

Záznamy vložené do ASEP za UI (1. 2. – 28. 2. 2023)

New ICS records in ASEP (1. 2. – 28. 2. 2023)

0567877 - ÚI 2023 US eng J - Journal Article

[Fabián, Zdeněk](#)

A measure of variability within parametric families of continuous distributions.

Communications in Statistics - Theory and Methods. Online 11 January 2023 (2023). ISSN 0361-0926.

E-ISSN 1532-415X

Institutional support: RVO:67985807

Keywords : Scalar-valued score * score mean * score variance * distance in the sample space

OECD category: Statistics and probability

Impact factor: 0.863, year: 2021

Method of publishing: Open access

<https://dx.doi.org/10.1080/03610926.2022.2155792>

[DOI: 10.1080/03610926.2022.2155792](https://doi.org/10.1080/03610926.2022.2155792)

A new approach to theory of continuous probability distributions, based on scalar-valued score functions, offers the score mean as a finite typical value of distributions including the heavy-tailed ones. In the article, we define the score variance as a finite measure of variability of distributions with respect to the typical value and discuss its properties and methods of its estimation. By means of the square root of the score variance we introduce a generalized Rao distance in the sample space.

Permanent Link: <https://hdl.handle.net/11104/0339131>

0568726 - ÚI 2023 US eng J - Journal Article

[Martinková, Patrícia](#) - [Bartoš, František](#) - [Brabec, Marek](#)

Assessing Inter-rater Reliability With Heterogeneous Variance Components Models: Flexible Approach Accounting for Contextual Variables.

Journal of Educational and Behavioral Statistics. Online February 9 (2023). ISSN 1076-9986. E-ISSN 1935-1054

Grant - others: GA MŠk(CZ) LM2015042

Institutional support: RVO:67985807

Keywords : Bayesian inference * inter-rater reliability * mixed-effect models * heterogeneous variance components * grant peer review

Impact factor: 2.116, year: 2021

Method of publishing: Limited access

[DOI: 10.3102/10769986221150517](https://doi.org/10.3102/10769986221150517)

Inter-rater reliability (IRR), which is a prerequisite of high-quality ratings and assessments, may be affected by contextual variables, such as the rater's or ratee's gender, major, or experience.

Identification of such heterogeneity sources in IRR is important for the implementation of policies with the potential to decrease measurement error and to increase IRR by focusing on the most relevant subgroups. In this study, we propose a flexible approach for assessing IRR in cases of heterogeneity due to covariates by directly modeling differences in variance components. We use Bayes factors (BFs) to select the best performing model, and we suggest using Bayesian model averaging as an alternative approach for obtaining IRR and variance component estimates, allowing us to account for

model uncertainty. We use inclusion BFs considering the whole model space to provide evidence for or against differences in variance components due to covariates. The proposed method is compared with other Bayesian and frequentist approaches in a simulation study, and we demonstrate its superiority in some situations. Finally, we provide real data examples from grant proposal peer review, demonstrating the usefulness of this method and its flexibility in the generalization of more complex designs.

Permanent Link: <https://hdl.handle.net/11104/0339989>

0568776 - ÚI 2023 US eng J - Journal Article

Liczbińska, G. - Brabec, Marek - Gautam, R. K. - Jhariya, J. - Kumar, A.

From little girls to adult women: Changes in age at marriage in Scheduled Castes from Madhya Pradesh and Uttar Pradesh, India.

PLoS ONE. Roč. 18, č. 2 (2023), č. článku e0281506. ISSN 1932-6203. E-ISSN 1932-6203

Institutional support: RVO:67985807

Keywords : GAM * semiparametric statistical analysis * penalized splines

OECD category: Statistics and probability

Impact factor: 3.752, year: 2021

Method of publishing: Open access

<https://dx.doi.org/10.1371/journal.pone.0281506>

[DOI: 10.1371/journal.pone.0281506](https://doi.org/10.1371/journal.pone.0281506)

BACKGROUND: Research confirms the negative relationship between early marriage and mothers' and children's health outcomes. This is why studies of the changes in age at marriage are an important task from the point of view of the health status and well-being of a mother and her offspring, especially in groups represented by extremely disadvantaged social strata in India. The results of such studies may influence the future family planning policy in the country. **OBJECTIVES:** This study aims to investigate the trend of age at marriage among the Scheduled Castes (SCs) women from two Indian states: Madhya Pradesh and Uttar Pradesh relative to the level of education and also to socioeconomic changes in the states. These states manifest the highest proportion of girls getting married below the age of 18 years—far above the proportion observed in entire India. **METHODS:** Women from Scheduled Caste, N = 1,612, aged 25–65, born in 1950–1990 were investigated. A modern semiparametric regression approach was used. To capture the relationship between age at marriage and year of birth, categories of women's level of education (illiterate; primary: 1st–5th standards; middle school: 6th–8th standards; high school: 9th–10th standards; higher secondary: 11th–12th standards), and categories of the profession (women working in the agricultural sector or the non-agricultural sector), flexible framework of the Generalized Additive Model (GAM) was applied. **RESULTS:** A significant impact of the cohort defined by the year of birth (<0.001), and women's education (<0.001) on age at marriage was noted, while the influence of women's occupation was not significant ($p = 0.642$). Mean age at marriage differed significantly with different education level. Women who graduated from primary school married 0.631 years later on average than illiterate ones, while those who graduated from middle schools, high schools (9th–10th standards) and higher secondary schools married significantly later than illiterate ones by 1.454 years and 2.463 years, respectively. Age at marriage increased over time: from slightly above 15 years in the cohort of illiterate women born in 1950 to almost 19 years in quite well-educated women born in 1990. The average age at marriage estimated for four education levels in 1990 ranged between 16.39 years (95%CI: 15.29–17.50) in the group of illiterate women and 18.86 years (95%CI: 17.76–19.95) in women graduated from high and higher secondary schools. **CONCLUSION:** The rise of age at marriage can be partly explained by the increase of females enrolled in schools, the alleviation of poverty, and the implementation of social programs for women.

Permanent Link: <https://hdl.handle.net/11104/0340036>

0568761 - ÚI 2023 RIV NL eng J - Journal Article

Lehnert, M. - Pánek, J. - Kopp, J. - [Geletič, Jan](#) - Květoňová, V. - Jurek, M.

Thermal comfort in urban areas on hot summer days and its improvement through participatory mapping: A case study of two Central European cities.

Landscape and Urban Planning. Roč. 233, May 2023 (2023), č. článku 104713. ISSN 0169-2046. E-ISSN 1872-6062

Institutional support: RVO:67985807

Keywords : Urban climate * Heat stress * Citizen science * Mental map * GeoParticipation

OECD category: Meteorology and atmospheric sciences

Impact factor: 8.119, year: 2021

Method of publishing: Limited access

<https://dx.doi.org/10.1016/j.landurbplan.2023.104713>

[DOI: 10.1016/j.landurbplan.2023.104713](https://doi.org/10.1016/j.landurbplan.2023.104713)

With increasing urbanisation and climate change, citizens are more frequently exposed to heat stress. In the current pragmatists' discourse, efforts to adapt cities to deteriorating climate conditions should reflect not only the objective (physical) effects of the proposed measures, but also citizens' preferences, which influence the perception schemata and mental image of a place. This study employs the innovative approach of mental mapping, using an online survey to identify mental hotspots and coolspots in two Central European cities of Plzeň and Olomouc (Czechia). Map points and polygons, indicating locations thermally (un)comfortable to individual respondents, are combined into aggregate mental maps. Personal behavioural adaptation measures and citizens' preferences for measures ameliorating thermal discomfort in thermally uncomfortable areas are analysed. The results show that the most preferred measures for improving thermal comfort are trees and parks, and a combination of greenery with blue elements. Other measures, such as temporary greenery, green roofs and facades, exterior shading elements, water spraying and misting, and street sprinkling, are substantially less frequently proposed. However, there are spatial differences between the preferred measures. The character of mental coolspots confirms citizens' preferences for trees and parks and its synergy with blue elements and provides inspiration for positive change in (mental) hotspots. Moreover, the uneven spatial distribution of mental coolspots in the studied cities revealed neighbourhoods with few or no cooling opportunities in public areas.

Permanent Link: <https://hdl.handle.net/11104/0340026>

0568186 - ÚI 2023 CH eng J - Journal Article

Filip, P. - Kokošová, V. - [Valenta, Zdeněk](#) - Baláž, M. - Mangia, S. - Michaeli, S. - Vojtíšek, L.

Utility of quantitative MRI metrics in human brain ageing research.

Frontiers in Aging Neuroscience. Accepted February 2023 (2023). ISSN 1663-4365. E-ISSN 1663-4365

R&D Projects: GA MŠk(CZ) LM2018129

Institutional support: RVO:67985807

Keywords : Ageing * quantitative MRI * relaxometry * diffusion weighted imaging * resting-state functional MR

Impact factor: 5.702, year: 2021

Method of publishing: Open access

The advent of new, advanced quantitative MRI metrics allows for in vivo evaluation of multiple biological processes highly relevant for ageing. The presented study combines several MRI parameters hypothesised to detect distinct biological characteristics as myelin density, cellularity, cellular membrane integrity and iron concentration. 116 healthy volunteers, continuously distributed over the whole adult age span, underwent a multi-modal MRI protocol acquisition. Scatterplots of individual MRI metrics revealed that certain MRI protocols offer much higher sensitivity to early adulthood changes while plateauing in higher age (e.g. global functional connectivity in cerebral cortex or orientation dispersion index in white matter), while other MRI metrics provided reverse ability – stable

levels in young adulthood with sharp changes with rising age (e.g. T1p and T2p). Nonetheless, despite the previously published validations of specificity towards microstructural biology based on cytoarchitectonic maps in healthy population or alterations in certain pathologies, several metrics previously hypothesised to be selective to common measures failed to show similar scatterplot distributions, pointing to further confounding factors directly related to age. Furthermore, other metrics, previously shown to detect different biological characteristics, exhibited substantial intercorrelations, be it due to the nature of the MRI protocol itself or co-dependence of relevant biological microstructural processes. All in all, the presented study provides a unique basis for the design and choice of relevant MRI parameters depending on the age group of interest. Furthermore, it calls for caution in simplistic biological inferences in ageing based on one simple MRI metric, even though previously validated under other conditions. Complex multi-modal approaches combining

Permanent Link: <https://hdl.handle.net/11104/0339519>

0568306 - ÚI 2023 RIV CH eng J - Journal Article

Korel, L. - Yorsh, U. - Behr, A. S. - Kockmann, N. - [Holeňa, Martin](#)

Text-to-Ontology Mapping via Natural Language Processing with Application to Search for Relevant Ontologies in Catalysis.

Computers. Roč. 12, č. 1 (2023), č. článku 14. ISSN 2073-431X

Institutional support: RVO:67985807

Keywords : text representation learning * text classification * text preprocessing * text data * ontology

OECD category: Computer sciences, information science, bioinformatics (hardware development to be 2.2, social aspect to be 5.8)

Method of publishing: Open access

DOI: [10.3390/computers12010014](https://doi.org/10.3390/computers12010014)

The paper presents a machine-learning based approach to text-to-ontology mapping. We explore a possibility of matching texts to the relevant ontologies using a combination of artificial neural networks and classifiers. Ontologies are formal specifications of the shared conceptualizations of application domains. While describing the same domain, different ontologies might be created by different domain experts. To enhance the reasoning and data handling of concepts in scientific papers, finding the best fitting ontology regarding description of the concepts contained in a text corpus. The approach presented in this work attempts to solve this by selection of a representative text paragraph from a set of scientific papers, which are used as data set. Then, using a pre-trained and fine-tuned Transformer, the paragraph is embedded into a vector space. Finally, the embedded vector becomes classified with respect to its relevance regarding a selected target ontology. To construct representative embeddings, we experiment with different training pipelines for natural language processing models. Those embeddings in turn are later used in the task of matching text to ontology. Finally, the result is assessed by compressing and visualizing the latent space and exploring the mappings between text fragments from a database and the set of chosen ontologies. To confirm the differences in behavior of the proposed ontology mapper models, we test five statistical hypotheses about their relative performance on ontology classification. To categorize the output from the Transformer, different classifiers are considered. These classifiers are, in detail, the Support Vector Machine (SVM), k-Nearest Neighbor, Gaussian Process, Random Forest, and Multilayer Perceptron. Application of these classifiers in a domain of scientific texts concerning catalysis research and respective ontologies, the suitability of the classifiers is evaluated, where the best result was achieved by the SVM classifier.

Permanent Link: <https://hdl.handle.net/11104/0339633>

0569239 - ÚI 2023 CZ cze J - Journal Article

Lehnert, M. - [Geletič, Jan](#) - Jurek, M.

Tepelný ostrov města očima současného výzkumu.

Geografické rozhledy. Roč. 32, č. 3 (12), s. 15. ISSN 1210-3004

Grant - others: AV ČR(CZ) StrategieAV21/23

Program: StrategieAV

Institutional support: RVO:67985807

Keywords : městské klima * tepelné prostředí člověka * tepelná expozice * pocitová teplota * tepelný komfort * urban climate * human thermal environment * thermal exposure * apparent temperature * thermal comfort

OECD category: Meteorology and atmospheric sciences

Method of publishing: Limited access

Energetická bilance prostoru města se významně liší od okolní krajiny. Tepelné prostředí městské krajiny má značný dopad na lidské zdraví a chování, flóru a faunu a celkovou udržitelnost měst. Nejznámějším projevem těchto specifik je tepelný ostrov města, současný výzkum se však stále více zaměřuje také na problematiku tepelné expozice a tepelného komfortu člověka.

Urban heat island in the perspective of current research. The energy balance of urban areas differs significantly from their surroundings. The thermal environment of urban landscape influences human health and behaviour, the flora and fauna, and the overall sustainability of cities. A well-known manifestation of those specifics is the urban heat island, yet current research focuses also on the topic of thermal exposure and human thermal comfort.

Permanent Link: <https://hdl.handle.net/11104/0340629>

0568737 - ÚI 2023 RIV DE ger J - Journal Article

[Porubský, Štefan](#)

Stefan Schwarz und die Entstehung der Halbgruppentheorie.

Sieger Beiträge zur Geschichte und Philosophie der Mathematik. Roč. 16, č. 1 (2022), s. 221-234. ISSN 2197-5590

Institutional support: RVO:67985807

Keywords : Štefan Schwarz * algebra * pologrupy * semigroups

OECD category: Pure mathematics

Method of publishing: Limited access

Stefan Schwarz war ein slowakischer Wissenschaftler, der während des 2. Weltkrieges in der Kriegsisolation als einer der ersten Mathematiker den Begriff der Halbgruppe definierte und aktiv als Gegenstand unabhängiger Forschung nutzte, die Grundeigenschaften studierte und den Ausbau ihrer Theorie nach dem Kriegsende massgebend beeinflusste.

Stefan Schwarz was a Slovak researcher who, in the war isolation during World War II, as one of the first mathematicians defined the concept of semigroups and actively used it as a subject of independent research, studying the basic properties and decisively influencing the development of their theory after the end of the war.

Permanent Link: <https://hdl.handle.net/11104/0340003>

0568283 - ÚI 2023 RIV GB eng J - Journal Article

Aguilera, J. P. - Bydžovský, J. - [Fernández-Duque, David](#)

Noetherian Godel logics.

Journal of Logic and Computation. Roč. 32, č. 8 (2022), s. 1487-1503. ISSN 0955-792X. E-ISSN 1465-363X

Institutional support: RVO:67985807

Keywords : Godel logic * fuzzy logic * hyperarithmetical set

OECD category: Pure mathematics

Impact factor: 0.509, year: 2021

Method of publishing: Limited access

<https://dx.doi.org/10.1093/logcom/exac064>

[DOI: 10.1093/logcom/exac064](https://doi.org/10.1093/logcom/exac064)

We introduce Noetherian Godel logics, Godel logics where the set of truth values is a closed subset of $[0,1]$ containing 0 and 1 and without any infinite ascending sequences. There are infinitely many such logics, including the well-known logic $G(\downarrow)$ whose set of truth values is $T(\downarrow) = \{0\}$ boolean OR $\{1/n : n \text{ is an element of } \mathbb{N} \setminus \{0\}\}$. We compute the complexity of satisfiability and validity for each Noetherian Godel logic and, in particular, in the logic $G(\downarrow)$. This yields optimal strengthening of the results of Baaz-Leitsch-Zach and Hajek

Permanent Link: <https://hdl.handle.net/11104/0339615>

0567920 - ÚI 2023 RIV eng J - Journal Article

[Keikha, Vahideh](#) - [Saumell, Maria](#)

On Voronoi visibility maps of 1.5D terrains with multiple viewpoints.

Information Processing Letters. Roč. 181, March 2023 (2023), č. článku 106362.

R&D Projects: GA ČR(CZ) GJ19-06792Y

Grant - others: AV ČR(CZ) AP1901

Program: Akademická prémie - Praemium Academiae

Institutional support: RVO:67985807

Keywords : Computational geometry * Visibility1.5D terrains * Voronoi diagrams * Multiple viewpoints

OECD category: Computer sciences, information science, bioinformatics (hardware development to be 2.2, social aspect to be 5.8)

Method of publishing: Limited access

[DOI: 10.1016/j.ipl.2023.106362](https://doi.org/10.1016/j.ipl.2023.106362)

Permanent Link: <https://hdl.handle.net/11104/0339185>

0568579 - ÚI 2023 RIV CZ eng L4 - Software

[Hlinka, Jaroslav](#) - [Pidnebesna, Anna](#) - [Tani Raffaelli, Giulio](#) - [Hartman, David](#) -

[Převorovský, Zdeněk](#) - [Chlada, Milan](#) - [Kovanda, Martin](#) - [Prášek, P.](#) - [Berka, Z.](#) - [Svoboda, R.](#)

Library of software modules for detecting extreme events.

Internal code: TN01000024/13-V02 ; 2022

Technical parameters: K dosažení popsaných detekcí jsou použity pokročilé metody využívající konkrétní strukturu problému. Knihovna je navržena v programovacím jazyce Python. Má strukturu centrální části (TN01000024/13-)V2.1 s obecnými analytickými moduly, doplněné specializovaným modulem V2.2 pro analýzu dat z non-destructive testing (NDT), a specializovaným modulem V2.3 pro analýzu video dat.

Economic parameters: Výsledkem je knihovna softwarových modulů schopných detekovat náhlé události a detekovat přechody mezi různými režimy studovaného systému. Klíčovou funkcionalitou je detekce zásadních změn v systému zvolené kritické infrastruktury. Tato schopnost umožňuje operátorům efektivně detekovat extrémní události a stavové přechody. LICENCE: Modul V2.1: GNU Affero General Public License v3.0. Modul V2.2: bez licence, avšak všechna práva vyhrazena. Modul V2.3: Modul pro analýzu videodat je dostupný účastníkům projektu v neveřejném repozitáři, ostatním zájemcům bude nabízen pod komerční licenci.

R&D Projects: GA TA ČR(CZ) TN01000024

Institutional support: RVO:67985807 ; RVO:61388998

Keywords : anomaly detection * non-destructive testing * video analysis * crowd dynamics

OECD category: Computer sciences, information science, bioinformathics (hardware development to be 2.2, social aspect to be 5.8); Audio engineering, reliability analysis (UT-L)

<https://www.ciirc.cvut.cz/research-education/projects/nck-kui/sub13/v2/>

The result is a library of software modules capable of detecting abrupt events and detecting transitions between different regimes of the system under study. A key functionality is the detection of crucial changes in the system of the selected critical infrastructure. This capability allows operators to effectively detect extreme events and state transitions. However, this problem is complicated by the usually limited amount of data available. To achieve the described detections, advanced methods are used that exploit the specific structure of the problem. The library is designed in the Python programming language. It has a central part structure (TN01000024/13-)V2.1 with general analysis modules, complemented by a specialized module V2.2 for the analysis of non-destructive testing (NDT) data, and a specialized module V2.3 for the analysis of video data. The result was achieved by implementing the stages of the sub-project, i.e. identification of the target functionality, preparation of pilot data and method development, initial implementation and its optimization by testing on new data.

Výsledkem je knihovna softwarových modulů schopných detekovat náhlé události a detekovat přechody mezi různými režimy studovaného systému. Klíčovou funkcionalitou je detekce zásadních změn v systému zvolené kritické infrastruktury. Tato schopnost umožňuje operátorům efektivně detekovat extrémní události a stavové přechody. Tento problém je však komplikovaný kvůli obvykle omezenému množství dostupných dat. K dosažení popsaných detekcí jsou použity pokročilé metody využívající konkrétní strukturu problému. Knihovna je navržena v programovacím jazyce Python. Má strukturu centrální části (TN01000024/13-)V2.1 s obecnými analytickými moduly, doplněné specializovaným modulem V2.2 pro analýzu dat z non-destructive testing (NDT), a specializovaným modulem V2.3 pro analýzu video dat. Výsledkem bylo dosažení realizací etap dílčího projektu, tj. identifikací cílové funkcionality, přípravy pilotních dat a vývoje metod, iniciální implementace a její optimalizace testováním na nových datech.

Permanent Link: <https://hdl.handle.net/11104/0339865>

Research data: [Github](#), [Gitlab](#) ÚT AVČR

0567939 - ÚI 2023 RIV CH eng C - Conference Paper (international conference)

[Keikha, Vahideh](#)

Large k-Gons in a 1.5D Terrain.

Computing and Combinatorics: 28th International Conference, COCOON 2022 Proceedings. Cham, 2023 - (Zhang, Y.; Miao, D.; Möhring, R.), s. 49-60. Lecture Notes in Computer Science, 13595. ISBN 978-3-031-22104-0. ISSN 0302-9743. E-ISSN 1611-3349.

[COCOON 2022: International Computing and Combinatorics Conference /28./, Shenzhen (CN), 22.10.2022-24.10.2022]

R&D Projects: GA ČR(CZ) GJ19-06792Y

Institutional support: RVO:67985807

OECD category: Computer sciences, information science, bioinformatics (hardware development to be 2.2, social aspect to be 5.8)

[DOI: 10.1007/978-3-031-22105-7_5](https://doi.org/10.1007/978-3-031-22105-7_5)

Permanent Link: <https://hdl.handle.net/11104/0339206>

0568613 - ÚI 2023 RIV CH eng C - Conference Paper (international conference)

Vidnerová, Petra - Kalina, Jan

Multi-objective Bayesian Optimization for Neural Architecture Search.

Artificial Intelligence and Soft Computing. 21st International Conference, ICAISC 2022. Proceedings, Part I. Cham: Springer, 2023 - (Rutkowski, L.; Scherer, R.; Korytkowski, M.; Pedrycz, W.;

Tadeusiewicz, R.; Zurada, J.), s. 144-153. Lecture Notes in Computer Science, 13588. ISBN 978-3-031-23491-0. ISSN 0302-9743.

[ICAISC 2022: International Conference on Artificial Intelligence and Soft Computing /21./. Zakopane (PL), 18.06.2022-22.06.2022]

R&D Projects: GA ČR(CZ) GA22-02067S

Institutional support: RVO:67985807

Keywords : Bayesian optimization * Multi-objective optimization * Neural architecture search * Number of parameters

OECD category: Computer sciences, information science, bioinformatics (hardware development to be 2.2, social aspect to be 5.8)

https://dx.doi.org/10.1007/978-3-031-23492-7_13

[DOI: 10.1007/978-3-031-23492-7_13](https://doi.org/10.1007/978-3-031-23492-7_13)

A novel multi-objective algorithm denoted as MO-BayONet is proposed for the Neural Architecture Search (NAS) in this paper. The method based on Bayesian optimization encodes the candidate architectures directly as lists of layers and constructs an extra feature vector for the corresponding surrogate model. The general method allows to accompany the search for the optimal network by additional criteria besides the network performance. The NAS method is applied to combine classification accuracy with network size on two benchmark datasets here. The results indicate that MO-BayONet is able to outperform an available genetic algorithm based approach.

Permanent Link: <https://hdl.handle.net/11104/0339882>

0568675 - ÚTIA 2023 RIV CZ eng C - Conference Paper (international conference)

Papáček, Štěpán - Matonoha, Ctirad - Duintjer Tebbens, Jurjen

Bohl-Marek decomposition applied to a class of biochemical networks with conservation properties.

Proceedings of the Seminar on Numerical Analysis & Winter School /SNA' 23/. Ostrava: Institute of Geonics of the Czech Academy of Sciences, 2023 - (Stary, J.; Sysala, S.; Sysalová, D.), s. 56-59. ISBN 978-80-86407-85-2.

[SEMINAR ON NUMERICAL ANALYSIS - SNA'23 In memoriam of professor Radim Blaheta. Ostrava (CZ), 23.01.2023-27.01.2023]

R&D Projects: GA ČR(CZ) GA21-03689S

Institutional support: RVO:67985556 ; RVO:67985807

Keywords : Mathematical modeling * Biochemical network * Pharmacokinetic (PBPK) models

OECD category: Applied mathematics

<http://library.utia.cas.cz/separaty/2023/TR/papacek-0568675.pdf>

This study presents an application of one special technique, further called as Bohl-Marek decomposition, related to the mathematical modeling of biochemical networks with mass conservation properties. We continue in direction of papers devoted to inverse problems of parameter estimation for mathematical models describing the drug-induced enzyme production networks [3]. However, being aware of the complexity of general physiologically based pharmacokinetic (PBPK) models, here we focus on the case of enzyme-catalyzed reactions with a substrate transport chain [5]. Although our ultimate goal is to develop a reliable method for fitting the model parameters to given experimental data, here we study certain numerical issues within the framework of optimal experimental design [6]. Before starting an experiment on a real biochemical network, we formulate an optimization problem aiming to maximize the information content of the corresponding experiment. For the above-sketched optimization problem, the computational costs related to the two formulations of the same biochemical network, being (i) the classical formulation $\dot{x}(t) = Ax(t) + b(t)$ and (ii) the 'quasi-linear' Bohl-Marek formulation $\dot{M}(t) = M(x(t))xM(t)$, can be determined and compared.

Permanent Link: <https://hdl.handle.net/11104/0339944>

0568775 - ÚI 2023 RIV IT eng A - Abstract

[Hlinka, Jaroslav](#) - [Pidnebesna, Anna](#) - [Caputi, Luigi](#)

Persistent homology to analyse disruptions of functional and effective brain connectivity.

The 11th International Conference on Complex Networks and their Applications - Book of Abstracts. Palermo: 12th International Conference on Complex Networks and their Applications, 2023. s. 513-514. ISBN 978-2-9557050-6-3.

[COMPLEX NETWORKS 2023: The 12th International Conference on Complex Networks and their Applications. 28.11.2023-30.11.2023, French Riviera]

R&D Projects: GA ČR(CZ) GA21-17211S

Institutional support: RVO:67985807

Keywords : Persistent homology * Connectivity * fMRI * Electrophysiology * Epilepsy * Schizophrenia

OECD category: Neurosciences (including psychophysiology)

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ZÁKLADNÍ ÚDAJE: The 11th International Conference on Complex Networks and their Applications - Book of Abstracts. Palermo: 12th International Conference on Complex Networks and their Applications, 2023. s. 513-514. ISBN 978-2-9557050-6-3. KONFERENCE: COMPLEX NETWORKS 2023: The 12th International Conference on Complex Networks and their Applications. 28.11.2023-30.11.2023, French Riviera]. ABSTRAKT: Topological Data Analysis (TDA [1]), despite its relative novelty, has already been applied to study network connectivity structure across fields. We propose that its prominent tool of persistent homology (PH) may apart from the more common dependence networks (functional connectivity – FC) be applied also to directed, causal, networks – known as effective connectivity (EC) in neuroscience. We test the PH discriminatory power in two archetypal examples of disease-related brain connectivity alterations: during epilepsy seizures (captured by electrophysiology – EEG) and in schizophrenia patients (using functional magnetic resonance imaging - fMRI). We employ a range of PH-based features and quantify ability to distinguish healthy from diseased brain states by applying a support vector machine (SVM), a relatively standard method of choice for similar data situations, used also previously in similar context. We compare this novel approach to using standard undirected PH applied to the functional connectivity matrix, as well as comparing the (D)PH approach to using the raw EC/FC matrices [2]

Permanent Link: <https://hdl.handle.net/11104/0340035>

0568772 - ÚI 2023 RIV US eng A - Abstract

[Geletič, Jan](#) - [Belda, M.](#) - [Bureš, Martin](#) - [Krč, Pavel](#) - [Resler, Jaroslav](#) - [Řezníček, Hynek](#) - [Krayenhoff, E. S.](#)

Complexity of adaptation and mitigation measures in urban canyon – microscale modeling approach. *AMS 2023: 103rd Annual Meeting Program Book*. Denver: AMS, 2023.

[AMS 2023: American Meteorological Society Annual Meeting /103./ 08.01.2023-12.01.2023, Denver / Online]

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Keywords : PALM * urban planning * biometeorology * air quality * vulnerability

OECD category: Meteorology and atmospheric sciences

ZÁKLADNÍ ÚDAJE: AMS 2023: 103rd Annual Meeting Program Book. Denver: AMS, 2023.

KONFERENCE: AMS 2023: 103rd Annual Meeting Program Book. Denver: AMS, 2023. ANOTACE: Cities worldwide, specifically in times of climate change, facing increasing global temperature. Higher temperatures have a negative effect on citizens, because heat-waves episodes are still longer and more intensive. Moreover, climate change is one of the most current and probably the most difficult challenges local governments face. Although a large number of adaptation strategies and climate plans have emerged recently, many have a common result (at least in Central Europe); the simplest and economically most advantageous solution is usually represented by urban greenery, primarily planting of trees or shrubs. Very popular are the implementation of high-reflective surfaces, green roofs or green walls. Usually known prejudice is that all adaptation and mitigation measures will improve the current situation. On the other hand, modern cities are very complex - and somehow also living - (eco)systems of various relations and their interactions. As an example, greenery in urban environments is perceived as an essential element of the face of cities and its characteristics are automatically accepted by residents as positive. The negative effects of greenery in urban areas, apart from possible allergies, are practically not considered in urban planning. For example, trees negatively affect air pollution concentrations, because they significantly modify distribution of micro and local scale eddies in urban canyons. However, the impact of adaptation and mitigation measures in cities, positive and negative, should be a significant consequence of adaptation policies, as well as the associated costs of care. Many models, mostly micro-scale, analyze the potential effect of selected adaptation measures in a realistic urban environment. But the commonly used models are rarely complex enough to model air quality and thermal properties on a fine enough scale. They are typically focused on one problem only, mostly on energy-related variables (surface/air temperature, biometeorological indices or mean radiant temperature, etc.). Situation in the street canyon is more complicated, because trees change energy balance and directly affect wind velocity. Moreover, to get valid results, proper models are not a guarantee; without good quality and precise enough input data. Main purpose of this presentation is to explain and summarize the latest findings on the positive and negative effects of adaptation and mitigation measures at the street level, which were analyzed using the LES-based PALM modeling system. Selected scenarios, discussed in detail with local municipality, were considered for a typical urban environment in Dejvice, a quarter in the Czech capital, Prague, confirming the inverse effect of greenery on biometeorological versus air quality indicators (ie. improving thermal comfort may bring about an increase of air pollution concentrations). Results suggest minimal effect of green roofs or green walls on pedestrian level, despite the fact that greenery has optimal conditions. Moreover, high-reflective surfaces also significantly change the energy balance of the surface; it strongly decreases convection, which represents potential problems in streets with heavy traffic. Thanks to detailed input and output geodata it is easy to analyze all results and describe all effects of adaptation and mitigation measures in their surroundings, same as in their neighborhood. Finally, microscale modeling systems show their huge potential for evaluation of future scenarios, as could be complex developer projects and re-organization of public transport (e.g., new tunnel or highway).

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Belda, M. - Resler, Jaroslav - Krč, Pavel - Geletič, Jan - Maronga, B. - Sühning, M. - Kurppa, M. - Kanani-Sühning, F. - Fuka, V. - Eben, Kryštof - Benešová, N.

Trade-offs Between Improvement of Thermal Comfort and Air Quality in Urban Environment Indicated by LES Model PALM Simulations in Prague Case Study.

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Keywords : PALM * adaptation measures * sensitivity * modeling * urban planning

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KONFERENCE: AMS 2023: American Meteorological Society Annual Meeting /103./ 08.01.2023-

12.01.2023, Denver / Online. ABSTRAKT: Thermal comfort of city dwellers is at the forefront of the urban studies especially in connection with climate change. Many studies analyze the impact of urbanistic measures to counter the phenomenon known as Urban Heat Island (UHI) with one of the most popular being urban greenery. However, impact of these measures on air quality is not always considered. In this study an LES-based modeling system PALM 6.0 featuring an improved urban surface model (USM) was used to analyze micro-climate sensitivity with respect to potential UHI mitigation measures in a densely built-up residential area in Prague, Czech Republic, particularly in the vicinity of a typical crossroads. The use of an integrated modeling system allowed the analysis of the effects both on biothermal indicators and air quality. Two types of scenario simulations were designed. First, a set of synthetic scenarios changing surface and material parameters such as albedo or emissivity, by which the sensitivity of the model itself to potentially erroneous input data was tested. These showed the highest sensitivity to correct setting of surface parameters used in radiation balance equations. Second, a set of urbanistic scenarios was designed to assess the limits of effects of commonly considered UHI mitigation measures such as greening of the streets or altering surface materials. In this case, urban greenery is confirmed to be the most effective measure, especially when considering both physical and biophysical temperature indicators. On the other hand, analysis of air quality, specifically with respect to PM_{2.5} dispersion, showed opposite behavior to that of thermal indicators; i.e. improved thermal comfort brings deterioration of PM_{2.5} concentrations due to decreased ventilation of the street canyon and decreased vertical turbulent transport.

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