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Detecting connectivity of small, dense oscillator networks from dynamical measurements based on a phase modeling approach

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ABSTRACT

An approach is presented for detecting the connectivity between the oscillator elements from the measured multivariate time series data. Our methodology is based upon the phase equation modeling of the oscillator networks, where not only the connection matrix but also the natural frequencies and the interaction function of the oscillators are estimated. Application of this technique to simulated data as well as experimental ones from electrochemical oscillators shows its capability for precise detection of defects in the connection matrix for *small-size networks*. Dependence of the methodology on the observational noise, the network size, the number of defects, and the data length is also examined.

1. Introduction

A network of interacting oscillators can be found in diverse fields of natural science and engineering [1–3]. Here, connectivity of the network elements plays a crucial role on the formation of the collective dynamics. Effect of the complex network topology on the dynamics of coupled oscillators has been intensively investigated [4]. To deal with the real-world systems, however, it is extremely rare that the detailed connectivity of the network can be directly and noninvasively investigated. In many systems especially in biology, direct measurement of the connectivity may destroy the true nature of the coupling functions that underlie the real network dynamics. For instance, in the studies of circadian rhythms, fundamental mechanisms for connecting the circadian cells in the superchiasmitic nucleus remain largely unknown [5,6]. Detailed physiological investigation of the *in vitro* tissue may not reveal the true network function that is inherent *in situ*. Because of these difficulties, estimation of the network connectivity from time series data recorded in a noninvasive manner is an awaited technique. Along this line, several approaches have been proposed up to date. Information transfer [7], mutual predictability [8], recurrence properties [9], and permutation-based asymmetric association measure [10] have been utilized to identify the coupling directions. Index for partial phase synchronization has been developed to distinguish direct from indirect interactions [11–13]. A graph theoretic approach to detect causalities in multivariate time series has been recently developed [14]. Response properties of the network dynamics to external stimuli have been also exploited [15,16].

Here, we focus on a phase description of the oscillator networks [2]. Under certain conditions, which are described in detail in Section 2, a network of weakly coupled self-sustained oscillators can be reduced to a dynamics of interacting phase oscillators. This drastically simplifies the modeling assumptions and enables straightforward estimation of the phase dynamics. We have applied the multiple-shooting method to fit the phase equations to multivariate time series to show that the interaction functions as well as the natural frequencies can be well identified from a globally coupled populations [17]. Kralemann et al. [18,19], on the other hand, carried out a data fitting using the probability density function of a modified phase to estimate the phase dynamics from time series and Blaha et al. [20] applied it to two interacting electrochemical oscillators. Our approach has the practical advantage of algorithmic simplicity and hence it is straightforward to implement. It has been, however, applied only to the simplest case of all-to-all coupling, where all oscillator elements are connected to all the others. The aim of the present Letter is to extend our previous approach to a network dynamics of an arbitrary topology. In particular, we focus on the case that the network has zero-or-unity connections, where the zero connections are referred to as defects in the coupling. We examine the capability of our approach to reveal the network connectivity from multivariate data recorded from coupled systems.

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2. Method

Our problem can be stated as follows. Consider a system of N weakly coupled nearly identical limit cycle oscillators:

$$\dot{\boldsymbol{x}}_i = \boldsymbol{F}_i(\boldsymbol{x}_i) + \frac{C}{N}\sum_{j=1,\, j\neq i}^{N} T_{i,j} G(\boldsymbol{x}_i, \boldsymbol{x}_j), \tag{1}$$

where $\boldsymbol{x}_i$ and $\boldsymbol{F}_i$ $(i = 1, 2, \ldots, N)$ stand for state variables and *autonomous* dynamics of the ith oscillator, respectively, C represents the coupling constant, and G is an interaction function between ith and jth oscillators. The matrix $\{T_{i,j}\}$ describes connectivity between the oscillators, where *the present problem is applicable to both uni- and bi-directionally coupled oscillators*. Our assumption is that in isolated condition (i.e., $C = 0$) each oscillator $\boldsymbol{F}_i$ generates a stable limit cycle with similar natural frequencies ω_i. The functions F_i should be similar among the N oscillators near the limit cycle trajectory. Then the phase reduction theory [2] states that for a weak coupling C the network dynamics can be reduced to the phase equations: $\dot{\theta}_i = \omega_i + \frac{C}{N}\sum_{j=1,\, j\neq i}^{N} T_{i,j} H(\theta_j - \theta_i)$ (θ_i: phase of ith oscillator; H: interaction function). As a recording condition, we assume that simultaneous measurement of all oscillators is made as $\{\xi_i(n\Delta t) = g(\boldsymbol{x}_i(n\Delta t))\colon n = 1, \ldots, M\}_{i=1}^{N}$ (g: observation function, Δt: sampling time).

Our objective of inferring the network connectivity through recovering the phase dynamics is accomplished under conditions that (i) the underlying dynamics (1) are unknown, (ii) the interaction function is based upon a difference coupling (i.e., $H(0) = 0$), (iii) the coupling constant C associated with the measured data is in a non-synchronized regime, and (iv) the connection matrix is composed of zero-or-unity elements (i.e., $T_{i,j} = 0$ or 1), where most of the connections exist (non-sparse matrix). Number of the defects ($T_{i,j} = 0$) is denoted by β.

Concerning the condition (ii), the difference coupling provides a good assumption, because, in many systems, the phase interaction disappears when the oscillators are in a complete in-phase relationship.

Concerning the condition (iv), such a non-sparsely connected system can be found in real-world systems. For instance, all-to-all connections are assumed in various systems including arrays of Josephson junctions [21] and lasers [22], population of circadian oscillators [5,6], ensembles of electrochemical oscillators [23], and neuronal populations [24]. It can easily happen that a small portion of the connections is destroyed by some damage to the system, resulting in a non-sparsely connected system.

Our approach to the problem is based upon the following four steps.

1. Extract phase signals $\theta_i(t)$ from the data $\xi_i(t)$. The phase θ is defined by a simple *piecewise linear* formula, in which it is increased by 2π at every local maximum of $\xi(t)$ and between the local maxima it grows in proportion to time [3].
2. Fit the phases $\{\theta_i(t)\}$ to the phase equations:

$$\dot{\theta}_i = \tilde{\omega}_i + \frac{C}{N}\sum_{j=1}^{N} \tilde{T}_{i,j} \tilde{H}(\theta_j - \theta_i), \tag{2}$$

where $\{\tilde{\omega}_i\}$ and $\{\tilde{T}_{i,j}\}$ represent approximate values for the natural frequencies and those for the connection matrix, respectively. $\tilde{H}$ stands for an *approximate function for the interaction* H, which is in general nonlinear and periodic with respect to 2π. The approximation is based on a *Fourier* expansion up to the order of D as $\tilde{H}(\Delta\theta) = \sum_{j=1}^{D}[a_j \sin j\Delta\theta + b_j(\cos j\Delta\theta - 1)]$.

The above phase equations have unknown parameters of $\{\tilde{\omega}_i, a_j, b_j, \tilde{T}_{i,j}\}$, which should be optimized to be fitted to the data. Simultaneous estimation of the unknown parameters all at once is, however, an ill-conditioned problem *because of the redundancy of the unknown parameters*. Therefore, we divide the parameters into two groups as $\{\tilde{\omega}_i, a_j, b_j\}$ and $\{\tilde{T}_{i,j}\}$ and estimate them separately in the next two steps.
3. In the first step, the connection matrix is assumed to be of all-to-all type ($\tilde{T}_{i,j} = 1$) and estimate the rest of the parameters denoted by $\boldsymbol{p} = \{\tilde{\omega}_i, a_j, b_j\}$. This provides a reasonable assumption for densely connected systems, in which most of the oscillators are coupled to each other. The parameters $\boldsymbol{p}$ are estimated by the multiple-shooting method [25]. We denote the time evolution of the phase equations (2) with respect to an initial condition $\boldsymbol{\theta}$ by $\boldsymbol{\phi}^t(\boldsymbol{\theta}, \boldsymbol{p})$. Then, at each sampling time $t = n\Delta t$, the phase equation must satisfy the boundary conditions: $\boldsymbol{\theta}((n+1)\Delta t) = \boldsymbol{\phi}^{\Delta t}(\boldsymbol{\theta}(n\Delta t), \boldsymbol{p})$. With respect to the unknown parameters $\boldsymbol{p}$, we solve these nonlinear equations by the generalized Newton method. The evolution function $\boldsymbol{\phi}^t$ is integrated numerically. For the computation of the gradients $\partial\boldsymbol{\phi}/\partial\boldsymbol{p}$ which are needed for the Newton method, variational equations of the phase equations (2) are also solved numerically.

A necessary condition to solve the nonlinear equations is that the number of the unknown parameters $\boldsymbol{p}$ is less than the number of the equations, that is, $N + 2D < N(M-1)$. This always holds in the case we have enough data points M.
4. In the second step, the parameters $\{\tilde{\omega}_i, a_j, b_j\}$ estimated in the previous step are fixed. With respect to the connection matrix $\boldsymbol{p} = \{\tilde{T}_{i,j}\}$ as the rest of the unknown parameters, the multiple-shooting method was applied again in a similar manner as in the previous step.

It should be noted that, in the above method, the first and the second steps can be repeated in an iterative manner to improve the estimates. We do not employ such a procedure, because our preliminary study indicated that the iterative algorithm simply increased the computational cost but did not show a clear improvement.

3. Results

We applied this technique to a prototypical example of weakly coupled limit cycle oscillators. We considered the following *system* of Rössler equations with diffusive coupling:

$$\begin{aligned}
\dot{x}_i &= -\alpha_i y_i - z_i, \\
\dot{y}_i &= \alpha_i x_i + 0.15 y_i + \frac{C}{N}\sum_{j=1}^{N} T_{i,j}(y_j - y_i), \\
\dot{z}_i &= 0.2 + z_i(x_i - 2),
\end{aligned} \tag{3}$$

where $i = 1, \ldots, N$. To consider an inhomogeneity of the network elements, parameter values α_i, which determine rotation speed in the (x, y)-space, were varied among the oscillators as $\alpha_i = 1 + 0.01 \cdot i$ $(i = 1, \ldots, N)$. Each Rössler oscillator generates a limit cycle attractor for the chosen parameter values in the absence of coupling (i.e., $C = 0$). The multivariate data were recorded as $\{y_i(t)\}_{i=1}^{N}$.

We started with the case of $N = 5$. As the coupling matrix, all-to-all connections were assumed ($T_{i,j} = 1$). The data $\{y_i(t)\}_{i=1}^{5}$ were recorded at a coupling strength of $C = 0.01$, which corresponds to non-synchronized regime. The sampling interval was set to be $\Delta t = 0.32$ for the extraction of the phases $\{\theta_i(t)\}$. Then to apply the multiple-shooting method the data have been down sampled to $\Delta t = 250 \cdot 0.32$ and the total of 1000 data points have been collected for the parameter estimation. As an initial condition, the unknown parameter values were all set to be zero, i.e.,