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Soft Sensing Method of Marine Enzyme Based on Dynamic Neural Network

Yuhan Ding[a], Xianglin Zhu[a,*], Jianhua Hao[b], Bo Wang[a], Zheyu Jiang[a]

[a]Jiangsu University, Zhenjiang, 212013, Jiangsu, China
[b]Yellow Sea Fisheries Research Institute, Chinese Academy of Fishery Sciences, 266071, Qingdao, China
zxl4390@126.com

Enzyme activity is very important information during marine enzyme fermentation control process while it cannot be detected online by physical sensors. Various soft sensing technologies have been proposed to solve this problem including neural network (NN) soft sensing. However, the current exist NN soft sensing methods are usually static ones and cannot reflect the dynamic characteristics of the fermentation process. To solve this problem, a kind of dynamic neural network (DNN) soft sensing model was proposed in this paper. The model was composed of a series of differentiators to represent the dynamic character and a multilayer feedforward NN to represent the nonlinear relation. The dynamic characteristics of the variables were reflected in the model through the differentiation of the variables and the nonlinear relation was well established through the reasonable structure of the NN. It was verified by the experiment that this kind of DNN soft sensing model obtained better result compared with the traditional static neural network (SNN) one. The relative mean square error (RMSE) of the DNN model is 130.1 g/L, which is less than 1/2 of the SNN model. The max relative error (MRE) of the DNN model is also decreased dramatically from 846.2 g/L of SNN model to 350.2 g/L.

1. Introduction

In many chemical and biochemical process control situations, there are variables which are closely related to the quality of the product and need to be strictly controlled. However, due to the technique or commercial reasons, most of these important variables are still hard to get. For instance, the enzyme activity is hard to obtain during the marine enzyme fermentation process (Huan et al., 2013). In order to solve the measurement problem of this kind of variables, many soft sensing methods are presented and widely used at present (Yang and Yan, 2012).

The basic idea of soft sensing is to estimate the important variables of the process which cannot be directly measured, based on the process auxiliary variables, which are easy to be measured (Chen et al., 2017). Soft sensing technology is mainly composed of four parts, i.e., the selection of auxiliary variables, data acquisition and processing, soft sensing model and online correction (Jin et al., 2015). The theoretical root is based on the inference control (Brosilow and Tong, 1978) and soft instruments (Joseph and Brosilow, 1978).

There are many soft sensing methods such as mass and energy balances method (Zhao, 1996), adaptive observer method (Wei and Karimi, 2013), regressive method (Teran and Machado, 2011), pattern recognition method (Mei et al., 2015), Kalman filter method (Fu et al., 2012), support vector machine (SVM) method (Liu et al., 2013), and artificial neural network (NN) method (Pappu and Gummadi, 2017). Researches indicated that NN soft sensing methods were better than other methods in accuracy and generalization ability in case the historical data are sufficient (Yu and Cheng, 2015), so it is more widely applied.

However, the NNs used in the current soft sensing methods are usually static ones and they cannot reflect the dynamic characteristics of the fermentation system. The soft sensing accuracy will deteriorate when the large changes occur. To solve this problem a kind of dynamic NN soft sensing model was proposed. This model was composed of a static NN to represent the nonlinear characteristics and a series of differentiators to represent the dynamic behavior. The complete characteristics of the system can be described and realized by this structure. Soft sensing experiment of marine enzyme fermentation process was then performed to validate the effectiveness of the proposed method.

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The remainder of this paper is organized as follows. In Section 2, the principle of dynamic soft sensing model is presented and its advantage is discussed. Then the fermentation and data acquisition experiments are introduced in Section 3. The soft sensing experiments and the results are presented and discussed in Section 4. Finally, conclusions are provided in Section 5.

2. Principles of dynamic neural network soft sensing

Currently, most of the NN soft sensing systems use the following static model:

$$Y = f(\boldsymbol{X}) \tag{1}$$

where Y represents the soft sensing result of the key variables, $\boldsymbol{X}$ represents the auxiliary input variables of the soft sensing mode, and f represents the nonlinear relations between the inputs and output, which is usually realized by a multilayer feedforward NN.

It can be seen from Eq(1) that most of the NN soft sensing models only adopt the current information of the auxiliary variables and exclude the dynamic information of the system, which makes them static models unable to reflect the dynamic characteristics of the system. Such models may get good result when the input variables are relatively steady while the predicting accuracy will deteriorate when large changes of input variables occur.

To solve this problem, a kind of dynamic NN is introduced to construct the soft sensing models. This kind of dynamic NN uses differentiators units to represent the dynamic characteristics, which can be described as follows:

$$Y = f_{NN}(\boldsymbol{X}, \dot{\boldsymbol{X}}, \ddot{\boldsymbol{X}}) \tag{2}$$

where $\dot{\boldsymbol{X}}, \ddot{\boldsymbol{X}}$ represent the first order and second order derivatives of the input variables, f_{NN} represent a static neural network to approximate a nonlinear function. For the marine enzyme fermentation process, $\boldsymbol{X}$ can be temperature, pH, dissolved oxygen, tank pressure, air flow and stirring speed, so $\dot{\boldsymbol{X}}, \ddot{\boldsymbol{X}}$ are the first and second order derivatives of these variables. As the first order and second order derivatives reflect the changing trends of the inputs, such kind of model can approximate most of the general nonlinear dynamic systems as well as soft sensing model of marine enzyme fermentation process, which is likely to obtain satisfactory soft sensing results.

3. Experiments

In this paper, Pa040523 (Chi et al., 2006) strains are the research object which was isolated and obtained from Bohai and the Yellow Sea. Pa040523 strain is a kind of marine bacteria producing enzyme. It is very strict with the fermentation environment. Only in limited temperature, pH value, fermentation time, amount of inoculation, ventilation and other growing condition can the marine microorganism grow best. Through the preliminary analysis of bacterial culture experiments, the optimum pH value, temperature, fermentation time, inoculation amount and aeration rate of the marine enzyme producing strain are 5.5, 12 °C, 72 h, 7 % and 170 mL. Under the optimum fermentation conditions, the enzyme activity in the fermentation tank of 50 L strain would reach the highest.

The fermentation tank was sterilized before using. The time of sterilization lasted about 30 min when the sterilization temperature was set to 121 °C and sterilization pressure was set to 0.11 MPa. Through material feeding system, the right amount of dextrin, soybean oil, alcohol, ammonia and other nutrients were poured into the fermentation tank. The fermentation lasted for about 72 h under the condition of 12 °C, pH value being about 5.5, inoculation amount being 7 %, broth content being 170 mL. The external controller needed to ensure the following conditions: the tank pressure was 0.03-0.07 MPa, ventilation ratio was from 0.5 to 1.2, coefficient of charge was 0.5 to 0.7 and regulating mode was set to adjustable-speed.

Different kinds of sensors, such temperature sensor, pH sensor, dissolved oxygen sensor, tank pressure sensor, air flow sensor, speed sensor, were connected to the fermentation tank, which can dynamically monitor the fermentation and obtain sensory results in real time. In a fermentation period, the enzyme activity was tested offline at intervals of 4 h. The enzyme activity data were then interpolated by polynomial difference with interval being 5 min. By this means, 4 batches of experimental data were collected, among which 3 batches were used as training samples, and the other one batch was used as the test samples.

4. Results and discussions

First, the static NN soft sensing model is investigated. From the previous analysis, there are 6 original variables that can be used as input of the soft sensor model, i.e. the temperature, pH, dissolved oxygen, tank pressure, air flow and stirring speed.

Denote them as $X_1 \sim X_6$ and take them as the input of a 6-12-1 structure NN as shown in Figure 1. Denote the enzyme activity as Y and take it as the output of the NN. The activated function of the hidden layer of the NN is “tansig” and one of output layer is “purelin”. Then the NN was trained with Levenberg-Marquardt training algorithm for 300 times and the training error was getting less than 10^{-6}. The trained NN can then be used to constitute a soft sensing model and realize the soft sensing in the enzyme fermentation process.

As the soft sensing model shown in Figure 1 is without any of the dynamic units and is only composed of an NN representing the nonlinear function, it is indeed a static NN soft sensing model.

The soft sensing result is shown in Figure 2, where the solid line represents the actual enzyme activity and the dashed line represents the soft sensing result.

The soft sensing result is also shown in Table 1 by relative mean square error (RMSE), which is calculated according to the following equation:

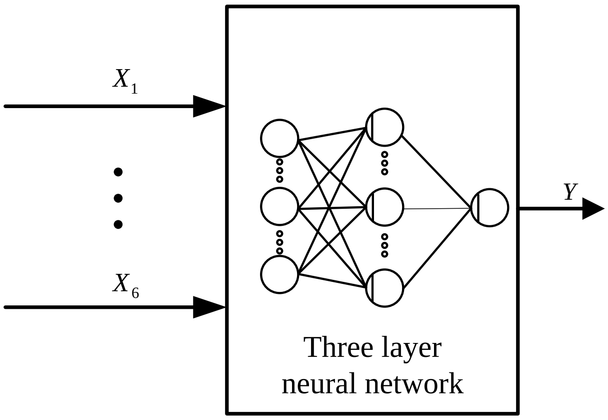

Figure 1: Static neural network soft sensing model

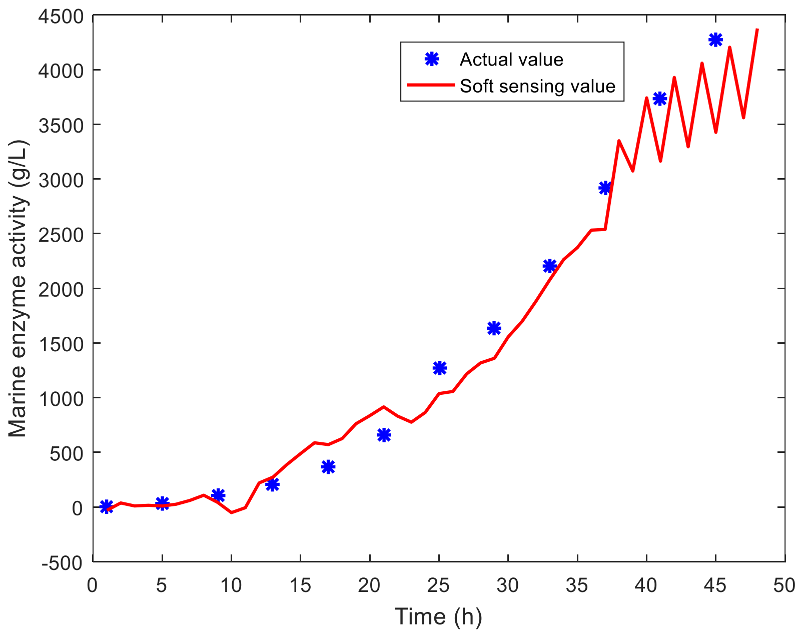

Figure 2: Soft sensing result obtained by static neural network

Table 1: Data error comparison between two soft sensing methods

SS model	RMSE (g/L)	MRE (g/L)
Static NN	347.2	846.2
Dynamic NN	130.1	350.2

$$RMSE = \frac{1}{\bar{P}}\sqrt{\frac{1}{n}\sum_{i=1}^{n}(Y_i - P_i)^2} \times 100\% \tag{3}$$

where Y_i represents the i^{th} soft sensing value of enzyme activity, P_i represents i^{th} actual value, n is the sample number, $\bar{P}$ is the mean value of actual enzyme activity.
Meanwhile, to evaluate the soft sensing error when big changes occur, max relative error (MRE) is also given in Table 1:

$$MRE = \frac{1}{\bar{P}}\max\left|Y_i - P_i\right| \times 100\% \,. \tag{4}$$

From Table 1, one can see that the RMSE and MRE of the static NN soft sensing result are both not small.
To improve the accuracy, a dynamic NN soft sensing model is constructed according to Eq(2). In this model, the dynamic information, i.e., the derivatives of the variables are taken into account. The inputs of the model will include $X_1 \sim X_6$ and their derivatives $\dot{X}_1 \sim \dot{X}_6, \ddot{X}_1 \sim \ddot{X}_6$, and a 18-25-1 structure NN should be used as shown in Figure 3, where the derivatives are obtained by the differentiators *S*.
Set the activating functions of hidden layer and output layer as same as the ones used in Figure 1 and train the NN with Levenberg-Marquardt algorithm for 300 times, the dynamic NN soft sensing model was finally constructed.
The ultimate dynamic NN model can be expressed as follows:

$$Y = f_{NN}(X_1, \dot{X}_1, \ddot{X}_1, ..., X_6, \dot{X}_6, \ddot{X}_6) \,. \tag{5}$$

The soft sensing result of the model is as shown in Figure 4, and the detailed RMSE and MRE are also shown in Table 1.
From Figure 2, Figure 4 and Table 1, the RMSE and MRE of the dynamic NN model are both smaller than those of the static one. This is because the derivatives existed in the model reflect the dynamic characters of the process, making the soft sensing model more sensitive to the input changes and improve the accuracy of the soft sensing result.
The RMSE of the DNN model is 130.1 g/L, which is less than 1/2 of the SNN model. The MRE of the DNN model is also decreased dramatically from 846.2 g/L of SNN model to 350.2 g/L.

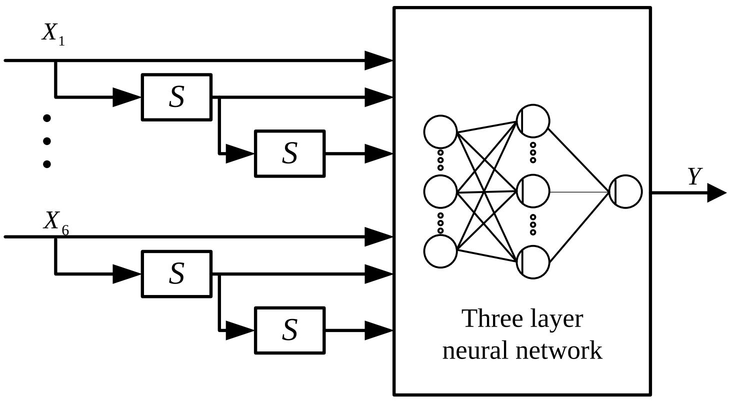

Figure 3: Dynamic neural network soft sensing model composed of a three-layer feedforward neural network and differentiators S

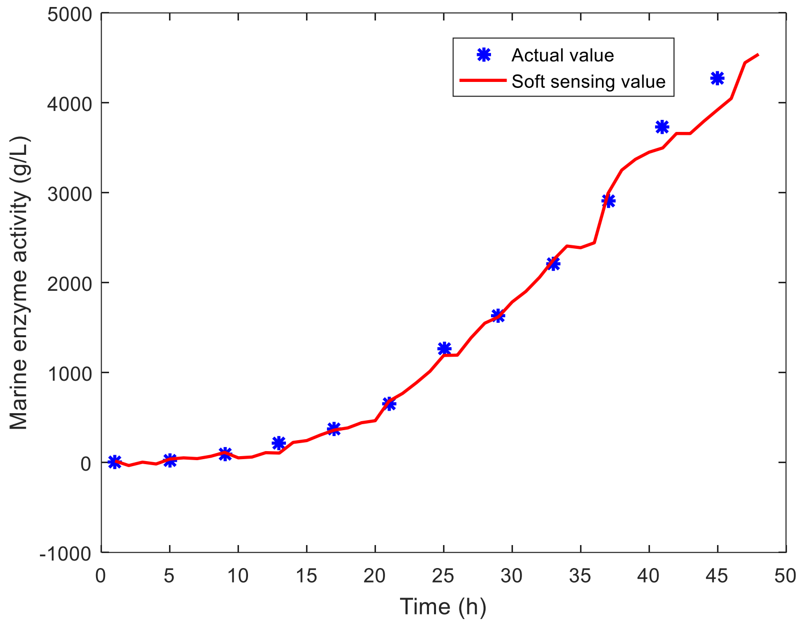

Figure 4: Soft sensing result obtained by dynamic NN model

5. Conclusions

Soft sensing method is an effective way to realize the real-time estimation of crucial process variables during the marine enzyme fermentation process. Static NN is one of the important soft sensing methods. This kind of NN model can give relatively good result when the marine enzyme fermentation process is relatively steady while the soft sensing result deteriorates when large changes occur. To solve this problem, a dynamic NN soft sensing model is proposed, which is composed a multilayer feedforward NN to approximate the nonlinear relationship between the input variables and output variable of the enzyme fermentation process, and a series of differentiators to represent the dynamic character. As the derivatives can be obtained by the differentiators, the dynamic information will be reflected in the model, so as to make the soft sensing result more accurate. The experimental results show that the dynamic NN model can not only reduce the RMSE but also the MRE and make it suitable to be used in the feedback control.

This method provides an effective way to solve the measurement problem of the complex systems with directly immeasurable variables, and makes these systems possible to be controlled and optimized. To fulfil this mission, some further work should be done. As mentioned in the introduction, the fourth part of soft sensing technology is online correction, which is very important for the long-time application. Since fermentation system changes more or less as time goes by, the accuracy of soft sensing model gets worse if it cannot reflect these changes. Online correction is such a technology that can follow the system change. It adjusts the inner structure or parameters of the NN model by sample new data and train the model with them. By this means, the NN soft sensing model can work more stably and correctly in a long period, and is more suitable to be used in the close loop control.

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