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Original Article

Application of Self-Organizing map for Time-Varying Biological to Predicting of Complexity Systems

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Abstract - *One of the problems in biochemistry is how to estimate the biological system's behaviour changes over time. The types of recursive identification methods like recursive least square error (RLSE) estimation and Kalman filter is used in previous, the speed of estimation is still a limiting factor in biological systems. It is especially noticeable when the identifier has to estimate the parameters in the situation that it had estimated before but has later lost the estimated values because of the changes in the behaviour of the biological system. To overcome this problem and speed up the identification process, the multiple model identification using the self-organizing map neural network (MMSOM) has been introduced. In multiple modelling, there is more than one estimated model for biological systems. In each step of time, the best model is selected for the biological systems according to previously defined criteria of identifications which is adaptive during different times.*

Keywords - *Biological Prediction. Deep learning. Neural Network. SOM*

I. INTRODUCTION

The modern approaches of complexity and self-organization to understanding dynamical biological systems concepts can inform current interest in systems biology [1], [2]. In the field of identification theory, plenty of methods have been developed to estimate model parameters of biological systems, such as least square error estimation, predictive error estimation and so on [3]. Many of the works in this field are for the case that the desired model is nonlinear biological modelling. Though the theory of linear modelling has significantly been studied, there are still a lot of related problems regarding it. The recent advances in machine learning algorithms have made data-driven approaches more competitive and powerful than ever [4]. Arguably, machine learning is one of the most important developments in biological data analysis. Machine learning has become an indispensable tool in bimolecular data analysis and prediction. Virtually every computational problem in computational biology and biophysics, such as the predictions of solvation free energies, protein-ligand binding affinities, mutation impacts, has a class of knowledge-based approaches that are either parallel or complementary to physics-based approaches [5], [6].

With its ability to recognize nonlinear and high-order interactions among features as well as the capability of handling data with underlying spatial dimensions, deep convolutional neural networks have led to breakthroughs in image processing, video, audio, and computer vision, whereas recurrent nets shed light on sequential data such as text and speech. Deep learning has fueled rapid growth in several areas of data science [7], [8], [9], [10], [11]. Machine learning-based approaches are advantageous because of their ability to handle very large data sets and nonlinear relationships in physically derived descriptors [12]. In particular, deep learning can automatically extract optimal features and discover intricate structures in large data sets. Multiple modelling and multiple control found their ways in industrial applications [13]. Target tracking, Aircraft control, and Failure detection and compensation are among the interesting topics in the aircraft-related fields. A wide variety of applications in bioengineering are also found for this method, like blood pressure control, arterial oxygen control and electrically stimulated muscle.

When there are multiple learning tasks, multi-task learning (MTL) provides a powerful tool to exploit the intrinsic relatedness among learning tasks, transfer predictive information among tasks, and achieve better-generalized performance. During the learning stage, MTL algorithms seek to learn a shared representation (e.g. Shared distribution of a given hyper-parameter, shared low-rank subspace, shared feature subset and clustered task structure) and use the shared representation to bridge between tasks and transfer knowledge. MTL has found applications to the bioactivity of small molecular drugs and genomics [14]. Linear regression-based MTL heavily depends on the well-crafted features, while neural network-based MTL allows more flexible task coupling and can deliver decent results with a large number of low-level features as long as such features have the representation power of the problem.

A self-organizing map (SOM) neural network is a kind of unsupervised learning neural network, which maps and classifies the characteristics of a collection of objects to several classes [15]. Most of the applications of this network are in signal processing or related topics [16]. There are few works related to the application of SOM in the identification of process systems. In this paper, an algorithm is introduced to use the multiple modelling by self-organizing map (MMSOM) neural network for computing and adapting the set of multiple models. It is applied to linear time-varying systems, and some of its mathematical properties have been investigated. One of the most striking characteristics of cells is the sheer complexity of metabolism.

II. METHODOLOGY

In this research, as shown in fig 1, a method for model identification of biological complexity as a method of stimulating new chemistry using the self-organizing map neural network (SOM) is presented. Different variations of that are introduced, and some of its properties are investigated. Inputs to the neural network are parameters of the instantaneous model evaluated adaptively in each instant of time. The neural network learns these models. Artificial Neural Networks (ANNs) are one example of a successful transfer of information about a complex biological system on biological applications. ANNs were developed, in part, as a tool with which to model the brain. To what extent current ANNs do so is a continuing subject of discussion, but the effort to make the connection between ANNs and brains (and to learn from the brain) has unquestionably expanded the capabilities of computation. The model with the closest output to the biological systems, the output is chosen as the model of ANNs systems.

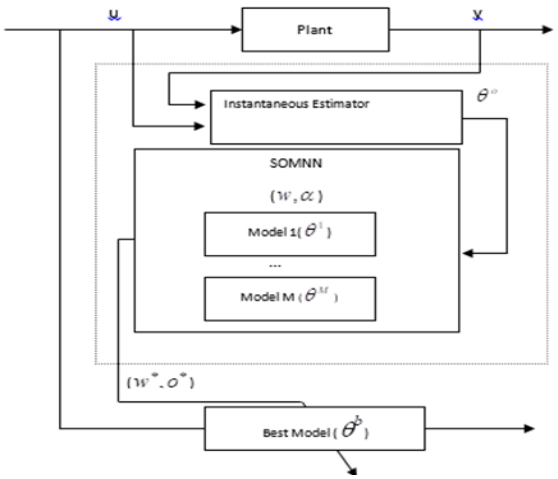

Fig. 1 Structure of the MMSOM identification algorithm

After that, the identification method of multiple modelling by the irregular self-organizing map (MMISOM) neural network is presented, which improves the original method of MMSOM that uses the rectangular SOM. The irregular SOM used in MMISOM is a graph of all the nodes and some of the links that make a minimum spanning tree (MST) graph. Using ISOM, the neighbourhood between the nodes may change to keep it MST. Therefore, ISOM has more flexibility to cover concave space while SOM is more suitable for convex spaces. Also, using a method introduced in this research, it is possible to add new models if the number of models is initially less than the suitable one. One of the opportunities in fundamental chemical research is to learn from biology and to use what is learned to design non-biological systems that dissipate energy, replicate, and adapt [17]. There is also the inverse opportunity: Learning from biological complexity as a method of stimulating new chemistry. With this opportunity, there is a great reason for optimism. Biological systems display such a large number of remarkable capabilities (And capabilities that are so clearly complex). Artificial Neural Networks (ANNs) are one example of a successful transfer of information about a complex biological system on biological applications. ANNs were developed, in part, as a tool with which to model the brain. To what extent current ANNs do so is a continuing subject of discussion, but the effort to make the connection between ANNs and brains (and to learn from the brain) has unquestionably expanded the capabilities of computation [18].

In this same sense, biology (and perhaps also complex materials) offers examples of complex systems that show types of behaviour that are now uncommon in molecular chemistry. A self-organizing map (SOM) neural network is a kind of unsupervised learning neural network, which maps and classifies. The characteristics of a collection of objects to some classes. Most of the applications of this network are in signal processing or related topics. There are few works related to the application of SOM in the identification of a process state [19]. In this thesis, an algorithm is introduced to use SOM neural networks for computing and adapting the set of multiple models in SMM. It is applied to linear time-varying systems, and some of its mathematical properties have been investigated.

The multiple modelling by self-organizing map (MMSOM) neural network is utilized. Inputs to the SOM are the parameters of an instantaneous model computed adaptively at each instant. The set of the reference vectors (RV) of the nodes in SOM is the set of multiple models. This method is useful specifically when the parameters change within a convex space. After introducing the algorithm, some of its properties are explained by an illustrative example.

SOM is a neural network, which maps the input data from the nm dimensional input space I to the M nodes output space O. O represents the quantization space of I, fig 2. Each of the nm input nodes Ii links to every of the M output nodes O_j with a weighted linkw_{ij}As shown in fig 2. In this study, the SOM neural network is utilized to produce the optimum set Θm of M linear models of the plant. The number of SOM inputs is equal to the number of estimation parameters. It has M output nodes, where M is the desired number of the local models. During this manuscript, the term node is used for the output node or

neuron. Otherwise, it is mentioned [20]. SOM learns its input and classifies them to some classes. At first, the Euclidean distance between the present input vector value and weights of the reference vectors of each output node is computed [21]. The network chooses the output node with the minimum distance as the winner node. The reference vectors of the neighbouring output nodes of the winner node are updated such that the new RV set of them is closer to the present input vector value. This training procedure is applied to all input vectors.

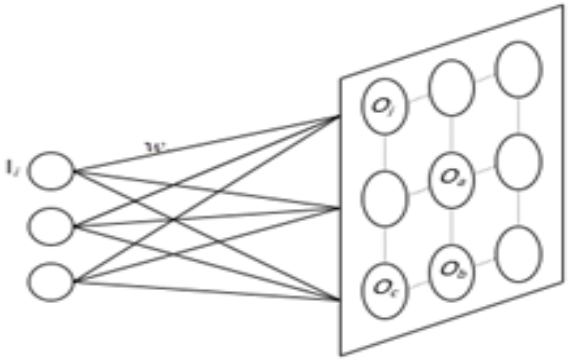

Fig. 2 SOM neural network illustration

SOM produces the local models by which the plant is to be modelled. It constantly gathers and combines the information about the plant from the IM. IM is identified for every step. These different values for IM are categorized by the SOM into some classes. Each of the local models represents one of these classes. To put it another way, SOM quantizes the space of the plant models Dm into some quantization sets

$$\theta_i = \{1 \dots M\}$$

The IM parameters at the time t that is $\theta^0(t)$, are the inputs to the SOM at that time. The number of the SOM input nodes should be nm, which is the same as the number of unknown parameters of the model. SOM compares these parameters with its reference vectors to find the winner node. The reference vectors of the neighbour nodes of the winner node learn the IM parameters change according to some learning rule. As a consequence, SOM classifies the produced values of the parameters of IM at different times into M classes. Each of the SOM nodes O_i with reference vector weights $w_i = \theta^i$ represent one of the subsets d_M^i of the space d_M reference vector is the nearest one to the parameters set in d_M^i Definition of the borders on $\{d_M^i\}_{i=1}^M$ depends on the relative values of Θ_l As shown in Fig 2, this definition. If the whole square is D_M and each dot denotes a local model θ^i, then the borders $\{d_M^i\}_{i=1}^M$ areas are shown in fig3.

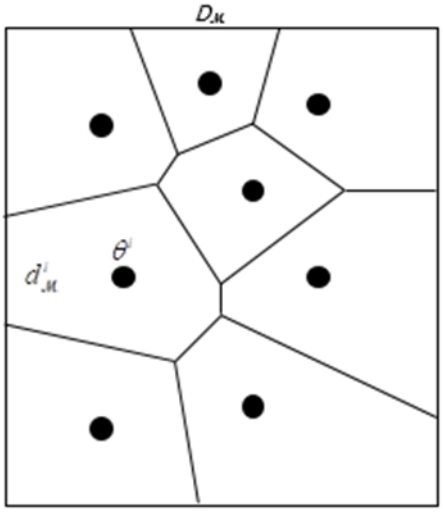

Fig. 3 Voronoi partition

For every point in d_M^i,θ^i It is the nearest dot to it. This kind of partitioning is called Voronoi partitioning 20. More specifically, the training steps of the SOM are as follows:

Assign an initial value to the weights W_{ij} , Apply the input vector IM to the input nodes; Find the winner output node O* by the following criterion:

$$d_j = \left\|\theta^0(t) - W_j\right\|$$

which describes the distance between the reference vector of the node j and the IM parameters $\theta^0(t)$ where $\|.\|$ denotes the Euclidean norm, $W_j = \left(W_{1j}, \dots W_{n_{mj}}\right)$ Is the reference vector connecting all input nodes to the output node j. Defining $d^* = \min_j d$ The winner neuron will be, $O^* = \{O_j | d_j = d^*\}$ Update the reference vectors by the learning rule:

$$W_{ij}(t+1) = W_{ij}(t) + \eta(t)\left[\theta_i^0(t) - W_{ij}(t)\right]\mathcal{H}(O^*, O_j, t)$$

Where W_{ij} is the ith component of the reference vector W_j, $\eta(t)$ is the learning rate and $\mathcal{H}(O^*, O_j, t)$ is the neighbourhood function for the winner node O^* in the output node O_j At time t. In the above procedure, the neighbourhood function and the learning rate should be defined according to the problem. The neighbourhood function $\mathcal{H}(O^*, O_i, t)$ is a kind of radius window, which is centred on the winner node O^*, found in step 3, and is described in this study as:

$$\mathcal{H}(O_k, O_j, t) = \begin{cases} 1 & , \quad is\ (O_k, O_j) = 0 \\ 1/2 & , \quad 0 < dits\ (O_k, O_j) \le max\left(1, m^{\left(\frac{10-\sqrt{i}}{10}\right)}\right) \\ 0 & , \quad otherwise \end{cases}$$

Where m denotes the total number of the nodes. Dist (O_k ,O_j) is the distance between nodes Ok and,O_j . The output nodes have net topology. Each node, based on the defined topology, is a one-step neighbour of some other nodes. The distance between the two output nodes is the minimum number of steps between them.

III. RESULTS AND DISCUSSION

As can be seen, the node O_b in fig 4 is a one-step neighbour of the nodes O_a and O_c . As a result, O_c is a 2 steps neighbour of O_a . The distance between the nodes O_a and O_b is one and between the nodes O_a and O_c Are two. The radius of the neighbourhood window decreases with time. The rate of change in the weights of the reference vector of a node The reference vectors are eventually distributed in a straight line between the two values $\theta_{\Im}$ The distribution of the reference vector's weights is proved to be dependent on the distribution of θ^0 which itself depends on the distribution of $\theta_{\Im}$. SOM stores 16 models in its reference vectors. One of these models should be selected as the model of the plant. As explained in Section, the output error criterion compares the models and introduces the best one at each step. The input u to the plant is also given as the input to all of the 16 models in SOM. The outputs of the models are obtained, as is illustrated in figure 4. Then the performance measures are computed for these models. α Is 0.95 in this example using the designed parameters (β,γ) = (1, 0.02). This research is on developing a method to establish a set of multiple models for linear time-varying biological systems by using the self-organizing map neural network [22]. Two versions of the method are introduced: MMSOM and MMISOM algorithms. Inputs to the neural network are parameters of the instantaneous model, evaluated adaptively in each instant of time. The neural network learns these models. So, the reference vectors of its output nodes are the estimation of the parameters of the multiple local models. At each time, it depends on the value of the neighbourhood function for that node. The magnitude change of the weights decreases as the distance of the node to the winner node increases. Fig 4 and 5. b is shown the clustering and predicting of the growing molecular networks [23]. The neighbourhood function for the SOM nodes is as described in the learning rate η=0.03, which is constant all through time. The obtained SOM after 2000 steps learning is shown in fig. 4

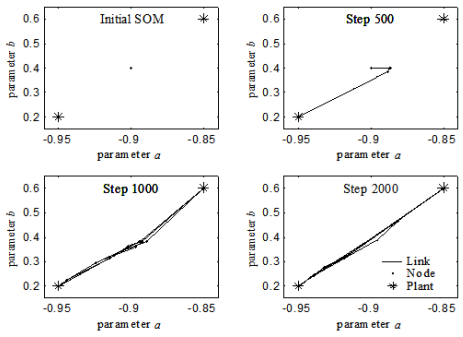

Fig. 4 the obtained SOM after 2000 steps learning is shown

A model with the closest output to the plant output is chosen as the model of the plant. MMSOM utilizes the rectangular SOM. It is suitable for the case that the space of its input is convex. On the other hand, The MMISOM utilizes an irregular self-organizing map (ISOM). The suitable number of models in MMISOM is not needed to be known at the beginning of the algorithm. It is variable, and the algorithm finds the number of suitable models for the plant. MMISOM has more flexibility than the MMSOM when the space of the linear model is not convex. Both methods are specifically suitable for plants with abruptly changed parameters. For instance, a robot arm should handle different loads one after another.

MMSOM and MMISOM have improved on the identification of the time-varying plants compared to the identifications with just one adaptive model for biological systems. The major improvement is in the transient period where the single-model adaptive identifier adapts to the new situation of the biological system by some significant delay. Simulation results as shown in fig 5. b that the best model on MMSOM (and MMISOM) is introduced for the plant much faster than the adaptive neural network has been sufficiently trained.

A stochastic property of the local models is obtained. The parameters of the plant at each step are selected randomly with a specified distribution. Based on this distribution, the distribution of the parameters of the local models is derived for this plant and compared with the plant parameters distribution. Comparing these PDF's shows that the distribution of the local models approaches to some function of the plant parameters distribution, and not exactly to them. Three factors affect this function and help the distribution to approach the plant one. The first factor is the quality of the IM identification, which affects the relationship between the plant parameters and the training inputs to SOM.

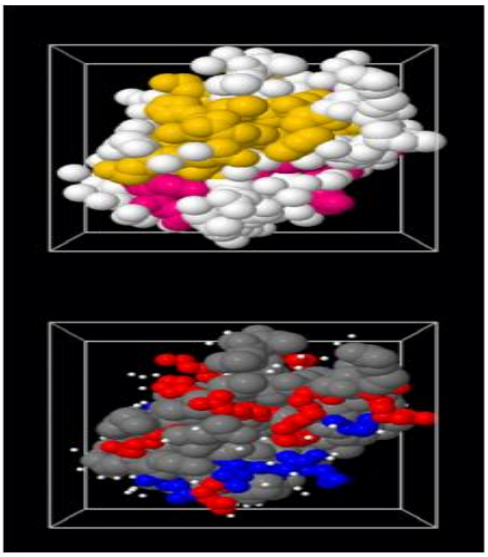

Fig.5 (TOP) Molecular Clustering by using SOM Algorithms predict the trend of features Fig.5.b (DOWN) SOM can be Predicting the trend of growing molecular networks

Inputs to the neural network are parameters of the instantaneous model, evaluated adaptively in each instant of time. The neural network learns these models. So, the reference vectors of its output nodes are the estimation of the parameters of the multiple local models. MMSOM utilizes the rectangular SOM. It is suitable for the case that the space of its input is convex. On the other hand, The MMISOM utilizes an irregular self-organizing map (ISOM). The suitable number of models in MMISOM is not needed to be known at the beginning of the algorithm. It is variable, and the algorithm finds the number of suitable models for the Biological systems. MMISOM has more flexibility than the MMSOM when the space of the Biological systems linear model is not convex. Both methods are specifically suitable for plants with abruptly changed parameters.

MMSOM and MMISOM have an improvement in the identification of the time-varying systems compared to the identifications with just one adaptive mode. The major improvement is in the transient period where the single-model adaptive identifier adapts to the new situation of the Biological systems by some significant delay. Simulation results show that the best model on MMSOM (and MMISOM) is introduced for the plant much faster than the adaptive IM after the neural network has been sufficiently trained.

Training of the neural network can be online or offline. The algorithms can introduce the model of the plant in situations that they have been experienced a few times. Therefore, none of the models is suitable at the early steps before sufficient training. Fortunately, the algorithm can take advantage of the adaptive IM identifier as the best model during that learning period. Hence, the quality of identification is at least the single adaptive IM one. Although these algorithms introduce the model of the plant faster than the IM identifier, the quality of the local models is directly related to the introduced IM to the SOM.

IV. CONCLUSION

In this paper, the goal is on developing a method to establish a set of multiple models for linear time-varying Biological systems by using the self-organizing map neural network. Two versions of the method are introduced: MMSOM and MMISOM algorithms. A stochastic property of the local models is obtained in the paper. The parameters of the Biological systems at each step are selected randomly with a specified distribution. Based on this distribution, the distribution of the parameters of the local models is derived for this system and compared with the Biological systems parameters distribution. At each time, the model with the closest output to the plant output is chosen as the model of the plant.

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