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A Gaussian mixture model based cost function for parameter estimation of chaotic biological systems

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ABSTRACT

As we know, many biological systems such as neurons or the heart can exhibit chaotic behavior. Conventional methods for parameter estimation in models of these systems have some limitations caused by sensitivity to initial conditions. In this paper, a novel cost function is proposed to overcome those limitations by building a statistical model on the distribution of the real system attractor in state space. This cost function is defined by the use of a likelihood score in a Gaussian mixture model (GMM) which is fitted to the observed attractor generated by the real system. Using that learned GMM, a similarity score can be defined by the computed likelihood score of the model time series. We have applied the proposed method to the parameter estimation of two important biological systems, a neuron and a cardiac pacemaker, which show chaotic behavior. Some simulated experiments are given to verify the usefulness of the proposed approach in clean and noisy conditions. The results show the adequacy of the proposed cost function.

1. Introduction

In biology, many systems exhibit chaos, and the study of such systems and their signals have progressed in recent decades. It has been claimed that many biological systems including the heart [1,2], brain (both in microscopic and macroscopic aspects) [3–5], and the human speech production system [6–8] have chaotic features. Also, carefully controlled experiments have clearly demonstrated chaotic dynamics in neurons [4]. Although traditional models of neurons like the Hodgkin and Huxley model [9] and the FitzHugh–Nagumo model [10] are so popular and useful in many applications, the Hindmarsh and Rose (HR) model [11] is one of the simplest mathematical representations of the oscillatory burst discharges that occur in real neurons. The HR model is a proper model to study spike trains in individual neurons and the cooperative behavior that arises when neurons are coupled together.

There are two main methods for parameter identification of chaotic systems. The first is the synchronization method [12–15], and the second is the optimization method [16–26]. When we talk about biological systems, there will be major limitations in the use of approaches that require control and synchronization. For example, since estimating parameters in chaotic systems has many difficulties, some approaches try first to control the system and bring it out of the chaotic mode.

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However, doing control in biological systems is usually impossible, and when possible, it causes serious problems. Furthermore, the experimental data may have been gathered previously, and there is no longer access to the system that produced it. Therefore, it seems that optimization methods are more proper for these kinds of problems.

In the optimization methods, the problem of parameter estimation is formulated as a cost function to be minimized. Although there are many optimization approaches used for this problem e.g., genetic algorithms [16], particle swarm optimization [19,22], evolutionary programming [26]. There is one thing common to all of them: they define a cost function based on similarity between the time series obtained from the real system and ones obtained from the model. They use time correlation between two chaotic time series as the similarity indicator. However, we believe that this indicator has limitations. For example, it is well known that chaotic systems are sensitive to initial conditions [27]. Thus there can be two completely identical (both in structure and parameters) chaotic systems that produce time series with no correlation due to a small difference in initial conditions [28–32]. One way to overcome this problem is using near term correlation and reinitiating the system frequently (i.e., not allowing significant divergence of the trajectories). However, this approach also has limitations. In many systems, we do not have access to a time series for all of the system variables. Thus we cannot reinitialize the model frequently since we do not know the value all the variables. Hence we prefer a new kind of similarity indicator and corresponding cost function.

Although chaotic systems have random-like behavior in the time domain, they are ordered in state space and have a specific topology usually in the form of strange attractors. In this work, we propose a similarity indicator between these attractors as an objective function for parameter estimation. To do this, we model the attractor of the real system by a statistical and parametric model. In [33–36] a Gaussian mixture model (GMM) was proposed as a parametric model of a phoneme attractor in state space. Their results of isolated phoneme classification showed that the GMM is a useful model to capture structure and topology of phoneme attractors in state space. Also, in [35–38], useful RPS-based features were attained via the modeling of the embedded phoneme attractor in the RPS. Thus we propose the use of a GMM as a parametric model of the strange attractor obtained from a real system. Based on the learned GMM, a similarity indicator can be achieved by matching the time series obtained from the model of a real system with different sets of parameters to evaluate the properness of each set. Hence our proposed cost function will consist of two steps; first, a training stage which includes fitting a GMM to the attractor of the real system in state space, and second, an evaluation step to compute the similarity between the learned GMM and attractors of the model with estimated parameters.

The rest of this paper is organized as follows: In Section 2, using the logistic map as a benchmark example of chaotic systems, we show that defining a similarity index in the time domain has major limitations and cannot be proper for the task of parameter estimation of chaotic systems. Section 3 details the proposed GMM based cost function and its result for the benchmark example. Section 4 introduces the HR Model as a commonly used neuron model that can exhibit chaotic properties. In Section 5, our experimental results are introduced and discussed. Finally, we draw conclusions in the last section.

2. Time domain vs. state space

Consider a set of difference equations (or alternately, a set of differential equations) known to be chaotic:

$$\vec{s}_{k+1} = \vec{f}(\vec{s}_k, \vec{\theta}) \tag{2.1}$$

in which $\vec{s} = (s_1, s_2, \ldots, s_n)$ is the state vector of the system and $\vec{\theta} = (\theta_1, \theta_2, \ldots, \theta_m)$ is a set of its parameters. It is assumed that we know the structure of the system, and the only unknown part is the parameter set. So we have a model of the following form:

$$\vec{v}_{k+1} = \vec{f}(\vec{v}_k, \vec{\tilde{\theta}}) \tag{2.2}$$

in which $\vec{v} = (v_1, v_2, \ldots, v_n)$ is the state vector of the model and $\vec{\tilde{\theta}} = (\tilde{\theta}_1, \tilde{\theta}_2, \ldots, \tilde{\theta}_m)$ is the set of estimated parameters. Our goal is to find values of $\tilde{\theta}$ that are close to θ when we do not know θ but only have access to a measured scalar time series from the system.A simple and well-known cost function is defined by the following equation (or something similar with the same concept) [16–26]:

$$\text{Cost Function} = \sum_{k=1}^{N} \left\| \overline{\vec{v}_k} - \overline{\vec{s}_k} \right\| \tag{2.3}$$

where N denotes the length of the time series used for parameter estimation, $\|\cdot\|$ is the Euclidean norm, and $\overline{\vec{s}_k}$ is those elements of $\vec{s}$ to which we have experimental access.

Owing to the limitations of the measurement instruments and the environment, all experimental data are mixed with noise to some extent [2]. Thus we can never have the exact initial conditions of the system (the error may be small, but not zero). Here we deal with chaotic systems whose main characteristic is their sensitive dependence on initial conditions and thus for which errors in the time domain are not a good indicator as clarified by the following simple example. Consider the logistic equation, which is a benchmark example of chaotic systems:

$$s_{k+1} = A s_k (1 - s_k) \tag{2.4}$$