

### **A comparison between joint regression analysis and the AMMI model: A case study with barley**

Joint regression analysis (JRA) and additive main effects and multiplicative interaction (AMMI) models are compared in order to (i) assess the ability of describing a genotype by environment interaction effects and (ii) evaluate the agreement between the winners of mega-environments obtained from the AMMI analysis and the genotypes in the upper contour of the JRA. An iterative algorithm is used to obtain the environmental indexes for JRA, and standard multiple comparison procedures are adapted for genotype comparison and selection. This study includes three data sets from a spring barley (*Hordeum vulgare* L.) breeding programme carried out between 2004 and 2006 in Czech Republic. The results from both techniques are integrated in order to advise plant breeders, farmers and agronomists for better genotype selection and prediction for new years and/or new environments.

#### **General information**

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Organisations: Research Community on Data-to-Decision (D2D), Depto. de Matemática, NOVA University of Lisbon, Dept. of Mathematical and Statistical Methods

Contributors: Pereira, D. G., Rodrigues, P. C., Mejza, S., Mexia, J. T.

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### **Ageing first passage time density in continuous time random walks and quenched energy landscapes**

We study the first passage dynamics of an ageing stochastic process in the continuous time random walk (CTRW) framework. In such CTRW processes the test particle performs a random walk, in which successive steps are separated by random waiting times distributed in terms of the waiting time probability density function  $\varphi(t) \sim t^{-1-\alpha}$  ( $0 \leq \alpha \leq 2$ ). An ageing stochastic process is defined by the explicit dependence of its dynamic quantities on the ageing time  $t_{\text{inf}}^a$ , the time elapsed between its preparation and the start of the observation. Subdiffusive ageing CTRWs with  $0 < \alpha < 1$  describe systems such as charge carriers in amorphous semiconductors, tracer dispersion in geological and biological systems, or the dynamics of blinking quantum dots. We derive the exact forms of the first passage time density for an ageing subdiffusive CTRW in the semi-infinite, confined, and biased case, finding different scaling regimes for weakly, intermediately, and strongly aged systems: these regimes, with different scaling laws, are also found when the scaling exponent is in the range  $1 < \alpha < 2$ , for sufficiently long  $t_{\text{inf}}^a$ . We compare our results with the ageing motion of a test particle in a quenched energy landscape. We test our theoretical results in the quenched landscape against simulations: only when the bias is strong enough, the correlations from returning to previously visited sites become insignificant and the results approach the ageing CTRW results. With small bias or without bias, the ageing effects disappear and a change in the exponent compared to the case of a completely annealed landscape can be found, reflecting the build-up of correlations in the quenched landscape.

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Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam, National Institute of Chemistry Ljubljana

Contributors: Krüsemann, H., Godec, A., Metzler, R.

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Original language: English

ASJC Scopus subject areas: Mathematical Physics, Physics and Astronomy(all), Statistical and Nonlinear Physics, Modelling and Simulation, Statistics and Probability

Keywords: anomalous diffusion, first passage, random walks

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

### Aging scaled Brownian motion

Scaled Brownian motion (SBM) is widely used to model anomalous diffusion of passive tracers in complex and biological systems. It is a highly nonstationary process governed by the Langevin equation for Brownian motion, however, with a power-law time dependence of the noise strength. Here we study the aging properties of SBM for both unconfined and confined motion. Specifically, we derive the ensemble and time averaged mean squared displacements and analyze their behavior in the regimes of weak, intermediate, and strong aging. A very rich behavior is revealed for confined aging SBM depending on different aging times and whether the process is sub- or superdiffusive. We demonstrate that the information on the aging factorizes with respect to the lag time and exhibits a functional form that is identical to the aging behavior of scale-free continuous time random walk processes. While SBM exhibits a disparity between ensemble and time averaged observables and is thus weakly nonergodic, strong aging is shown to effect a convergence of the ensemble and time averaged mean squared displacement. Finally, we derive the density of first passage times in the semi-infinite domain that features a crossover defined by the aging time.

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MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Max-Planck Institute for the Physics of Complex Systems, Institute for Physics and Astronomy, University of Potsdam, Nordic Institute for Theoretical Physics NORDITA, Shahid Beheshti University, Kharkov Institute of Physics and Technology

Contributors: Safdari, H., Chechkin, A. V., Jafari, G. R., Metzler, R.

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ASJC Scopus subject areas: Condensed Matter Physics, Statistical and Nonlinear Physics, Statistics and Probability

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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`.

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

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### **A stochastic model for survival of early prostate cancer with adjustments for leadtime, length bias, and over-detection**

To compare the survival between screen-detected and clinically detected cancers, we applied a series of non-homogeneous stochastic processes to deal with leadtime, length bias, and over-detection by using full information on detection modes obtained from the Finnish randomized controlled trial for prostate cancer screening. The results show after 9-year follow-up the hazard ratio of prostate cancer death for screen-detected cases against clinically detected cases increased from 0.24 (95% CI: 0.16-0.35) without correction for these biases, to 0.76 after correction for leadtime and length biases, and finally to 1.03 (95% CI: 0.79-1.33) for a further adjustment for over-detection. Adjustment for leadtime and length bias but no over-detection led to a 24% reduction in prostate cancer death as a result of prostate-specific antigen test. The further calibration of over-detection indicates no gain in survival of screen-detected prostate cancers (excluding over-detected case as stayer considered in the mover-stayer model) as compared with the control group in the absence of screening that is considered as the mover. However, whether the model assumption on over-detection is robust should be validated with other data sets and longer follow-up.

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MoE publication type: A1 Journal article-refereed

Organisations: Prostate cancer research center (PCRC), National Taiwan University, Finnish Cancer Institute, Taipei Medical University, McMaster University

Contributors: Wu, G. H. M., Auvinen, A., Yen, A. M. F., Hakama, M., Walter, S. D., Chen, H. H.  
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Original language: English

ASJC Scopus subject areas: Statistics and Probability, Medicine(all), Statistics, Probability and Uncertainty

Keywords: Leadtime and length bias, Mass screening, Prostate neoplasms, Prostate-specific antigen, Stochastic processes

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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

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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.

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Original language: English

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

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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**

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

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

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

### **Clustering-based method for developing a genomic copy number alteration signature for predicting the metastatic potential of prostate cancer**

The transition of cancer from a localized tumor to a distant metastasis is not well understood for prostate and many other cancers, partly, because of the scarcity of tumor samples, especially metastases, from cancer patients with long-term clinical follow-up. To overcome this limitation, we developed a semi-supervised clustering method using the tumor genomic DNA copy number alterations to classify each patient into inferred clinical outcome groups of metastatic potential. Our data set was comprised of 294 primary tumors and 49 metastases from 5 independent cohorts of prostate cancer patients. The alterations were modeled based on Darwins evolutionary selection theory and the genes overlapping these altered genomic regions were used to develop a metastatic potential score for a prostate cancer primary tumor. The function of the proteins encoded by some of the predictor genes promote escape from anoikis, a pathway of apoptosis, deregulated in metastases. We evaluated the metastatic potential score with other clinical predictors available at diagnosis using a Cox proportional hazards model and show our proposed score was the only significant predictor of metastasis free survival. The metastasis gene signature and associated score could be applied directly to copy number alteration profiles from patient biopsies positive for prostate cancer.

#### **General information**

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Organisations: Prostate cancer research center (PCRC), Albert Einstein College of Medicine of Yeshiva University, NYU Langone Medical Center, Baylor College of Medicine, Johns Hopkins School of Medicine, Department of Surgery

Contributors: Pearlman, A., Campbell, C., Brooks, E., Genshaft, A., Shajahan, S., Ittman, M., Bova, G. S., Melamed, J., Holcomb, I., Schneider, R. J., Ostrer, H.

Publication date: 2012

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Original language: English

ASJC Scopus subject areas: Statistics and Probability

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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

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Organisations: Faculty of Biomedical Sciences and Engineering, Mechanical Engineering and Industrial Systems, Signal Processing, Research group: Data-analytics and Optimization, Tampere University Hospital, Faculty of Medicine and Life Sciences, BioMediTech, Fimlab Laboratories Ltd, BioMediTech Institute

Contributors: Kartasalo, K., Latonen, L., Vihinen, J., Visakorpi, T., Nykter, M., Ruusuvoori, P.

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### Conformational properties of complex polymers: Rosette versus star-like structures

Multiple loop formation in polymer macromolecules is an important feature of the chromatin organization and DNA compactification in the nuclei. We analyse the size and shape characteristics of complex polymer structures, containing in general  $f_1$  loops (petals) and  $f_2$  linear chains (branches). Within the frames of continuous model of Gaussian macromolecule, we apply the path integration method and obtain the estimates for gyration radius  $R_g$  and asphericity  $\bar{A}$  of typical conformation as functions of parameters  $f_1$ ,  $f_2$ . In particular, our results qualitatively reveal the extent of anisotropy of star-like topologies as compared to the rosette structures of the same total molecular weight.

#### General information

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Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam, Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine

Contributors: Blavatska, V., Metzler, R.

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Keywords: conformational properties, path integration, polymers

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

### Diffusion through thin membranes: Modeling across scales

From macroscopic to microscopic scales it is demonstrated that diffusion through membranes can be modeled using specific boundary conditions across them. The membranes are here considered thin in comparison to the overall size of the system. In a macroscopic scale the membrane is introduced as a transmission boundary condition, which enables an effective modeling of systems that involve multiple scales. In a mesoscopic scale, a numerical lattice-Boltzmann scheme with a partial-bounceback condition at the membrane is proposed and analyzed. It is shown that this mesoscopic approach provides a consistent approximation of the transmission boundary condition. Furthermore, analysis of the mesoscopic scheme gives rise to an expression for the permeability of a thin membrane as a function of a mesoscopic transmission parameter. In a microscopic model, the mean waiting time for a passage of a particle through the membrane is in accordance with this permeability. Numerical results computed with the mesoscopic scheme are then compared successfully with analytical solutions derived in a macroscopic scale, and the membrane model introduced here is used to simulate diffusive transport between the cell nucleus and cytoplasm through the nuclear envelope in a realistic cell model based on fluorescence microscopy data. By comparing the simulated fluorophore transport to the experimental one, we determine the permeability of the nuclear envelope of HeLa cells to enhanced yellow fluorescent protein.

#### General information

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MoE publication type: A1 Journal article-refereed

Organisations: Physics, Department of Physics, Research area: Computational Physics, University of Jyväskylä, University of Eastern Finland, University of Helsinki, University of Oxford, ITMO University

Contributors: Aho, V., Mattila, K., Kühn, T., Kekäläinen, P., Pulkkinen, O., Minussi, R. B., Vihinen-Ranta, M., Timonen, J.

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ASJC Scopus subject areas: Condensed Matter Physics, Statistical and Nonlinear Physics, Statistics and Probability

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INT=fys,"Mattila, Keijo"

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### Dynamics of coupled repressilators: The role of mRNA kinetics and transcription cooperativity

Oscillatory regulatory networks have been discovered in many cellular pathways. An especially challenging area is studying dynamics of cellular oscillators interacting with one another in a population. Synchronization is only one of and the simplest outcome of such interaction. It is suggested that the outcome depends on the structure of the network. Phase-attractive (synchronizing) and phase-repulsive coupling structures were distinguished for regulatory oscillators. In this paper, we question this separation. We study an example of two interacting repressilators (artificial regulatory oscillators based on cyclic repression). We show that changing the cooperativity of transcription repression (Hill coefficient) and reaction timescales dramatically alter synchronization properties. The network becomes birhythmic-it chooses between the in-phase and antiphase synchronization. Thus, the type of synchronization is not characteristic for the network structure. However, we conclude that the specific scenario of emergence and stabilization of synchronous solutions is much more characteristic.

### General information

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Organisations: Mathematical modelling with wide societal impact (MathImpact), Department of Theoretical Physics, Lebedev Physical Institute, IUPUI

Contributors: Potapov, I., Volkov, E., Kuznetsov, A.

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Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Statistical and Nonlinear Physics, Statistics and Probability

DOIs:

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



## Dynamics of intracranial electroencephalographic recordings from epilepsy patients using univariate and bivariate recurrence networks

Recently Andrezejak et al. combined the randomness and nonlinear independence test with iterative amplitude adjusted Fourier transform (iAAFT) surrogates to distinguish between the dynamics of seizure-free intracranial electroencephalographic (EEG) signals recorded from epileptogenic (focal) and nonepileptogenic (nonfocal) brain areas of epileptic patients. However, stationarity is a part of the null hypothesis for iAAFT surrogates and thus nonstationarity can violate the null hypothesis. In this work we first propose the application of the randomness and nonlinear independence test based on recurrence network measures to distinguish between the dynamics of focal and nonfocal EEG signals. Furthermore, we combine these tests with both iAAFT and truncated Fourier transform (TFT) surrogate methods, which also preserves the nonstationarity of the original data in the surrogates along with its linear structure. Our results indicate that focal EEG signals exhibit an increased degree of structural complexity and interdependency compared to nonfocal EEG signals. In general, we find higher rejections for randomness and nonlinear independence tests for focal EEG signals compared to nonfocal EEG signals. In particular, the univariate recurrence network measures, the average clustering coefficient  $C$  and assortativity  $R$ , and the bivariate recurrence network measure, the average cross-clustering coefficient  $C_{\text{cross}}$ , can successfully distinguish between the focal and nonfocal EEG signals, even when the analysis is restricted to nonstationary signals, irrespective of the type of surrogates used. On the other hand, we find that the univariate recurrence network measures, the average path length  $L$ , and the average betweenness centrality  $BC$  fail to distinguish between the focal and nonfocal EEG signals when iAAFT surrogates are used. However, these two measures can distinguish between focal and nonfocal EEG signals when TFT surrogates are used for nonstationary signals. We also report an improvement in the performance of nonlinear prediction error  $N$  and nonlinear interdependence measure  $L$  used by Andrezejak et al., when TFT surrogates are used for nonstationary EEG signals. We also find that the outcome of the nonlinear independence test based on the average cross-clustering coefficient  $C_{\text{cross}}$  is independent of the outcome of the randomness test based on the average clustering coefficient  $C$ . Thus, the univariate and bivariate recurrence network measures provide independent information regarding the dynamics of the focal and nonfocal EEG signals. In conclusion, recurrence network analysis combined with nonstationary surrogates can be applied to derive reliable biomarkers to distinguish between epileptogenic and nonepileptogenic brain areas using EEG signals.

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Organisations: Department of Electronics and Communications Engineering, Research group: Computational Biophysics and Imaging Group, BioMediTech, Integrated Technologies for Tissue Engineering Research (ITTE), BioMediTech

Contributors: Subramaniam, N. P., Hyttinen, J.

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Source ID: 84924359654

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

## Ergodicity breaking, ageing, and confinement in generalized diffusion processes with position and time dependent diffusivity

We study generalized anomalous diffusion processes whose diffusion coefficient  $D(x, t) \sim$

$D \propto |x|^\alpha t^\beta$  depends on both the position  $x$  of the test particle and the process time  $t$ .

This process thus combines the features of scaled Brownian motion and heterogeneous diffusion parent processes. We compute the ensemble and time averaged mean squared displacements of this generalized diffusion process. The scaling exponent of the ensemble averaged mean squared displacement is shown to be the product of the critical exponents of the parent processes, and describes both subdiffusive and superdiffusive systems. We quantify the amplitude fluctuations of the time averaged mean squared displacement as function of the length of the time series and the lag time. In particular, we observe a weak ergodicity breaking of this generalized diffusion process: even in the long time limit the ensemble and time averaged mean squared displacements are strictly disparate. When we start to observe this process some time after its initiation we observe distinct features of ageing. We derive a universal ageing factor for the time averaged mean squared displacement containing all information on the ageing time and the measurement time. External confinement is shown to alter the magnitudes and statistics of the ensemble and time averaged mean squared

displacements.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam

Contributors: Cherstvy, A. G., Metzler, R.

Publication date: 15 May 2015

Peer-reviewed: Yes

### Publication information

Journal: Journal of Statistical Mechanics: Theory and Experiment

Volume: 2015

Issue number: 5

Article number: P05010

ISSN (Print): 1742-5468

Ratings:

Scopus rating (2015): CiteScore 3.7 SJR 0.689 SNIP 0.829

Original language: English

ASJC Scopus subject areas: Statistics and Probability, Statistical and Nonlinear Physics, Statistics, Probability and Uncertainty

Keywords: diffusion

DOIs:

10.1088/1742-5468/2015/05/P05010

URLs:

<http://www.scopus.com/inward/record.url?scp=84930653082&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84930653082

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<br/>Portfolio EDEND: 2014-09-15<br/>Publisher name: Oxford University Press  
Source: researchoutputwizard

Source ID: 396

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

### **Exploratory analysis of spatiotemporal patterns of cellular automata by clustering compressibility**

In this paper we study the classification of spatiotemporal pattern of one-dimensional cellular automata (CA) whereas the classification comprises CA rules including their initial conditions. We propose an exploratory analysis method based on the normalized compression distance (NCD) of spatiotemporal patterns which is used as dissimilarity measure for a hierarchical clustering. Our approach is different with respect to the following points. First, the classification of spatiotemporal pattern is comparative because the NCD evaluates explicitly the difference of compressibility among two objects, e.g., strings corresponding to spatiotemporal patterns. This is in contrast to all other measures applied so far in a similar context because they are essentially univariate. Second, Kolmogorov complexity, which underlies the NCD, was used in the classification of CA with respect to their spatiotemporal pattern. Third, our method is semiautomatic allowing us to investigate hundreds or thousands of CA rules or initial conditions simultaneously to gain insights into their organizational structure. Our numerical results are not only plausible confirming previous classification attempts but also shed light on the intricate influence of random initial conditions on the classification results.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Biology and Machine Learning Lab., Faculty of Medicine, Health and Life Sciences, Queen's University, Belfast, Northern Ireland

Contributors: Emmert-Streib, F.

Publication date: 8 Feb 2010

Peer-reviewed: Yes

### **Publication information**

Journal: Physical Review E

Volume: 81

Issue number: 2

Article number: 026103

ISSN (Print): 1539-3755

Ratings:

Scopus rating (2010): SJR 1.692 SNIP 1.213

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Statistical and Nonlinear Physics, Statistics and Probability

DOIs:

10.1103/PhysRevE.81.026103

URLs:

<http://www.scopus.com/inward/record.url?scp=76749153776&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 76749153776

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

### **Fault tolerance of information processing in gene networks**

The major objective of this paper is to study the fault tolerance of gene networks. For single gene knockouts we investigate the disturbance of the communication abilities of gene networks globally. For our study we use directed scale-free networks resembling important properties of gene networks, e.g., signaling, or transcriptional regulatory networks, as well as metabolic networks and define a Markov chain on the network to model the communication dynamics. This allows us to evaluate the spread of information in the network and, hence, detect differences due to single gene knockouts in the gene-to-gene communication asymptotically regarding the limiting stationary distributions governed by the Markov chain. Further, we study the connection of the global effect of the perturbations with local properties of the network topology by means of statistical hypothesis tests.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Computational Biology and Machine Learning, School of Biomedical Sciences, Department of Biostatistics, TU Vienna

Contributors: Emmert-Streib, F., Dehmer, M.  
Number of pages: 8  
Pages: 541-548  
Publication date: 15 Feb 2009  
Peer-reviewed: Yes

#### Publication information

Journal: Physica A: Statistical Mechanics and Its Applications

Volume: 388

Issue number: 4

ISSN (Print): 0378-4371

Ratings:

Scopus rating (2009): SJR 0.829 SNIP 1.026

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Statistics and Probability

Keywords: Information processing, Markov chain, Robustness, Scale-free network

DOIs:

10.1016/j.physa.2008.10.032

URLs:

<http://www.scopus.com/inward/record.url?scp=57349185507&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 57349185507

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

#### First-principles data set of 45,892 isolated and cation-coordinated conformers of 20 proteinogenic amino acids

We present a structural data set of the 20 proteinogenic amino acids and their amino-methylated and acetylated (capped) dipeptides. Different protonation states of the backbone (uncharged and zwitterionic) were considered for the amino acids as well as varied side chain protonation states. Furthermore, we studied amino acids and dipeptides in complex with divalent cations ( $\text{Ca}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Pb}^{2+}$ , and  $\text{Hg}^{2+}$ ). The database covers the conformational hierarchies of 280 systems in a wide relative energy range of up to 4 eV (390 kJ/mol), summing up to a total of 45,892 stationary points on the respective potential-energy surfaces. All systems were calculated on equal first-principles footing, applying density-functional theory in the generalized gradient approximation corrected for long-range van der Waals interactions. We show good agreement to available experimental data for gas-phase ion affinities. Our curated data can be utilized, for example, for a wide comparison across chemical space of the building blocks of life, for the parametrization of protein force fields, and for the calculation of reference spectra for biophysical applications.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Fritz Haber Institute of the Max Planck Society, COMP Centre of Excellence, Department of Applied Physics, Aalto University, Aalto University, Duke University

Contributors: Ropo, M., Schneider, M., Baldauf, C., Blum, V.

Publication date: 16 Feb 2016

Peer-reviewed: Yes

#### Publication information

Journal: Scientific Data

Volume: 3

Article number: 160009

ISSN (Print): 2052-4463

Ratings:

Scopus rating (2016): CiteScore 4.7 SJR 3.261 SNIP 2.208

Original language: English

ASJC Scopus subject areas: Education, Library and Information Sciences, Computer Science Applications, Information Systems, Statistics, Probability and Uncertainty, Statistics and Probability

Electronic versions:

ropo et al - First-principles data set

DOIs:

10.1038/sdata.2016.9

URLs:

<http://urn.fi/URN:NBN:fi:tty-201607294339>

Source: Scopus

Source ID: 84961184519

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

### Forecasting mortality rate by singular spectrum analysis

Singular spectrum analysis (SSA) is a relatively new and powerful non-parametric time series analysis technique that has demonstrated its capability in forecasting different time series in various disciplines. In this paper, we study the feasibility of using the SSA to perform mortality forecasts. Comparisons are made with the Hyndman–Ullah model, which is a new powerful tool in the field of mortality forecasting, and will be considered as a benchmark to evaluate the performance of the SSA for mortality forecasting. We use both SSA and Hyndman–Ullah models to obtain 10 forecasts for the period 2000–2009 in nine European countries including Belgium, Denmark, Finland, France, Italy, The Netherlands, Norway, Sweden and Switzerland. Computational results show a superior accuracy of the SSA forecasting algorithms, when compared with the Hyndman–Ullah approach.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research Community on Data-to-Decision (D2D), Statistical Research and Training Center (SRTC), Shahid Beheshti University

Contributors: Mahmoudvand, R., Alehosseini, F., Rodrigues, P. C.

Number of pages: 14

Pages: 193-206

Publication date: 1 Nov 2015

Peer-reviewed: Yes

#### Publication information

Journal: REVSTAT STATISTICAL JOURNAL

Volume: 13

Issue number: 3

ISSN (Print): 1645-6726

Ratings:

Scopus rating (2015): CiteScore 2.6 SJR 1.333 SNIP 2.109

Original language: English

ASJC Scopus subject areas: Statistics and Probability

Keywords: Hyndman–Ullah model, Mortality rate, Singular spectrum analysis

URLs:

<http://www.scopus.com/inward/record.url?scp=84947785922&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84947785922

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

### Generative modeling for maximizing precision and recall in information visualization

Information visualization has recently been formulated as an information retrieval problem, where the goal is to find similar data points based on the visualized nonlinear projection, and the visualization is optimized to maximize a compromise between (smoothed) precision and recall. We turn the visualization into a generative modeling task where a simple user model parameterized by the data coordinates is optimized, neighborhood relations are the observed data, and straightforward maximum likelihood estimation corresponds to Stochastic Neighbor Embedding (SNE). While SNE maximizes pure recall, adding a mixture component that "explains away" misses allows our generative model to focus on maximizing precision as well. The resulting model is a generative solution to maximizing tradeoffs between precision and recall. The model outperforms earlier models in terms of precision and recall and in external validation by unsupervised classification.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Peltonen, J., Kaski, S.

Number of pages: 9

Pages: 579-587

Publication date: 2011

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Machine Learning Research

Volume: 15

ISSN (Print): 1532-4435

Ratings:

Scopus rating (2011): CiteScore 7.7 SJR 1.18 SNIP 2.912

Original language: English

ASJC Scopus subject areas: Artificial Intelligence, Software, Control and Systems Engineering, Statistics and Probability

URLs:

<http://www.scopus.com/inward/record.url?scp=84862299625&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84862299625

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](https://doi.org/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

### **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

#### Hermitian one-particle density matrix through a semiclassical gradient expansion

We carry out the semiclassical expansion of the one-particle density matrix up to the second order in  $\hbar$ . We use the method of Grammaticos and Voros based on the Wigner transform of operators. We show that the resulting density matrix is Hermitian and idempotent in contrast with the well-known result of the semiclassical Kirzhnits expansion. Our density matrix leads to the same particle density and kinetic energy density as in the literature, and it satisfies the consistency criterion of the Euler equation. The derived Hermitian density matrix clarifies the ambiguity in the usefulness of gradient expansion approximations and might reignite the development of density functionals with semiclassical methods.

#### 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, Computational Science X (CompX), Université Ferhat

Contributors: Bencheikh, K., Räsänen, E.

Publication date: 9 Dec 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physics A: Mathematical and Theoretical

Volume: 49

Issue number: 1

Article number: 015205

ISSN (Print): 1751-8113

Ratings:

Scopus rating (2015): CiteScore 3.5 SJR 1.028 SNIP 1.04

Original language: English

ASJC Scopus subject areas: Mathematical Physics, Physics and Astronomy(all), Statistical and Nonlinear Physics, Modelling and Simulation, Statistics and Probability

Keywords: density matrix, density-functional theory, Wigner transform

DOIs:

10.1088/1751-8113/49/1/015205

Source: Scopus

Source ID: 84961361098

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

### High-Reynolds-number turbulent cavity flow using the lattice Boltzmann method

We present a boundary condition scheme for the lattice Boltzmann method that has significantly improved stability for modeling turbulent flows while maintaining excellent parallel scalability. Simulations of a three-dimensional lid-driven cavity flow are found to be stable up to the unprecedented Reynolds number  $Re=5 \times 10^4$  for this setup. Excellent agreement with energy balance equations, computational and experimental results are shown. We quantify rises in the production of turbulence and turbulent drag, and determine peak locations of turbulent production.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Duke University, State University of Santa Catarina, Centro S3, University Tor Vergata, Jyväskylän yliopisto, Pontifical Catholic University of Paraná

Contributors: Hegele, L. A., Scagliarini, A., Sbragaglia, M., Mattila, K. K., Philippi, P. C., Puleri, D. F., Gounley, J., Randles, A.

Number of pages: 13

Publication date: 4 Oct 2018

Peer-reviewed: Yes

#### Publication information

Journal: Physical Review E

Volume: 98

Issue number: 4

Article number: 043302

ISSN (Print): 2470-0045

Ratings:

Scopus rating (2018): CiteScore 4.3 SJR 0.992 SNIP 1.188

Original language: English

ASJC Scopus subject areas: Statistical and Nonlinear Physics, Statistics and Probability, Condensed Matter Physics  
DOIs:

10.1103/PhysRevE.98.043302

Source: Scopus

Source ID: 85054599510

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

### Information retrieval perspective to meta-visualization

In visual data exploration with scatter plots, no single plot is sufficient to analyze complicated high-dimensional data sets. Given numerous visualizations created with different features or methods, meta-visualization is needed to analyze the visualizations together. We solve how to arrange numerous visualizations onto a meta-visualization display, so that their similarities and differences can be analyzed. We introduce a machine learning approach to optimize the meta-visualization, based on an information retrieval perspective: Two visualizations are similar if the analyst would retrieve similar neighborhoods between data samples from either visualization. Based on the approach, we introduce a nonlinear embedding method for meta-visualization: it optimizes locations of visualizations on a display, so that visualizations giving similar information about data are close to each other.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Peltonen, J., Lin, Z.

Number of pages: 16

Pages: 165-180

Publication date: 2013

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Machine Learning Research

Volume: 29

ISSN (Print): 1532-4435

Ratings:

Scopus rating (2013): CiteScore 6.2 SJR 1.235 SNIP 2.293



Original language: English

ASJC Scopus subject areas: Artificial Intelligence, Software, Control and Systems Engineering, Statistics and Probability

Keywords: Meta-visualization, Neighbor embedding, Nonlinear dimensionality reduction

URLs:

<http://www.scopus.com/inward/record.url?scp=84908485499&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84908485499

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

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

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

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Luukko, P. J. J., 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](https://doi.org/10.1007/s00180-015-0603-9)

URLs:

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

#### **Bibliographical note**

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

Source: Scopus

Source ID: 84963783252

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

### **Investigation of an entropic stabilizer for the lattice-Boltzmann method**

The lattice-Boltzmann (LB) method is commonly used for the simulation of fluid flows at the hydrodynamic level of description. Due to its kinetic theory origins, the standard LB schemes carry more degrees of freedom than strictly needed, e.g., for the approximation of solutions to the Navier-stokes equation. In particular, there is freedom in the details of the so-called collision operator. This aspect was recently utilized when an entropic stabilizer, based on the principle of maximizing local entropy, was proposed for the LB method [I. V. Karlin, F. Bösch, and S. S. Chikatamarla, Phys. Rev. E 90, 031302(R) (2014)]. The proposed stabilizer can be considered as an add-on or extension to basic LB schemes. Here the entropic stabilizer is investigated numerically using the perturbed double periodic shear layer flow as a benchmark case. The investigation is carried out by comparing numerical results obtained with six distinct LB schemes. The main observation is that the unbounded, and not explicitly controllable, relaxation time for the higher-order moments will directly influence the leading-order error terms. As a consequence, the order of accuracy and, in general, the numerical behavior

of LB schemes are substantially altered. Hence, in addition to systematic numerical validation, more detailed theoretical analysis of the entropic stabilizer is still required in order to properly understand its properties.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Department of Petroleum Engineering, State University of Santa Catarina, Federal University of Santa Catarina

Contributors: Mattila, K. K., Hegele, L. A., Philippi, P. C.

Publication date: 19 Jun 2015

Peer-reviewed: Yes

#### Publication information

Journal: Physical Review E

Volume: 91

Issue number: 6

Article number: 063010

ISSN (Print): 1539-3755

Ratings:

Scopus rating (2015): CiteScore 1.89 SJR 1.183 SNIP 2.283

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Statistical and Nonlinear Physics, Statistics and Probability

DOIs:

10.1103/PhysRevE.91.063010

#### Bibliographical note

INT=fys,"Mattila, Keijo K."

Source: Scopus

Source ID: 84936946902

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

#### Majorization-minimization for manifold embedding

Nonlinear dimensionality reduction by manifold embedding has become a popular and powerful approach both for visualization and as preprocessing for predictive tasks, but more efficient optimization algorithms are still crucially needed. Majorization-Minimization (MM) is a promising approach that monotonically decreases the cost function, but it remains unknown how to tightly majorize the manifold embedding objective functions such that the resulting MM algorithms are efficient and robust. We propose a new MM procedure that yields fast MM algorithms for a wide variety of manifold embedding problems. In our majorization step, two parts of the cost function are respectively upper bounded by quadratic and Lipschitz surrogates, and the resulting upper bound can be minimized in closed form. For cost functions amenable to such QL-majorization, the MM yields monotonic improvement and is efficient: In experiments, the newly developed MM algorithms outperformed five state-of-the-art optimization approaches in manifold embedding tasks.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

Contributors: Yang, Z., Peltonen, J., Kaski, S.

Number of pages: 10

Pages: 1088-1097

Publication date: 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Machine Learning Research

Volume: 38

ISSN (Print): 1532-4435

Ratings:

Scopus rating (2015): CiteScore 4.5 SJR 1.431 SNIP 2.032

Original language: English

ASJC Scopus subject areas: Control and Systems Engineering, Software, Statistics and Probability, Artificial Intelligence

URLs:

<http://www.scopus.com/inward/record.url?scp=84954311496&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84954311496

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

### **Nonlinear continuous-wave optical propagation in nematic liquid crystals: Interplay between reorientational and thermal effects**

We investigate nonlinear optical propagation of continuous-wave (CW) beams in bulk nematic liquid crystals. We thoroughly analyze the competing roles of reorientational and thermal nonlinearity with reference to self-focusing/defocusing and, eventually, the formation of nonlinear diffraction-free wavepackets, the so-called spatial optical solitons. To this extent we refer to dye-doped nematic liquid crystals in planar cells excited by a single CW beam in the highly nonlocal limit. To adjust the relative weight between the two nonlinear responses, we employ two distinct wavelengths, inside and outside the absorption band of the dye, respectively. Different concentrations of the dye are considered in order to enhance the thermal effect. The theoretical analysis is complemented by numerical simulations in the highly nonlocal approximation based on a semi-analytic approach. Theoretical results are finally compared to experimental results in the Nematic Liquid Crystals (NLC) 4-trans-4'-n-hexylcyclohexylisothiocyanatobenzene (6CHBT) doped with Sudan Blue dye.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Photonics, Politechnika Warszawska, University "Roma Tre", NooEL-Nonlinear Optics

Contributors: Alberucci, A., Laudyn, U. A., Piccardi, A., Kwasny, M., Klus, B., Karpierz, M. A., Assanto, G.

Publication date: 11 Jul 2017

Peer-reviewed: Yes

#### **Publication information**

Journal: Physical Review E

Volume: 96

Issue number: 1

Article number: 012703

ISSN (Print): 2470-0045

Ratings:

Scopus rating (2017): CiteScore 4.3 SJR 0.979 SNIP 0.953

Original language: English

ASJC Scopus subject areas: Statistical and Nonlinear Physics, Statistics and Probability, Condensed Matter Physics  
DOIs:

10.1103/PhysRevE.96.012703

Source: Scopus

Source ID: 85026478719

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

### **Optimization and universality of Brownian search in a basic model of quenched heterogeneous media**

The kinetics of a variety of transport-controlled processes can be reduced to the problem of determining the mean time needed to arrive at a given location for the first time, the so-called mean first-passage time (MFPT) problem. The occurrence of occasional large jumps or intermittent patterns combining various types of motion are known to outperform the standard random walk with respect to the MFPT, by reducing oversampling of space. Here we show that a regular but spatially heterogeneous random walk can significantly and universally enhance the search in any spatial dimension. In a generic minimal model we consider a spherically symmetric system comprising two concentric regions with piecewise constant diffusivity. The MFPT is analyzed under the constraint of conserved average dynamics, that is, the spatially averaged diffusivity is kept constant. Our analytical calculations and extensive numerical simulations demonstrate the existence of an optimal heterogeneity minimizing the MFPT to the target. We prove that the MFPT for a random walk is completely dominated by what we term direct trajectories towards the target and reveal a remarkable universality of the spatially heterogeneous search with respect to target size and system dimensionality. In contrast to intermittent strategies, which are most profitable in low spatial dimensions, the spatially inhomogeneous search performs best in higher dimensions. Discussing our results alongside recent experiments on single-particle tracking in living cells, we argue that the observed spatial heterogeneity may be beneficial for cellular signaling processes.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam, National Institute of Chemistry Ljubljana

Contributors: Godec, A., Metzler, R.

Publication date: 21 May 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Physical Review E

Volume: 91

Issue number: 5

Article number: 052134

ISSN (Print): 1539-3755

Ratings:

Scopus rating (2015): CiteScore 1.89 SJR 1.183 SNIP 2.283

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Statistical and Nonlinear Physics, Statistics and Probability  
DOIs:

10.1103/PhysRevE.91.052134

URLs:

<http://www.scopus.com/inward/record.url?scp=84930652975&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84930652975

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

### **Parity-time-symmetric solitons in trapped Bose-Einstein condensates and the influence of varying complex potentials: A variational approach**

Dynamics and properties of nonlinear matter waves in a trapped BEC subject to a PT-symmetric linear potential, with the trap in the form of a super-Gaussian potential, are investigated via a variational approach accounting for the complex nature of the soliton. In the process, we address how the shape of the imaginary part of the potential, that is, a gain-loss mechanism, affects the self-localization and the stability of the condensate. Variational results are found to be in good agreement with full numerical simulations for predicting the shape, width, and chemical potential of the condensate until the PT breaking point. Variational computation also predicts the existence of solitary solution only above a threshold in the particle number as the gain-loss is increased, in agreement with numerical simulations.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research group: Nonlinear Optics, Frontier Photonics, Universidade do Porto, Univ Roma Tre, Roma Tre University, Dept Elect Engr, NooEL, Cochin University of Science and Technology, Centro de Física Do Porto

Contributors: Devassy, L., Jisha, C. P., Alberucci, A., Kuriakose, V. C.

Number of pages: 12

Publication date: 19 Aug 2015

Peer-reviewed: Yes

### Publication information

Journal: Physical Review E

Volume: 92

Issue number: 2

Article number: 022914

ISSN (Print): 1539-3755

Ratings:

Scopus rating (2015): CiteScore 1.89 SJR 1.183 SNIP 2.283

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Statistical and Nonlinear Physics, Statistics and Probability

DOIs:

10.1103/PhysRevE.92.022914

URLs:

<http://www.scopus.com/inward/record.url?scp=84939612865&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84939612865

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

### Quantifying the non-ergodicity of scaled Brownian motion

We examine the non-ergodic properties of scaled Brownian motion (SBM), a non-stationary stochastic process with a time dependent diffusivity of the form  $D(t) \propto t^{\alpha-1}$ . We compute the ergodicity breaking parameter EB in the entire range of scaling exponents  $\alpha$ , both analytically and via extensive computer simulations of the stochastic Langevin equation. We demonstrate that in the limit of long trajectory lengths  $T$  and short lag times  $\Delta$  the EB parameter as function of the scaling exponent  $\alpha$  has no divergence at  $\alpha = 1/2$  and present the asymptotes for EB in different limits. We generalize the analytical and simulations results for the time averaged and ergodic properties of SBM in the presence of ageing, that is, when the observation of the system starts only a finite time span after its initiation. The approach developed here for the calculation of the higher time averaged moments of the particle displacement can be applied to derive the ergodic properties of other stochastic processes such as fractional Brownian motion.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam, Akhiezer Institute for Theoretical Physics, Kharkov Institute of Physics and Technology, Institute for Physics AndAstronomy, Humboldt-Universität zu Berlin, Shahid Beheshti University

Contributors: Safdari, H., Cherstvy, A. G., Chechkin, A. V., Thiel, F., Sokolov, I. M., Metzler, R.

Publication date: 18 Sep 2015

Peer-reviewed: Yes

### Publication information

Journal: Journal of Physics A: Mathematical and Theoretical

Volume: 48

Issue number: 37

Article number: 375002

ISSN (Print): 1751-8113

Ratings:

Scopus rating (2015): CiteScore 3.5 SJR 1.028 SNIP 1.04

Original language: English

ASJC Scopus subject areas: Mathematical Physics, Physics and Astronomy(all), Statistical and Nonlinear Physics, Modelling and Simulation, Statistics and Probability

Keywords: ageing, anomalous diffusion, scaled Brownian motion

DOIs:

10.1088/1751-8113/48/37/375002

URLs:

<http://www.scopus.com/inward/record.url?scp=84940069543&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84940069543

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

### **Reorientational versus Kerr dark and gray solitary waves using modulation theory**

We develop a modulation theory model based on a Lagrangian formulation to investigate the evolution of dark and gray optical spatial solitary waves for both the defocusing nonlinear Schrödinger (NLS) equation and the nematicon equations describing nonlinear beams, nematicons, in self-defocusing nematic liquid crystals. Since it has an exact soliton solution, the defocusing NLS equation is used as a test bed for the modulation theory applied to the nematicon equations, which have no exact solitary wave solution. We find that the evolution of dark and gray NLS solitons, as well as nematicons, is entirely driven by the emission of diffractive radiation, in contrast to the evolution of bright NLS solitons and bright nematicons. Moreover, the steady nematicon profile is nonmonotonic due to the long-range nonlocality associated with the perturbation of the optic axis. Excellent agreement is obtained with numerical solutions of both the defocusing NLS and nematicon equations. The comparisons for the nematicon solutions raise a number of subtle issues relating to the definition and measurement of the width of a dark or gray nematicon.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Frontier Photonics, Univ Roma Tre, Roma Tre University, Dept Elect Engn, NooEL, University "Roma Tre", University of Wollongong, Department of Electrical Engineering, University of Edinburgh

Contributors: Assanto, G., Marchant, T. R., Minzoni, A. A., Smyth, N. F.

Publication date: 9 Dec 2011

Peer-reviewed: Yes

#### **Publication information**

Journal: Physical Review E

Volume: 84

Issue number: 6

Article number: 066602

ISSN (Print): 1539-3755

Ratings:

Scopus rating (2011): CiteScore 2.28 SJR 1.48 SNIP 0

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Statistical and Nonlinear Physics, Statistics and Probability

DOIs:

10.1103/PhysRevE.84.066602

URLs:

<http://www.scopus.com/inward/record.url?scp=84555189254&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84555189254

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

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

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

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 3

Pages: 3345-3347

Publication date: 1 Nov 2016

Peer-reviewed: Yes

### Publication information

Journal: Bioinformatics

Volume: 32

Issue number: 21

ISSN (Print): 1367-4803

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

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

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

Summary: Each cell is a phenotypically unique individual that is influenced by internal and external processes, operating in parallel. To characterize the dynamics of cellular processes one needs to observe many individual cells from multiple points of view and over time, so as to identify commonalities and variability. With this aim, we engineered a software, 'SCIP', to analyze multi-modal, multi-process, time-lapse microscopy morphological and functional images. SCIP is capable of automatic and/or manually corrected segmentation of cells and lineages, automatic alignment of different microscopy channels, as well as detect, count and characterize fluorescent spots (such as RNA tagged by MS2-GFP),

nucleoids, Z rings, Min system, inclusion bodies, undefined structures, etc. The results can be exported into \*.mat files and all results can be jointly analyzed, to allow studying not only each feature and process individually, but also find potential relationships. While we exemplify its use on Escherichia coli, many of its functionalities are expected to be of use in analyzing other prokaryotes and eukaryotic cells as well. We expect SCIP to facilitate the finding of relationships between cellular processes, from small-scale (e.g. gene expression) to large-scale (e.g. cell division), in single cells and cell lineages. Availability and implementation: [http://www.ca3-uninova.org/project\\_scip](http://www.ca3-uninova.org/project_scip). Supplementary information: Supplementary data are available at Bioinformatics online.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

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

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

Number of pages: 3

Pages: 4318-4320

Publication date: 15 Dec 2018

Peer-reviewed: Yes

### Publication information

Journal: Bioinformatics

Volume: 34

Issue number: 24

ISSN (Print): 1367-4803

Ratings:

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

Original language: English

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

DOIs:

10.1093/bioinformatics/bty505

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

### Search reliability and search efficiency of combined Lévy-Brownian motion: Long relocations mingled with thorough local exploration

A combined dynamics consisting of Brownian motion and Lévy flights is exhibited by a variety of biological systems performing search processes. Assessing the search reliability of ever locating the target and the search efficiency of doing so economically of such dynamics thus poses an important problem. Here we model this dynamics by a one-dimensional fractional Fokker-Planck equation combining unbiased Brownian motion and Lévy flights. By solving this equation both analytically and numerically we show that the superposition of recurrent Brownian motion and Lévy flights with stable exponent  $\alpha < 1$ , by itself implying zero probability of hitting a point on a line, leads to transient motion with finite probability of hitting any point on the line. We present results for the exact dependence of the values of both the search reliability and the search efficiency on the distance between the starting and target positions as well as the choice of the scaling exponent  $\alpha$  of the Lévy flight component.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Research area: Computational Physics, Technische Universität München, Università degli Studi di Padova, Italy, School of Mathematical Sciences, Institute for Physics and Astronomy, Universität Potsdam

Contributors: Palyulin, V. V., Chechkin, A. V., Klages, R., Metzler, R.

Publication date: 8 Sep 2016

Peer-reviewed: Yes

### Publication information

Journal: Journal of Physics A: Mathematical and Theoretical

Volume: 49

Issue number: 39

Article number: 394002

ISSN (Print): 1751-8113

Ratings:

Scopus rating (2016): CiteScore 3.7 SJR 0.935 SNIP 0.941

Original language: English

ASJC Scopus subject areas: Statistical and Nonlinear Physics, Statistics and Probability, Modelling and Simulation, Mathematical Physics, Physics and Astronomy(all)



Keywords: Brownian motion, first arrival, first passage, Lévy flights, random search process

DOIs:

10.1088/1751-8113/49/39/394002

URLs:

<https://arxiv.org/abs/1609.03822>

URLs:

<http://www.scopus.com/inward/record.url?scp=84989172145&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84989172145

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

### Signal focusing through active transport

The accuracy of molecular signaling in biological cells and novel diagnostic devices is ultimately limited by the counting noise floor imposed by the thermal diffusion. Motivated by the fact that messenger RNA and vesicle-engulfed signaling molecules transiently bind to molecular motors and are actively transported in biological cells, we show here that the random active delivery of signaling particles to within a typical diffusion distance to the receptor generically reduces the correlation time of the counting noise. Considering a variety of signaling particle sizes from mRNA to vesicles and cell sizes from prokaryotic to eukaryotic cells, we show that the conditions for active focusing - faster and more precise signaling - are indeed compatible with observations in living cells. Our results improve the understanding of molecular cellular signaling and novel diagnostic devices.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Institute for Physics and Astronomy, University of Potsdam, Laboratory for Molecular Modeling, National Institute of Chemistry Ljubljana

Contributors: Godec, A., Metzler, R.

Number of pages: 6

Publication date: 2 Jul 2015

Peer-reviewed: Yes

### Publication information

Journal: Physical Review E

Volume: 92

Issue number: 1

Article number: 010701

ISSN (Print): 1539-3755

Ratings:

Scopus rating (2015): CiteScore 1.89 SJR 1.183 SNIP 2.283

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Statistical and Nonlinear Physics, Statistics and Probability

DOIs:

10.1103/PhysRevE.92.010701

URLs:

<http://www.scopus.com/inward/record.url?scp=84937010360&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84937010360

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

### Structured orthogonal families of one and two strata prime basis factorial models

The models in structured families correspond to the treatments of a fixed effects base design  $\pi$ , on the fixed effects parameters of the models, is studied. Analyzing such a families enables the study of the action of nesting factors on the effects and interactions of nested factors. When  $\pi$  has an orthogonal structure, the family of models is said to be orthogonal. The models in the family can have one, two or more strata. Models with more than one stratum are obtained through nesting of one stratum models. A general treatment of the case in which the base design has orthogonal structure is presented and a special emphasis is given to the families of prime basis factorials models. These last models are, as it is well known, widely used in fertilization trials.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research Community on Data-to-Decision (D2D), ISLA Campus Lisbon, Laureate International Universities , Campus FCT-UNL

Contributors: Rodrigues, P. C., Moreira, E. E., Jesus, V. M., Mexia, J. T.  
Number of pages: 12  
Pages: 603-614  
Publication date: 2014  
Peer-reviewed: Yes

#### Publication information

Journal: Statistical Papers  
Volume: 55  
Issue number: 3  
ISSN (Print): 0932-5026  
Ratings:

Scopus rating (2014): CiteScore 1.7 SJR 1.037 SNIP 1.55

Original language: English

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

Keywords: Factorial designs, Families of models, Nested models, Orthogonal models, Two strata models

DOIs:

10.1007/s00362-013-0507-0

URLs:

<http://www.scopus.com/inward/record.url?scp=84903887341&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84903887341

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

### Using multi-step proposal distribution for improved MCMC convergence in Bayesian network structure learning

Bayesian networks have become popular for modeling probabilistic relationships between entities. As their structure can also be given a causal interpretation about the studied system, they can be used to learn, for example, regulatory relationships of genes or proteins in biological networks and pathways. Inference of the Bayesian network structure is complicated by the size of the model structure space, necessitating the use of optimization methods or sampling techniques, such as Markov Chain Monte Carlo (MCMC) methods. However, convergence of MCMC chains is in many cases slow and can become even a harder issue as the dataset size grows. We show here how to improve convergence in the Bayesian network structure space by using an adjustable proposal distribution with the possibility to propose a wide range of steps in the structure space, and demonstrate improved network structure inference by analyzing phosphoprotein data from the human primary T cell signaling network.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Signal Processing, Aalto University, Department of Computer Science and Information Systems

Contributors: Larjo, A., Lähdesmäki, H.

Publication date: 27 Dec 2015

Peer-reviewed: Yes

#### Publication information

Journal: Eurasip Journal on Bioinformatics and Systems Biology

Volume: 2015

Issue number: 1

Article number: 6

ISSN (Print): 1687-4145

Ratings:

Scopus rating (2015): CiteScore 1.8 SJR 0.314 SNIP 0.371

Original language: English

ASJC Scopus subject areas: Medicine(all), Computer Science(all), Signal Processing, Statistics and Probability, General

Keywords: Bayesian network, MCMC, Proposal distribution, Structure learning

DOIs:

10.1186/s13637-015-0024-7

#### Bibliographical note

EXT="Lähdesmäki, Harri"

Source: Scopus

Source ID: 84932633872

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

### Performance of Variable Partial Factor approach in a slope design

Most of the design codes have moved from traditional total factor of safety method to the partial factor approach, aiming to cover the uncertainties better. The target has been to reach more consistent safety levels, but it has not always been obtained. This has raised more interest towards reliability based design and its applications. In this paper, the performance of two partial factor approaches were compared from the reliability point of view; eurocode 7 design approach 3 and proposed Variable Partial Factor approach. The results show that the partial factor method with fixed partial factors cannot fully cover the uncertainties related to the design. The partial factors should be dependent on the level of uncertainty of the parameters. The results also show that RBD can be applied in a designer friendly way. In addition, some challenges in the determination of the characteristic values were pointed out.

#### General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Civil Engineering

Contributors: Knuuti, M., Lämsivaara, T.

Publication date: 2019

#### Host publication information

Title of host publication: 13th International Conference on Applications of Statistics and Probability in Civil Engineering (ICASP13), Seoul, South Korea, May 26-30, 2019

ASJC Scopus subject areas: Civil and Structural Engineering, Statistics and Probability

DOIs:

10.22725/ICASP13.475

