Estimating the Phase Response Function Only from Noisy Multivariate Time Series

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Abstract—The phase reduction method is a strong tool to analyze collective behaviors of various biological, physical or chemical oscillatory components. In this method, the response of a reduced system to external forces is described by the phase response function (PRF). In this paper, we propose a method for estimating the PRF only from noisy multivariate time series. To confirm the validity of our method, we estimate the PRFs of the Stuart-Landau and FitzHugh-Nagumo oscillators. As a result, estimated PRFs from multivariate time series show good agreement with the theoretical ones. We also show that the estimation method is robust against noisy environment.

1. Introduction

Rhythmic phenomena are ubiquitous in the real world, for example, the synchronization of frog calls [1], the Belousov-Zhabotinsky reaction [2] and the Josephson junction [3]. These collective orders are organized through interactions between oscillatory components, whose behaviors are described by ordinary differential equations. When we analytically investigate the collective behavior of interacting components, the phase reduction method becomes a strong tool [4], because a model of the components is too complex to investigate analytically. However, if we use the phase reduction method, we can reduce these models to a simple model with one degree of freedom. In this method, the response of a reduced system to external forces is described by a phase response function (PRF). If the PRF of a nonlinear dynamical system such as a neuron is obtained, we can understand its behavior. Thus, it is important to estimate the PRF in various fields including the computational neuroscience. The methods for estimating the PRF have been studied in many previous works [5].

In this paper, we propose a method for estimating the PRF only from noisy multivariate time series. In conventional methods, it is necessary to perturb a dynamical system repeatedly and observe its responses. For example, in case of a neuron, we have to inject impulsive or fluctuating drive currents to the neuron repeatedly and record its spike times. However, we cannot apply the same strategy to many other dynamical systems. This is the reason why most of the conventional methods, which are developed to estimate the PRF of neurons, do not work well for the other dynamical systems. Our method only needs multivariate time series and can be applied to a general class of dynamical systems. Namely, we can omit complicated experimental procedures in the conventional methods and estimate the PRF of various dynamical systems.

Several methods [6], which are based on the embedding theory [7], have been proposed to estimate the PRF only from a time series. However, their methods are valid only for the type I oscillator, whose PRF is estimated only from the vector field on the unperturbed limit-cycle attractor, because the vector field around the attractor is neglected in their methods. Thus, their methods are not valid for the type II oscillator. On the other hand, in our method, we estimate the Jacobian matrix on the limit-cycle attractor, which is a linear approximation of the vector field around the attractor, by utilizing fluctuations of the orbit. Therefore, we can estimate the PRF considering the vector field around the attractor, which makes our method valid for a general class of limit-cycle oscillators.

2. Theoretical aspects

The phase reduction method was established by Kuramoto [4]. Let us define $x \in \mathbb{R}^n$ as an *n*-dimensional state variable and consider the following system:

$$\dot{\boldsymbol{x}} = \boldsymbol{F}(\boldsymbol{x}) + \boldsymbol{p}(t), \qquad (1)$$

where $\mathbf{F}(\mathbf{x}) \in \mathbb{R}^n$ is an unperturbed vector field, which has a *T*-periodic limit-cycle solution $\mathbf{x}_0(t)$, and $\mathbf{p}(t)$ is an external force. Here, we call $\mathbf{p}(t)$ the dynamical noise. The phase coordinate $\theta(\mathbf{x})$ is defined in a neighborhood of $\mathbf{x}_0(t)$ so that the phase θ may always increase at the constant speed ω (= 1/T = $\operatorname{grad}_{\mathbf{x}} \theta(\mathbf{x}) \cdot \mathbf{F}(\mathbf{x})$), where $\operatorname{grad}_{\mathbf{x}}$ represents the gradient operator. The constant ω is called the phase speed or angular velocity. Kuramoto defined the PRF $\boldsymbol{Z}(\theta) \in \mathbb{R}^n$:

$$\boldsymbol{Z}(\boldsymbol{\theta}) = \operatorname{grad}_{\boldsymbol{x}} \boldsymbol{\theta}(\boldsymbol{x}_0(\boldsymbol{\theta})). \tag{2}$$

According to the Malkin theorem, the PRF $Z(\theta)$ satisfies the adjoint equation [8]:

$$\dot{\boldsymbol{Z}} = D\boldsymbol{F}(\boldsymbol{x}_0(\theta))^\top \boldsymbol{Z},\tag{3}$$

and the normalization condition:

$$\boldsymbol{Z}(\theta) \cdot \boldsymbol{F}(\boldsymbol{x}_0(\theta)) = \omega, \qquad (4)$$

where $D\mathbf{F}(\mathbf{x}) \in \mathbb{R}^{n \times n}$ is the Jacobian matrix on the point \mathbf{x} . If the Jacobian matrix is estimated, integrating the adjoint equation (3), we can obtain the PRF. In our method, instead of estimating the Jacobian matrix itself, we estimate the tangent map as in Ref. [9]. Let us define $\Delta \mathbf{x}(t) \in \mathbb{R}^n$ as a very small displacement vector from a point $\mathbf{x}(t)$. The evolution of $\Delta \mathbf{x}(t)$ can be approximated with

$$\Delta \dot{\boldsymbol{x}}(t) = D\boldsymbol{F}(\boldsymbol{x}(t))\Delta \boldsymbol{x}(t).$$
(5)

We define the tangent map $G \in \mathbb{R}^{n \times n}$:

$$+ \Delta t) = \Delta \boldsymbol{x}(t) + \int_{t}^{t+\Delta t} D\boldsymbol{F}(\boldsymbol{x}(s)) \Delta \boldsymbol{x}(s) ds \equiv \boldsymbol{G} \Delta \boldsymbol{x}(t),$$
 (6)

which can be used to integrate the adjoint equation (3) as follows

$$\boldsymbol{Z}(t + \Delta t) = \boldsymbol{G}^{\top} \boldsymbol{Z}(t).$$
(7)

3. Proposed method

 $\Delta \boldsymbol{x}(t)$

In our method, we estimate the tangent maps defined in Eq. (6) and integrate the adjoint equation (3) by using Eq. (7). The solution of the adjoint equation is the estimated PRF.

(i) Estimation of the tangent maps: Let $x_t \in \mathbb{R}^n$ (t = 1, 2, ..., N) be a noisy *n*-dimensional multivariate time series observed from a dynamical system that has a stable limit-cycle solution. We first assume that we can observe only a noisy time series x_t . We do not need any additional information or restrictive assumptions. We define $y_t \in \mathbb{R}^n$ (t = 1, 2, ..., M) as the unperturbed limit-cycle orbit of one oscillatory period and $F_t \in \mathbb{R}^n$ (i = 1, 2, ..., M) as the vector field on the point y_t , which are estimated by averaging x_t . For simplicity of notation, $y_t \in \mathbb{R}^n$ is defined so that the periodic boundary condition $y_{M+1} = y_1$ may hold. We set the initial point y_1 on the limit-cycle orbit, estimate y_t and F_t by the following equations:

$$\boldsymbol{F}_{t} = \frac{1}{L\Delta t} \sum_{j=1}^{L} \left[\boldsymbol{x}_{k(j)+1} - \boldsymbol{x}_{k(j)} \right], \qquad (8)$$

$$\boldsymbol{y}_{t+1} = \boldsymbol{y}_t + \boldsymbol{F}_t \Delta t, \qquad (9)$$

where Δt is the time step of \boldsymbol{x}_t and \boldsymbol{y}_t , and $\boldsymbol{x}_{k(j)}$ $(j = 1, 2, \ldots, L)$ is one of the L neighbor points of the point \boldsymbol{y}_t satisfying $||\boldsymbol{x}_{k(j)} - \boldsymbol{y}_t|| < \epsilon$, where $||\cdot||$ denotes the Euclidean norm, and ϵ is the threshold. In Eq. (8), we simply average the noisy one-step evolutions of data points $\boldsymbol{x}_{k(j)+1} - \boldsymbol{x}_{k(j)}$ $(j = 1, \ldots, L)$, which yields the averaged vector field \boldsymbol{F}_t . In Eq. (9), we use a simple linear time series prediction by using \boldsymbol{F}_t and estimate \boldsymbol{y}_{t+1} . If the unperturbed limit cycle attractor is sufficiently stable, the original orbit is well fitted by the estimated orbit \boldsymbol{y}_t $(t = 1, 2, 3, \ldots)$.

Since the neighbor points y_t and $x_{k(j)}$ evolve into y_{t+1} and $x_{k(j)+1}$, respectively, we define the displacement vectors $\Delta x_j, \Delta x'_j \in \mathbb{R}^n$:

$$\Delta \boldsymbol{x}_j \equiv \boldsymbol{x}_{k(j)} - \boldsymbol{y}_t, \ \Delta \boldsymbol{x}'_j \equiv \boldsymbol{x}_{k(j)+1} - \boldsymbol{y}_{t+1}. \tag{10}$$

From Eq. (6), we can estimate the tangent map $G_t \in \mathbb{R}^{n \times n}$ (i = 1, 2, ..., M) minimizing the square error S:

$$S \equiv \sum_{j=1}^{L} \left| \Delta \boldsymbol{x}_{j}^{\prime} - \boldsymbol{G}_{t} \Delta \boldsymbol{x}_{j} \right|^{2}$$
(11)

by the least-squares optimization. In other words, the tangent map G_t can be obtained as

$$\boldsymbol{G}_t = \boldsymbol{C}_t \boldsymbol{W}_t^{-1}, \qquad (12)$$

where $C_t \in \mathbb{R}^{n \times n}$ $(\equiv L^{-1} \sum_{j=1}^{L} \Delta x'_j \Delta x^{\top}_j)$ is the covariance matrix between Δx_j and $\Delta x'_j$, and $W_t \in \mathbb{R}^{n \times n}$ $(\equiv L^{-1} \sum_{j=1}^{L} \Delta x_j \Delta x^{\top}_j)$ is the variance matrix of Δx_j .

(ii) Integration of the adjoint equation: We define $\tilde{Z}_t \in \mathbb{R}^n$ (i = 1, 2, ..., M) as the estimated PRF before the normalization so that the periodic boundary condition $\tilde{Z}_{M+1} = \tilde{Z}_1$ may hold. Instead of directly integrating the adjoint equation, we use Eq. (7) and iteratively calculate the following equation:

$$\tilde{\boldsymbol{Z}}_{t-1} = \boldsymbol{G}_t^\top \tilde{\boldsymbol{Z}}_t, \tag{13}$$

for t = M, M - 1, M - 2, ... for several periods. The initial value \tilde{Z}_M is arbitrary. To achieve numerical stability, the adjoint equation must be integrated *backward* as mentioned in Ref. [8]. Finally, we normalize the PRF by

$$\boldsymbol{Z}_t = \frac{\omega}{Z_0} \tilde{\boldsymbol{Z}}_t,\tag{14}$$

where $Z_0 \equiv M^{-1} \sum_{i=1}^{M} \mathbf{F}_t \cdot \tilde{\mathbf{Z}}_t$. The estimate $\mathbf{Z}_t \in \mathbb{R}^n$ of the PRF is obtained.

4. Simulation settings

To confirm the validity of our method, we applied our method to the Stuart-Landau [4] and the FitzHugh-Nagumo [10] oscillators.

The Stuart-Landau oscillator [4] has a normal form of the Hopf bifurcation and is described by

$$\dot{x} = x - \eta y - (x^2 + y^2)(x - \alpha y) + \sigma_{\rm dyn}\xi_1(t), \ (15)$$

$$\dot{y} = y + \eta x - (x^2 + y^2)(y + \alpha x) + \sigma_{\rm dyn}\xi_2(t), \ (16)$$

where x and y are state variables, $\sigma_{\rm dyn}$ is the strength of the dynamical noise, and $\xi_i(t)$ (i = 1, 2) is the Gaussian white noise satisfying $\langle \xi_i(t) \rangle = 0$ and $\langle \xi_i(t)\xi_j(s) \rangle = \delta_{ij}\delta(t-s)$, where $\langle \cdot \rangle$ represents the temporal average, and $\delta(t)$ is Dirac's delta function. We set the parameters $\eta = 2$ and $\alpha = -1$. For these parameters, we analytically obtain the PRF $\mathbf{Z}(\theta) =$ $(\sqrt{2}\pi)^{-1}[\sin(\theta + 3\pi/4), \sin(\theta + \pi/4)]^{\top}$ (Fig. 1 (a)).

The FitzHugh-Nagumo oscillator [10] is described by

$$\dot{v} = v - \frac{v^3}{3} - u + I_0 + \sigma_{\rm dyn} \xi_1(t),$$
 (17)

$$\dot{u} = \epsilon(u+a-bu) + \sigma_{\rm dyn}\xi_2(t), \qquad (18)$$

where v and u are state variables, and we set the parameters $I_0 = 0.8$, $\epsilon = 0.08$, a = 0.7 and b = 0.8. We numerically calculate the theoretical PRF of this model by using the method proposed in Ref. [8] (Fig. 1 (b)).

In numerical simulations, we assumed that all variables of the dynamical systems are observed, and that the observed multivariate time series is subject to the observational noise, which is the Gaussian white noise with the mean 0 and the variance $\sigma_{\rm obs}^2$. We estimated the PRFs only from the multivariate time series.

5. Results

Theoretical PRF and estimated PRF are compared in Fig. 1. They show good agreements with each other. From Fig. 1, we can effectively estimate the PRFs of both the Stuart-Landau and FitzHugh-Nagumo oscillators.

To confirm the robustness of our method, we investigated the estimation accuracy for various parameters. In Fig. 2, we show the mean square errors (MSEs) between the theoretically calculated and estimated PRFs. As shown in Fig. 2 (a) and (b), when the strength of the observational noise σ_{obs} is large, the MSEs tend to be large. It is natural to consider that the observational noise is an obstacle for the accurate estimation. As shown in Fig. 2 (c) and (d), when the time step Δt is large, the MSEs also tend to be large. This result indicates that Δt must be sufficiently smaller than the decay time of the orbit into the limit-cycle attractor for the accurate estimation.

Figure 2 shows that the dynamical noise improves estimation accuracy. When the strength of the dynamical noise σ_{dyn} is sufficiently large, even if σ_{obs} or Δt is large to a certain extent, the PRFs can be precisely



Figure 1: Theoretically calculated (lines) and estimated (circles) PRFs. We set the parameters $\sigma_{\rm dyn} = 10^{-2}$, $\sigma_{\rm obs} = 0$, $N = 10^6$, $\Delta t = 10^{-3}$ and $\epsilon = 0.1$ for (a) the Stuart-Landau oscillator, and $\sigma_{\rm dyn} = 10^{-2}$, $\sigma_{\rm obs} = 0$, $N = 10^5$, $\Delta t = 10^{-2}$ and $\epsilon = 0.1$ for (b) the FitzHugh-Nagumo oscillator.

estimated as demonstrated in Fig. 2. When $\sigma_{\rm dyn}$ is small, we cannot estimate the PRF even if $\sigma_{\rm obs}$ and Δt are sufficiently small. These results indicate that the dynamical noise plays a key role in estimating the PRF. The strong dynamical noise lengthens the decay time of the orbit, which ebables us to estimate the evolution of displacement vectors in the estimation of the tangent maps.

6. Summary

In this paper, we proposed an approach to estimate the PRF only from noisy multivariate time series. Although several methods [6] have already been proposed to estimate the PRF only from a time series, their methods are valid only for the limited systems. On the other hand, in our method, we estimate the Jacobian matrix utilizing fluctuations of the orbit induced by the dynamical noise. Thus, our method is valid for the general class of limit-cycle oscillators. We demonstrated the numerical results for the Stuart-Landau and FitzHugh-Nagumo oscillators.

When we observe the response of real systems such as a neuron, the dynamical noise is inevitable and inherent in the system. It has been considered that the noise in real systems is an obstacle for estimating the PRF. On the other hand, we utilize the dynamical noise rather than reduce it. We demonstrated that the robust estimation is realized by the dynamical noise. One of the important works is to estimate PRFs only from a single variable time series.

The authors would like to thank Mr. S. Ogawa and AGS Corp. for their encouragement on this research project.

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(d) MSE of $Z_y(\theta)$ (σ_{dyn} vs. Δt)

Figure 2: The MSEs between the theoretical and estimated PRFs $\mathbf{Z}(\theta) = [Z_x(\theta), Z_y(\theta)]^{\top}$ of the Stuart-Landau oscillator for various parameters. We use the heat maps on the $(\sigma_{\rm dyn}, \sigma_{\rm obs})$ and $(\sigma_{\rm dyn}, \Delta t)$ planes, and the color represents the MSE. We set the parameters $N = 10^5$, $\Delta t = 10^{-3}$, $\epsilon = 0.1$ for (a) and (b), and $N = 10^5$, $\sigma_{\rm obs} = 10^{-5}$, $\epsilon = 0.1$ for (c) and (d).