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

Yasser Shekofteh [a,b], Sajad Jafari [a,*], Julien Clinton Sprott [c], S. Mohammad Reza Hashemi Golpayegani [a], Farshad Almasganj [a]

[a] *Biomedical Engineering Department, Amirkabir University of Technology, Tehran 15875-4413, Iran*
[b] *Research Center of Intelligent Signal Processing (RCISP), Tehran, Iran*
[c] *Department of Physics, University of Wisconsin, Madison, WI 53706, USA*

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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.

* Corresponding author. Tel.: +98 9357874169.
E-mail address: sajadjafari@aut.ac.ir (S. Jafari).

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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:

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

Suppose that the value of A in the real system is 3.76 (for which the system is chaotic) and we have a model exactly like our system:

$$v_{k+1} = \mathrm{A}v_k(1 - v_k) \tag{2.5}$$

If we even consider the true value for A in the model, a little difference in the initial conditions in the system and its model can lead to two different time series. Fig. 1 shows the effect of a difference in the initial conditions of 0.1%.

If we calculate the cost function from Eq. (2.3) with that 0.1% difference in the initial conditions, we see that this method does not give a proper result (Fig. 2) because it does not have a global minimum at 3.76, and it is not monotonic on both sides of that minimum, because it is not convex. Furthermore, we expect discontinuities in the cost function due to the bifurcations that typically occur in chaotic systems. Especially in the periodic windows, we may see local maxima in the cost function since the behavior will be very different from the chaotic case with $A = 3.76$. As can be seen in Fig. 2, the global minimum occurs near $A = 3$, which is far from the correct value.

Although chaotic systems have random-like behavior in the time domain, they are ordered in state space and have a specific topology. In other words, there exists an attractor from which the system trajectories do not escape, even though the initial conditions change (of course initial conditions should be in the basin of attraction of that attractor). For example, if we plot those random-like signals in Fig. 1 in the state space, we obtain ordered patterns (attractors) which are the same geometrically (Fig. 3). Even two completely different initial conditions result in similar patterns (Fig. 4). In this work we propose using the similarity between these attractors of the state space as the objective function for parameter estimation. In the next section we describe the proposed method.

3. Proposed GMM-based cost function

As mentioned before, state space is a suitable domain to represent chaotic and nonlinear behaviors of a chaotic and complex system. One of the advantages of considering the signal in state space is its time-independent distribution. Based on this characteristic, a statistical distribution of observed vectors in state space can capture the attractor topology and nonlinear system characteristics. The distribution of attractor points is invariant and independent of initial conditions provided the initial conditions are in the basin of attraction [2,39]. Thus we propose a similarity indicator using a likelihood score between a learned statistical model of a real system attractor and a new distribution for an attractor obtained by a model of the system. Here, we use a GMM as the statistical model. The GMM is a parametric probability density function represented by a weighted sum of Gaussian component densities [40]. GMMs are commonly used as a parametric model of the probability distribution of the state space vectors in many different systems such as vocal-tract related features in a speech recognition system [41] or ECG signal classification methods [42]. One of the powerful characteristics of the GMM is its ability to form smooth approximations of attractors in state space [43].

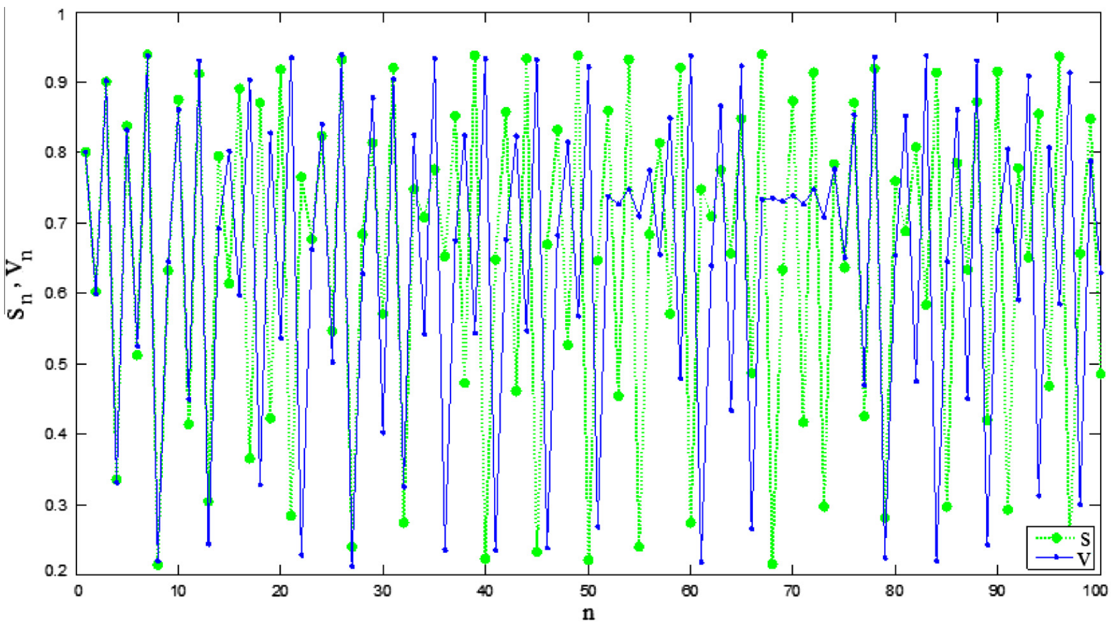

Fig. 1. Chaotic evolution of the logistic map with $A = 3.76$ showing the effect of a difference in the initial conditions of 0.1%. The initial conditions are $s_1 = 0.8$ and $v_1 = 0.8008$.

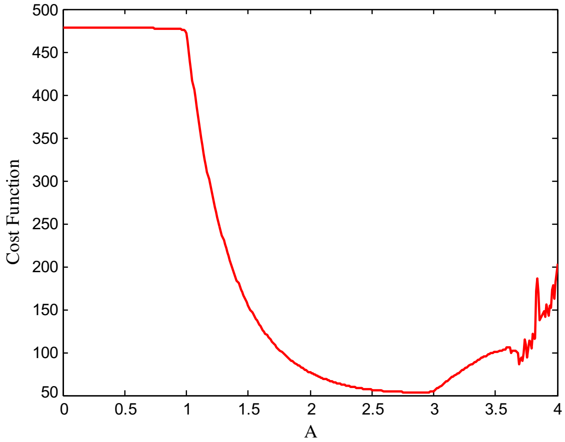

Fig. 2. Cost function obtained from Eq. (2.3). The initial conditions are $s_1 = 0.8$ and $v_1 = 0.8008$ with $N = 1000$. Global minimum occurs near $A = 3$, which is far from the correct value of $A = 3.76$.

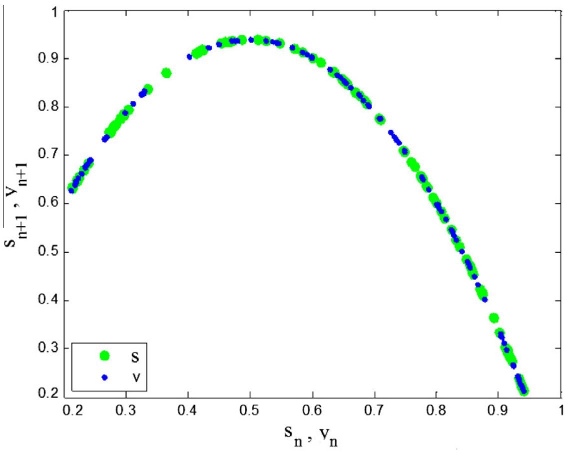

Fig. 3. State space for the logistic map with $A = 3.76$ showing independence of initial conditions. The initial conditions are $s_1 = 0.8$ and $v_1 = 0.8008$.

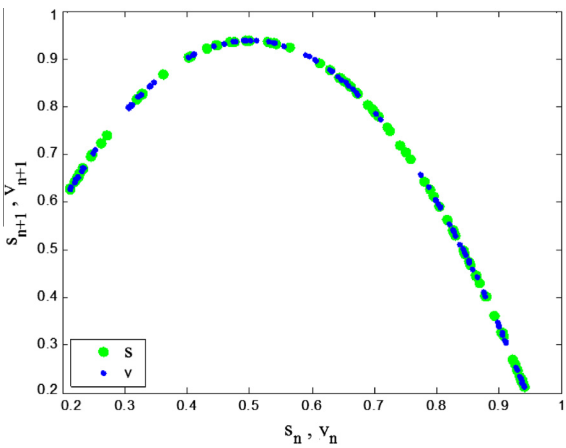

Fig. 4. State space for the logistic map with $A = 3.76$ showing independence of initial conditions. The initial conditions are $s_1 = 0.5$ and $v_1 = 0.9$.

To find the similarity between the attractor of a real system and the state space points of the model, we calculate a likelihood score which comes from GMM computations. Our algorithm consists of two steps; a training stage which includes fitting the GMM to the attractor of the real system, and an evaluation stage to select the best set of parameters in the model which causes the best similarity score in the learned GMM. Following are those steps in detail:

Step 1: The first step of the proposed approach is the learning phase. A GMM learns the probability distribution of the attractor of the real system. A GMM is a weighted sum of M individual Gaussian densities. It can be represented by a set of its parameters, λ, as follows,

$$\lambda = \{w_m, \mu_m, \Sigma_m\}, \quad m = 1, \ldots, M$$

$$p(\boldsymbol{v}|\lambda) = \sum_{m=1}^{M} w_m \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma_m|^{1/2}} \exp\left\{\frac{-1}{2}(v - \mu_m)^T \Sigma_m^{-1} (v - \mu_m)\right\} \tag{3.1}$$

where M is the number of mixtures (Gaussian components), μ_m is the D-dimensional mean vector of the mth mixtures, Σ_m is the $D \times D$ covariance matrix, $|\cdot|$ denotes the determinant operator, and y is the observation vector in state space. Also, $p(v|\lambda)$ is the likelihood score for the observed vector v. This score is obtained by giving y to the learned GMM with its parameters of λ. Using the prepared training data for the attractor of the real system, the parameters of the GMM will be specialized in order to model the geometry of that attractor. As a popular and well-established method, a maximum likelihood (ML) estimation is used to identify the GMM parameters [40,44]. However, there are no analytical solutions to determine the optimum number of GMM mixtures needed for a specific problem because it depends on the complexity of the involved data set [37]. Fig. 5 shows a visualization of GMM modeling of the chaotic attractor of the logistic system (with $A = 3.76$) in a two-dimensional state space using 16 Gaussian components ($M = 16$), where every two-dimensional ellipsoid corresponds to one of the Gaussian components of the GMM.

Step 2: The second step of the proposed approach is finding the best model parameters using the learned GMM in step 1. Here, the search space will be formed from a set of acceptable value of the model parameters. Then, for each set of model parameters, the model will be simulated, and a new trajectory in the state space will be obtained. Finally, the similarity score will be computed using an average point-by-point likelihood score obtained from the learned GMM, λ, as follows,

$$p(\boldsymbol{V^k}|\lambda) = \frac{1}{N}\sum_{n=1}^{N} \log\{p(\boldsymbol{v_n^k}|\lambda)\} \tag{3.2}$$

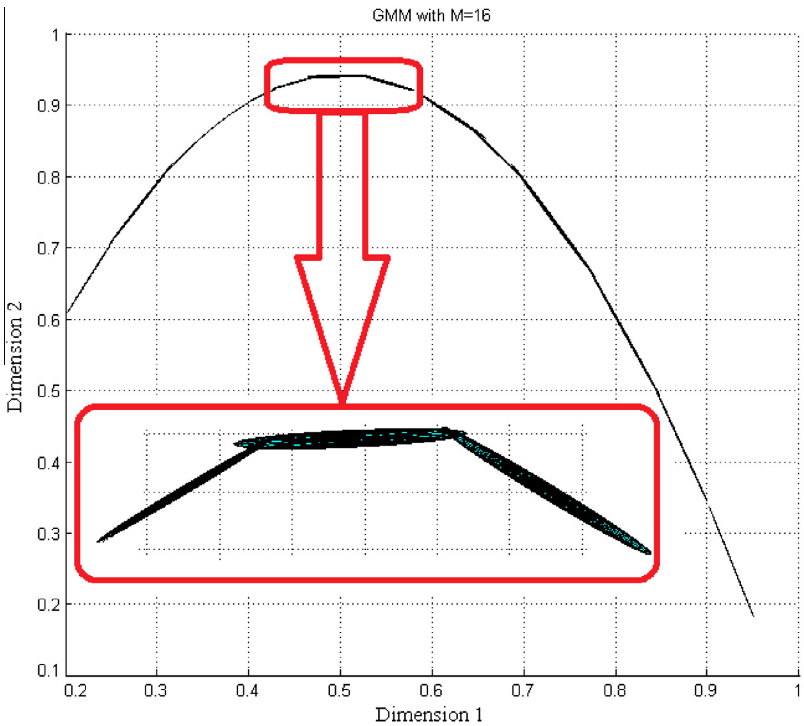

Fig. 5. GMM modeling (with $M = 16$ component) of the real system attractor for the logistic system.

where $\boldsymbol{V}^k$ is a matrix whose rows are composed from the state space vector of the model trajectory with the model's parameters $\tilde{\theta}$, and N is the number of state space points in the $\boldsymbol{V}^k$ matrix. The model selection is accomplished by computing the conditional likelihoods of the observed vectors under learned GMM and selecting the parameters of a model which can gain the best similarity score.

Selection of the best model's parameters $\tilde{\theta}^*$ is conducted by the following criteria: If we use the negative of the similarity score, then the parameter estimation becomes a cost function minimization. Eq. (3.3) shows the final cost function, $J(k)$, based on the negative of the mean log-likelihood score,

$$\tilde{\theta}^* = argmin\{J(\tilde{\theta})\} \quad \& \quad J(\tilde{\theta}) = -p\left(\mathbf{Y}^k|\lambda_{\tilde{\theta}}\right) \tag{3.3}$$

where $\tilde{\theta}$ is the set of model parameters and $\lambda_{\tilde{\theta}}$ is its learned GMM for the real system attractor. Our objective is to determine parameters of the model in such a way that the value of J is minimized.

The proposed cost function for the case of the logistic map is shown in Figs. 6 and 7 along with a bifurcation diagram for the logistic map. As can be seen, this cost function has the desired ideal properties. It shows the effect of changing the parameter of the model, including the bifurcations and the monotonic trend along with a global minimum at exactly at the right value of A (here $A = 3.76$). Fig. 7 shows the effect of increasing the number of components used in the GMM. As shown, all of the cost functions are proper and acceptable.

4. Hindmarsh–Rose model

In 1984, Hindmarsh and Rose introduced a model (the HR model) for neurons described by three first order ordinary differential equations. The model can exhibit a variety of dynamic behaviors for the membrane potential which include chaotic dynamics [11]. This model has three variables: membrane potential, a spiking variable (the rate of sodium and potassium transport through the fast ion channels), and a bursting variable (the transport of other ions thorough slow channels). Eq. (4.1) shows this model in which all of the parameters have values commonly used in the literature. The only exceptions are the main bifurcation parameters of the model which are the current that enters the neuron, I, and the efficiency of the slow channels to exchange ions, r.

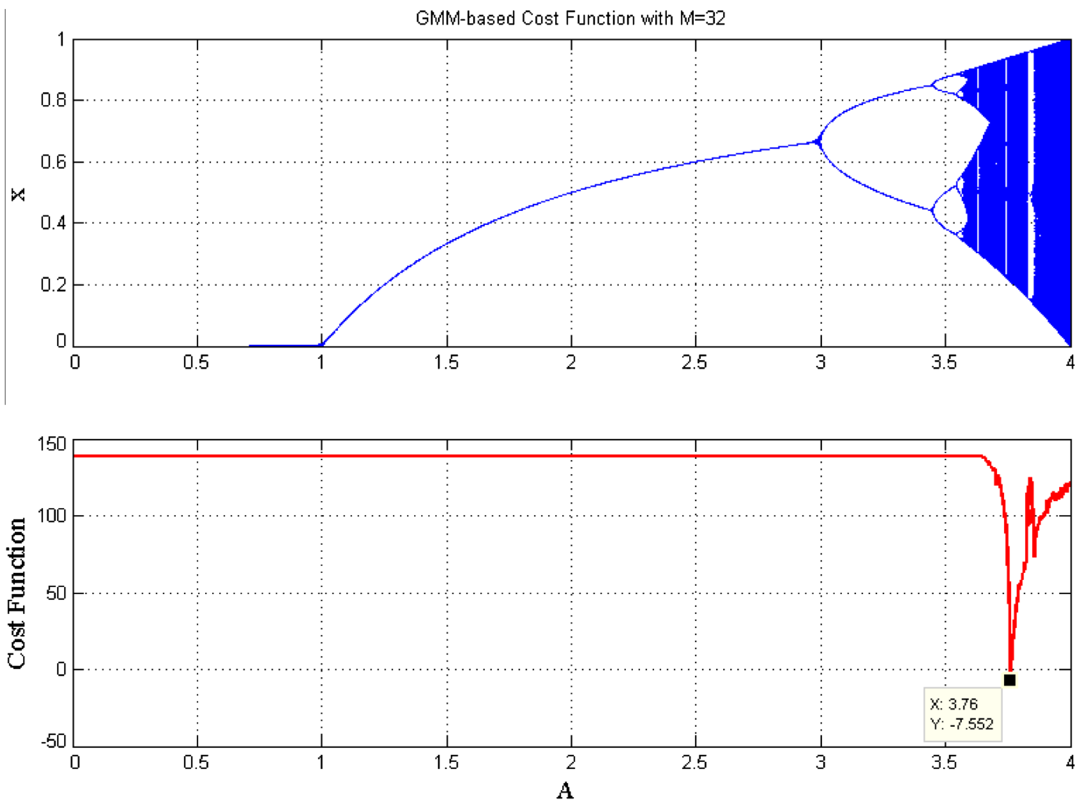

Fig. 6. New GMM-based cost function obtained by the proposed algorithm with $M = 32$. The initial conditions are random numbers between 0 and 1. Transient parts of the data are omitted.

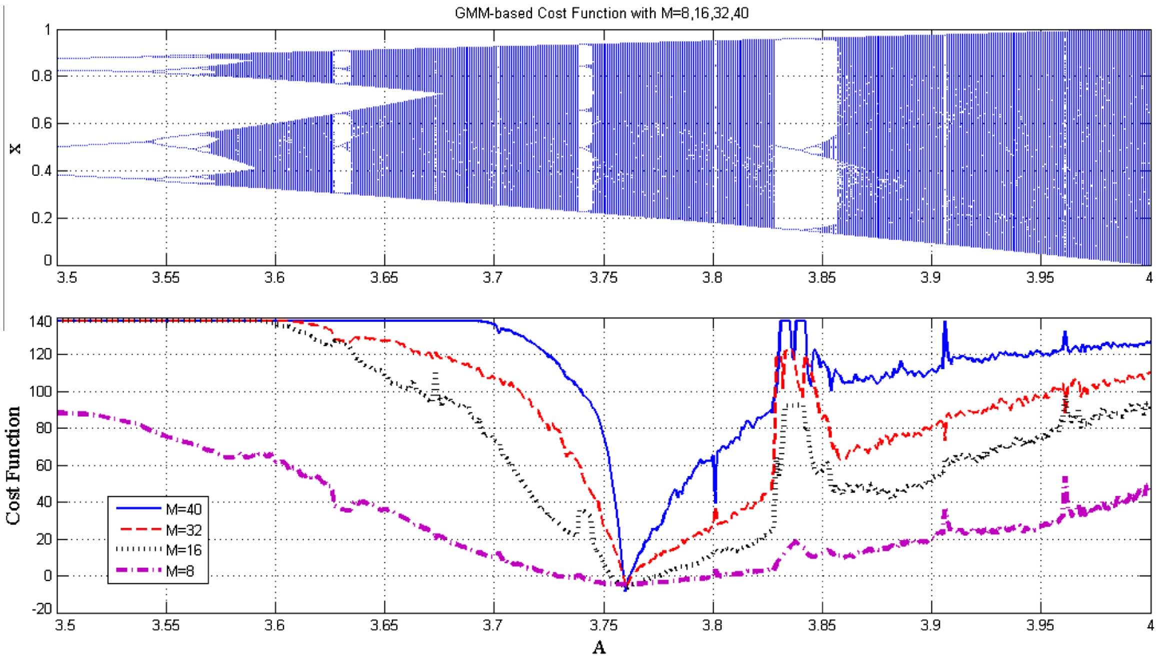

Fig. 7. New cost function obtained by the proposed algorithm with $M = 8$, $M = 16$, $M = 32$, and $M = 40$ shown with violet, black, red, and blue lines, respectively.

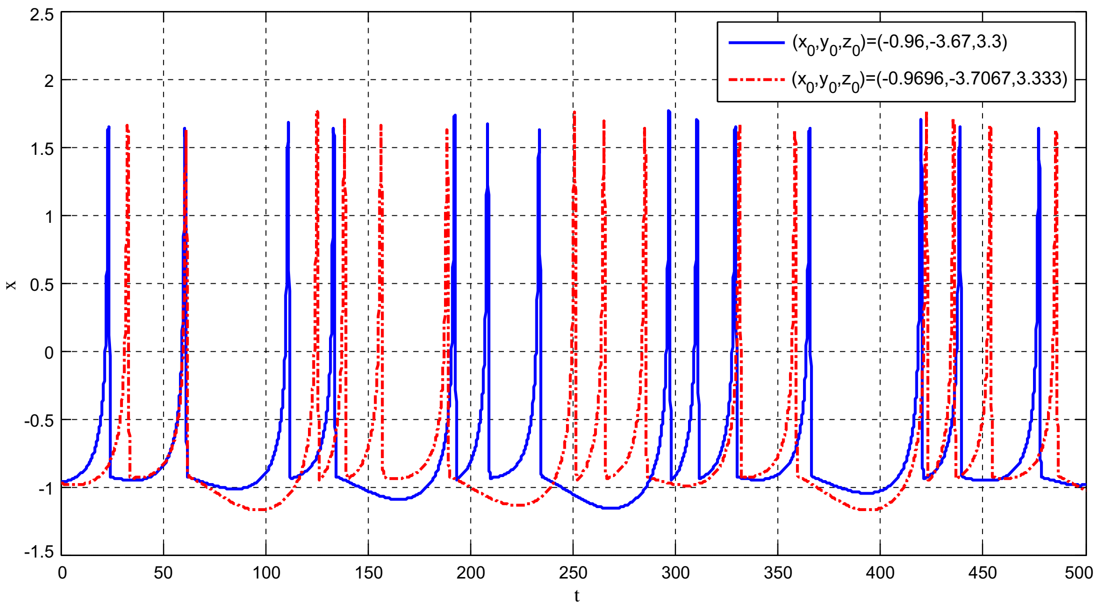

Fig. 8. Chaotic evolution of x showing the effect of changing the initial conditions by 1%.

$$\begin{aligned}
\dot{x} &= 3x^2 - x^3 + y - z + I \\
\dot{y} &= 1 - 5x^2 - y \\
\dot{z} &= r[4(x + 1.6) - z]
\end{aligned} \tag{4.1}$$

where x, y, and z are membrane potential, spiking variable, and bursting variable, respectively. Using these three variables, we can construct a three-dimensional state space that shows the dynamic of the HR model. We consider these variables as a three-dimensional vector $v = [x,y,z]$. This vector determines the system state, which can be viewed as a point in state space. The trajectory, starting from some initial point $v_0 = v(t_0)$ and followed as $t \to \pm\infty$, produces a corresponding attractor in state space [2].

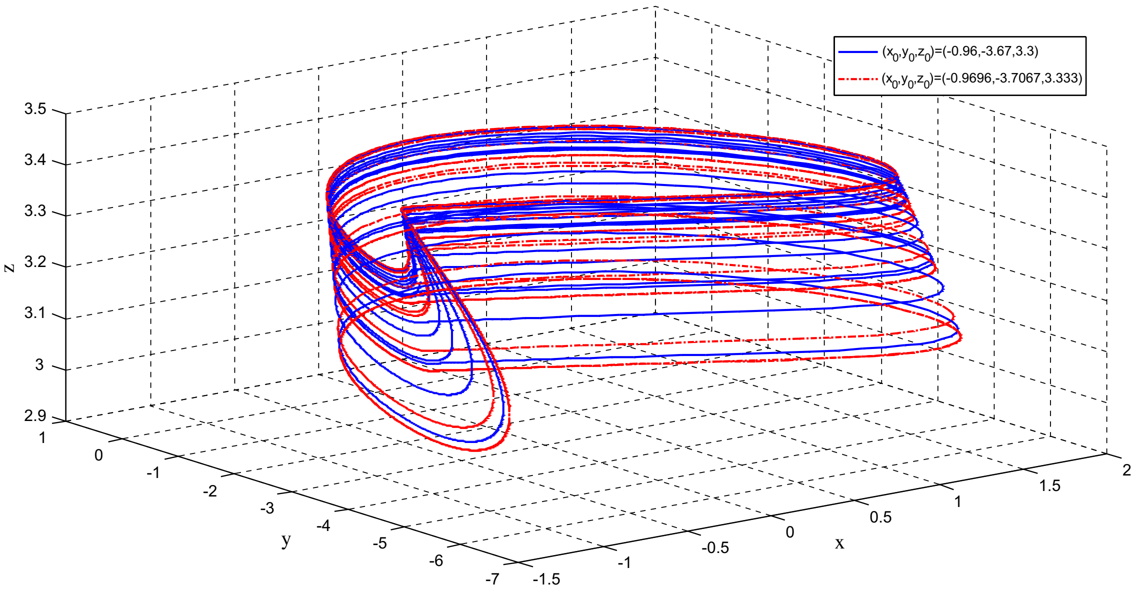

Fig. 9. Attractor of the HR model in 3-D state space with two nearby initial conditions.

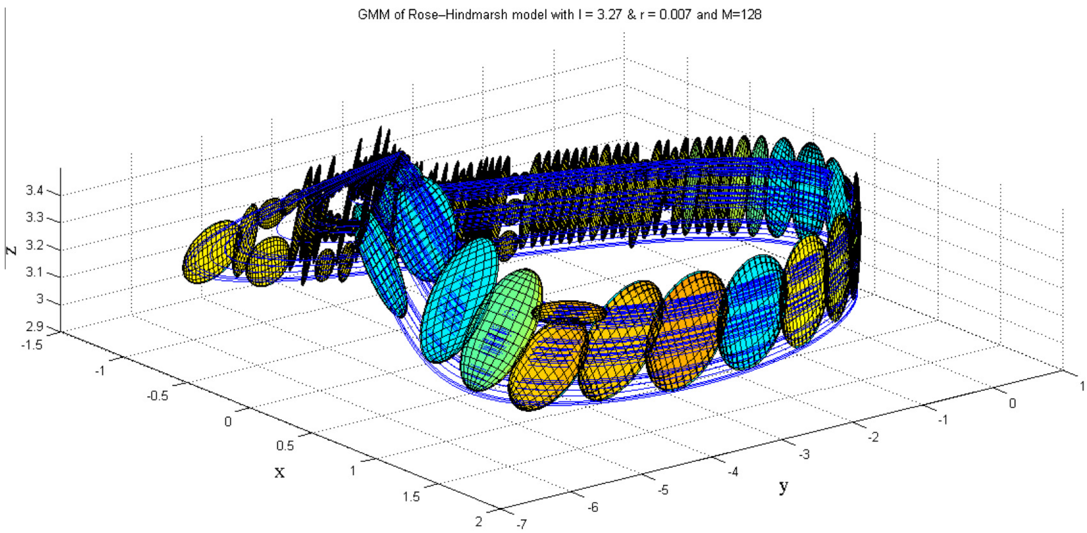

Fig. 10. GMM modeling (with $M = 128$ components) of the real system attractor for the HR system in 3-D state space. Each three-dimensional ellipsoid shows a Gaussian component of the GMM.

The HR model has been investigated widely in the chaos literature [45–52]. Especially, it has been a benchmark for different parameter estimation strategies for chaotic real-world problems [53–57]. We considered $I = 3.27$ and $r = 0.007$ as the real values of the parameters to be estimated.

Fig. 8 shows the effect of a 1% change in the initial conditions of $(x_0, y_0, z_0) = (-0.96, -3.67, 3.3) \rightarrow (x_0, y_0, z_0) = (-0.9696, -3.7067, 3.333)$ on the membrane potential time series. As can be seen, there is no correlation between the time series in the time domain due to sensitive dependence on initial conditions. On the other hand, Fig. 9 shows those time series in a 3-D state space. We can see that they both create geometrically similar attractors.

5. Simulation results and discussion

In this section, we show simulations to assess the acceptability of the proposed cost function in estimating parameters of the HR neuron. We used a fourth-order Runge–Kutta method with an adaptive step size whose average value is 0.06 s and a total of 32925 samples corresponding to a time of 2000 s.

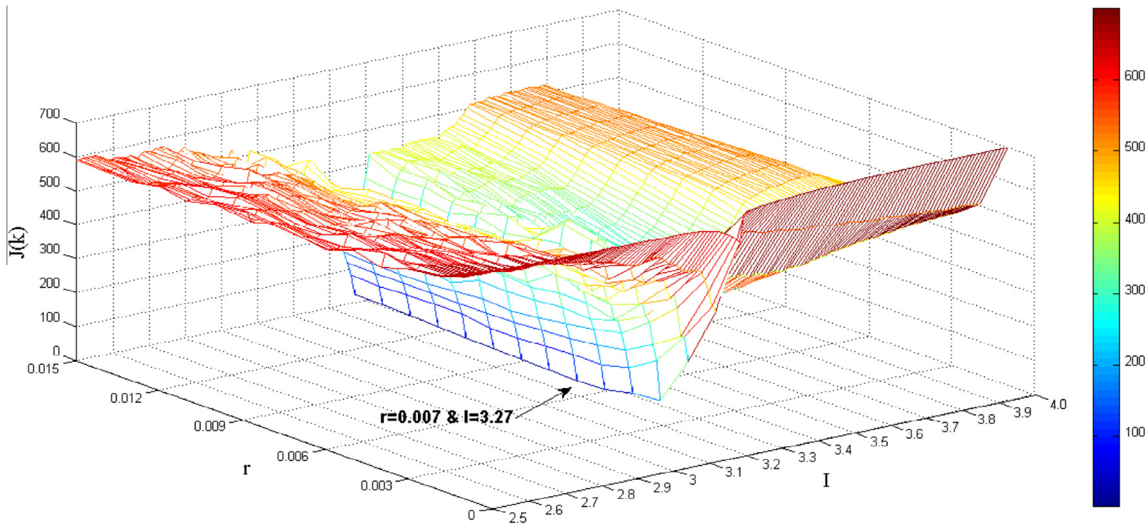

Fig. 11. The surface of the GMM based cost function for the HR model for a variation in the parameters, r and I.

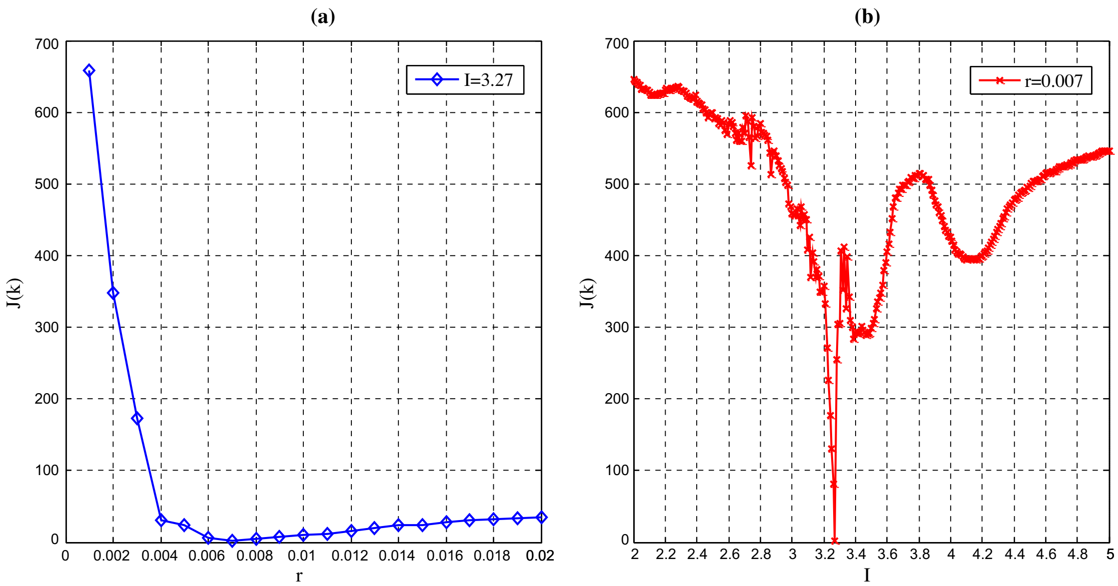

Fig. 12. Cross sections of the surface in Fig. 4 for (a) $I = 3.27$, (b) and $r = 0.007$.

Here, we assume that the original chaotic system of (4.1) has the following real value of the parameters $I = 3.27$ and $r = 0.007$ which are to be estimated by minimization of the proposed cost function. Experimentally, we use $M = 128$ mixtures to model the system attractor in state space. Based on the observation vector y, in this work, $D = 3$ is selected for the HR model.

Fig. 10 shows the chaotic attractor of the HR model in the three-dimensional state space. Also shown is a visualization of its GMM modeling using 128 Gaussian components ($M = 128$), where every three-dimensional ellipsoid corresponds to one of the Gaussian components of the GMM.

If we plot the value of the negative of the mean log-likelihood for each pair of parameters, a cost "surface" can be obtained that shows dissimilarity between the real system attractor and each model attractor. In Fig. 11, such a surface is shown for the proposed cost function. The minimum point on that surface gives the parameters for the best model. Fig. 12 shows one-dimensional sections of that surface. As can be seen in those figures, the global minimum of the cost function is in the right place ($I = 3.27$ and $r = 0.007$). Moreover, the surface is almost convex, which makes it is a simple case for any optimization approach than moves downhill.

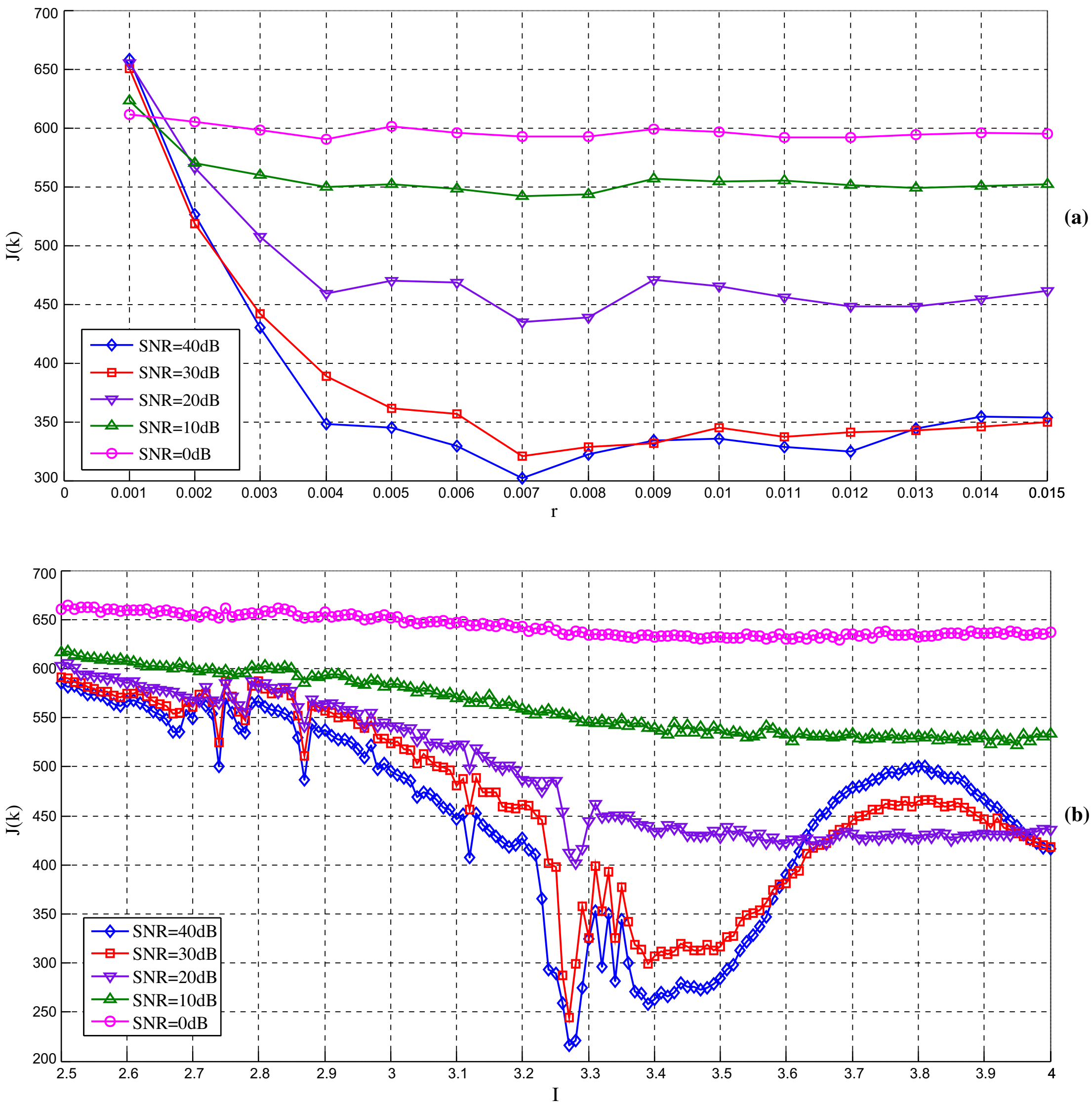

Fig. 13. GMM based cost function obtained by the proposed algorithm in the presence of different amounts of additive noise: (a) cross sections of the surface for $I = 3.27$ (b) cross sections of the surface for $r = 0.007$.

5.1. The effect of noise

Since all real data are contaminated by some degree of noise, we have investigated the effect of different noise levels in data on the GMM based cost function. Fig. 13 shows the cross sections of the proposed cost function in the presence of some additive white Gaussian noise (AWGN) with different values of signal-to-noise ratio (SNR). As can be seen, the proposed method is robust against low levels of noise (SNR $\geqslant$ 20 dB). However, noise with low SNR values (SNR < 20 dB) affects the accuracy of the global minimum and moves it away from the exact value. Fortunately, many different noise reduction techniques [58–62] can be used to clean the data.

5.2. High dimension parameter estimation

In the parameter estimation of chaotic systems, we are dealing with systems whose behavior may change greatly and suddenly with small changes in the parameters. Thus we expect rugged surfaces with possibly many local optima. As the number of parameters increases, the curse of dimensionality appears. Therefore, we have chosen a model for the natural cardiac pacemaker [63] which has many parameters as another example. This system is a modification of the forced van der Pol equation and can be described by the equation

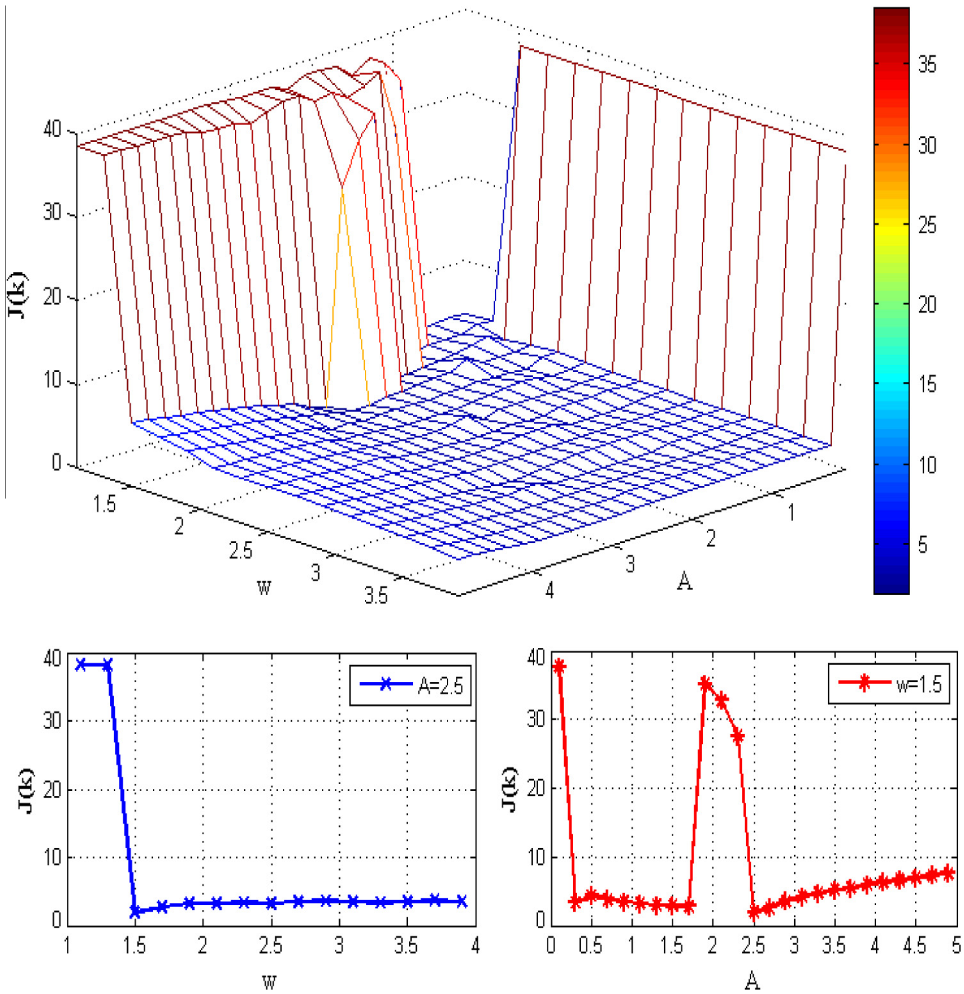

Fig. 14. 2-D and 1-D sections of the cost function surface for the natural cardiac pacemaker.

$$\ddot{x} + \alpha(x - v_1)(x - v_2)\dot{x} + \frac{x(x + d)(x + e)}{ed} = F(t)$$
$$F(t) = A\sin(\omega t) \tag{5.1}$$

where α modifies the pulse shape, which changes the time that the heart receives the stimulus, v_1 and v_2 compose an asymmetric term that replaces the damping term in the classic van der Pol equation, e controls the atrial or ventricular contraction period, d is a parameter that arises when the harmonic forcing of the classic equation is replaced by a cubic term, and $F(t)$ is an external forcing function [63]. The system thus has seven parameters. Considering the values of the parameters that result in chaotic behavior ($\alpha = 0.5$, $v_1 = 0.97$, $v_2 = -1, d = 3, e = 6, A = 2.5,$ and $\omega = 1.9$), we applied the GMM method to obtain a cost function. The global minimum of the surface is in the correct place. Fig. 14 shows some 2-D and 1-D sections of that cost function.

6. Conclusions

In this paper an appropriate and new cost function has been introduced to be used in parameter estimation of chaotic neurons (and in general other complex chaotic systems), based on a statistical model of the real system attractor in state space. Since Gaussian mixture models are strong tools for use as parametric models of the probability distribution of state space vectors in many different systems, we have used them in this work for that statistical model. The proposed cost function is the negative of a similarity metric which is formed by averaging some log-likelihood scores. Overall results indicate that the global minimum of the proposed cost function is the true value of the model's parameters in the clean and low-noise noisy condition. Since this method is based on the topology of strange attractors, one virtue is that the sample time is not critical, and even with short and piecewise time series, the GMM can be trained even when the data do not completely cover the attractor.

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