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

In this paper, we prove bounds for the unique, positive zero of $O_G^{\star}(z):=1-O_G(z)$, 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 $O_G^{\star}(z)$ 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 δ.

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.
Publication date: 1 Sep 2020
Peer-reviewed: Yes

Publication information

Journal: Applied Mathematics and Computation
Volume: 380
Article number: 125239
ISSN (Print): 0096-3003
Original language: English
ASJC Scopus subject areas: Computational Mathematics, Applied Mathematics
Keywords: Data science, Graph measures, Graphs, Networks, Quantitative graph theory, Symmetry
DOIs:

10.1016/j.amc.2020.125239
Source: Scopus
Source ID: 85083681263
Research output: Contribution to journal › Article › 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

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), 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.
Number of pages: 7
Publication date: 2020
Peer-reviewed: Yes

Publication information

Journal: Applied Mathematics and Computation
Volume: 380
Article number: 125302
ISSN (Print): 0096-3003
Original language: English
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

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.
Number of pages: 21
Publication date: 2020
Peer-reviewed: Yes

Publication information
Journal: Applied Mathematics and Computation
Volume: 386
Article number: 125517
ISSN (Print): 0096-3003
Original language: English
ASJC Scopus subject areas: Computational Mathematics, Applied Mathematics
Keywords: Complex dynamical networks, Demographics, Equilibrium analysis, Intercity commuting, Two-city epidemic model
DOIs:
10.1016/j.amc.2020.125517
Source: Scopus
Source ID: 85087990407
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
Peer-reviewed: Yes

Publication information
Journal: Applied Mathematics and Computation
Volume: 363
Article number: 124616
ISSN (Print): 0096-3003
Ratings:
Scopus rating (2019): CiteScore 5.6 SJR 0.969 SNIP 1.766

Original language: English
ASJC Scopus subject areas: Computational Mathematics, Applied Mathematics
Keywords: Graph entropy, Spanning forest, Subgraph
DOIs:
10.1016/j.amc.2019.124616
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

Publication status: Published
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
Peer-reviewed: Yes

Publication information

Journal: Applied Mathematics and Computation
Volume: 362
Article number: 124521
ISSN (Print): 0096-3003
Ratings:
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 showhowfor 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
Peer-reviewed: Yes

Publication information

Journal: ACM TRANSACTIONS ON COMPUTATIONAL LOGIC
Volume: 21
Issue number: 1
Article number: 7

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

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: Mesaros, 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
Journal: IEEE/ACM Transactions on Audio Speech and Language Processing
Volume: 27
Issue number: 6
ISSN (Print): 2329-9290
Ratings:
Scopus rating (2019): CiteScore 9.2 SJR 1.335 SNIP 2.489
Original language: English
ASJC Scopus subject areas: Computer Science (miscellaneous), Acoustics and Ultrasonics, Computational Mathematics, Electrical and Electronic Engineering
Keywords: confidence intervals, jackknife estimates, pattern recognition, Sound event detection, weak labels
DOIs:
10.1109/TASLP.2019.2907016
Source: Scopus
Source ID: 85064625139
Research output: Contribution to journal › Article › Scientific › peer-review

Hypermonogenic solutions and plane waves of the Dirac operator in $R^p \times R^q$
In this paper we first define hypermonogenic solutions of the Dirac operator in $R^p \times R^q$ 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.
Number of pages: 14
Pages: 1-14
Publication date: 1 Apr 2019
Peer-reviewed: Yes
Early online date: 2018

Publication information
Journal: Applied Mathematics and Computation
Volume: 346
ISSN (Print): 0096-3003
Ratings:

Scopus rating (2019): CiteScore 5.6 SJR 0.969 SNIP 1.766
Original language: English
ASJC Scopus subject areas: Computational Mathematics, Applied Mathematics
Keywords: Cauchy's formula, Hypermonogenic solution, Plane wave
DOIs:

10.1016/j.amc.2018.09.058
Source: Scopus
Source ID: 85055664097
Research output: Contribution to journal › Article › 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
Pages: 121-128
Publication date: 2019
Peer-reviewed: Yes

Publication information
Journal: Computational Materials Science
Volume: 156
ISSN (Print): 0927-0256
Ratings:

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
ISSN (Print): 0898-1221
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

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

Publication status: Published
MoE publication type: A1 Journal article-refereed
Organisations: Computing Sciences, St Giles
Contributors: Batty, C., Paunonen, L., Seifert, D.
Number of pages: 12
Pages: 808-819
Publication date: 2019
Peer-reviewed: Yes

Publication information

Journal: SIAM JOURNAL ON MATHEMATICAL ANALYSIS
Volume: 51
Issue number: 2
ISSN (Print): 0036-1410
Ratings:

Scopus rating (2019): CiteScore 2.4 SJR 1.787 SNIP 1.379
Original language: English
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
DOIs:
10.1137/18M1195796
Source: Scopus
Source ID: 85065492247
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 Jyvaskyla
Contributors: Kuva, J., Voutilainen, M., Mattila, K.
Publication date: 2019
Peer-reviewed: Yes

Publication information
Journal: COMPUTATIONAL GEOSCIENCES
ISSN (Print): 1420-0597
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
Electronic versions:
Kuva2019_Article_ModelingMassTransferInFracture
DOIs:
10.1007/s10596-019-09852-5
URLs:
http://urn.fi/URN:NBN:fi:tty-201909062074
Source: Scopus
Source ID: 85069698468
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. 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., Ruusuvuori, P.
Number of pages: 9
Pages: 3013-3021
Publication date: 1 Sep 2018
Peer-reviewed: Yes

Publication information
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:tty-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

Publication information

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

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

Homogeneous (α,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

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 bootstraping) 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
Ratings:

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

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., Helske, 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

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

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., Șicleru, 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

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
Journal: Bioinformatics
Volume: 31
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/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
Portfolio EDEND: 2014-09-15
Publisher name: Oxford University Press
Source: researchoutputwizard
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_{60} 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_{60} 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_{60} 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_{60}. 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_{60} 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
Journal: Applied Mathematics and Computation
Volume: 242
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
Journal: Bioinformatics
Volume: 30
Issue number: 19
ISSN (Print): 1367-4803
Ratings:

Scopus rating (2014): CiteScore 9 SJR 4.171 SNIP 1.838
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
Issue number: 3
ISSN (Print): 1367-4803
Ratings:

Scopus rating (2014): CiteScore 9 SJR 4.171 SNIP 1.838
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/btt687
URLs:

http://www.scopus.com/inward/record.url?scp=84893275855&partnerID=8YFLogxK (Link to publication in Scopus)

Source: Scopus
Source ID: 84893275855
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 & Engn
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

A full-potential linearized augmented plane wave study of the interaction of CO2 with α-Pu (020) surface nanolayers

Adsorption of CO_2 on α-Pu (020) surface nanolayers is investigated using GGA-DFT and the suite of software DMOL^3 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_2 configurations (5.18 and 1.90 eV, respectively). For initial vertically upright orientations, final configuration of the CO_2 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

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

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_nO_m clusters remain the O_h symmetry after DFT relaxation. The largest binding energy corresponds to the cluster with the smallest deviation from the bulk (UO_2) 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
URLs:

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

Density functional theory study of $FePd_n$ (n = 2-14) clusters and interactions with small molecules

First-principles calculations have been conducted to investigate the properties of $FePd_n$ (n = 2-14) clusters. In the lowest energy structures of $FePd_n$ 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_n clusters have been enhanced by the doping of Fe impurity. Furthermore, the adsorption of small molecules, including NH_3, H_2O, CO, H_2, and O_2, on the higher stability of $FePd_n$ (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 $E_a(H_2O) < E_a(H_2) < E_a(NH_3) < E_a(O_2) < E_a(CO)$. NH_3, CO and H_2 molecules prefer to adsorb on the $FePd_{10}$ cluster with the highest adsorption energy, while H_2O and O_2 are more like to adsorb on the $FePd_5$. The magnetic moments of $FePd_n$ 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.commatsci.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

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
Ratings:

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 mechanism 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

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

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

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
URLs:
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 stings. 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 - α-helix, antiparallel β-sheet, and parallel β-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

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

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 telescopc movement and the hydraulic fluid field. Both models are embeded with a friction model based on a bristle approach. The models are implemented in a finite element enviroment. 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

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
Title of host publication: European Control Conference 2020, ECC 2020
Publisher: IEEE
ISBN (Print): 978-1-7281-8813-3
ISBN (Electronic): 9783907144015, 978-3-90714-402-2
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

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
Pages: 1178-1185
Publication date: 2020

Host publication information
Title of host publication: European Control Conference 2020, ECC 2020
Publisher: IEEE
ISBN (Print): 978-1-7281-8813-3
ISBN (Electronic): 9783907144015, 978-3-90714-402-2
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

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

Host publication information

Title of host publication: 9th International Conference on Information Science and Technology, ICIST 2019
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

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
ISBN (Print): 978-1-5386-7187-0
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:

10.23919/ACESS.2018.8669363
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

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

Title of host publication: 2018 International Applied Computational Electromagnetics Society Symposium in China, ACES-China 2018
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/ACESS.2018.8669314
Source: Scopus
Source ID: 85063790306
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › 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

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

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