection of outliers among continuous functions on a compact domain $[0, 1]$ or $[0, 1]^d$. Special attention is paid to functions outlying not only in location but also in their shape.

The procedure is based on functional data depth, either integrated or infimal. It is an alternative to the outlier detection based on the Jth order depth suggested in [1]. The idea is to use one dimensional functional depth to function x "decomposed" to polynomials.

The suggested procedure is simple and computationally feasible. Moreover, it gives the information about the *order* of outlyingness, i.e., that a function is outlier in the sense of location, trend, convexity and so on.

References:

[1] Nagy, S., Gijbels, I. and Hlubinka, D.: Depth-based recognition of shape outlying functions. *Journal of Computational and Graphical Statistics* **26**, 4 (2017), 883–893.

Relative Energy Inequality and Weak-strong Uniqueness for an Isothermal Non-Newtonian Compressible Fluid

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Our presentation deals with three-dimensional nonsteady NavierStokes equations for non-Newtonian compressible fluids. We show how to derive the relative energy inequality for the weak solutions to these equations and how prove that the standard energy inequality implies the relative energy inequality. Consequently, the relative energy inequality allows us to achieve a weak-strong uniqueness result. In other words, we present that the weak solution of the Navier-Stokes system coincides with the strong solution emanated from the same initial conditions as long as the strong solution exists. For this purpose, a new assumption on the coercivity of the viscous stress tensor was introduced along with two natural examples satisfying it.

Straight-Line Errors-in-Variables Calibration Model

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We are considering the measurement model of linear comparative calibration which is from the point of view of mathematical statistics a nonlinear regression model of direct measurements. The measurement vectors are normally distributed random vectors, μ and ν are vectors of their mean values and are related by the equation $\nu = a\mathbf{1} + b\mu$. The covariance matrix of the model is a known positive definite matrix. We develop the mean value function of the model using Taylor expansion in appropriately chosen prior values μ_0,a_0,b_0 of the model parameters. In the case under consideration a linear-quadratic regression model of direct measurements is obtained with new parameters $\delta\mu, \delta a, \delta b$. This model is referred to us as a weakly nonlinear model [1]. We aim to determine the conditions under which the nonlinear regression model representing the straight-line calibration model can be treated as a conventional linear regression model. The influence of nonlinearity in the model is demonstrated by testing the consistency of a realization of the observation vector with the linearized version of the model. If the second-order terms in the Taylor expansion of the function of mean values are statistically nonsignificant, we get a linear regression model and linear methods can be applied. On the other hand, we recommend (in agreement with [2] and [4]) utilizing the Weighted Total Least Squares method for parameter estimation and covariance matrix determination, following the law of propagation of uncertainty. The Monte Carlo method [3] can be used as an alternative approach.
Acknowledgement: The project was supported by projects APVV-21-0216, SK-CZ-RD-21-0109, APVV-21-0195, VEGA 2/0096/21, VEGA 2/0023/22.

References:

[1] Kubáček L., Tesaříková, E.: *Weakly Nonlinear Regression Models.* Olomouc 2008.

[2] JCGM 100:2008 (GUM): *Evaluation of measurement data – Guide to the expression of uncertainty in measurement.* (2008).

[3] JCGM 101:2008 (GUM S1): *Evaluation of measurement data – Supplement 1 to the Guide to the expression of uncertainty in measurement – Propagation of distributions using a Monte Carlo method.* (2008).

[4] JCGM 102:2011 (GUM S2): *Evaluation of measurement data – Supplement 2 to the Guide to the expression of uncertainty in measurement.* (2011).

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