

### Relations and bounds for the zeros of graph polynomials using vertex orbits

In this paper, we prove bounds for the unique, positive zero of  $O_G^*(z) = 1 - O_G(z)$ , where  $O_G(z)$  is the so-called orbit polynomial [1]. The orbit polynomial is based on the multiplicity and cardinalities of the vertex orbits of a graph. In [1], we have shown that the unique, positive zero  $\delta \leq 1$  of  $O_G^*(z)$  can serve as a meaningful measure of graph symmetry. In this paper, we study special graph classes with a specified number of orbits and obtain bounds on the value of  $\delta$ .

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computing Sciences, Swiss Distance University of Applied Sciences, Nankai University, Institute for Bioinformatics and Translational Research, The City College of New York (CUNY), Facebook Inc, Guizhou University of Finance and Economics, Teacher Training University, TU Vienna, Aalto University, Peking University

Contributors: Dehmer, M., Emmert-Streib, F., Mowshowitz, A., Ilić, A., Chen, Z., Yu, G., Feng, L., Ghorbani, M., Varmuza, K., Tao, J.

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ASJC Scopus subject areas: Computational Mathematics, Applied Mathematics

Keywords: Data science, Graph measures, Graphs, Networks, Quantitative graph theory, Symmetry

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Research output: Contribution to journal > Article > Scientific > peer-review

### A novel epidemic model considering demographics and intercity commuting on complex dynamical networks

In order to characterize the impact of demographics and intercity commuting between cities on epidemic propagation, we propose a novel two-city epidemic model, where the spreading process is depicted by using SIR (susceptible-infected-recovered) model. The infectious diseases can spread in two cities at the same time, and be taken from one city to the other through intercity commuters. Firstly, we take use of the spectral analysis method to obtain the basic reproduction number  $R_0$  of the model. Then, the equilibria including the endemic equilibrium and disease-free one of the proposed model are analyzed and calculated, and the results indicate that they are globally asymptotic stable. Moreover, the degree distribution of the population changes over time, forming a complex dynamical networks before the system reaches a steady state. Finally, through a large number of numerical simulations, we show that demographics, intercity commuting rates and exposed individuals during commuting have great effects on the epidemic spreading behavior between two cities. The analysis of the proposed model can further help to understand the transmission behavior of epidemics in reality, and it is also of great practical significance to predict the epidemic trends among cities and design effective measures to curb the infectious diseases.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computing Sciences, Research group: Predictive Society and Data Analytics (PSDA), Research group: Computational Medicine and Statistical Learning Laboratory (CMSL), Tianjin University of Technology, University of Applied Sciences Upper Austria, Shanxi University

Contributors: Yin, Q., Wang, Z., Xia, C., Dehmer, M., Emmert-Streib, F., Jin, Z.

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ASJC Scopus subject areas: Computational Mathematics, Applied Mathematics

Keywords: Complex dynamical networks, Demographics, Equilibrium analysis, Intercity commuting, Two-city epidemic model

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Research output: Contribution to journal > Article > Scientific > peer-review

### **Introducing Multi-Convexity in Path Constrained Trajectory Optimization for Mobile Manipulators**

Mobile manipulators have a highly non-linear and non-convex mapping between the end-effector path and the manipulator's joints and position and orientation of the mobile base. As a result, trajectory optimization with end-effector path constraints takes the form of a difficult non-linear optimization problem. In this paper, we present the first multi-convex approximation to this difficult optimization problem that eventually reduces to solving a sequence of globally valid convex quadratic programs (QPs). The proposed optimizer rests on two novel building blocks. First, we introduce a set of auxiliary variables in which the non-linear constraints that arise out of manipulator kinematics and its coupling with the mobile base have a multi-affine form. Projecting the auxiliary variables to the space of actual configuration variables of the mobile manipulator involves a non-convex optimization. Thus, the second building block involves computing a convex surrogate for this non-convex projection. We show how large parts of the proposed optimizer can be solved in parallel providing the possibility of exploiting multi-core CPUs. We validate our trajectory optimization on different benchmark examples. Specifically, we highlight how it solves the cyclicity problem and provides a holistic approach where a diverse set of trajectories can be obtained by trading-off different aspects of manipulator and mobile base motion.

#### **General information**

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Automation Technology and Mechanical Engineering, Research group: Robotics and Automation, University of Tartu, Johannes Kepler University

Contributors: Singh, A. K., Ahonen, A., Ghabcheloo, R., Mueller, A.

Number of pages: 8

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Publication date: 2020

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ASJC Scopus subject areas: Artificial Intelligence, Decision Sciences (miscellaneous), Control and Systems Engineering, Mechanical Engineering, Computational Mathematics, Control and Optimization

#### **Bibliographical note**

EXT="Singh, Arun Kumar"

Source: Scopus

Source ID: 85090156821

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

### **Resilient Cooperative Voltage Control for Distribution Network with High Penetration Distributed Energy Resources**

This paper considers the problem of designing a resilient distributed voltage control algorithm for distribution systems with high penetration of distributed energy resources in the presence of an unknown cyber-attack. The purpose of the attack is to force the system to violate the operating voltage limit by intercepting its communication channels and inserting exogenous signals to perturb and/or modify the information being exchanged. We first review the cooperative voltage control proposed in our previous work and provide a new stability analysis for it. Next, we present a resilient cooperative voltage control algorithm by introducing a virtual system interconnected with the original system such that the voltage can be maintained within the operational limit under unknown attacks. The resiliency of the proposed algorithm is demonstrated via simulations on the IEEE 8500-node system when subjected to an attack which consists of corrupting the data being exchanged in the communication network between two generation units.

#### **General information**

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Automation Technology and Mechanical Engineering, University of Central Florida

Contributors: Gusrialdi, A., Xu, Y., Qu, Z., Simaan, M. A.

Number of pages: 7

Pages: 1533-1539

Publication date: 2020

#### **Host publication information**

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Publisher: IEEE  
ISBN (Print): 978-1-7281-8813-3  
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ASJC Scopus subject areas: Artificial Intelligence, Decision Sciences (miscellaneous), Control and Systems Engineering, Mechanical Engineering, Computational Mathematics, Control and Optimization  
Keywords: cooperative control, cyber attacks, distribution network, resilient control, Voltage control  
Source: Scopus  
Source ID: 85090152084  
Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

### **The watching system as a generalization of identifying code**

The watching system, as a generalization of identifying code, has been defined by Auger in 2010. The identifying code has been used to wireless networks and it has been also applied to locate objects in the sensor networks. On the other hand, the graph product is employed in most of the mathematic branches such as network design to study the structure of network elements. In this paper, we give some upper bounds for the watching number of well-know product graphs.

#### **General information**

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Organisations: Computing Sciences, Research group: Predictive Society and Data Analytics (PSDA), Research group: Computational Medicine and Statistical Learning Laboratory (CMSL), Teacher Training University, Swiss Distance University of Applied Sciences, Institute for Bioinformatics and Translational Research, Nankai University  
Contributors: Ghorbani, M., Dehmer, M., Maimani, H., Maddah, S., Roozbayani, M., Emmert-Streib, F.  
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ASJC Scopus subject areas: Computational Mathematics, Applied Mathematics  
Keywords: Domination number, Graph products, Identifying code, Watching system  
DOIs:  
10.1016/j.amc.2020.125302  
Source: Scopus  
Source ID: 85083340308  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Graph entropy based on the number of spanning forests of c-cyclic graphs**

Graph entropies have been introduced to quantitatively measure the structural information content of graphs and networks; they have plenty of applications in various fields. Utilizing the number of subgraphs to establish measures for determining the complexity of molecular graphs are also prevalent in the study of mathematical chemistry. In this paper, we develop a new graph entropy measure that is based on the number of spanning forests. We prove explicit expressions for the entropy for trees, unicyclic and bicyclic graphs, and show that the cycle graph  $C_n$  attains the maximal value of the entropy for unicyclic graphs with order  $n$  and large cycle lengths. Based on generating numerical results, we conjecture extremal unicyclic graphs with respect to the entropy as well as we compare the values of our entropy for  $c$ -cyclic graphs, and generate graphs of bicyclic graphs and tricyclic graphs with 6 vertices for performing further research.

#### **General information**

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Computing Sciences, Research group: Predictive Society and Data Analytics (PSDA), Northwestern Polytechnical University, Yulin University, Beijing University of Chemical Technology, University of Applied Sciences Upper Austria, School of Management, Nankai University, Hall in Tyrol, Mathematics Faculty of Information Technology and Communication Sciences  
Contributors: Wan, P., Tu, J., Dehmer, M., Zhang, S., Emmert-Streib, F.  
Publication date: 15 Dec 2019  
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Original language: English  
ASJC Scopus subject areas: Computational Mathematics, Applied Mathematics  
Keywords: Graph entropy, Spanning forest, Subgraph  
DOIs:  
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Source: Scopus  
Source ID: 85073703315  
Research output: Contribution to journal › Article › Scientific › peer-review

### **On efficient network similarity measures**

This paper presents novel graph similarity measures which can be applied to simple directed and undirected networks. To define the graph similarity measures, we first map graphs to real numbers by utilizing structural graph measures. Then, we define measures of similarity between real numbers and prove that they can be used as proxies for graph similarity. Numerical results are derived to show the domain coverage of these measures as well as their clustering ability. The latter relates to the efficient grouping of graphs according to certain structural properties. Our numerical results are sensitive to these properties and offer insights useful for designing effective graph similarity measures.

### **General information**

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MoE publication type: A1 Journal article-refereed  
Organisations: Computing Sciences, Research group: Computational Medicine and Statistical Learning Laboratory (CMSL), Research group: Predictive Society and Data Analytics (PSDA), University of Applied Sciences Upper Austria, Nankai University, Hall in Tyrol, Shandong University at Weihai, Steyr School of Management, Shahid Rajaee Teacher Training University, The City College of New York (CUNY), Predictive Society and Data Analytics Lab, Institute of Biosciences and Medical Technology  
Contributors: Dehmer, M., Chen, Z., Shi, Y., Zhang, Y., Tripathi, S., Ghorbani, M., Mowshowitz, A., Emmert-Streib, F.  
Publication date: 1 Dec 2019  
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Scopus rating (2019): CiteScore 5.6 SJR 0.969 SNIP 1.766  
Original language: English  
ASJC Scopus subject areas: Computational Mathematics, Applied Mathematics  
Keywords: Distance measures, Graphs, Inequalities, Networks, Similarity measures  
DOIs:  
10.1016/j.amc.2019.06.035  
Source: Scopus  
Source ID: 85068221101  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Satisfiability of modal inclusion logic: Lax and strict semantics**

We investigate the computational complexity of the satisfiability problem of modal inclusion logic. We distinguish two variants of the problem: one for the strict and another one for the lax semantics. Both problems turn out to be EXPTIME-complete on general structures. Finally, we show how for a specific class of structures NEXPTIME-completeness for these problems under strict semantics can be achieved.

### **General information**

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Computing Sciences, Leibniz-Universität Hannover, Tampere University  
Contributors: Hella, L., Kuusisto, A., Meier, A., Vollmer, H.  
Publication date: 1 Oct 2019  
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ISSN (Print): 1529-3785

Ratings:

Scopus rating (2019): CiteScore 2.2 SJR 0.572 SNIP 1.095

Original language: English

ASJC Scopus subject areas: Theoretical Computer Science, Computer Science(all), Logic, Computational Mathematics

Keywords: Computational complexity, Modal inclusion logic, Satisfiability, Team semantics

DOIs:

10.1145/3356043

### Bibliographical note

DUPL=50949587

Source: Scopus

Source ID: 85075599859

Research output: Contribution to journal > Article > Scientific > peer-review

### Visibility-Aware Part Coding for Vehicle Viewing Angle Estimation

A number of spatially-localised semantic parts of vehicles sensitive to pose changes are encoded their visible probabilities into a mid-level feature vector. Car pose estimation is then formulated into a regression on concatenated low-and mid-level features to continuously changing viewing angles. Each dimension of our visibility-Aware part codes separates all the training samples into two groups according to its visual existence in images, which provides additional part-specific range constraint of viewing angles. Moreover, the proposed codes can alleviate the suffering from sparse and imbalanced data distribution in the light of modelling latent dependency across angle targets. Experimental evaluation for car pose estimation on the EPFL Multi-View Car benchmark demonstrates significant improvement of our method over the state-of-The-Art regression methods, especially when only sparse and imbalanced data is available.

### General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Computing Sciences, Research group: Vision, South China University of Technology

Contributors: Yang, D., Qian, Y., Cai, D., Yan, S., Kämäräinen, J., Chen, K.

Number of pages: 6

Pages: 65-70

Publication date: 1 Aug 2019

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Publisher: IEEE

ISBN (Electronic): 9781728121062

ASJC Scopus subject areas: Computer Science Applications, Computer Vision and Pattern Recognition, Information Systems, Computational Mathematics, Control and Optimization

Keywords: Car pose estimation, Coding, Pose-sensitive parts, Regression forests, Visibility-Aware

DOIs:

10.1109/ICIST.2019.8836907

### Bibliographical note

EXT="Chen, Ke"

jufoid=79229

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

### Sound Event Detection in the DCASE 2017 Challenge

Each edition of the challenge on Detection and Classification of Acoustic Scenes and Events (DCASE) contained several tasks involving sound event detection in different setups. DCASE 2017 presented participants with three such tasks, each having specific datasets and detection requirements: Task 2, in which target sound events were very rare in both training and testing data, Task 3 having overlapping events annotated in real-life audio, and Task 4, in which only weakly labeled data were available for training. In this paper, we present three tasks, including the datasets and baseline systems, and analyze the challenge entries for each task. We observe the popularity of methods using deep neural networks, and the still widely used mel frequency-based representations, with only few approaches standing out as radically different. Analysis of the systems behavior reveals that task-specific optimization has a big role in producing good performance; however, often this optimization closely follows the ranking metric, and its maximization/minimization does not result in universally good performance. We also introduce the calculation of confidence intervals based on a jackknife resampling

procedure to perform statistical analysis of the challenge results. The analysis indicates that while the 95% confidence intervals for many systems overlap, there are significant differences in performance between the top systems and the baseline for all tasks.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computing Sciences, Carnegie Mellon University, Tampere University

Contributors: Mesáros, A., Diment, A., Elizalde, B., Heittola, T., Vincent, E., Raj, B., Virtanen, T.

Number of pages: 15

Pages: 992-1006

Publication date: 1 Jun 2019

Peer-reviewed: Yes

#### Publication information

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Issue number: 6

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Keywords: confidence intervals, jackknife estimates, pattern recognition, Sound event detection, weak labels

DOIs:

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Source: Scopus

Source ID: 85064625139

Research output: [Contribution to journal](#) › [Article](#) › [Scientific](#) › [peer-review](#)

#### Hypermonogenic solutions and plane waves of the Dirac operator in $\mathbb{R}^p \times \mathbb{R}^q$

In this paper we first define hypermonogenic solutions of the Dirac operator in  $\mathbb{R}^p \times \mathbb{R}^q$  and study some basic properties, e.g., obtaining a Cauchy integral formula in the unit hemisphere. Hypermonogenic solutions form a natural function class in classical Clifford analysis. After that, we define the corresponding hypermonogenic plane wave solutions and deduce explicit methods to compute these functions.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Civil Engineering, Universiteit Gent

Contributors: Guzmán Adán, A., Orelma, H., Sommen, F.

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Pages: 1-14

Publication date: 1 Apr 2019

Peer-reviewed: Yes

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Original language: English

ASJC Scopus subject areas: Computational Mathematics, Applied Mathematics

Keywords: Cauchy's formula, Hypermonogenic solution, Plane wave

DOIs:

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Source: Scopus

Source ID: 85055664097

Research output: [Contribution to journal](#) › [Article](#) › [Scientific](#) › [peer-review](#)

### **Circularly Polarized Textile Tag Antenna for Wearable Passive UHF RFID Systems**

We present a circularly polarized tag antenna using textile materials for wearable passive ultra high frequency (UHF) radio frequency identification (RFID) system. A corner-truncated square patch with a shorting pin and an inductive feed network are used to achieve circularly polarization and conjugate impedance matching. The antenna has similar best axial ratio values of 2.1 dB and 2.2 dB for both in air and on-body conditions, and desirable corresponding read range of 9.1 m and 8.4 m.

#### **General information**

Publication status: Published  
MoE publication type: A4 Article in a conference publication  
Organisations: BioMediTech, Donghua University  
Contributors: Kuang, Y., Ma, S., Ukkonen, L., Virkki, J., Björninen, T.  
Publication date: 18 Mar 2019

#### **Host publication information**

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Publisher: IEEE  
ISBN (Electronic): 9780996007849  
ASJC Scopus subject areas: Computational Mathematics, Instrumentation, Electrical and Electronic Engineering, Computer Networks and Communications  
Keywords: Circularly polarized antenna, Radio frequency identification, Wearable antenna  
DOIs:  
10.23919/ACCESS.2018.8669314  
Source: Scopus  
Source ID: 85063790306  
Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

### **Comparison of Human Head Phantoms with Different Complexities for Implantable Antenna Development**

Human body phantom with electrical properties is widely used in electromagnetics solvers to model the lossy human tissue environment. The selection of the phantoms affects the computational efficiency and results accuracy. In this work, we evaluated four human head phantoms with an intracranial implantable antenna. Results of phantom complexity and antenna parameters are compared to provide the reference in phantom selection for implantable antenna development.

#### **General information**

Publication status: Published  
MoE publication type: A4 Article in a conference publication  
Organisations: BioMediTech  
Contributors: Ma, S., Ukkonen, L., Sydänheimo, L., Björninen, T.  
Publication date: 18 Mar 2019

#### **Host publication information**

Title of host publication: 2018 International Applied Computational Electromagnetics Society (ACES) Symposium : 29 July-1 Aug. 2018, China  
Publisher: IEEE  
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ISBN (Electronic): 978-0-9960078-4-9  
ASJC Scopus subject areas: Computational Mathematics, Instrumentation, Electrical and Electronic Engineering, Computer Networks and Communications  
Keywords: anatomical head phantom, implantable antenna, multilayer head phantom  
Electronic versions:  
Comparison of Human Head Phantoms 2019  
DOIs:  
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URLs:  
<http://urn.fi/URN:NBN:fi:tuni-202005155345>  
Source: Scopus  
Source ID: 85063771074  
Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

### **An automated algorithm for reliable equation of state fitting of magnetic systems**

In computational physics and materials science ground-state properties are often extracted from an equation of state fit to energy-volume data. Magnetic systems often have multiple magnetic phases present in the energy-volume data, which poses a challenge for the fitting approach because the results are sensitive to the selection of included fitting points. This is because practically all popular equation of state fitting functions, such as Murnaghan and Birch-Murnaghan, assume just

one phase and therefore cannot correctly fit magnetic energy-volume data that contains multiple phases. When fitting magnetic energy-volume data it is therefore important to select the range of fitting points in such a way that only points from the one relevant phase are included. We present a simple algorithm that makes the point selection automatically. Selecting fitting points automatically removes human bias and should also be useful for large-scale projects where selecting all fitting points by hand is not feasible.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research area: Computational Physics, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Uppsala University, Department of Physics and Astronomy, University of Turku, Royal Institute of Technology

Contributors: Levämäki, H., Tian, L., Vitos, L., Ropo, M.

Number of pages: 8

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Publication date: 2019

Peer-reviewed: Yes

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Scopus rating (2019): CiteScore 5 SJR 0.823 SNIP 1.115

Original language: English

ASJC Scopus subject areas: Computer Science(all), Chemistry(all), Materials Science(all), Mechanics of Materials, Physics and Astronomy(all), Computational Mathematics

Keywords: EOS, Equation of state fitting

DOIs:

10.1016/j.commatsci.2018.09.026

Source: Scopus

Source ID: 85053772857

Research output: Contribution to journal › Article › Scientific › peer-review

#### Cuts for 3-D magnetic scalar potentials: Visualizing unintuitive surfaces arising from trivial knots

A wealth of literature exists on computing and visualizing cuts for the magnetic scalar potential of a current carrying conductor via Finite Element Methods (FEM) and harmonic maps to the circle. By a cut we refer to an orientable surface bounded by a given current carrying path (such that the flux through it may be computed) that restricts contour integrals on a curl-zero vector field to those that do not link the current-carrying path, analogous to branch cuts of complex analysis. This work is concerned with a study of a peculiar contour that illustrates topologically unintuitive aspects of cuts obtained from a trivial loop and raises questions about the notion of an optimal cut. Specifically, an unknotted curve that bounds only high genus surfaces in its convex hull is analyzed. The current work considers the geometric realization as a current-carrying wire in order to construct a magnetic scalar potential. Moreover, we consider the problem of choosing an energy functional on the space of maps, suggesting an algorithm for computing cuts via minimizing a conformally invariant functional utilizing Newton iteration.

#### General information

Publication status: Accepted/In press

MoE publication type: A1 Journal article-refereed

Organisations: Electrical Engineering, Boston University

Contributors: Stockrahm, A., Lahtinen, V., Kangas, J. J., Kotiuga, P. R.

Publication date: 2019

Peer-reviewed: Yes

#### Publication information

Journal: Computers and Mathematics with Applications

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Ratings:

Scopus rating (2019): CiteScore 4.8 SJR 1.214 SNIP 1.42

Original language: English

ASJC Scopus subject areas: Modelling and Simulation, Computational Theory and Mathematics, Computational Mathematics

Keywords: Homology, Magnetic fields, Visualization

DOIs:

10.1016/j.camwa.2019.05.023



Source: Scopus

Source ID: 85067239229

Research output: Contribution to journal › Article › Scientific › peer-review

### Modeling mass transfer in fracture flows with the time domain-random walk method

The time domain-random walk method was developed further for simulating mass transfer in fracture flows together with matrix diffusion in surrounding porous media. Specifically, a time domain-random walk scheme was developed for numerically approximating solutions of the advection-diffusion equation when the diffusion coefficient exhibits significant spatial variation or even discontinuities. The proposed scheme relies on second-order accurate, central-difference approximations of the advective and diffusive fluxes. The scheme was verified by comparing simulated results against analytical solutions in flow configurations involving a rectangular channel connected on one side with a porous matrix. Simulations with several flow rates, diffusion coefficients, and matrix porosities indicate good agreement between the numerical approximations and analytical solutions.

#### General information

Publication status: E-pub ahead of print

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Geological Survey of Finland, University of Helsinki, University of Jyväskylä

Contributors: Kuva, J., Voutilainen, M., Mattila, K.

Publication date: 2019

Peer-reviewed: Yes

#### Publication information

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Ratings:

Scopus rating (2019): CiteScore 5.4 SJR 0.823 SNIP 1.424

Original language: English

ASJC Scopus subject areas: Computer Science Applications, Computers in Earth Sciences, Computational Theory and Mathematics, Computational Mathematics

Keywords: Advection, Breakthrough curve, Matrix diffusion, Porous media, Simulation, Solute transport

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URLs:

<http://urn.fi/URN:NBN:fi:ty-201909062074>

Source: Scopus

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Research output: Contribution to journal › Article › Scientific › peer-review

### Optimal energy decay for the wave-heat system on a rectangular domain

We study the rate of energy decay for solutions of a coupled wave-heat system on a rectangular domain. Using techniques from the theory of  $C_0$ -semigroups, and in particular a well-known result due to Borichev and Tomilov, we prove that the energy of classical solutions decays like  $t^{-2/3}$  as  $t \rightarrow \infty$ . This rate is moreover shown to be sharp. Our result implies in particular that a general estimate in the literature, which predicts at least logarithmic decay and is known to be best possible in general, is suboptimal in the special case under consideration here. Our strategy of proof involves direct estimates based on separation of variables and a refined version of the technique developed in our earlier paper for a one-dimensional wave-heat system.

#### General information

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MoE publication type: A1 Journal article-refereed

Organisations: Computing Sciences, St Giles

Contributors: Batty, C., Paunonen, L., Seifert, D.

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ASJC Scopus subject areas: Analysis, Computational Mathematics, Applied Mathematics

Keywords: C -semigroups, Coupled, Energy, Heat equation, Rates of decay, Rectangular domain, Resolvent estimates, Wave equation

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10.1137/18M1195796

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Source ID: 85065492247

Research output: Contribution to journal › Article › Scientific › peer-review

### **SCIP: a single-cell image processor toolbox**

**Summary:** Each cell is a phenotypically unique individual that is influenced by internal and external processes, operating in parallel. To characterize the dynamics of cellular processes one needs to observe many individual cells from multiple points of view and over time, so as to identify commonalities and variability. With this aim, we engineered a software, 'SCIP', to analyze multi-modal, multi-process, time-lapse microscopy morphological and functional images. SCIP is capable of automatic and/or manually corrected segmentation of cells and lineages, automatic alignment of different microscopy channels, as well as detect, count and characterize fluorescent spots (such as RNA tagged by MS2-GFP), nucleoids, Z rings, Min system, inclusion bodies, undefined structures, etc. The results can be exported into \*.mat files and all results can be jointly analyzed, to allow studying not only each feature and process individually, but also find potential relationships. While we exemplify its use on Escherichia coli, many of its functionalities are expected to be of use in analyzing other prokaryotes and eukaryotic cells as well. We expect SCIP to facilitate the finding of relationships between cellular processes, from small-scale (e.g. gene expression) to large-scale (e.g. cell division), in single cells and cell lineages. Availability and implementation: [http://www.ca3-uninova.org/project\\_scip](http://www.ca3-uninova.org/project_scip). Supplementary information: Supplementary data are available at Bioinformatics online.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Campus FCT-UNL

Contributors: Martins, L., Neeli-Venkata, R., Oliveira, S. M., Häkkinen, A., Ribeiro, A. S., Fonseca, J. M.

Number of pages: 3

Pages: 4318-4320

Publication date: 15 Dec 2018

Peer-reviewed: Yes

### **Publication information**

Journal: Bioinformatics

Volume: 34

Issue number: 24

ISSN (Print): 1367-4803

Ratings:

Scopus rating (2018): CiteScore 9.7 SJR 4.549 SNIP 1.908

Original language: English

ASJC Scopus subject areas: Statistics and Probability, Biochemistry, Molecular Biology, Computer Science Applications, Computational Theory and Mathematics, Computational Mathematics

DOIs:

10.1093/bioinformatics/bty505

Research output: Contribution to journal › Article › Scientific › peer-review

### **Comparative analysis of tissue reconstruction algorithms for 3D histology**

**Motivation:** Digital pathology enables new approaches that expand beyond storage, visualization or analysis of histological samples in digital format. One novel opportunity is 3D histology, where a three-dimensional reconstruction of the sample is formed computationally based on serial tissue sections. This allows examining tissue architecture in 3D, for example, for diagnostic purposes. Importantly, 3D histology enables joint mapping of cellular morphology with spatially resolved omics data in the true 3D context of the tissue at microscopic resolution. Several algorithms have been proposed for the reconstruction task, but a quantitative comparison of their accuracy is lacking. **Results:** We developed a benchmarking framework to evaluate the accuracy of several free and commercial 3D reconstruction methods using two whole slide image datasets. The results provide a solid basis for further development and application of 3D histology algorithms and indicate that methods capable of compensating for local tissue deformation are superior to simpler approaches.

### **General information**

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Faculty of Biomedical Sciences and Engineering, Mechanical Engineering and Industrial Systems, Signal Processing, Research group: Data-analytics and Optimization, Tampere University Hospital, Faculty of Medicine and Life Sciences, BioMediTech, Fimlab Laboratories Ltd, BioMediTech Institute  
Contributors: Kartasalo, K., Latonen, L., Vihinen, J., Visakorpi, T., Nykter, M., Ruusuvoori, P.  
Number of pages: 9  
Pages: 3013-3021  
Publication date: 1 Sep 2018  
Peer-reviewed: Yes

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Journal: Bioinformatics  
Volume: 34  
Issue number: 17  
ISSN (Print): 1367-4803  
Ratings:  
Scopus rating (2018): CiteScore 9.7 SJR 4.549 SNIP 1.908  
Original language: English  
ASJC Scopus subject areas: Statistics and Probability, Biochemistry, Molecular Biology, Computer Science Applications, Computational Theory and Mathematics, Computational Mathematics  
Electronic versions:  
bty210  
DOIs:  
10.1093/bioinformatics/bty210  
URLs:  
<http://urn.fi/URN:NBN:fi:ty-201811162594>  
Source: Scopus  
Source ID: 85055091427  
Research output: Contribution to journal > Article > Scientific > peer-review

#### Multichannel Blind Sound Source Separation using Spatial Covariance Model with Level and Time Differences and Non-Negative Matrix Factorization

This paper presents an algorithm for multichannel sound source separation using explicit modeling of level and time differences in source spatial covariance matrices (SCM). We propose a novel SCM model in which the spatial properties are modeled by the weighted sum of direction of arrival (DOA) kernels. DOA kernels are obtained as the combination of phase and level difference covariance matrices representing both time and level differences between microphones for a grid of predefined source directions. The proposed SCM model is combined with the NMF model for the magnitude spectrograms. Opposite to other SCM models in the literature, in this work, source localization is implicitly defined in the model and estimated during the signal factorization. Therefore, no localization pre-processing is required. Parameters are estimated using complex-valued non-negative matrix factorization (CNMF) with both Euclidean distance and Itakura Saito divergence. Separation performance of the proposed system is evaluated using the two-channel SiSEC development dataset and four channels signals recorded in a regular room with moderate reverberation. Finally, a comparison to other state-of-the-art methods is performed, showing better achieved separation performance in terms of SIR and perceptual measures.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Signal Processing, Universidad de Jaen  
Contributors: Carabias Orti, J. J., Nikunen, J., Virtanen, T., Vera-Candeas, P.  
Pages: 1512-1527  
Publication date: Sep 2018  
Peer-reviewed: Yes  
Early online date: 26 Apr 2018

#### Publication information

Journal: IEEE/ACM Transactions on Audio Speech and Language Processing  
Volume: 26  
Issue number: 9  
ISSN (Print): 2329-9290  
Ratings:  
Scopus rating (2018): CiteScore 6.9 SJR 1.045 SNIP 2.428  
Original language: English  
ASJC Scopus subject areas: Computer Science (miscellaneous), Acoustics and Ultrasonics, Computational Mathematics, Electrical and Electronic Engineering

Keywords: Covariance matrices, direction of arrival estimation, Direction-of-arrival estimation, interaural level difference, interaural time difference, Kernel, Microphones, multichannel source separation, non-negative matrix factorization, Source separation, spatial covariance model, Spectrogram, Time-frequency analysis

DOIs:

10.1109/TASLP.2018.2830105

Source: Scopus

Source ID: 85046357571

Research output: Contribution to journal › Article › Scientific › peer-review

### Hypermonogenic Functions of Two Vector Variables

In this paper we introduce the modified Dirac operators (Formula presented.) and (Formula presented.), where (Formula presented.) is differentiable function, and (Formula presented.) is the Clifford algebra generated by the basis vectors of (Formula presented.). We look for solutions (Formula presented.) of the system (Formula presented.), where the first and third variables are invariant under rotations. These functions are called (Formula presented.)-hypermonogenic functions. We discuss about axially symmetric functions with respect to the symmetric group (Formula presented.). Some examples of axially symmetric (Formula presented.)-hypermonogenic functions generated by homogeneous functions and hypergeometric functions are presented.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Civil Engineering, University of Helsinki, Laboratory of Civil Engineering, Universidade de Aveiro

Contributors: Eriksson, S. L., Orelma, H., Vieira, N.

Number of pages: 16

Pages: 555–570

Publication date: 2018

Peer-reviewed: Yes

Early online date: 26 Sep 2017

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Journal: Complex Analysis and Operator Theory

Volume: 12

Issue number: 2

ISSN (Print): 1661-8254

Ratings:

Scopus rating (2018): CiteScore 1.2 SJR 0.459 SNIP 0.889

Original language: English

ASJC Scopus subject areas: Computational Theory and Mathematics, Computational Mathematics, Applied Mathematics

Keywords: Axially symmetric functions, Hypermonogenic functions, Modified Dirac operator, Several vector variables

DOIs:

10.1007/s11785-017-0728-7

### Bibliographical note

EXT="Eriksson, S. L."

Source: Scopus

Source ID: 85029901048

Research output: Contribution to journal › Article › Scientific › peer-review

### Chipless graphene tag and dual-CP reader for Internet of Things

This paper proposes a printable chipless tag that encodes more bits than a conventional tag, and also a dual circularly polarized (CP) reader that achieves high isolation as well as insensitive orientation. To demonstrate this concept, a radio-frequency identification (RFID) tag with a compact size of 12mm × 12mm is designed to encode 8 bits covering 6-9 GHz, and is investigated with dual-CP backscattering characteristics. Using conductive ink such as graphene, it is possible to directly print this kind of chipless tag on A4 papers, clothes, plastics, etc. This flexible low-cost tag and dual-CP reader are promising to significantly benefit the Internet of Things (IoT).

### General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Faculty of Biomedical Sciences and Engineering, Research group: Wireless Identification and Sensing Systems Research Group, BioMediTech, Southeast University, BioMediTech Institute

Contributors: Dong, G., Shen, Y., He, H., Virkki, J., Hu, S.

Publication date: 26 Sep 2017

### Host publication information

Title of host publication: 2017 International Applied Computational Electromagnetics Society Symposium in China, ACES-China 2017

Publisher: IEEE

ISBN (Electronic): 9780996007856

ASJC Scopus subject areas: Electrical and Electronic Engineering, Computational Mathematics, Instrumentation, Computer Networks and Communications

Keywords: Chipless tag, dual circular polarization, Internet of Things (IoT), radar cross section (RCS), radio-frequency identification (RFID)

Source: Scopus

Source ID: 85032786773

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

### Homogeneous $(\alpha, k)$ -Polynomial Solutions of the Fractional Riesz System in Hyperbolic Space

In this paper we study the fractional analogous of the Laplace–Beltrami equation and the hyperbolic Riesz system studied previously by H. Leutwiler, in (Formula presented.). In both cases we replace the integer derivatives by Caputo fractional derivatives of order (Formula presented.). We characterize the space of solutions of the fractional Laplace–Beltrami equation, and we calculate its dimension. We establish relations between the solutions of the fractional Laplace–Beltrami equation and the solutions of the hyperbolic fractional Riesz system. Some examples of the polynomial solutions will be presented. Moreover, the behaviour of the obtained results when (Formula presented.) is presented, and a final remark about the consideration of Riemann–Liouville fractional derivatives instead of Caputo fractional derivatives is made.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Mathematics, Universidade de Aveiro

Contributors: Orelma, H., Vieira, N.

Number of pages: 15

Pages: 1253–1267

Publication date: 2017

Peer-reviewed: Yes

Early online date: 1 Apr 2017

### Publication information

Journal: Complex Analysis and Operator Theory

Volume: 11

Issue number: 5

ISSN (Print): 1661-8254

Ratings:

Scopus rating (2017): CiteScore 1.3 SJR 0.663 SNIP 1.072

Original language: English

ASJC Scopus subject areas: Computational Theory and Mathematics, Computational Mathematics, Applied Mathematics

Keywords: Caputo fractional derivative, Hyperbolic, Hyperbolic fractional Riesz system, Hypermonogenic functions, Laplace–Beltrami fractional differential operator

DOIs:

10.1007/s11785-017-0666-4

Source: Scopus

Source ID: 85016641794

Research output: Contribution to journal › Article › Scientific › peer-review

### Integral kernels for $k$ -hypermonogenic functions

We consider the modified Cauchy–Riemann operator (Formula presented.) in the universal Clifford algebra (Formula presented.) with the basis (Formula presented.). The null-solutions of this operator are called  $k$ -hypermonogenic functions. We calculate the  $k$ -hyperbolic harmonic fundamental solutions, i.e. solutions to (Formula presented.), and use these solutions to find  $k$ -hypermonogenic kernels for a Cauchy-type integral formula in the upper half-space.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Mathematics, University of Helsinki

Contributors: Vuojamo, V., Eriksson, S.

Number of pages: 12

Pages: 1-12

Publication date: 2017

Peer-reviewed: Yes  
Early online date: 21 Feb 2017

### Publication information

Journal: Complex Variables and Elliptic Equations

Volume: 62

Issue number: 9

ISSN (Print): 1747-6933

Ratings:

Scopus rating (2017): CiteScore 1.4 SJR 0.616 SNIP 1.018

Original language: English

ASJC Scopus subject areas: Analysis, Numerical Analysis, Computational Mathematics, Applied Mathematics

Keywords: Cauchy integral formula, Clifford algebra, hyperbolic Laplace–Beltrami, k-hyperbolic harmonic, k-hypermonogenic

DOIs:

10.1080/17476933.2016.1250402

### Bibliographical note

EXT="Eriksson, Sirkka-Liisa"

Source: Scopus

Source ID: 85013192611

Research output: Contribution to journal › Article › Scientific › peer-review

### SamExploreR: Exploring reproducibility and robustness of RNA-seq results based on SAM files

Motivation: Data from RNA-seq experiments provide us with many new possibilities to gain insights into biological and disease mechanisms of cellular functioning. However, the reproducibility and robustness of RNA-seq data analysis results is often unclear. This is in part attributed to the two counter acting goals of (i) a cost efficient and (ii) an optimal experimental design leading to a compromise, e.g. in the sequencing depth of experiments. Results: We introduce an R package called samExploreR that allows the subsampling (m out of n bootstrapping) of short-reads based on SAM files facilitating the investigation of sequencing depth related questions for the experimental design. Overall, this provides a systematic way for exploring the reproducibility and robustness of general RNA-seq studies. We exemplify the usage of samExploreR by studying the influence of the sequencing depth and the annotation on the identification of differentially expressed genes.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Signal Processing, BioMediTech, Queen's University, Belfast, Northern Ireland, University of Arkansas for Medical Sciences, Nankai University

Contributors: Stupnikov, A., Tripathi, S., De Matos Simoes, R., McArt, D., Salto-Tellez, M., Glazko, G., Dehmer, M., Emmert-Streib, F.

Number of pages: 3

Pages: 3345-3347

Publication date: 1 Nov 2016

Peer-reviewed: Yes

### Publication information

Journal: Bioinformatics

Volume: 32

Issue number: 21

ISSN (Print): 1367-4803

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Scopus rating (2016): CiteScore 10.8 SJR 5.21 SNIP 2.336

Original language: English

ASJC Scopus subject areas: Statistics and Probability, Medicine(all), Biochemistry, Molecular Biology, Computer Science Applications, Computational Theory and Mathematics, Computational Mathematics

DOIs:

10.1093/bioinformatics/btw475

Source: Scopus

Source ID: 84994666672

Research output: Contribution to journal › Article › Scientific › peer-review

### Introducing libeemd: a program package for performing the ensemble empirical mode decomposition

The ensemble empirical mode decomposition (EEMD) and its complete variant (CEEMDAN) are adaptive, noise-assisted data analysis methods that improve on the ordinary empirical mode decomposition (EMD). All these methods decompose

possibly nonlinear and/or nonstationary time series data into a finite amount of components separated by instantaneous frequencies. This decomposition provides a powerful method to look into the different processes behind a given time series data, and provides a way to separate short time-scale events from a general trend. We present a free software implementation of EMD, EEMD and CEEMDAN and give an overview of the EMD methodology and the algorithms used in the decomposition. We release our implementation, libeemd, with the aim of providing a user-friendly, fast, stable, well-documented and easily extensible EEMD library for anyone interested in using (E)EMD in the analysis of time series data. While written in C for numerical efficiency, our implementation includes interfaces to the Python and R languages, and interfaces to other languages are straightforward.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research group: Quantum Control and Dynamics, Research area: Computational Physics, University of Jyväskylä

Contributors: Luukko, P. J. J., Helse, J., Räsänen, E.

Number of pages: 13

Pages: 545-557

Publication date: 1 Jun 2016

Peer-reviewed: Yes

### Publication information

Journal: Computational Statistics

Volume: 31

Issue number: 2

ISSN (Print): 0943-4062

Ratings:

Scopus rating (2016): CiteScore 2 SJR 0.706 SNIP 0.951

Original language: English

ASJC Scopus subject areas: Statistics and Probability, Computational Mathematics, Statistics, Probability and Uncertainty

Keywords: Adaptive data analysis, Detrending, Hilbert–Huang transform, Intrinsic mode function, Noise-assisted data analysis, Time series analysis

DOIs:

10.1007/s00180-015-0603-9

URLs:

<http://urn.fi/URN:NBN:fi:jyu-201604272338>

### Bibliographical note

EXT="Luukko, P. J. J."

Source: Scopus

Source ID: 84963783252

Research output: Contribution to journal > Article > Scientific > peer-review

### Characterizing rate limiting steps in transcription from RNA production times in live cells

Motivation: Single-molecule measurements of live *Escherichia coli* transcription dynamics suggest that this process ranges from sub- to super-Poissonian, depending on the conditions and on the promoter. For its accurate quantification, we propose a model that accommodates all these settings, and statistical methods to estimate the model parameters and to select the relevant components. Results: The new methodology has improved accuracy and avoids overestimating the transcription rate due to finite measurement time, by exploiting unobserved data and by accounting for the effects of discrete sampling. First, we use Monte Carlo simulations of models based on measurements to show that the methods are reliable and offer substantial improvements over previous methods. Next, we apply the methods on measurements of transcription intervals of different promoters in live *E. coli*, and show that they produce significantly different results, both in low- and high-noise settings, and that, in the latter case, they even lead to qualitatively different results. Finally, we demonstrate that the methods can be generalized for other similar purposes, such as for estimating gene activation kinetics. In this case, the new methods allow quantifying the inducer uptake dynamics as opposed to just comparing them between cases, which was not previously possible. We expect this new methodology to be a valuable tool for functional analysis of cellular processes using single-molecule or single-event microscopy measurements in live cells.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Laboratory of Biosystem Dynamics-LBD, Department of Signal Processing

Contributors: Häkkinen, A., Ribeiro, A. S.

Number of pages: 7

Pages: 1346-1352

Publication date: 1 May 2016

Peer-reviewed: Yes

### Publication information

Journal: Bioinformatics

Volume: 32

Issue number: 9

ISSN (Print): 1367-4803

Ratings:

Scopus rating (2016): CiteScore 10.8 SJR 5.21 SNIP 2.336

Original language: English

ASJC Scopus subject areas: Biochemistry, Molecular Biology, Computational Theory and Mathematics, Computer Science Applications, Computational Mathematics, Statistics and Probability

DOIs:

10.1093/bioinformatics/btv744

Source: Scopus

Source ID: 84966359423

Research output: [Contribution to journal](#) › [Article](#) › [Scientific](#) › [peer-review](#)

### Modeling probability densities with sums of exponentials via polynomial approximation

**Abstract** We propose a method for optimization with semi-infinite constraints that involve a linear combination of functions, focusing on shape-constrained optimization with exponential functions. Each function is lower and upper bounded on sub-intervals by low-degree polynomials. Thus, the constraints can be approximated with polynomial inequalities that can be implemented with linear matrix inequalities. Convexity is preserved, but the problem has now a finite number of constraints. We show how to take advantage of the properties of the exponential function in order to build quickly accurate approximations. The problem used for illustration is the least-squares fitting of a positive sum of exponentials to an empirical probability density function. When the exponents are given, the problem is convex, but we also give a procedure for optimizing the exponents. Several examples show that the method is flexible, accurate and gives better results than other methods for the investigated problems.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Signal Processing, Research group: SGN-SPAG, Department of Automatic Control and Computers, University Politehnica of Bucharest, Université de Pau et des Pays de l'Adour

Contributors: Dumitrescu, B., Şicleru, B. C., Avram, F.

Pages: 513–525

Publication date: 2016

Peer-reviewed: Yes

Early online date: 30 Jul 2015

### Publication information

Journal: Journal of Computational and Applied Mathematics

Volume: 292

ISSN (Print): 0377-0427

Ratings:

Scopus rating (2016): CiteScore 2.9 SJR 1.087 SNIP 1.315

Original language: English

ASJC Scopus subject areas: Computational Mathematics, Applied Mathematics

Keywords: Density fitting, Optimization, Polynomial approximation, Semi-infinite programming, Sum of exponentials

DOIs:

10.1016/j.cam.2015.07.032

Source: Scopus

Source ID: 84939247768

Research output: [Contribution to journal](#) › [Article](#) › [Scientific](#) › [peer-review](#)

### On k-Hypermonogenic Functions and Their Mean Value Properties

We study a hyperbolic version of holomorphic functions to higher dimensions. In this frame work, a generalization of holomorphic functions are called (Formula presented.)-hypermonogenic functions. These functions are depending on several real variables and their values are in a Clifford algebra. They are defined in terms of hyperbolic Dirac operators. They are connected to harmonic functions with respect to the Riemannian metric (Formula presented.) in the same way as the usual harmonic function to holomorphic functions. We present the mean value property for (Formula presented.)-hypermonogenic functions and related results. Earlier the mean value properties has been proved for hypermonogenic functions. The key tools are the invariance properties of the hyperbolic metric.



### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Department of Mathematics, Research group: MAT Clifford analysis  
Contributors: Eriksson, S., Orelma, H.  
Number of pages: 15  
Pages: 311-325  
Publication date: 2016  
Peer-reviewed: Yes  
Early online date: 8 Mar 2015

### Publication information

Journal: Complex Analysis and Operator Theory  
Volume: 10  
Issue number: 2  
ISSN (Print): 1661-8254  
Ratings:  
Scopus rating (2016): CiteScore 1.4 SJR 0.554 SNIP 0.776  
Original language: English  
ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics, Computational Theory and Mathematics  
Keywords: Dirac operator, Hyperbolic metric, Hypermonogenic, Monogenic  
DOIs:  
10.1007/s11785-015-0445-z  
Source: Scopus  
Source ID: 84955725749  
Research output: Contribution to journal > Article > Scientific > peer-review

### Two models for hydraulic cylinders in flexible multibody simulations

In modelling hydraulic cylinders interaction between the structural response and the hydraulic system needs to be taken into account. In this chapter two approaches for modelling flexible multibody systems coupled with hydraulic actuators i.e. cylinders are presented and compared. These models are the truss-elementlike cylinder and bending flexible cylinder models. The bending flexible cylinder element is a super-element combining the geometrically exact Reissner-beam element, the  $C^1$ -continuous slide-spring element needed for the telescopic movement and the hydraulic fluid field. Both models are embedded with a friction model based on a bristle approach. The models are implemented in a finite element environment. In time the coupled stiff differential equation system is integrated using the L-stable Rosenbrock method.

### General information

Publication status: Published  
MoE publication type: A3 Part of a book or another research book  
Organisations: Department of Civil Engineering, Research group: Structural Mechanics, Department of Mechanical Engineering and Industrial Systems, Research area: Applied Mechanics, FS Dynamics Finland Oy Ab  
Contributors: Ylinen, A., Mäkinen, J., Kouhia, R.  
Number of pages: 31  
Pages: 463-493  
Publication date: 2016

### Host publication information

Title of host publication: Computational Methods for Solids and Fluids : Multiscale Analysis, Probability Aspects and Model Reduction  
Publisher: Springer  
ISBN (Print): 978-3-319-27994-7  
ISBN (Electronic): 978-3-319-27996-1

### Publication series

Name: Computational Methods in Applied Sciences  
Volume: 41  
ISSN (Print): 1871-3033  
ASJC Scopus subject areas: Computational Mathematics, Modelling and Simulation, Fluid Flow and Transfer Processes, Computer Science Applications, Civil and Structural Engineering, Electrical and Electronic Engineering, Biomedical Engineering  
DOIs:  
10.1007/978-3-319-27996-1\_17

### Bibliographical note

JUFOID=79940  
EXT="Ylinen, Antti"

Source: Scopus

Source ID: 84964233721

Research output: Chapter in Book/Report/Conference proceeding › Chapter › Scientific › peer-review

### **A robust AMMI model for the analysis of genotype-by-environment data**

Motivation: One of the most widely used models to analyse genotype-by-environment data is the additive main effects and multiplicative interaction (AMMI) model. Genotype-by-environment data resulting from multi-location trials are usually organized in two-way tables with genotypes in the rows and environments (location-year combinations) in the columns. The AMMI model applies singular value decomposition (SVD) to the residuals of a specific linear model, to decompose the genotype-by-environment interaction (GEI) into a sum of multiplicative terms. However, SVD, being a least squares method, is highly sensitive to contamination and the presence of even a single outlier, if extreme, may draw the leading principal component towards itself resulting in possible misinterpretations and in turn lead to bad practical decisions. Since, as in many other real-life studies the distribution of these data is usually not normal due to the presence of outlying observations, either resulting from measurement errors or sometimes from individual intrinsic characteristics, robust SVD methods have been suggested to help overcome this handicap. Results: We propose a robust generalization of the AMMI model (the R-AMMI model) that overcomes the fragility of its classical version when the data are contaminated. Here, robust statistical methods replace the classic ones to model, structure and analyse GEI. The performance of the robust extensions of the AMMI model is assessed through a Monte Carlo simulation study where several contamination schemes are considered. Applications to two real plant datasets are also presented to illustrate the benefits of the proposed methodology, which can be broadened to both animal and human genetics studies. Availability and implementation: Source code implemented in R is available in the supplementary material under the function `r-AMMI`.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research Community on Data-to-Decision (D2D), Centro de Matemática e Aplicações (CMA, NOVA University of Lisbon

Contributors: Rodrigues, P. C., Monteiro, A., Lourenço, V. M.

Number of pages: 9

Pages: 58-66

Publication date: 1 Jul 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Bioinformatics

Volume: 32

Issue number: 1

ISSN (Print): 1367-4803

Ratings:

Scopus rating (2015): CiteScore 9.7 SJR 4.97 SNIP 2.16

Original language: English

ASJC Scopus subject areas: Biochemistry, Molecular Biology, Computational Theory and Mathematics, Computer Science Applications, Computational Mathematics, Statistics and Probability, Medicine(all)

DOIs:

10.1093/bioinformatics/btv533

URLs:

<http://www.scopus.com/inward/record.url?scp=84959872026&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84959872026

Research output: Contribution to journal › Article › Scientific › peer-review

### **Graph distance measures based on topological indices revisited**

Graph distance measures based on topological indices have been already explored by Dehmer et al. Also, inequalities for those graph distance measures have been proved. In this paper, we continue studying such comparative graph measures based on the well-known Wiener index, graph energy and Randić index, respectively. We prove extremal properties of the graph distance measures for some special classes of graphs. To demonstrate useful properties of the measures, we also discuss numerical results. To conclude the paper we state some open problems.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Signal Processing, BioMediTech, Research Community on Data-to-Decision (D2D), BioMediTech - Institute of Biosciences and Medical Technology, Department of Mechatronics and Biomedical Computer Science, Universität der Bundeswehr München, UMIT, Center for Combinatorics and LPMC-TJKLC, Eduard Wallnoefer Zentrum 1, Nankai University

Contributors: Dehmer, M., Emmert-Streib, F., Shi, Y.  
Number of pages: 11  
Pages: 623-633  
Publication date: 18 Jun 2015  
Peer-reviewed: Yes

#### Publication information

Journal: Applied Mathematics and Computation  
Volume: 266  
ISSN (Print): 0096-3003  
Ratings:  
Scopus rating (2015): CiteScore 2.9 SJR 0.95 SNIP 1.239  
Original language: English  
ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics  
Keywords: Distance measure, Edit distance, Extremal graph, Topological index  
DOIs:  
10.1016/j.amc.2015.05.072  
Source: Scopus  
Source ID: 84935922526  
Research output: Contribution to journal > Article > Scientific > peer-review

#### Estimation of GFP-tagged RNA numbers from temporal fluorescence intensity data

Motivation: MS2-GFP-tagging of RNA is currently the only method to measure intervals between consecutive transcription events in live cells. For this, new transcripts must be accurately detected from intensity time traces. Results: We present a novel method for automatically estimating RNA numbers and production intervals from temporal data of cell fluorescence intensities that reduces uncertainty by exploiting temporal information. We also derive a robust variant, more resistant to outliers caused e.g. by RNAs moving out of focus. Using Monte Carlo simulations, we show that the quantification of RNA numbers and production intervals is generally improved compared with previous methods. Finally, we analyze data from live Escherichia coli and show statistically significant differences to previous methods. The new methods can be used to quantify numbers and production intervals of any fluorescent probes, which are present in low copy numbers, are brighter than the cell background and degrade slowly. Availability: Source code is available under Mozilla Public License at <http://www.cs.tut.fi/%7ehakkin22/jumpdet/>. Contact:

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Department of Signal Processing, Research group: Laboratory of Biosystem Dynamics-LBD, Multi-scaled biodata analysis and modelling (MultiBAM)  
Contributors: Häkkinen, A., Ribeiro, A. S.  
Number of pages: 7  
Pages: 69-75  
Publication date: 1 Jan 2015  
Peer-reviewed: Yes

#### Publication information

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Scopus rating (2015): CiteScore 9.7 SJR 4.97 SNIP 2.16  
Original language: English  
ASJC Scopus subject areas: Biochemistry, Molecular Biology, Computational Theory and Mathematics, Computer Science Applications, Computational Mathematics, Statistics and Probability, Medicine(all)  
DOIs:  
10.1093/bioinformatics/btu592  
URLs:  
<http://www.scopus.com/inward/record.url?scp=84922352843&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

Contribution: organisation=sgn,FACT1=1<br/>Portfolio EDEND: 2014-09-15<br/>Publisher name: Oxford University Press  
Source: researchoutputwizzard  
Source ID: 396  
Research output: Contribution to journal > Article > Scientific > peer-review

### Van der Waals interactions are critical in Car-Parrinello molecular dynamics simulations of porphyrin-fullerene dyads

The interplay between electrostatic and van der Waals (vdW) interactions in porphyrin-C<sub>60</sub> dyads is still under debate despite its importance in influencing the structural characteristics of such complexes considered for various applications in molecular photovoltaics. In this article, we sample the conformational space of a porphyrin-C<sub>60</sub> dyad using Car-Parrinello molecular dynamics simulations with and without empirical vdW corrections. Long-range vdW interactions, which are poorly described by the commonly used density functional theory functionals, prove to be essential for a proper dynamics of the dyad moieties. Inclusion of vdW corrections brings porphyrin and C<sub>60</sub> close together in an orientation that is in agreement with experimental observations. The structural differences arising from the vdW corrections are shown to be significant for several properties and potentially less important for others. Additionally, our Mulliken population analysis reveals that contrary to the common belief, porphyrin is not the primary electron donating moiety for C<sub>60</sub>. In the considered dyad, fullerene's affinity for electrons is primarily satisfied by charge transfer from the amide group of the linker. However, we show that in the absence of another suitable bound donor, C<sub>60</sub> can withdraw electrons from porphyrin if it is sufficiently close.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Computational Science X (CompX), Frontier Photonics, VTT Technical Research Centre of Finland

Contributors: Karilainen, T., Cramariuc, O., Kuisma, M., Tappura, K., Hukka, T. I.

Number of pages: 10

Pages: 612-621

Publication date: 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Computational Chemistry

Volume: 36

Issue number: 9

ISSN (Print): 0192-8651

Ratings:

Scopus rating (2015): CiteScore 6.7 SJR 1.382 SNIP 1.368

Original language: English

ASJC Scopus subject areas: Chemistry(all), Computational Mathematics

Keywords: Car-Parrinello molecular dynamics, Fullerene, Porphyrin, Time-dependent-density functional theory

DOIs:

10.1002/jcc.23834

URLs:

<http://www.scopus.com/inward/record.url?scp=84923259668&partnerID=8YFLogxK> (Link to publication in Scopus)

#### Bibliographical note

ORG=fys,0.5

ORG=keb,0.5

Source: Scopus

Source ID: 84923259668

Research output: Contribution to journal > Article > Scientific > peer-review

#### Entropy bounds for dendrimers

Many graph invariants have been used for the construction of entropy-based measures to characterize the structure of complex networks. When considering Shannon entropy-based graph measures, there has been very little work to find their extremal values. A reason for this might be the fact that Shannon's entropy represents a multivariate function and all probability values are not equal to zero when considering graph entropies. Dehmer and Kraus proved some extremal results for graph entropies which are based on information functionals and express some conjectures generated by numerical simulations to find extremal values of graph entropies. Dehmer and Kraus discussed the extremal values of entropies for dendrimers. In this paper, we continue to study the extremal values of graph entropy for dendrimers, which has most interesting applications in molecular structure networks, and also in the pharmaceutical and biomedical area. Among all dendrimers with  $n$  vertices, we obtain the extremal values of graph entropy based on different well-known information functionals. Numerical experiments verifies our results.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research Community on Data-to-Decision (D2D), Nankai University, Universität der Bundeswehr München, Computational Biology and Machine Learning, Queen's University, Belfast, Northern Ireland  
Contributors: Chen, Z., Dehmer, M., Emmert-Streib, F., Shi, Y.  
Number of pages: 11  
Pages: 462-472  
Publication date: 1 Sep 2014  
Peer-reviewed: Yes

#### Publication information

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ISSN (Print): 0096-3003

Ratings:

Scopus rating (2014): CiteScore 2.9 SJR 0.961 SNIP 1.467

Original language: English

ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics

Keywords: Dendrimers, Extremal values, Graph entropy, Information theory, Shannon's entropy

DOIs:

10.1016/j.amc.2014.05.105

URLs:

<http://www.scopus.com/inward/record.url?scp=84903150191&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84903150191

Research output: Contribution to journal › Article › Scientific › peer-review

#### NetBioV: An R package for visualizing large network data in biology and medicine

NetBioV (Network Biology Visualization) is an R package that allows the visualization of large network data in biology and medicine. The purpose of NetBioV is to enable an organized and reproducible visualization of networks by emphasizing or highlighting specific structural properties that are of biological relevance.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research Community on Data-to-Decision (D2D), Prostate cancer research center (PCRC), Queen's University, Belfast, Northern Ireland, Universität der Bundeswehr München, Computational Biology and Machine Learning

Contributors: Tripathi, S., Dehmer, M., Emmert-Streib, F.

Number of pages: 3

Pages: 2834-2836

Publication date: 2 Apr 2014

Peer-reviewed: Yes

#### Publication information

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ISSN (Print): 1367-4803

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Original language: English

ASJC Scopus subject areas: Biochemistry, Molecular Biology, Computational Theory and Mathematics, Computer Science Applications, Computational Mathematics, Statistics and Probability, Medicine(all)

DOIs:

10.1093/bioinformatics/btu384

URLs:

<http://www.scopus.com/inward/record.url?scp=84911403383&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84911403383

Research output: Contribution to journal › Article › Scientific › peer-review

#### Gene Sets Net Correlations Analysis (GSNCA): A multivariate differential coexpression test for gene sets

Motivation: To date, gene set analysis approaches primarily focus on identifying differentially expressed gene sets (pathways). Methods for identifying differentially coexpressed pathways also exist but are mostly based on aggregated pairwise correlations or other pairwise measures of coexpression. Instead, we propose Gene Sets Net Correlations Analysis (GSNCA), a multivariate differential coexpression test that accounts for the complete correlation structure

between genes. Results: In GSNCA, weight factors are assigned to genes in proportion to the genes' cross-correlations (intergene correlations). The problem of finding the weight vectors is formulated as an eigenvector problem with a unique solution. GSNCA tests the null hypothesis that for a gene set there is no difference in the weight vectors of the genes between two conditions. In simulation studies and the analyses of experimental data, we demonstrate that GSNCA captures changes in the structure of genes' cross-correlations rather than differences in the averaged pairwise correlations. Thus, GSNCA infers differences in coexpression networks, however, bypassing method-dependent steps of network inference. As an additional result from GSNCA, we define hub genes as genes with the largest weights and show that these genes correspond frequently to major and specific pathway regulators, as well as to genes that are most affected by the biological difference between two conditions. In summary, GSNCA is a new approach for the analysis of differentially coexpressed pathways that also evaluates the importance of the genes in the pathways, thus providing unique information that may result in the generation of novel biological hypotheses.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research Community on Data-to-Decision (D2D), University of Arkansas for Medical Sciences, Computational Biology and Machine Learning, Queen's University, Belfast, Northern Ireland

Contributors: Rahmatallah, Y., Emmert-Streib, F., Glazko, G.

Number of pages: 9

Pages: 360-368

Publication date: 1 Feb 2014

Peer-reviewed: Yes

#### Publication information

Journal: Bioinformatics

Volume: 30

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ISSN (Print): 1367-4803

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ASJC Scopus subject areas: Biochemistry, Molecular Biology, Computational Theory and Mathematics, Computer Science Applications, Computational Mathematics, Statistics and Probability, Medicine(all)

DOIs:

[10.1093/bioinformatics/btt687](https://doi.org/10.1093/bioinformatics/btt687)

URLs:

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Source: Scopus

Source ID: 84893275855

Research output: Contribution to journal > Article > Scientific > peer-review

#### A full-potential linearized augmented plane wave study of the interaction of CO<sub>2</sub> with $\alpha$ -Pu (020) surface nanolayers

Adsorption of CO<sub>2</sub> on  $\alpha$ -Pu (020) surface nanolayers is investigated using GGA-DFT and the suite of software DMOL<sup>3</sup> and WIEN2k. Completely dissociated configurations (C+O+O) exhibit the strongest binding with the surface (7.94 eV), followed by partially dissociated (CO+O) and molecular CO<sub>2</sub> configurations (5.18 and 1.90 eV, respectively). For initial vertically upright orientations, final configuration of the CO<sub>2</sub> molecule does not change after optimization. For initial flat lying orientations, the final states correspond to bent geometry with a bond angle of ~130°. For CO+O coadsorptions, the stable configurations correspond to CO dipole moment orientations of 105°-167° with respect to the normal surface.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), University of Texas at Arlington

Contributors: Wang, J., Ray, A. K.

Number of pages: 8

Pages: 1710-1717

Publication date: 2014

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Computational and Theoretical Nanoscience

Volume: 11

Issue number: 7

ISSN (Print): 1546-1955

Ratings:

Scopus rating (2014): CiteScore 1.9 SJR 0.326 SNIP 0.773

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Electrical and Electronic Engineering, Materials Science(all), Computational Mathematics, Chemistry(all)

Keywords: Adsorption, Alpha-Plutonium, Carbon Dioxide, Density Functional Theory, Nanolayers

DOIs:

10.1166/jctn.2014.3555

URLs:

<http://www.scopus.com/inward/record.url?scp=84898458971&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84898458971

Research output: Contribution to journal > Article > Scientific > peer-review

### **A microscopic view of the mechanisms of active transport across the cellular membrane**

Membrane transporters are molecular machines that couple active transport of their specific substrates to various sources of cellular energy through a set of highly coordinated protein conformational changes. The alternating-access mechanism of transport in these proteins, which ensures that the substrate is only accessible from one side of the membrane at any given time, relies on complex and global protein conformational changes that are also closely coupled to molecular events such as substrate binding and translocation. In this review, we describe the application of advanced molecular modeling and simulation technologies to a number of membrane transport proteins studied in our laboratory. The goal is to demonstrate the power of the methods in describing functionally relevant molecular events ranging from more localized events such as substrate binding and gating motions to large, global protein conformational changes governing the transition of the protein between major functional states.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Department of Biochemistry, Univ Illinois, University of Illinois System, University of Illinois Urbana-Champaign, Frederick Seitz Mat Res Lab, Dept Mat Sci & Engr

Contributors: Enkavi, G., Li, J., Wen, P., Thangapandian, S., Moradi, M., Jiang, T., Han, W., Tajkhorshid, E.

Number of pages: 49

Pages: 77-125

Publication date: 2014

Peer-reviewed: Yes

### **Publication information**

Journal: Annual Reports in Computational Chemistry

Volume: 10

ISSN (Print): 1574-1400

Ratings:

Scopus rating (2014): CiteScore 2.3 SJR 0.74 SNIP 0

Original language: English

ASJC Scopus subject areas: Chemistry(all), Computational Mathematics

Keywords: Conformational changes, Membrane transporters, Molecular dynamics, Nonequilibrium simulation, Primary transporters, Secondary transporters, Substrate binding

DOIs:

10.1016/B978-0-444-63378-1.00004-5

URLs:

<http://www.scopus.com/inward/record.url?scp=84919386963&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84919386963

Research output: Contribution to journal > Article > Scientific > peer-review

### **Magnetic origin of the chemical balance in alloyed Fe-Cr stainless steels: First-principles and Ising model study**

Iron-chromium is the base material for most of the stainless steel grades. Recently, new insights into the origins of fundamental physical and chemical characteristics of Fe-Cr based alloys have been achieved. Some of the new results are quite unexpected and call for further investigations. The present study focuses on the magnetic contribution in the atomic driving forces related to the chemical composition in Fe-Cr when alloyed with Al, Ti, V, Mn, Co, Ni, and Mo. Using the ab initio exact muffin-tin orbitals method combined with an Ising-type spin model, we demonstrate that the magnetic moment of the solute atoms with the induced changes in the magnetic moments of the host atoms form the main factor in determining the mixing energy and chemical potentials of low-Cr Fe-Cr based alloys. The results obtained in the present work are related to the designing and tuning of the microstructure and corrosion protection of low-Cr steels.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Turun Yliopisto/Turun Biomateriaalikeskus, Department of Physics and Astronomy, University of Turku, Abo Akad Univ, Abo Akademi University, Dept Phys, Uppsala University, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences

Contributors: Airiskallio, E., Nurmi, E., Väyrynen, I. J., Kokko, K., Ropo, M., Punkkinen, M. P. J., Johansson, B., Vitos, L.

Number of pages: 6

Pages: 135-140

Publication date: 2014

Peer-reviewed: Yes

### Publication information

Journal: Computational Materials Science

Volume: 92

ISSN (Print): 0927-0256

Ratings:

Scopus rating (2014): CiteScore 3.6 SJR 1.098 SNIP 1.612

Original language: English

ASJC Scopus subject areas: Computer Science(all), Chemistry(all), Materials Science(all), Mechanics of Materials, Physics and Astronomy(all), Computational Mathematics

Keywords: Al, Chemical potential, Co, Corrosion protection, Cr, Fe, First principles calculation, Ising model, Magnetic moment, Mixing energy, Mn, Mo, Ni, Stainless steel, Ti, V

DOIs:

10.1016/j.commatsci.2014.05.036

URLs:

<http://www.scopus.com/inward/record.url?scp=84902660256&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84902660256

Research output: Contribution to journal > Article > Scientific > peer-review

### An efficient heuristic approach to detecting graph isomorphism based on combinations of highly discriminating invariants

The search for an easily computable, finite, complete set of graph invariants remains a challenging research topic. All measures characterizing the topology of a graph that have been developed thus far exhibit some degree of degeneracy, i.e., an inability to distinguish between non-isomorphic graphs. In this paper, we show that certain graph invariants can be useful in substantially reducing the computational complexity of isomorphism testing. Our findings are underpinned by numerical results based on a large scale statistical analysis.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research Community on Data-to-Decision (D2D), Institute for Bioinformatics and Translational Research, The City College of New York (CUNY), Computational Biology and Machine Learning Lab., Faculty of Medicine, Health and Life Sciences, Queen's University, Belfast, Northern Ireland

Contributors: Dehmer, M., Grabner, M., Mowshowitz, A., Emmert-Streib, F.

Number of pages: 15

Pages: 311-325

Publication date: Aug 2013

Peer-reviewed: Yes

### Publication information

Journal: Advances in Computational Mathematics

Volume: 39

Issue number: 2

ISSN (Print): 1019-7168

Ratings:

Scopus rating (2013): CiteScore 2.7 SJR 1.063 SNIP 1.644

Original language: English

ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics

Keywords: Graph isomorphism, Graph measures, Graph topology, Graphs, Uniqueness

DOIs:

10.1007/s10444-012-9281-0

URLs:

<http://www.scopus.com/inward/record.url?scp=84884974800&partnerID=8YFLogxK> (Link to publication in Scopus)



Source: Scopus

Source ID: 84884974800

Research output: Contribution to journal › Article › Scientific › peer-review

### Density functional theory study of FePd<sub>n</sub> (n = 2-14) clusters and interactions with small molecules

First-principles calculations have been conducted to investigate the properties of FePd<sub>n</sub> (n = 2-14) clusters. In the lowest energy structures of FePd<sub>n</sub> clusters, the Fe atom gradually moves from the convex to the surface, and then to the interior site with the number of Pd atoms increasing from 2 to 14. The magnetic moments of Pd<sub>n</sub> clusters have been enhanced by the doping of Fe impurity. Furthermore, the adsorption of small molecules, including NH<sub>3</sub>, H<sub>2</sub>O, CO, H<sub>2</sub>, and O<sub>2</sub>, on the higher stability of FePd<sub>n</sub> (n = 5, 7, 10, and 12) clusters were studied. The lowest energy adsorption structures are obtained for each molecule. On the whole, the adsorption energies vary as the order of  $E_a(\text{H}_2\text{O}) < E_a(\text{H}_2) < E_a(\text{NH}_3) < E_a(\text{O}_2) < E_a(\text{CO})$ . NH<sub>3</sub>, CO and H<sub>2</sub> molecules prefer to adsorb on the FePd<sub>10</sub> cluster with the highest adsorption energy, while H<sub>2</sub>O and O<sub>2</sub> are more like to adsorb on the FePd<sub>5</sub>. The magnetic moments of FePd<sub>n</sub> clusters are reduced with the adsorption of molecules.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), Northwest University China, National Laboratory of Solid State Microstructures, Nanjing University, Institute of Photonics and Photo-technology

Contributors: Ma, L., Wang, J., Hao, Y., Wang, G.

Number of pages: 8

Pages: 166-173

Publication date: Feb 2013

Peer-reviewed: Yes

#### Publication information

Journal: Computational Materials Science

Volume: 68

ISSN (Print): 0927-0256

Ratings:

Scopus rating (2013): CiteScore 3.5 SJR 0.951 SNIP 1.306

Original language: English

ASJC Scopus subject areas: Computer Science(all), Chemistry(all), Materials Science(all), Mechanics of Materials, Physics and Astronomy(all), Computational Mathematics

Keywords: Cluster, Density functional theory, Small molecule adsorption

DOIs:

10.1016/j.commat.2012.10.014

URLs:

<http://www.scopus.com/inward/record.url?scp=84869874680&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84869874680

Research output: Contribution to journal › Article › Scientific › peer-review

### Growth behavior and magnetic properties of spherical uranium oxide nanoclusters

The growth behavior and magnetic properties of spherical uranium oxide nanoclusters have been investigated using the generalized gradient approximation (GGA) to density functional theory (DFT). The geometries of U<sub>n</sub>O<sub>m</sub> clusters remain the O<sub>n</sub> symmetry after DFT relaxation. The largest binding energy corresponds to the cluster with the smallest deviation from the bulk (UO<sub>2</sub>) ratio. The electronic structures and magnetic properties of these nanoclusters are presented. We find the chemical bonding between the U and O atoms has a significant ionic character. The reduction of magnetism in the inner positions can be understood by the charge transfer and the hybridization between U atoms and the neighboring O atoms.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Science X (CompX), University of Texas at Arlington

Contributors: Ma, L., Ray, A. K.

Number of pages: 7

Pages: 334-340

Publication date: Feb 2013

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Computational and Theoretical Nanoscience

Volume: 10

Issue number: 2

ISSN (Print): 1546-1955

Ratings:

Scopus rating (2013): CiteScore 1.4 SJR 0.384 SNIP 0.593

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Electrical and Electronic Engineering, Materials Science(all), Computational Mathematics, Chemistry(all)

Keywords: Growth behavior, Magnetism, Nanoclusters, Uranium oxide

DOIs:

10.1166/jctn.2013.2701

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<http://www.scopus.com/inward/record.url?scp=84876525693&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84876525693

Research output: Contribution to journal > Article > Scientific > peer-review

### **Gene set analysis for self-contained tests: Complex null and specific alternative hypotheses**

Motivation: The analysis of differentially expressed gene sets became a routine in the analyses of gene expression data.

There is a multitude of tests available, ranging from aggregation tests that summarize gene-level statistics for a gene set to true multivariate tests, accounting for intergene correlations. Most of them detect complex departures from the null hypothesis but when the null hypothesis is rejected the specific alternative leading to the rejection is not easily identifiable.

Results: In this article we compare the power and Type I error rates of minimum-spanning tree (MST)-based non-parametric multivariate tests with several multivariate and aggregation tests, which are frequently used for pathway analyses. In our simulation study, we demonstrate that MST-based tests have power that is for many settings comparable with the power of conventional approaches, but outperform them in specific regions of the parameter space corresponding to biologically relevant configurations. Further, we find for simulated and for gene expression data that MST-based tests discriminate well against shift and scale alternatives. As a general result, we suggest a two-step practical analysis strategy that may increase the interpretability of experimental data: first, apply the most powerful multivariate test to find the subset of pathways for which the null hypothesis is rejected and second, apply MST-based tests to these pathways to select those that support specific alternative hypotheses.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Prostate cancer research center (PCRC), University of Arkansas for Medical Sciences, Computational Biology and Machine Learning, Queen's University, Belfast, Northern Ireland

Contributors: Rahmatallah, Y., Emmert-Streib, F., Glazko, G.

Number of pages: 8

Pages: 3073-3080

Publication date: Dec 2012

Peer-reviewed: Yes

### **Publication information**

Journal: Bioinformatics

Volume: 28

Issue number: 23

ISSN (Print): 1367-4803

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Scopus rating (2012): CiteScore 10.5 SJR 5.275 SNIP 2.051

Original language: English

ASJC Scopus subject areas: Biochemistry, Molecular Biology, Computational Theory and Mathematics, Computer Science Applications, Computational Mathematics, Statistics and Probability, Medicine(all)

DOIs:

10.1093/bioinformatics/bts579

URLs:

<http://www.scopus.com/inward/record.url?scp=84870441671&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84870441671

Research output: Contribution to journal > Article > Scientific > peer-review

### **Universal construction mechanism for networks from one-dimensional symbol sequences**

In this paper we introduce construction mechanisms to generate directed networks from one-dimensional symbol sequences. We prove that any of these construction mechanisms leads to the same undirected network. Further, we prove that the introduced construction mechanisms are universal in the sense that any undirected network can be generated by such a mechanism. In addition, we provide various numerical examples to demonstrate the applicability of the introduced mechanism.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research Community on Data-to-Decision (D2D), Computational Biology and Machine Learning, Queen's University, Belfast, Northern Ireland

Contributors: Emmert-Streib, F.

Number of pages: 11

Pages: 1020-1030

Publication date: 15 Oct 2012

Peer-reviewed: Yes

#### **Publication information**

Journal: Applied Mathematics and Computation

Volume: 219

Issue number: 3

ISSN (Print): 0096-3003

Ratings:

Scopus rating (2012): CiteScore 2.8 SJR 1.02 SNIP 1.295

Original language: English

ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics

Keywords: Complex networks, Network construction, Random networks, Symbol sequences, Universal network construction

DOIs:

10.1016/j.amc.2012.07.006

URLs:

<http://www.scopus.com/inward/record.url?scp=84867336661&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84867336661

Research output: Contribution to journal > Article > Scientific > peer-review

### **Evolutionary dynamics of the spatial Prisoner's Dilemma with self-inhibition**

In this paper we study the influence of interventions on self-interactions in a spatial Prisoner's Dilemma on a two-dimensional grid with periodic boundary conditions and synchronous updating of the dynamics. We investigate two different types of self-interaction modifications. The first type (FSIP) is deterministic, effecting each self-interaction of a player by a constant factor, whereas the second type (PSIP) performs a probabilistic interventions. Both types of interventions lead to a reduction of the payoff of the players and, hence, represent inhibiting effects. We find that a constant but moderate reduction of self-interactions has a very beneficial effect on the evolution of cooperators in the population, whereas probabilistic interventions on self-interactions are in general counter productive for the coexistence of the two different strategies.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research Community on Data-to-Decision (D2D), Computational Biology and Machine Learning, Queen's University, Belfast, Northern Ireland

Contributors: Emmert-Streib, F.

Number of pages: 7

Pages: 6482-6488

Publication date: 5 Feb 2012

Peer-reviewed: Yes

#### **Publication information**

Journal: Applied Mathematics and Computation

Volume: 218

Issue number: 11

ISSN (Print): 0096-3003

Ratings:

Scopus rating (2012): CiteScore 2.8 SJR 1.02 SNIP 1.295

Original language: English

ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics

Keywords: Evolutionary dynamics, Evolutionary game theory, Game theory, Prisoner's dilemma

DOIs:

10.1016/j.amc.2011.12.018

URLs:

<http://www.scopus.com/inward/record.url?scp=84855904251&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84855904251

Research output: Contribution to journal › Article › Scientific › peer-review

### **Machine learning: How it can help nanocomputing**

We examine possibilities for making advances in nanocomputing by bringing in ideas from the field of machine learning. The potential from combining machine learning with nanocomputing seems to be underutilized. We review three complementary approaches. Firstly, machine learning can be used in the different phases of developing complicated nanocomputing devices: in modeling, designing, constructing, and programming the devices. Secondly, machine learning methods implemented by nanocomputing hardware can be a competitive solution especially for specialized application areas like sensory information processing; working towards such implementations advances nanocomputing by guiding development of the nanocomponents and architectures required for such applications. Thirdly, nanotechnology enabled quantum computing can significantly increase our capacity to solve NP-complete optimization problems; although this increase is not specific to machine learning, several such problems occur in machine learning and artificial intelligence, hence solving such problems is a useful goal that partly motivates development of quantum computing. The main value of this paper is to provide new ideas for researchers working on nanocomputing, nanoarchitectures, development and design of nanoprocessors and other nanocomponents, or nanomanufacturing.

### **General information**

Publication status: Published

MoE publication type: A2 Review article in a scientific journal

Organisations: Research Community on Data-to-Decision (D2D), Nokia, Aalto University

Contributors: Uusitalo, M. A., Peltonen, J., Ryhänen, T.

Number of pages: 17

Pages: 1347-1363

Publication date: Aug 2011

Peer-reviewed: Yes

### **Publication information**

Journal: Journal of Computational and Theoretical Nanoscience

Volume: 8

Issue number: 8

ISSN (Print): 1546-1955

Ratings:

Scopus rating (2011): CiteScore 1.5 SJR 0.398 SNIP 0.477

Original language: English

ASJC Scopus subject areas: Chemistry(all), Materials Science(all), Condensed Matter Physics, Computational Mathematics, Electrical and Electronic Engineering

Keywords: Machine Learning, Nanoarchitectures, Nanocomputing, Nanotechnology, Neural Networks, Quantum Computing

DOIs:

10.1166/jctn.2011.1821

URLs:

<http://www.scopus.com/inward/record.url?scp=84856844597&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84856844597

Research output: Contribution to journal › Review Article › Scientific › peer-review

### **BACOM: In silico detection of genomic deletion types and correction of normal cell contamination in copy number data**

Motivation: Identification of somatic DNA copy number alterations (CNAs) and significant consensus events (SCEs) in cancer genomes is a main task in discovering potential cancer-driving genes such as oncogenes and tumor suppressors. The recent development of SNP array technology has facilitated studies on copy number changes at a genome-wide scale with high resolution. However, existing copy number analysis methods are oblivious to normal cell contamination and cannot distinguish between contributions of cancerous and normal cells to the measured copy number signals. This contamination could significantly confound downstream analysis of CNAs and affect the power to detect SCEs in clinical samples. Results: We report here a statistically principled in silico approach, Bayesian Analysis of COpy number Mixtures (BACOM), to accurately estimate genomic deletion type and normal tissue contamination, and accordingly recover the true copy number profile in cancer cells. We tested the proposed method on two simulated datasets, two prostate cancer

datasets and The Cancer Genome Atlas high-grade ovarian dataset, and obtained very promising results supported by the ground truth and biological plausibility. Moreover, based on a large number of comparative simulation studies, the proposed method gives significantly improved power to detect SCEs after in silico correction of normal tissue contamination. We develop a cross-platform open-source Java application that implements the whole pipeline of copy number analysis of heterogeneous cancer tissues including relevant processing steps. We also provide an R interface, *bacomR*, for running BACOM within the R environment, making it straightforward to include in existing data pipelines.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Prostate cancer research center (PCRC), Virginia Tech, Johns Hopkins School of Medicine, Wake Forest University School of Medicine

Contributors: Yu, G., Zhang, B., Bova, G. S., Xu, J., Shih, I. M., Wang, Y.

Number of pages: 8

Pages: 1473-1480

Publication date: Jun 2011

Peer-reviewed: Yes

#### Publication information

Journal: Bioinformatics

Volume: 27

Issue number: 11

Article number: btr183

ISSN (Print): 1367-4803

Ratings:

Scopus rating (2011): CiteScore 8.9 SJR 4.118 SNIP 1.83

Original language: English

ASJC Scopus subject areas: Biochemistry, Molecular Biology, Computational Theory and Mathematics, Computer Science Applications, Computational Mathematics, Statistics and Probability, Medicine(all)

DOIs:

10.1093/bioinformatics/btr183

URLs:

<http://www.scopus.com/inward/record.url?scp=79957859881&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 79957859881

Research output: Contribution to journal > Article > Scientific > peer-review

#### The different levels of magneto-mechanical coupling in energy conversion machines and devices

This paper reviews the methods for coupling the magnetic and mechanical problems in magnetic materials and their application to electrical machines. The reviewed methods include both the material models and the computing methods as well as the methods for computing the magnetic forces. The paper shows that there are different levels of coupling the magnetic system with the mechanical one and that the use of a method or another depends on the application and the level of accuracy aimed at. The paper also clarifies some terms and concepts related to the coupling terminology such as strong, weak, local, global, direct and indirect coupling and put these terms in a coherent context. Most of the examples are related to the two dimensional analysis but some three dimensional ones are also shown.

#### General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Life Cycle Effectiveness of the Built Environment (LCE@BE), Aalto University

Contributors: Belahcen, A., Kouhia, R., Fonteyn, K.

Number of pages: 12

Pages: 472-483

Publication date: 2011

#### Host publication information

Title of host publication: Proceedings of the 4th International Conference on Computational Methods for Coupled Problems in Science and Engineering, COUPLED PROBLEMS 2011

ISBN (Print): 9788489925786

ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics

Keywords: Computing Methods, Coupled problems, Electrical machines, Magnetic forces, Magneto-mechanics, Magnetostriction

URLs:

<http://www.scopus.com/inward/record.url?scp=84857432902&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84857432902

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

### **Revealing differences in gene network inference algorithms on the network level by ensemble methods**

Motivation: The inference of regulatory networks from large-scale expression data holds great promise because of the potentially causal interpretation of these networks. However, due to the difficulty to establish reliable methods based on observational data there is so far only incomplete knowledge about possibilities and limitations of such inference methods in this context. Results: In this article, we conduct a statistical analysis investigating differences and similarities of four network inference algorithms, ARACNE, CLR, MRNET and RN, with respect to local network-based measures. We employ ensemble methods allowing to assess the inferability down to the level of individual edges. Our analysis reveals the bias of these inference methods with respect to the inference of various network components and, hence, provides guidance in the interpretation of inferred regulatory networks from expression data. Further, as application we predict the total number of regulatory interactions in human B cells and hypothesize about the role of Myc and its targets regarding molecular information processing.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: School of Medicine, Computational Biology and Machine Learning

Contributors: Altay, G., Emmert-Streib, F.

Number of pages: 7

Pages: 1738-1744

Publication date: 25 May 2010

Peer-reviewed: Yes

#### **Publication information**

Journal: Bioinformatics

Volume: 26

Issue number: 14

Article number: btq259

ISSN (Print): 1367-4803

Ratings:

Scopus rating (2010): SJR 3.661 SNIP 1.886

Original language: English

ASJC Scopus subject areas: Biochemistry, Molecular Biology, Computational Theory and Mathematics, Computer Science Applications, Computational Mathematics, Statistics and Probability, Medicine(all)

DOIs:

10.1093/bioinformatics/btq259

URLs:

<http://www.scopus.com/inward/record.url?scp=77954484005&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 77954484005

Research output: Contribution to journal > Article > Scientific > peer-review

### **Unite and conquer: Univariate and multivariate approaches for finding differentially expressed gene sets**

Motivation: Recently, many univariate and several multivariate approaches have been suggested for testing differential expression of gene sets between different phenotypes. However, despite a wealth of literature studying their performance on simulated and real biological data, still there is a need to quantify their relative performance when they are testing different null hypotheses. Results: In this article, we compare the performance of univariate and multivariate tests on both simulated and biological data. In the simulation study we demonstrate that high correlations equally affect the power of both, univariate as well as multivariate tests. In addition, for most of them the power is similarly affected by the dimensionality of the gene set and by the percentage of genes in the set, for which expression is changing between two phenotypes. The application of different test statistics to biological data reveals that three statistics (sum of squared t-tests, Hotelling's  $T^2$ , N-statistic), testing different null hypotheses, find some common but also some complementing differentially expressed gene sets under specific settings. This demonstrates that due to complementing null hypotheses each test projects on different aspects of the data and for the analysis of biological data it is beneficial to use all three tests simultaneously instead of focusing exclusively on just one.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: University of Rochester Medical Center, Computational Biology and Machine Learning, Queen's University, Belfast, Northern Ireland

Contributors: Glazko, G. V., Emmert-Streib, F.  
Number of pages: 7  
Pages: 2348-2354  
Publication date: Sep 2009  
Peer-reviewed: Yes

#### Publication information

Journal: Bioinformatics

Volume: 25

Issue number: 18

ISSN (Print): 1367-4803

Ratings:

Scopus rating (2009): SJR 3.111 SNIP 1.834

Original language: English

ASJC Scopus subject areas: Biochemistry, Molecular Biology, Computational Theory and Mathematics, Computer Science Applications, Computational Mathematics, Statistics and Probability

DOIs:

10.1093/bioinformatics/btp406

Source: Scopus

Source ID: 69849105388

Research output: Contribution to journal › Article › Scientific › peer-review

#### A comparative analysis of multidimensional features of objects resembling sets of graphs

In the present paper, we introduce a notion of a style representing abstract, complex objects having characteristics that can be represented as structured objects. Furthermore, we provide some mathematical properties of such styles. As a main result, we present a novel approach to perform a meaningful comparative analysis of such styles by defining and using graph-theoretic measures. We compare two styles by comparing the underlying feature sets representing sets of graph structurally. To determine the structural similarity between the underlying graphs, we use graph similarity measures that are computationally efficient. More precisely, in order to compare styles, we map each feature set to a so-called median graph and compare the resulting median graphs. As an application, we perform an experimental study to compare special styles representing sets of undirected graphs and present numerical results thereof.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: TU Vienna, Department of Biostatistics, Visiting Graduate Student in Department of Urban Design and Planning, University of Washington, Seattle, USA 1.1.2012-15.6.2012 (12.9.2011 alkaen), University of Veterinary Medicine Vienna

Contributors: Dehmer, M., Emmert-Streib, F., Gesell, T.

Number of pages: 15

Pages: 221-235

Publication date: 15 Feb 2008

Peer-reviewed: Yes

#### Publication information

Journal: Applied Mathematics and Computation

Volume: 196

Issue number: 1

ISSN (Print): 0096-3003

Ratings:

Scopus rating (2008): SJR 0.778 SNIP 0.983

Original language: English

ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics, Numerical Analysis

Keywords: Classification, Object comparison, Similarity, Structural similarity, Structured objects

DOIs:

10.1016/j.amc.2007.05.058

Source: Scopus

Source ID: 38049038817

Research output: Contribution to journal › Article › Scientific › peer-review

#### Structural similarity of directed universal hierarchical graphs: A low computational complexity approach

In the present paper we mainly introduce an efficient approach to measure the structural similarity of so called directed universal hierarchical graphs. We want to underline that directed universal hierarchical graphs can be obtained from generalized trees which are already introduced. In order to classify these graphs, we state our novel graph similarity method. As a main result we notice that our novel algorithm has low computational complexity.

### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: University of Veterinary Medicine Vienna, Stowers Institute for Medical Research  
Contributors: Dehmer, M., Emmert-Streib, F.  
Number of pages: 14  
Pages: 7-20  
Publication date: 1 Dec 2007  
Peer-reviewed: Yes

### Publication information

Journal: Applied Mathematics and Computation  
Volume: 194  
Issue number: 1  
ISSN (Print): 0096-3003  
Ratings:  
Scopus rating (2007): SJR 0.869 SNIP 1.113  
Original language: English  
ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics, Numerical Analysis  
Keywords: Complexity analysis, Graph classes, Graph classification, Graph similarity, Hierarchical models, Structured objects  
DOIs:  
10.1016/j.amc.2007.04.006  
URLs:  
<http://www.scopus.com/inward/record.url?scp=35648968162&partnerID=8YFLogxK> (Link to publication in Scopus)  
Source: Scopus  
Source ID: 35648968162  
Research output: Contribution to journal > Article > Scientific > peer-review

### Information theoretic measures of UHG graphs with low computational complexity

We introduce a novel graph class we call universal hierarchical graphs (UHG) whose topology can be found numerous in problems representing, e.g., temporal, spacial or general process structures of systems. For this graph class we show, that we can naturally assign two probability distributions, for nodes and for edges, which lead us directly to the definition of the entropy and joint entropy and, hence, mutual information establishing an information theory for this graph class. Furthermore, we provide some results under which conditions these constraint probability distributions maximize the corresponding entropy. Also, we demonstrate that these entropic measures can be computed efficiently which is a prerequisite for every large scale practical application and show some numerical examples.

### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Stowers Institute for Medical Research, University of Veterinary Medicine Vienna  
Contributors: Emmert-Streib, F., Dehmer, M.  
Number of pages: 12  
Pages: 1783-1794  
Publication date: 15 Jul 2007  
Peer-reviewed: Yes

### Publication information

Journal: Applied Mathematics and Computation  
Volume: 190  
Issue number: 2  
ISSN (Print): 0096-3003  
Ratings:  
Scopus rating (2007): SJR 0.869 SNIP 1.113  
Original language: English  
ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics, Numerical Analysis  
Keywords: Entropy, Graph classes, Graph measures, Hierarchical graphs, Information theory  
DOIs:  
10.1016/j.amc.2007.02.095  
URLs:  
<http://www.scopus.com/inward/record.url?scp=34250623666&partnerID=8YFLogxK> (Link to publication in Scopus)  
Source: Scopus  
Source ID: 34250623666



### Comparing large graphs efficiently by margins of feature vectors

Measuring the structural similarity of graphs is a challenging and outstanding problem. Most of the classical approaches of the so-called exact graph matching methods are based on graph or subgraph isomorphic relations of the underlying graphs. In contrast to these methods in this paper we introduce a novel approach to measure the structural similarity of directed and undirected graphs that is mainly based on margins of feature vectors representing graphs. We introduce novel graph similarity and dissimilarity measures, provide some properties and analyze their algorithmic complexity. We find that the computational complexity of our measures is polynomial in the graph size and, hence, significantly better than classical methods from, e.g. exact graph matching which are NP-complete. Numerically, we provide some examples of our measure and compare the results with the well-known graph edit distance.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: University of Veterinary Medicine Vienna, Stowers Institute for Medical Research

Contributors: Dehmer, M., Emmert-Streib, F.

Number of pages: 12

Pages: 1699-1710

Publication date: 15 May 2007

Peer-reviewed: Yes

#### Publication information

Journal: Applied Mathematics and Computation

Volume: 188

Issue number: 2

ISSN (Print): 0096-3003

Ratings:

Scopus rating (2007): SJR 0.869 SNIP 1.113

Original language: English

ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics, Numerical Analysis

Keywords: Degree vectors, Directed and undirected graphs, Graph similarity, Similarity measures

DOIs:

10.1016/j.amc.2006.11.185

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<http://www.scopus.com/inward/record.url?scp=34248165422&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 34248165422

Research output: Contribution to journal › Article › Scientific › peer-review

### Topological mappings between graphs, trees and generalized trees

We present novel topological mappings between graphs, trees and generalized trees that means between structured objects with different properties. The two major contributions of this paper are, first, to clarify the relation between graphs, trees and generalized trees, a graph class recently introduced. Second, these transformations provide a unique opportunity to transform structured objects into a representation that might be beneficial for a processing, e.g., by machine learning techniques for graph classification.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Stowers Institute for Medical Research, Universität Rostock, Albert

Contributors: Emmert-Streib, F., Dehmer, M.

Number of pages: 8

Pages: 1326-1333

Publication date: 15 Mar 2007

Peer-reviewed: Yes

#### Publication information

Journal: Applied Mathematics and Computation

Volume: 186

Issue number: 2

ISSN (Print): 0096-3003

Ratings:

Scopus rating (2007): SJR 0.869 SNIP 1.113

Original language: English

ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics, Numerical Analysis

Keywords: Applied graph theory, Graph transformation, Hierarchical graphs

DOIs:

10.1016/j.amc.2006.07.162

URLs:

<http://www.scopus.com/inward/record.url?scp=33947616843&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 33947616843

Research output: Contribution to journal › Article › Scientific › peer-review

### **A similarity measure for graphs with low computational complexity**

We present and analyze an algorithm to measure the structural similarity of generalized trees, a new graph class which includes rooted trees. For this, we represent structural properties of graphs as strings and define the similarity of two graphs as optimal alignments of the corresponding property strings. We prove that the obtained graph similarity measures are so called Backward similarity measures. From this we find that the time complexity of our algorithm is polynomial and, hence, significantly better than the time complexity of classical graph similarity methods based on isomorphic relations.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Technical University Darmstadt, Stowers Institute for Medical Research

Contributors: Dehmer, M., Emmert-Streib, F., Kilian, J.

Number of pages: 13

Pages: 447-459

Publication date: 1 Nov 2006

Peer-reviewed: Yes

### **Publication information**

Journal: Applied Mathematics and Computation

Volume: 182

Issue number: 1

ISSN (Print): 0096-3003

Ratings:

Scopus rating (2006): SJR 0.809 SNIP 1.217

Original language: English

ASJC Scopus subject areas: Applied Mathematics, Computational Mathematics, Numerical Analysis

Keywords: Computational complexity, Dynamic programming, Graph similarity, Graph theory

DOIs:

10.1016/j.amc.2006.04.006

URLs:

<http://www.scopus.com/inward/record.url?scp=33750819438&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 33750819438

Research output: Contribution to journal › Article › Scientific › peer-review

### **Algorithmic computation of knot polynomials of secondary structure elements of proteins**

The classification of protein structures is an important and still outstanding problem. The purpose of this paper is threefold. First, we utilize a relation between the Tutte and homfly polynomial to show that the Alexander-Conway polynomial can be algorithmically computed for a given planar graph. Second, as special cases of planar graphs, we use polymer graphs of protein structures. More precisely, we use three building blocks of the three-dimensional protein structure -  $\alpha$ -helix, antiparallel  $\beta$ -sheet, and parallel  $\beta$ -sheet - and calculate, for their corresponding polymer graphs, the Tutte polynomials analytically by providing recurrence equations for all three secondary structure elements. Third, we present numerical results comparing the results from our analytical calculations with the numerical results of our algorithm - not only to test consistency, but also to demonstrate that all assigned polynomials are unique labels of the secondary structure elements. This paves the way for an automatic classification of protein structures.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Stowers Institute for Medical Research

Contributors: Emmert-Streib, F.

Number of pages: 10

Pages: 1503-1512

Publication date: 1 Oct 2006

Peer-reviewed: Yes

### Publication information

Journal: Journal of Computational Biology

Volume: 13

Issue number: 8

ISSN (Print): 1066-5277

Ratings:

Scopus rating (2006): SJR 1.421 SNIP 1.155

Original language: English

ASJC Scopus subject areas: Molecular Biology, Genetics, Computational Mathematics, Modelling and Simulation, Computational Theory and Mathematics

Keywords: Knot polynomial, Planar graph, Protein structure, Topological invariant, Tutte polynomial

DOIs:

10.1089/cmb.2006.13.1503

URLs:

<http://www.scopus.com/inward/record.url?scp=34547671421&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 34547671421

Research output: Contribution to journal > Article > Scientific > peer-review

### Melting of copper clusters

Melting of icosahedral and Wulff polyhedral copper clusters are studied using molecular dynamics and effective medium theory. Icosahedral closed shell copper clusters are most stable up to a cluster size of ~ 2500 atoms and their melting temperature is highest for small clusters, accordingly. Wulff polyhedra are most stable for larger clusters and, consequently, their melting temperature is highest for large clusters. The melting temperature decreases with decreasing cluster size and is proportional to the average coordination number of atoms. The whole icosahedral cluster melts simultaneously and can possibly be superheated. Icosahedral clusters with partially filled shells melt at lower temperatures than closed shell icosahedra, but no surface premelting is observed. (111) surface layers of large Wulff polyhedra are also solid up to the cluster melting temperatures, but (100) facets premelt at a lower temperature than the whole cluster.

### General information

Publication status: Published

MoE publication type: Not Eligible

Organisations: Jyväskylän yliopisto

Contributors: Valkealahti, S., Manninen, M.

Number of pages: 12

Pages: 123-134

Publication date: 1 Jan 1993

Peer-reviewed: Yes

### Publication information

Journal: Computational Materials Science

Volume: 1

Issue number: 2

ISSN (Print): 0927-0256

Original language: English

ASJC Scopus subject areas: Computer Science(all), Chemistry(all), Materials Science(all), Mechanics of Materials, Physics and Astronomy(all), Computational Mathematics

DOIs:

10.1016/0927-0256(93)90003-6

Source: Scopus

Source ID: 0027553804

Research output: Contribution to journal > Article > Scientific > peer-review