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Inference of functional dependence in coupled chaotic systems using feed-forward neural network

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ABSTRACT

We propose a new model-free method based on feed-forward artificial neuronal network for detecting functional connectivity in coupled systems. The developed method which does not require large computational costs and which is able to work with short data trials can be used for analysis and restoration of connectivity in experimental multichannel data of different nature. We test this approach on the chaotic Rössler system and demonstrate good agreement with the previous well-know results.

Keywords: Artificial neural network, machine learning, nonlinear dynamics, synchronization, functional connectivity

1. INTRODUCTION

Brain, being one of the most complex systems in nature, exhibits well-pronounced network properties on both anatomical and functional levels.[1–4] The latter implies the existence of functional dependence between the states of remote brain areas, which is believed to provide mechanisms for neuronal communication and information transfer within a distributed brain network. According to the recent theories,[5–9] neural interaction between distant brain regions through emergent functional connectivity structures determines normal brain functioning, including cognitive, motor-related activity etc. At the same time, abnormalities in functional brain networks stand behind various types of brain disorders like epilepsy, Parkinson's and Alzheimer's diseases, brain tumors etc.[10,11] Thus, prediction of functional connectivity between brain areas is a crucial approach for brain functioning diagnostics in modern neuroscience.[12]

In nonlinear dynamics, the presence of a functional relation between the dynamics of coupled chaotic systems is known as a particular type of synchronous behavior called *generalized synchronization* (GS).[13–16] This relation may be very complicated and its explicit form cannot be found in most cases. Recently, the phenomenon of GS has been an object of extensive research, having both theoretical and applied significance (e.g., for information transmission by means of chaotic signals[17–19]).

The definition of the GS regime in the case of unidirectional coupling accepted hitherto is the presence of a functional relation

$$\mathbf{y}(t) = \mathbf{F}(\mathbf{x}(t)) \tag{1}$$

between the drive $\mathbf{x}(t)$ and response $\mathbf{y}(t)$ oscillator states. In the Ref.[15] this definition has been generalized on mutual coupling systems as

$$\mathbf{F}(\mathbf{x}(t), \mathbf{y}(t)) = 0. \tag{2}$$

The concept of GS may be essentially applied in neuroscience for data-driven functional connectivity reconstruction based on multichannel EEG/MEG data. However, it has not been systematically used in this context so far. This is due to a number of substantial limitations of existing techniques for detecting the presence of GS in neurophysiological data, which is usually characterized by short duration of time series under analysis, the presence of artifacts and a high level of noise.[20,21] Actually, the most easy, clear, and powerful auxiliary

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system approach[22] is applicable only for systems with unidirectional coupling and requires the consideration of an identical replica of the response system, which is possible in extremely rare cases. The Lyapunov exponents calculation[15,23] is also effective only for model systems with known model equations for which it is possible to calculate the spectrum of Lyapunov exponents. Finally, the nearest-neighbor method[13,15,24] is convenient one for GS inference from experimental data but this approach requires long time series for statistical measure estimation in phase space.

Motivated by the above discussion, in this report we develop a model-free data-driven approach for detecting functional dependency inspired by the concepts of nonlinear dynamics and based on feed-forward (FF) artificial neuronal network (ANN). Machine learning techniques are the "cutting edge" of modern big data analysis. Currently, machine learning techniques are widely applied for the analysis and prediction of nonlinear systems dynamics.[25–27] In particular, reservoir computing is used for data-driven model-free estimation of the Lyapunov exponents[28] and for attractor reconstruction[29] of chaotic processes, multilayer perceptron (MLP) detects the nonlinear process of decision-making in the human brain,[30] etc. Recently, Ibáñez-Soria *et al*[31] applied echo state networks for the detection of functional interrelations in terms of GS. In their work they stated that architecture of feed-forward neural networks "*[...] is suitable for the analysis of stationary problems but, in general, is not adequate to deal with dynamical time-dependent problems*". Thus, their approach relied on a recurrent neural network (RNN) to provide the fading memory that allows processing dynamical signals. This approach required the extensive calculations for RNN training and relatively long time series for training and validation. On the contrary, in our recent study[32] we have demonstrated that inference of functional connectivity could be considered as a time-independent problem and, therefore, effectively solved by feed-forward artificial neuronal network. Based on the approximation theorem, MLP with nonlinear activators in hidden layers is able to approximate any arbitrary given function.[33,34] FF MLP may also approximate any function mapping from any finite dimensional discrete space to another.[35] This property of FF MLP is especially useful for the approximation of the functional relation $\mathbf{F}$ in (1) considering only an experimental data set of $\mathbf{x}(t_i)$ and $\mathbf{y}(t_i)$, where $t_i = i\Delta t$ is the discrete time moments and Δt is the sample rate.

Current paper aims at exploring the inference of functional connectivity in the pair of unidirectionally coupled chaotic oscillators in the vicinity of the GS threshold. As a base chaotic model we have taken classical Rössler oscillator. We have found that MLP perfectly distinguishes between systems state below and above synchronization threshold, however it is less sensitive to the establishment of synchronization near the threshold.

2. FEED-FORWARD ANN APPROACH

ANN is known to be a biologically inspired computational system, whose main purpose is to fit unknown and usually complex relationship between input and output data.[35] Since functional connectivity in coupled systems implies the existence of functional dependence between them, ANN seems to be an essential tool in this context.

Fig. 1 gives a schematic illustration of the proposed ANN-based method for data-driven functional connectivity detection. Considering two coupled processes, whose dynamics is represented by multivariate signals $\mathbf{x}(t)$ and $\mathbf{y}(t)$, functional connectivity implies $\mathbf{y}(t) = \mathbf{F}(\mathbf{x}(t))$. Since from a mathematical point of view ANN defines a function $f : \mathbf{x} \to \mathbf{y}$, one may use ANN to build a model of the unknown relation $\mathbf{F}(\bullet)$ and predict the $\mathbf{y}$ state based on the $\mathbf{x}$ state. Thus, if a true functional relation $\mathbf{y}(t) = \mathbf{F}[\mathbf{x}(t)]$ exists, ANN is able to approximate it and give a precise prediction $\mathbf{y}'(t)$ of the $\mathbf{y}(t)$ state on the basis of $\mathbf{x}(t)$. On the contrary, if functional dependence is not established, ANN fails to learn it and therefore is not able to predict the $\mathbf{y}$-state accurately enough. Summarizing the above, the criterion for functional connectivity inference is equality of predicted and actual values of $\mathbf{y}$ processes: $\mathbf{y}'(t) = \mathbf{y}(t)$.

As compared to a recent paper on the application of echo-state networks (ESNs) to detect GS,[31] our approach does not take into account systems behavior in time domain, but verifies the possibility for one-to-one mapping $\mathbf{F} : \mathbf{x} \to \mathbf{y}$. Thus, our method is not subjected to reproducing a systems replicas with exactly the same dynamical properties using networks with internal memory, and therefore requires a more simple architectures of the ANN. In many cases, deep ANNs provide high approximation accuracy and reduce number of nodes required for representation of desired function (see Ref.[35]). So, to achieve satisfying result one should carefully set ANN architecture, considering its depth, i.e. the number of hidden layers, as an important parameter. In particular,

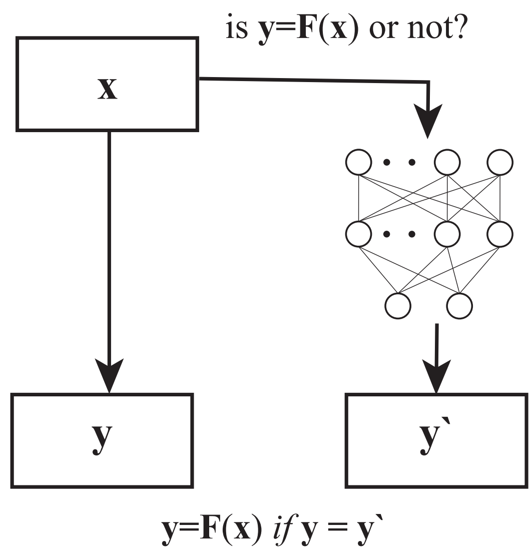

Figure 1. Inference of functional connectivity using proposed feed-forward ANN-based approach. Dependence of $\mathbf{y}$ on $\mathbf{x}$ is detected if ANN-model of functional relation $F(\bullet)$ provides accurate prediction $\mathbf{y}'(t)$ of $\mathbf{y}(t)$-state by the $\mathbf{x}(t)$-state.

throughout this study we use the traditional FF ANN architecture – multilayer perceptron. MLP consists of 2 hidden layers, each containing 10 softmax units. The number of both inputs and outputs is determined by the embedding dimensions of coupled systems. Output artificial neurons have a linear activation function.

To infer functional dependence we consider a pair of multivariate data trials collected from interacting systems $\mathbf{x} = \{\mathbf{x}(t_1), \mathbf{x}(t_2), \dots, \mathbf{x}(t_N)\}$ and $\mathbf{y} = \{\mathbf{y}(t_1), \mathbf{y}(t_2), \dots, \mathbf{y}(t_N)\}$, where N is the trial length. Each sample $\mathbf{x}(t_i)$ is assigned a sample $\mathbf{y}(t_i)$, so $\mathbf{x}(t_i)$ is considered as input data and $\mathbf{y}(t_i)$ — as target data. Then, the data is normalized in range $[0, 1]$, shuffled and separated equally into training and validation sets. To train the network we use Adam optimizer with learning rate 0.001 implemented in Keras API.[36] To avoid possible fails related with model overfitting we check the divergence between trainig and validation errors – if these values diverge for the past 10 training epochs, the process is terminated and starts over. To quantify the degree of functional dependence we use ANN validation accuracy as well as the coefficient of determination (R^2-score), which evaluates "goodness of fit" of the original data collected from a response system $\mathbf{y}(t)$ and its ANN prediction $\mathbf{y}'(t)$. In multivariate form R^2-score is defined as:

$$R^2 = 1 - \frac{\sum_{d=1}^{D} \sum_{i=1}^{N} \left(y_d(t_i) - y'_d(t_i)\right)^2}{\sum_{d=1}^{D} \sum_{i=1}^{N} \left(y_d(t_i) - \bar{y}_d\right)^2}, \quad (3)$$

where D is the number of dimensions, N is the length of the data set, overbar denotes mean value, $y_d(t)$ and $y'_d(t)$ are the d-th component of response system vector state $\mathbf{y}(t)$ and its prediction via ANN, respectively. R^2 ranges from 0 to 1 and quantifies the fraction of data being well predicted by the ANN model. As $R^2 = 0.5$ indicates that only a half of data is fitted by the model (almost random prediction), this value is further considered as a threshold value for functional dependence inference.

3. RESULTS

In this work we apply our MLP-based approach to quantify the transition from unsynchronized behavior to synchronization in the coupled model chaotic oscillators. For instance, we consider the pair of Rössler oscillators which is a classical nonlinear model for the study various aspects of synchronization, namely GS:[13, 22, 37]

$$\begin{aligned} \dot{x}_{1,2} &= -\omega_{1,2} y_{1,2} - z_{1,2} + \varepsilon_{1,2}\left(x_{2,1} - x_{1,2}\right) \\ \dot{y}_{1,2} &= \omega_{1,2} x_{1,2} + a y_{1,2}, \quad \dot{z}_{1,2} = p + z_{1,2}\left(x_{1,2} - c\right), \end{aligned} \quad (4)$$

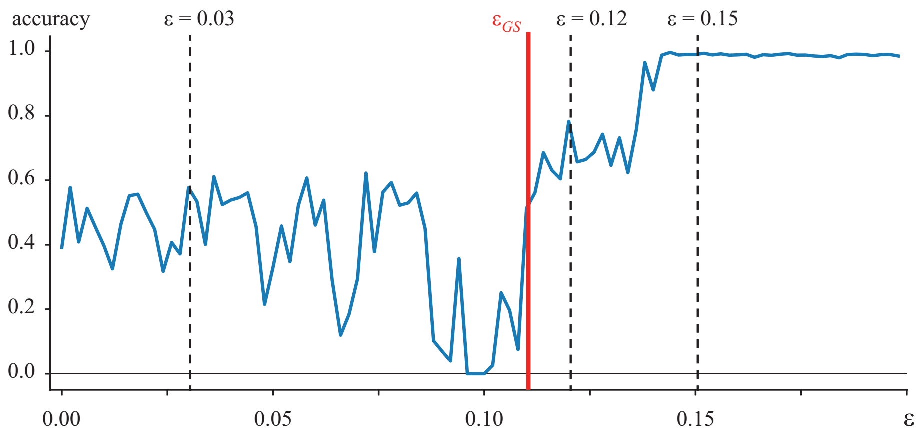

Figure 2. Dependence of MLP validation accuracy on the coupling parameter ε. Red vertical line indicates the GS threshold $\varepsilon_{GS} = 0.11$ according to Ref.[37] and verified using auxiliary system approach.[22] Vertical dashed lines show three values of coupling parameter ε for further consideration: $\varepsilon = 0.03$ (below ε_{GS}); $\varepsilon = 0.15$ (above ε_{GS}); $\varepsilon = 0.12$ (slightly above ε_{GS}).

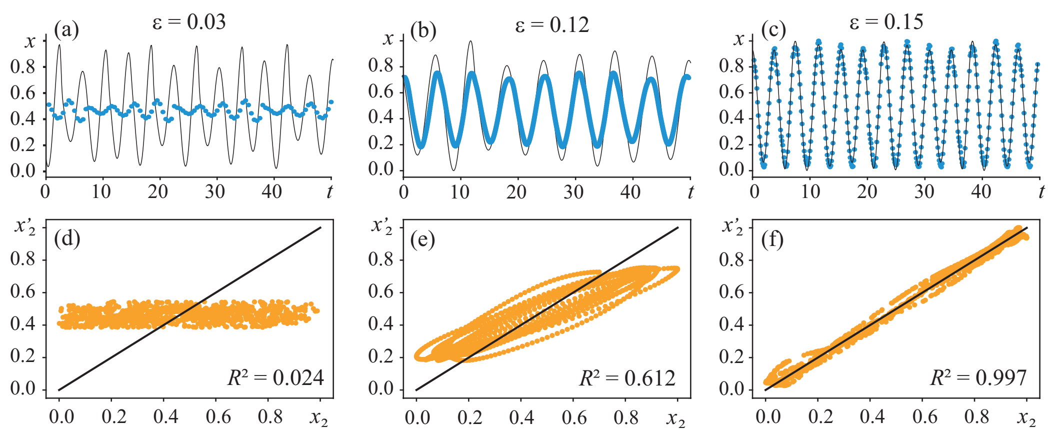

Figure 3. Inference of functional dependence in unidirectionally coupled Rössler oscillators below ($\varepsilon = 0.03$, left column), above ($\varepsilon = 0.15$, right column) and slightly above GS ($\varepsilon = 0.12$, middle column) threshold $\varepsilon_{GS} \approx 0.11$.[15] (a)-(c) Test sample of the second Rössler oscillator time series x_2 (black curve) and its prediction x'_2 via ANN (blue points). (d)-(f) Regression analysis of x_2 variable prediction by ANN model.

where $\mathbf{u}_{1,2} = (x_{1,2}, y_{1,2}, z_{1,2})^T$ are the vector states of interacting Rössler oscillators. The control parameters $a = 0.15$, $p = 0.2$ and $c = 10$ have been set identical for both systems, while $\omega_1 = 0.99$ and $\omega_2 = 0.95$ by the analogy with Refs.[15,37] In case of unidirectional coupling we suggest that master oscillator 1 drives response oscillator 2 and, therefore, $\varepsilon_1 = 0$ and $\varepsilon_2 = \varepsilon$. Eqs. (4) were integrated numerically by Runge-Kutta method of order 4 with $\Delta t = 10^{-3}$.

Fig. 2 illustrates the quantification of transition from asynchronous to synchronized dynamics in the pair of unidirectionally coupled Rössler oscillators by means of the proposed FF ANN-based approach. Here, we use the ANN accuracy of the response system state prediction based on the state of the driving one as a quantifying measure. Due to 3D phase spaces of drive and response systems we have used MLP with 3 inputs and 3 outputs corresponding to 3 variables $(x_{1,2}, y_{1,2}, z_{1,2})$. For the training process of the MLP, we selected time interval with a duration of 100 (10^5 samples) after long transient processes. Entire data set 10^5 pairs of ($\mathbf{u}_1$, $\mathbf{u}_2$) has been randomly separated in half into training and validation sets, each consisting of 5×10^4 pairs. As input data of MLP we considered the drive system states $\mathbf{u}_1(t_i)$ from the training set, and as target data — the corresponding response system states $\mathbf{u}_2(t_i)$. At the validation stage, we have applied the remaining 5×10^4 vectors $\mathbf{u}_1(t_i)$

as input data for the trained MLP and determined the validation accuracy by comparing the predicted vectors $\mathbf{u}'(t_i)$ with the numerically obtained vectors $\mathbf{u}_2(t_i)$. It is seen from Fig. 2 that the ANN accuracy below the threshold does not exceed 0.6 and even drops approximately to the zero level just slightly before the threshold. Slightly above the GS threshold ANN accuracy sharply increases up, but, however, does not demonstrate perfect prediction with typical values lying in the range $0.7 \div 0.8$. In case of $\varepsilon > 0.14$ ANN perfectly predicts the state of the response system with accuracy close to 1.0.

Let us consider closer the transition captured by ANN. Left column in Fig. 3 shows the dynamics of response Rössler system and its ANN prediction in the absence of functional relation between drive and response oscillators $\varepsilon = 0.03 < \varepsilon_{GS}$ Ref.[37] It is seen, that ANN fails to identify any functional relation between coupled systems and provides completely inaccurate prediction time series $x_2(t)$ and phase trajectory of the response oscillator (Fig. 3a). Regression analysis also evidences that predicted and original data are completely uncorrelated with $R^2 = 0.024$ (Fig. 3d). Slightly above the GS threshold at $\varepsilon = 0.12$ ANN does not provide identical representation od the response system state as shown in Fig. 3b. Despite inaccurate prediction of amplitude dynamics, ANN manages to reproduce precisely the phase behavior. It also coincides with the regression analysis, showing non-zero goodness of fit, but still far from perfect (Fig. 3e). By contrast, above GS threshold $\varepsilon = 0.15 > \varepsilon_{GS}$ ANN demonstrates precise prediction of response Rössler system with $R^2 = 0.997$ (Fig. 2c,f). This identifies the presence of functional dependence between the states of coupled systems.

4. CONCLUSION

In conclusion, we have applied the machine learning based method for detecting functional connectivity in unidirectionally coupled systems without additional information about analyzed systems. Aside from good agreement with the previous well-know results in GS studies we demonstrate some interesting features of the ANN-approach application in data-driven detecting of synchronized behavior in coupled chaotic oscillators. In particular, we show that ANN is able to distinguish between asynchronous and synchronized behavior below and above GS. However, in the vicinity of the GS threshold ANN perfectly reproduces phase dynamics and fails at amplitude prediction. We conclude, that close to the boundary of GS functional dependence between drive and response systems may be complex for rather simple ANN architecture. At the same time, phase relationship between the interacting systems is easier to learn from the analyzed chaotic time series. The developed feed-forward ANN method contributes to the approaches of analysis and prediction of connectivity in multichannel experimental data of different nature (e.g., biological, neurophysiological, climate, etc big data sets).

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