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Quantifying interactions between complex oscillatory systems: a topic in time series analysis

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1 State of the Art

Recently, new approaches to understanding the behavior of complex systems based on results of non-linear dynamics have come to the forefront of current research. This tendency is becoming clearer as more and more problems from geology, meteorology, physical, chemical and life sciences have been more satisfactorily understood after reformulating them in the framework of non-linear dynamics. Especially in life sciences and medicine important components of physiological systems, such as the human body, have been modeled as a set of coupled non-linear dynamical oscillators: the heart, the brain and the lungs. When trying to understand complex systems, scientific advances depend on developments in theoretical and experimental science and on building links between hypothesized models and experimental results.

Central to the analysis of self-sustained oscillators is the concept of phase. The motion of many oscillatory systems in their state space may be decomposed into two primary variables: amplitude and *phase*. The amplitude of the limit cycle represents the intensity of the oscillations and is stable. Phase represents the position of the system along the limit cycle and is free: it is neither stable nor unstable. It is an observable of the system that characterizes its motion along the attractor (in the direction of the zero Lyapunov exponent). Phase can be affected by very weak forces which is important for the analysis of weak couplings.

1.1 Quantifying directional influence

The first step in detecting directional influence is developing an index which reacts to the strength of directional coupling. Such an index does not as of itself constitute a complete method of detecting coupling directionality.

At present there are three main approaches to detecting directionality in bivariate time series. The first approach is based on state-space reconstruction and mutual prediction, the second approach is based on modeling functional relationships of phases and the third approach involves estimating information-theoretic functionals.

State space methods include various cross-prediction methods and methods based on statistics of nearest neighbors. Cross-prediction methods attempt to directly exploit Granger's ideas on mutual forecasting of series generated by coupled linear systems [9]. Generally the attractor in state space is reconstructed by means of a time-delay embedding [10, 11, 12]. However opposite opinions exist on how to interpret cross-prediction accuracy in the context of directionality detection [13, 14]. Alternative methods exploit statistics based on nearest neighbor distances [15], however in Ref. [16] the authors assert that other factors such as the effective dimension at typical neighborhood sizes may influence the result of the previously published algorithms.

The second group involves estimating functional relationships between phases of the systems. In Ref. [17] the authors try to estimate the Fourier coefficients of the coupling function and subsequently compute a norm based on a subset of the coefficients indicating the directionality. However this approach was found to be accurate only for long time series [18]. The method has been improved with a bias correcting term and an estimate of significance of the directionality by Smirnov and Bezruchko [19].

The last group of methods consists of algorithms based on information theory. Here, Schreiber [20] proposes to compute the *transfer entropy*, based on the Kullback-Leibler entropy measuring the deviation of the transition probability density function (PDF) from the generalized Markov property. Paluš [21, 4] has applied information theoretic functionals to phases to detect the "net flow of information" between processes. Recently it has been shown that the method of Schreiber can be identified with the method of Paluš for a certain set of parameters [1].

1.2 Quantifying dependent states

Quantification of various synchronization types is a much more intensively studied problem than the detection or quantification of directionality. One of the most important types of synchronization studied in oscillatory systems is *phase synchronization.* Phase synchronization is a process of mutual attunement of rhythms of two oscillating systems. It can occur under very weak coupling and has been found in stochastic systems and even in systems exhibiting deterministic chaos [22].

The only method which can detect phase synchronization with certainty is an *active experiment*: if the systems resume synchronous motion after a disturbance has been introduced into the coupled system, phase synchronization is taking place. Frequently, an active experiment cannot be performed (e.g. in health care it would be unethical). At this point, specialized techniques of time-series analysis are required to handle the problem.

When analyzing experimental data, indices quantifying the *degree of synchronization* are often applied to the time series in an attempt to detect phase synchronization. It should be noted that although these indices quantify the dependence between the two systems, they are generally not connected to a theoretical definition of phase synchronization. A better-suited name would thus be ‘dependence index’. Currently, there is a number of phase dependence indices in use, for example Conditional probability [23], Mean phase coherence [24], Mutual information [25], Shannon entropy of the phase differences [23] or Cross-correlation between probabilities of recurrence [26].

1.3 Testing the significance

Various methods to quantify directional interactions and the amount of statistical dependence between two time series have been listed above. However their results may be biased by estimator properties, by the amount of noise in the time series, by the complexity and characteristics of the individual dynamics of each system. The absolute values of the results of the above algorithms thus have no clear interpretation except under special circumstances.

Additional work is required to verify the significance of results from these methods. A frequently used approach to the verification of significance of an index value is the method of *surrogate data* [27]. Surrogate data in this context are time series which preserve all the properties of the original time series except the one which is being tested. In both cases (directionality and synchronization), the tested property is coupling.

Several surrogate generation algorithms have been proposed to date: Fourier transform surrogates [27], amplitude adjusted Fourier transform surrogates [28], permutation surrogates [29] and twin surrogates [30]. It should be noted that none of the methods is ideal: all of them have their advantages and disadvantages and surrogate testing is a problem that requires careful consideration.

Assuming that applicable surrogates are available, a standard one sided hypothesis test can be constructed to check whether an index value is significant and infer whether directional influence or phase synchronization is present.

2 Aims of the doctoral thesis

The present work is focused on building links between theoretical and practical aspects of complex systems modeling. The goal of the work is the analysis, comparison and further development of selected time series analysis algorithms aimed at uncovering interactions between coupled oscillatory systems with a minimum of assumptions on the form of the interactions.

The main problem was to find frequently used estimators of information-theoretic functionals, adapt them for evaluating conditional mutual information and test them against each other on selected model systems to find out if any one would exhibit markedly better performance in the problem of detecting directional coupling than the rest. The reference estimator was the equiquantal estimator of conditional mutual information [25].

Detection of directional coupling requires the use of surrogates. The choice of surrogates introduced a new degree of freedom in the comparison process and it was necessary to examine how surrogates interact with each estimator.

Under generalized synchronization, directionality of coupling cannot be reliably detected as a functional relationship between the phases and amplitudes exist. The detection of generalized synchronization in experimental time series is problematic. On the other hand, it is possible to detect phase synchronized states between two systems and consider these a warning that the systems may be coupled too tightly. In an effort to find a method of detecting synchronized states, the current phase "synchronization" indices had to be examined and tested.

Finally the methods for detecting directionality and for detecting synchronized states were applied to an experimental problem in the context of the EU FP6 project BRACCIA: the search for changes in phase dynamics of the human cardiorespiratory system. The application of different methods on a single set of experimental data will give us an idea of the variability and stability in the results.

3 Working methods

Progress in the field of nonlinear science is difficult as most random variables generally do not conform to any known probability distribution and fully analytical treatment of the problems is in many cases not possible. Ideally the proposed method should be theoretically connected to the phenomena it tries to quantify and rigorously tested on model systems to show that it can be expected to perform reasonably in practice. Yet better testing is possible by acquiring data from real systems with known coupling parameters: these can then be used to test the algorithm as well.

Most estimators of conditional mutual information have a free parameter which affects their results. The number of sample points supplied to the estimator has a decisive effect on the quality of estimates. The estimators were first investigated by applying them to coupled ARMA (autoregressive moving average) systems, linear parts of the Barnes sunspot model [31] where an analytical estimate of the conditional mutual information was available. Detailed numerical experiments have been performed to illuminate the properties of the estimators with respect to these parameters.

Detailed numerical studies involving the entire estimation and surrogate generation framework were performed using the coupled Rössler systems [32]. In these experiments the entire framework of estimation and significance testing was applied to judge the quality of the end result: the quality of detection of either directionality or phase synchronization.

The testing process described above is extremely computationally intensive and has been made possible by gaining access to various high-performance computing facilities, such as the HPCx (tightly coupled IBM p575 systems with 2608 CPUs) in Manchester and IBM Bluegene/L (1024 CPUs) system in the Edinburgh Parallel Computing Centre. Additionally for smaller jobs various clusters around the world were generously made available, for example at the University of Edmonton in Canada or the Joyce and Otmar cluster of the Institute of Computer Science in Prague. Distributed programs were created using the MPI standard (Message Passing Interface) that could be run on these clusters and on supercomputers alike. The source code was written in C++ and Python.

4 Results

4.1 Directionality analysis

Based on previous work of Kozachenko and Leonenko [33] on entropy estimates from nearest neighbor distances, Kraskov *et al.* [34] have derived an estimator of mutual information from k-th nearest neighbor distances. The original work of Kozachenko and Leonenko only deals with derivation of a consistent estimator of entropy from nearest neighbor distances. Recently, Goria *et al.* [35] has shown that entropy estimators based on k-th nearest neighbor distances are consistent. In this work, an estimator of conditional mutual information has been derived based on the work of the above authors. Use of the estimator requires a sophisticated processing system as fast methods for satisfying fixed mass hyper-sphere queries (finding the k-th nearest neighbor) and fixed range queries (finding all points inside a given hyper sphere) should be used. Among well-known algorithms used are k-D trees [36] and box indexing algorithms [37] for fast multi-dimensional nearest neighbor search. Methods for this purpose have been tested on high-dimensional spaces with samples drawn from different distributions and the results have been published in [2]. The estimator has been tested on the Barnes model [31]. It was expected that this functional will also be a consis-

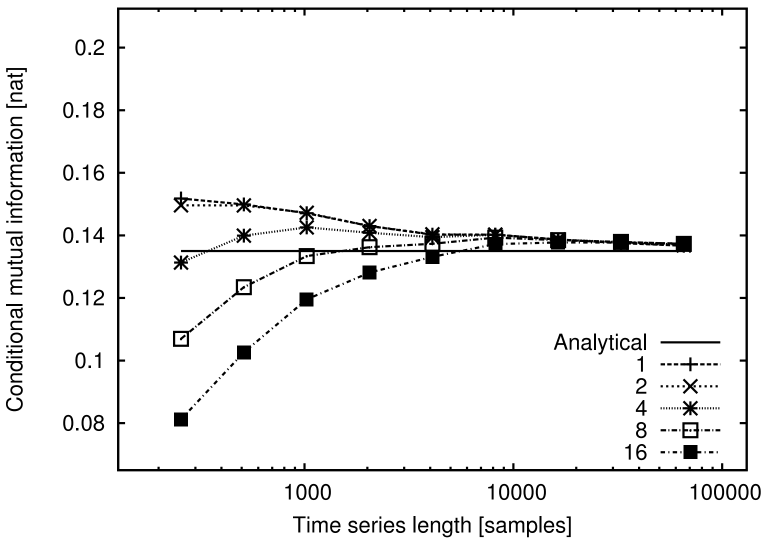

Figure 1: Convergence behavior of CMI estimates vs. length of input series with respect to the free parameter on the Barnes model using k-NN method. Analytical estimate of CMI indicated by horizontal line.

tent estimator of conditional mutual information as it is based on the theory behind an unbiased estimate of the entropy of a random sample. The numerical study supports this assumption and shows that the method seems to converge to the analytical estimate for many different values of the free parameter k (cf. Fig. 1). This is a unique behavior not seen in any of the previous methods.

This estimator however requires high quality data, i.e. not contaminated by nonlinear deformations sometimes found in experimental time series. Deformations of the sample space will not be reproduced in the surrogate time series properly and cause increased bias in the estimates. Since random sample distances are used to build the final estimate any such deformation presents a large problem and is the cause of diminished performance of this estimator in some situations. Methods based on random sample distances also show a decreased performance on systems with dissimilar dynamics [3].

4.2 Synchronization analysis

Close examination of the current phase synchronization detection methods has shown that these methods detect statistical dependencies rather than synchronized states. However this was not satisfactory with respect to our problem of detecting phase-synchronized states as an indication of increased coupling strength.

An algorithm has been constructed to detect phase-synchronized states that was based on the connection between the frequency locking condition and the gradient of a linear regression of the differences of phase values. A bootstrap test is proposed to test the significance of the estimated gradient. The null hypothesis of the bootstrap test is that the two systems are synchronized: this is a completely different approach that current methods.

To test the effectiveness of the proposed detector, previously published results have been replicated using large-scale testing. The results of synchronization detection using the proposed method are in excellent agreement with the results previously published in [22].

4.3 Experimental data study

One of the aims of the BRACCIA project is to apply recent findings in the analysis of coupling from time series to data recorded in the waking state and under general anesthesia and to discover factors differentiating between these two states. The methods developed in the framework of non-linear dynamics were applied to experimental data acquired from human volunteers. The underlying assumption is that the subsystems of the human cardiorespiratory system behave like noisy dynamical systems and can be analyzed as a set of weakly coupled non-linear oscillators. The central problem is then the detection of changes in coupling between respiratory, cardiac and cortical oscillations. In this work the interactions between the cardiac and respiratory oscillators were examined.

Data from human volunteers was acquired in a clinical setting in the Ulleval Hospital in Oslo and in the Royal Lancaster Infirmary. In this study, 25 patients were included. Measurements were carried out in the waking state and under general anesthesia for spontaneous and controlled respiration (depending on the choice of anesthetic for the subject) to record 20–30 minutes of the activity of the human organism in each state.

The data has then been preprocesed and analyzed using selected methods. The dependence indices paint a consistent picture of what is happening within the cardiorespiratory system: all of the used indices increase when the patient is in the anesthetized state.The analysis of directionality reveals another effect of general anesthesia on the cardiorespiratory system: the directional influence from the lungs to the heart is reduced and the opposite influence is increased. This is consistent with a shift in directionality in the cardiorespiratory system. In the waking state, directional influence is usually present from the lungs towards the heart, so called "Respiratory sinus arrhythmia" or variation of the heart rate according to the inspiration/expiration cycle of the lungs. Under general anesthesia, this influence is greatly reduced. On the other hand, directional influence from the heart to the lungs is not clear in the waking state but the proportion of significant results is much higher in the anesthetized state quite consistently. There is some variation between the methods and even with respect to the parameters within one method. The medians of the distributions are however very stable across parameter choices and even across different methods. There is also a clear agreement between the methods in the difference between general anesthesia and the waking state for both directionalities.

5 Conclusion

In this work the framework for analyzing systems of self-sustained non-linear oscillators was presented and the necessary concepts were introduced. The conditions for the application of the phase dynamics approach and it's advantages were described. The concept of weak interactions was presented and the problem of quantification of weak interactions was divided into two classes: synchronization detection and directionality analysis.

The core problem studied in this work is the problem of analyzing the full range of weak interactions in a pair of non-linear oscillators. Methods of quantifying strength of directional coupling have been introduced and information-theoretic methods have been studied in detail. Selected estimation procedures based on different types of information in the time series were theoretically investigated and numerically tested. A new estimator based on [33, 34] converging to the true value of conditional mutual information independently of its free parameter has been derived. The estimator was empirically shown to have the properties that were expected based on the derivation process. Although the estimator has favorable theoretical properties, caution is advised when applying the estimator to real data as noise and deformations of the measured signal can perturb the metric relationships in the sample space. Binning estimators seem to be less sensitive to the influence of measurement noise and signal deformations.

The current methodology for detecting phase synchronization was analyzed and it was ascertained that frequently applied methods detect phase synchronization in the weaker sense. These methods result in marking any dependent states as synchronized even if the coupling is not strong enough to actually cause the systems to enter a phase-synchronized state. Large-scale testing was conducted to verify this phenomenon for a selection of frequently applied methods. A new approach to detecting synchronized states using the null hypothesis of the phase-synchronized state was introduced and shown to detect phase-synchronized states satisfactorily. The effectiveness of the detector was shown using detailed numerical studies.

A selection of dependence analysis methods and directionality detection methods were applied to electrocardiogram and respiratory effort time series obtained within the project BRACCIA. Data from 25 patients were analyzed with the goal of finding differences in the functioning of the cardiorespiratory system between the waking state and under general anesthesia. Previous findings on stronger overall coupling between the two subsystems were confirmed by the present analysis. It was found that in the preliminary study there were clear changes of directional influence: in the waking state, the respiratory system affected the cardiac oscillator more than under general anesthesia and vice-versa the influence of the cardiac system on the respiratory system is stronger under anesthesia than in the waking state. The indication of directional influence was stable with respect to changing the free parameters of the methods.

Further work will concentrate on generalizing the above framework to a system of many coupled oscillators instead of studying the reduced situation of a pair of systems. This situation arises when measuring e.g. the activity of the human brain. If magnetic resonance imaging (MRI) is used to obtain a multivariate signal from the brain, the resulting data contains tens of thousands of time series, with each characterizing brain activity at a high spatial resolution using a BOLD (blood oxygen level dependent) signal. Another avenue of research consists in trying to derive an index capturing directional influence between systems that would be robust with respect to deformations of the time series which are theoretically difficult to analyze. A method that would be enormously helpful in practice would be an algorithm that would include an internal significance test thus eliminating the need for a separate surrogate generation algorithm.

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6 Resumé

Tato práce se zaměřuje na problém hledání interakcí mezi komplexními oscilačními procesy. Nalezení vnitřních souvislostí mezi jednotlivými procesy je důležitým krokem k hlubšímu pochopení funkce složitých systémů. Zde se soustředíme na dva hlavní problémy současné analýzy párů dynamických procesů: určení směru působení a testování synchronizace. Cílem analýzy směru působení je zjištění asymetrických vztahů mezi procesy. Odhalení synchronizace, sladění rytmů dynamických procesů, ukazuje na užší součinnost dvou procesů. V práci jsou testovány současné metody zpracování časových řad, které slouží k odhalování popsaných jevů. Pomocí detaliních numerických studií jsou analyzovány vlastnosti těchto přístupů a jsou předloženy nové možnosti řešení obou problémů. Závěrem práce je zpracována předběžná studie experimentálně získaných dat, která porovnává interakce v lidském kardiorespiračním systému při vědomí v klidovém stavu a během celkové anestézie. Nové metody lze využít v rámci aplikace teorie nelineární dynamiky k analýze vzájemného ovlivňování biologických, meteorologických, chemických a dalších systémů