6th International Workshop on Set-Oriented Numerics

Imperial College London, 28th September – 1st October 2015

Poster titles and abstracts

The poster session will take place in the lunch break on Wednesday, 30 September 2015 in Huxley Lecture Theater 130 from 12.00pm to 14.00pm. Lunch will be provided and is free of charge for all participants of the workshop.

Andreas Bittracher (TU Munich)

Pseudogenerators for Spatial Metastability Analysis

Metastable behavior in dynamical systems may be a significant challenge for a simulation based analysis, even in the autonomous case. In recent years, transfer operator based approaches to problems exhibiting metastability have matured, but in order to make these approaches computationally feasible for larger systems, various reduction techniques had to be proposed. For example, Schütte introduced a spatial transfer operator for Langevin dynamics, which acts on densities on configuration space, instead of the full phase space. This reduction unfortunately leads to the loss of the semigroup property of the operator, and the Markoviantity of the underlying system.

However, we were able to demonstrate that despite this, the family of spatial transfer operators possesses a well defined generating structure, largely analogous to the semigroup case. What is more, the underlying ”pseudogenerators” have particularly simple, explicit expressions, with interesting connections to the well-known Smoluchowski equation. Furthermore, their discretization involves no momentum averaging. This makes collocation methods particularly easy to implement and computationally efficient, which in turn may open the door for further efficiency improvements in, e.g., the computational treatment of conformation dynamics. Pseudogenerators for systems in molecular internal coordinates can also be defined, as well as the projection onto a principal one-dimensional reaction coordinate.

Gemma Lancaster (Lancaster University)

Identifying chronotaxic systems from single-variable time series

The recent introduction of chronotaxic systems provides a framework which describes nonautonomous systems with stable yet time-varying frequencies which are resistant to continuous external perturbations [1, 2, 3], characteristics which are often seen in living systems. This approach allows the underlying determinism of systems which have previously been considered stochastic to be appreciated. The novelty of this approach necessitated the development of a new set of methods for the extraction of information about the dynamics and interactions present in chronotaxic systems from real time series [4]. These inverse approach methods, based on time-frequency analysis, Bayesian inference [5], and detrended fluctuation analysis, can identify chronotaxicity in phase dynamics extracted from a single time series [6]. Here, coupled chronotaxic phase oscillators are simulated numerically and the reliability of the methods for the detection of chronotaxic systems from a single time series is demonstrated in different scenarios. Once shown to be successful in simulated data, the methods are applied to real experimental electroencephalography (EEG) data. The assumptions, limitations and future directions of the methods are also discussed.

References

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Philipp Rumschinski (Magdeburg University)

Determining reachable sets and the output energy of polynomial continuous-time systems

In this poster, we demonstrate how reachable sets and the initial conditions leading to a bounded L_2-norm of the output can be computed efficiently for polynomial models. Uncertainties are considered here as unknown-but-bounded variables, i.e. variables that are allowed to take any value from a semi-algebraic set. The presented methods are based on formulating the desired sets in terms of polynomial feasibility problems. The appearing continuous-time dynamics constraints are hereby treated with help of occupation measures. The resulting infinite dimensional linear programs are then addressed through Lasserre's converging hierarchy of LMI problems. The employed methods are exemplified with two academic examples.

Valentina Ticcinelli (Lancaster University)

Characterizing Coupling Functions in Networks of Oscillators

How to characterize and reconstruct networks from data is a challenge which pervades all of science [1-3]. Numerous methods have been introduced for detecting the existence of causal connections in networks, most of which focus on pairwise interactions [4]. Here, we present a new method, based on dynamical Bayesian inference, which is capable of detecting the effective phase connectivity within networks of time-evolving coupled oscillators subject to noise [5-8]. It can reconstruct not only pairwise, but also joint conductivities and conductivities of higher degree, including triplets and quadruplets of interacting oscillators. Moreover, one can infer details of the coupling functions from which, in turn, the existence of causal links can be determined as well as the underlying functional mechanisms.

We will illustrate the characteristics and potential of the method by application to a numerically-generated network of phase oscillators, with time-dependent coupling parameters, and subject to noise [8]. By the mean of an algorithm based on two-dimensional correlation, we are able to integrate the information carried by the form of the coupling functions in a polar representation. The procedure makes use of numerically-generated banks of comparison functions. As examples, results involving real data will be shown, including coupling functions between EEG brain waves for subjects with Autistic Spectrum Disorder.

References

[1] Strogatz S, *Nature* 410 268-276, 2001. [2] Achard S, Salvador R, Whitcher B, Suckling J and Bullmore E D, *J. Neurosci.* 26 63-72, 2006. [3] Donges J F, Zou Y, Marwan N and Kurths J, *Europhys. Lett.* 87 48007, 2009. [4] Park H J and Friston K, *Science* 342 1238411, 2013. [5] Kralemann B, Cimponeriu L, Rosenblum M, Pikovsky A and Mrowka R, *Physical Review E* 77 066205, 2008. [6] Duggento A, Stankovski T, McClintock P V E and Stefanovska A, *Phys. Rev. E* 86 061126, 2012. [7] Stankovski T, Duggento A, McClintock P V E and Stefanovska A, *Phys. Rev. Lett.* 109 024101, 2012. [8] Stankovski T, Ticcinelli V, McClintock P V E and Stefanovska A, *New J. Phys.* 17 035002, 2015.