DY 63: Modeling and Data Analysis

Time: Friday 10:00–11:30 Location: H20

DY 63.1 Fri 10:00 H20

Analyzing stochastic time serieses via Bayesian parameter estimation of Langevin models with correlated noise — Oliver Kamps and •Clemens Willers — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany

Over the last years, the estimation of stochastic evolution equations of complex systems has been applied in many scientific fields ranging from physics to biology and finance. Especially, Langevin models with delta-correlated noise terms, which realize a Markovian dynamic, have been used successfully in this context [1]. However, many real world data sets exhibit correlated noise and a non-Markovian dynamic, for example data sets from turbulence [2].

To tackle this problem, we use Langevin models containing an added hidden component which realizes a driving correlated noise. We develop a method for the systematic estimation of the drift- and diffusion functions, parameterized through spline functions. The method is based on a likelihood function which is constructed by a short-time propagator for the measured values of the visible component. A Markov Chain Monte Carlo procedure makes it possible to get access to both the parameters and their reliability. The method is demonstrated using the example of turbulent real world data sets as the country-wide wind power production [3].

[1] Friedrich et al., Phys. Rep. 506, 87 (2011) [2] Friedrich and Peinke, Phys. Rev. Lett. 78, 863 (1997) [3] Kamps O., in Wind Energy-Impact of Turbulence, edited by Hölling M. et al. (Springer) 2014, p. 67.

DY 63.2 Fri 10:15 H20

Phase walk analysis of leptokurtic time series — •Christoph Räth[1], Heike Modest[1], and Korbinian Schreiber[2] — [1]Institut für Materialphysik im Weltraum, DLR, Münchener Str. 20, 82234 Weßling, Germany — [2]Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

A very general definition of nonlinearity in data sets can be obtained from their representation in Fourier space: From the Wiener-Khintchine theorem and the bijectivity of the Fourier transformation it follows that the linear information is entirely represented by the Fourier amplitudes. Hence, all nonlinear information is contained solely in the Fourier phases. Yet, the direct study of the Fourier phases has so far attracted only little attention. Here, we present a novel method to quantify the phase information. In close analogy to random walk analyses, we propose the phase walk statistics as a way to quantify the phase information. We apply it to the analysis of nonlinearities in intermittent, leptokurtic time series like turbulent wind data, the Dow Jones (DJ) day-to-day returns and synthetic leptokurtic data. Testing for nonlinearities by means of surrogates shows that the new method yields strong significances for nonlinear behavior. Due to the drastically decreased computing time as compared to embedding space methods, the number of surrogate realizations can be increased by orders of magnitude [1]. Thereby, the probability distribution of the test statistics can very accurately be derived and parameterized, which allows for much more precise tests on nonlinearities. [1] K. Schreiber et al., Chaos, 28, 063120 (2018)

DY 63.3 Fri 10:30 H20

Data Science based Magnesium Corrosion Engineering — Tim Würger[1] and •Robert Meissner[1,2] — [1]MagIC Magnesium Innovation Centre, Institute of Materials Research, Helmholtz Zentrum Geesthacht, Geesthacht, Germany — [2]Hamburg University of Technology, Institute of Polymer and Composites, Hamburg, Germany

Magnesium is a material with high potential for a wide range of applications in areas such as transport, energy, and medicine. However, the corrosion properties of magnesium still limit its practical application. It is, therefore, necessary to develop new approaches that can prevent or control corrosion and degradation in order to adapt to the specific needs of the application. One way to accomplish this is to use inhibitor molecules that block or trap corrosive species that would otherwise further promote corrosion. As it is not possible to obtain a detailed atomistic understanding of the inhibition mechanisms for each additive due to the variety of different molecules, other inhibition prediction measures are required. We present a concept combining high throughput calculations with dimensionality reduction algorithms and corrosion experiments. Physical properties, e.g. HOMO/LUMO gaps or corrosion inhibition of inhibitor molecules, are presented next to a two-dimensional sketch map of the molecules based on their molecular similarity. This approach facilitates the search for new molecules with a positive or negative influence on corrosion inhibition efficiency by out-of-sample mapping and could thus contribute significantly to a better understanding of corrosion inhibition mechanisms and control of magnesium/electrolyte interface properties.

DY 63.4 Fri 10:45 H20

DyCA - Dynamical Component Analysis — Steffen Hartmann, •Katharina Korn, Bastian Seifert, and Christian Uhl — Center for Signal Analysis of Complex Systems, University of Applied Sciences Ansbach, Residenzstr. 8, 91522 Ansbach

Spatio-temporal patterns emerging from a certain class of low-dimensional differential equations can be decomposed by dynamical component analysis (DyCA), a new algorithm proposed in [1]. We present the method, which is based on a least-square-optimization leading to a generalized eigenvalue problem of correlation matrices of the signal and its derivative. The application of DyCA to simulated and real world data is demonstrated and the power of the algorithm is shown by comparing the results to principal and independent component analysis (PCA, ICA).

[1] B. Seifert, K. Korn, S. Hartmann, and C. Uhl, Dynamical Component Analysis (DyCA): Dimensionality reduction for high-dimensional deterministic time-series, 2018 IEEE 28th International Workshop on Machine Learning for Signal Processing (MLSP), Aalborg, 17.-20.09.2018

DY 63.5 Fri 11:00 H20

Data-driven modelling of spatio-temporal dynamics by means of artificial neural networks — •Sebastian Herzog[1,2], Florentin Wörgötter[2], and Ulrich Parlitz[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Germany — [2]Third Institute of Physics and Bernstein Center for Computational Neuroscience, University of Göttingen, Germany

We present a data driven modeling ansatz [1] which combines deep convolutional neural networks (CNNs) for feature extraction and dimension reduction with an adapted conditional random field (CRF) in order to model the properties of temporal sequences. To validate the proposed method we used the BOCF model describing electrical excitation waves in cardiac tissue where chaotic dynamics is associated with cardiac arrhythmias. Running the trained network in a closed loop(feedback) configuration iterated prediction provided forecasts of the complex dynamics that turned out to follow the true evolution of the BOCF simulation. The direct comparison between the forecasted data from the network and the real data from the BOCF simulation clearly shows that machine learning methods like those employed here provide faithful models of the underlying complex dynamics of excitable media that, when suitably trained can provide powerful tools for predicting the spatio-temporal evolution and for cross-estimating not directly observed variables. [1] S. Herzog, F. Wörgötter, U. Parlitz, Data-driven modelling and prediction of complex spatio-temporal dynamics in excitable media, in: Front. Appl. Math. Stat. - Dynamical Systems (2018), doi: 10.3389/fams.2018.00060

DY 63.6 Fri 11:15 H20

Estimating model parameters by attractor comparison — •Ulrich Parlitz — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — Institute for Nonlinear Dynamics, Georg-August-Universität, Göttingen, Germany

Time series based methods for estimating parameters of dynamical models are discussed which are based on a comparison of the asymptotic dynamics given by (reconstructed) attractors underlying the observed data and those generated by the model. The similarity of both distributions of (reconstructed) states is quantified by different measures of (dis-)similarity or "distance" (e.g., ordinal pattern distributions, nearest neighbor distances) and a good set of model parameters minimizes their "distance" or dissimilarity. We present different implementations of this approach for parameter estimation and evaluate their performance with several dynamical examples.