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Soft-Sensing Modeling Method of Vinyl Acetate Polymerization Rate

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Abstract

In the procedure of polyvinyl alcohol production, it is hardly accurate measuring the Vinyl Acetate (VAC) polymerization rate. To solve this awkward situation, this paper adopt Genetic Algorithm-Back Propagation (GA-BP) Neural Network to fit the nonlinear relation of the variables which derives from the production process by setting the VAC polymerization rate as the master variable and the initiator addition ratio, methanol ratio, polymerization temperature and VAC activity degree as auxiliary variables. Establish VAC polymerization rate soft-sensing model based on GA-BP network which the connection weights optimized by genetic algorithm. The comparison results with BP network based on the actual measured data show that the model this paper constructed is accurate and effective.

Keywords*: VAC polymerization rate; soft-sensing; GA-BP neural network; Genetic Algorithm*

1. Introduction

Vinyl Acetate (VAC) polymerization rate represents the level of VAC polymerization, it is the main measure of VAC polymerization and key parameter of the polymeric product and ramification. Therefore, realize VAC polymerization rate real-time online measurement and monitoring and then the whole production process optimally is a critical technique. But now no effective online measurements for VAC polymerization rate in China and hardly adjust control strategy in time, a soft-sensing model is needed for predicting.

In the study of VAC polymerization rate soft-sensing, with limited samples and high demand of generalization ability, it requests the system model high accuracy and prediction ability. Literature [1] adopted the RBF neural network based on k-means clustering algorithm to soft- sensing of vinyl acetate polymerization rate and obtained ideal results, but trial and error is not the best method to determine the number of the center points and makes it difficultly to model while high accuracy requirements for sample data. Literature [2] proposed a method to establish vinyl acetate polymerization rate soft-sensing model based on BP Neural Network. Although BP neural network has better accuracy to approximate non-linear function and fault tolerance, it is easy to entrap local minimum with weak generalization ability. Genetic Algorithm (GA) [3]~[6], which has high computational efficiency, is a parallel and global optimization method. This paper establishes an optimization model by combing GA and BP algorithm to obtain the optimal weights and threshold value, and simulation results prove that the inference is reasonable.

2. Establishing Soft-sensing Model

2.1. Selecting the Auxiliary Variables

VAC polymerization rate is affected by many factors, mainly include initiator addition rate, methanol ratio, polymerization time, polymerization temperature, raw materials (including essential VAC, polymeric methanol, initiator, recycled VAC, reuse liquid, etc) quality, the oxygen content of polymerization system and so on. In terms of the mechanism of Polyvinyl alcohol (PVA) polymerization reaction, monitoring data of production process, the principle of auxiliary variable selecting and consulting technician, set the initiator addition rate X1, methanol ratio X2, polymerization temperature X3, VAC activity degree X4 (main reflection of the VAC's quality) as

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the auxiliary variables and the soft-sensing model of VAC polymerization rate descript as follows:

$$y = f\{X_1, X_2, X_3, X_4, \omega\}. \tag{1}$$

Here, ω is the variable affects the polymerization rate, f{.} is the complex multi-variable non-linear function between input and output.

2.2. Data Preprocessing

In data preprocessing, if only use the original measurement data for network training, it may lead to information lost and instability of numerical calculation, which causes by the non-uniform of measurement data in engineering unit and order of magnitude. We adopt normalization method to normalize input data and target data and limit the data of network input in interval [0,1] in this paper. The data normalized transformation can be expressed by:

$$\overline{X_i} = \frac{X_i - X_{i\min}}{X_{i\max} - X_{i\min}}. \tag{2}$$

Here X_i is the untreated input (or target) value, $\overline{X_i}$ is the normalized value, $X_{i\min}$ and $X_{i\max}$ are the minimum and maximum of the input (or target) value, respectively.

2.3. Soft-sensing Model of VAC Polymerization Rate based on GA-BP Neural Network

BP neural network has better accuracy to approximate non-linear function and fault tolerance, can easy fit of a continuous function in any closed interval by using monolayer BP network and a three layer BP network can map from arbitrary n dimensional to m dimensional [7]. However, BP algorithm can convergence network weights to a final solution, but it is easy to entrap local minimum and cannot guarantee the final solution is the global optimal solution of the whole error set. Meanwhile, the training procedure entrap local minimum and hardly achieve rated accuracy.

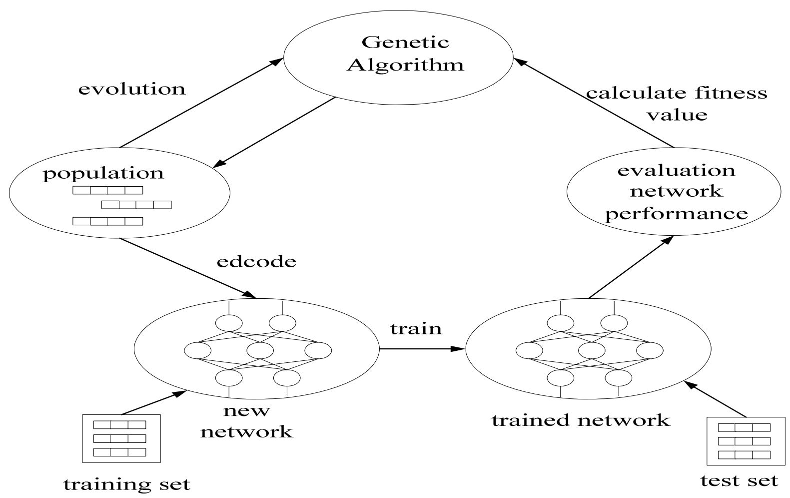

Figure 1. Genetic Algorithm Optimize BP Neural Network

Genetic Algorithm is a nontraditional optimization routine that uses the principles of natural selection and genetics, which has been successfully applied in various fields [8]. It can fast converge to optimal solution but can't accurately determine the position. If combined BP neural network with Genetic Algorithm and establish genetic neural network (GA-BP neural network), use GA algorithm to optimize the BP neural network initial weights and threshold value and converge the search space, then utilize BP algorithm for optimal solution, it can fully realize complementary of the two. With the previous method, we can obtain accurate soft-sensing model of VAC polymerization rate. In this model, set the initial weights and threshold value as the code and initialize population size, select a fitness function and change the individuals with selection, crossover and mutation. Finally, we obtain the optimal individual and decode it for the weights and threshold value of GA-BP network. The procedure of code and decode shows as Figure 1.

In the study of BP network topology, it is vital to confirm the cell number in hidden layer which influences the mapping relationship of different dimensions in BP network, and if only with three layers, BP network can achieve map arbitrary n dimension to m dimension. This paper adopts Kolmogrov theorem [3] to confirm neural network the layers of neural network, that is when the input is n, then the hidden layer is 2n+1.

Set the initiator addition rate, methanol ratio, polymerization temperature, VAC activity degree as the auxiliary variables and VAC polymerization rate as the output variable, and then construct soft-sensing model of VAC polymerization rate. The model shows as Figure 2.

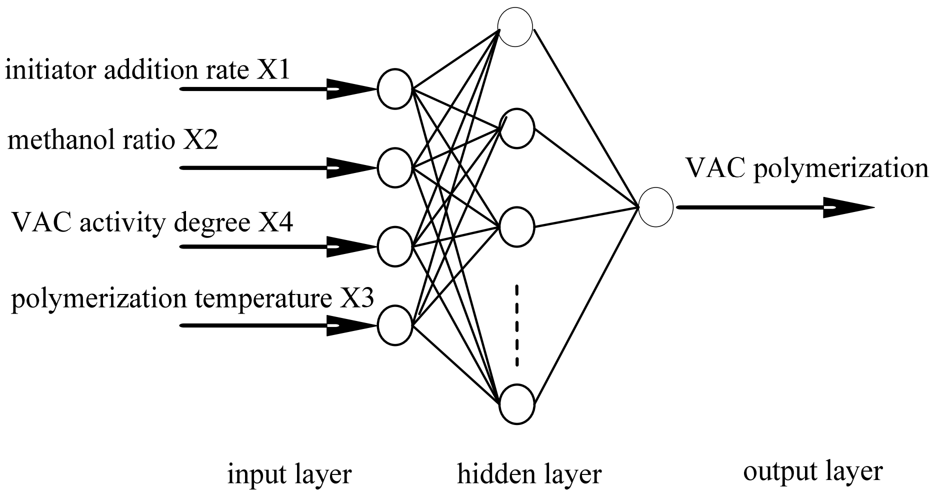

Figure 2. GA-BP Network Topology VAC Polymerization Rate

2.4. Genetic Coding

For coding the initial weights and threshold value of GA-BP network, it is easy to think that take the BP network weights and threshold value coding for binary string. This kind of coding scheme, the operation is simple and easy to implement, but still have some problems in it. In order to avoiding the disadvantages of binary code with slow evolution speed and unable to find the optimal solution, this paper directly code the weights and threshold value by mapping them to a real number respectively, and then form the set of chromosome [8]. Set W_1 as the connection weight matrix of input layer to hidden layer and W_2 as that of hidden layer to output layer. b_1 and b_2 are the threshold value of hidden layer and output layer. Then the four numerical value W_1, W_2, b_1 and b_2 unite and consist of the coded chromosome. The length of one chromosome is

$$S = R*S1 + S1*S2 + S1 + S2. \quad (3)$$

Here, R is the dimension of input matrix, S_1 and S_2 is the neuron number of hidden and output layer respectively.

2.5. Fitness Function

In the study of BP neural network, usually set its performance parameters as the mean square error (mse) emerged in the procedure of network training. Thus, many researchers assumed $f = 1/mse$ as the fitness evaluation function. The larger fitness value is, the more accuracy network. However, it is inconvenience to analyse the simulation results for the mean square error usually small and $f \to \infty$. An optimization method which can avoid this is proposed in equation (4), it replaces the mean square error with square sum of error and obtain a better fitness function.

$$f = \frac{1}{1 + MSE}. \quad (4)$$

2.6. Population Initialization

In the procedure of Genetic Algorithm, it is vital to set population size and iterations when initialize population [9]. Population size disturbs the results and efficiency of genetic algorithm. It is fast but less diversity and maybe not find the optimal solution with small population size, however, it will calculation slowly when the population size is large. So suitable population size is necessary and the conventional size is 20 to 100.

The same situation is also appeared in the setting of iterations, although genetic algorithm can search more optimal solution of high fitness continuously, but in the later period, when genetic algorithm searching near the optimal solution, the population average fitness close to individual best fitness, genetic process actually stagnated. So the conventional iterations can obtain according to the method of setting population size.

2.7. Genetic Operation

Genetic operation is a procedure which can obtain the fittest by sorting the fitness value and then select the optimal one. It can generational optimize the solution and approach the global optimal solution. It contains three genetic operators: selection, crossover and mutation.

Selecting operator is the genetic operation that can obtain the optimal fitness value and eliminate the inferiors from population. The rate of fitness values, which the probability of the selected individual is proportional to the fitness values of the population, usually use to select the genetic operator and the equation is

$$P(i) = \frac{f(i)}{\sum_{i=1}^{m} f(i)}. \quad (5)$$

Here m is the population size and $f(i)$ is the fitness value of i th individual. With the principle of selecting genetic operator, guaranteed the genetic algorithm with the diversity of individuals and easy for the subsequent genetic operation.

If only genetic algorithm does selecting operation, the offspring population will never surpass the initial population, let alone obtain optimal one. These make it of great importance of crossover operator and mutation operator in the procedure of genetic operation. Crossover operator, which can obtain new individual by exchanging the two genes that selected for reproduction with same position, is similar to the recombination of biological genetic chromosome, it is the main operation to obtain new individual and the suitable value space is 0.4~0.99. Mutation operation which is the mutation operator is also an influence aspect in generating new individual by disturb the position value of genes on chromosome with a small mutation rate and its usual value is 0.0001 to 0.1 [10].

The procedure of establishing soft-sensing model of VAC polymerization rate based on GA - BP network can summarize as follows:

(1) Select the auxiliary variables and preprocess the data.
(2) Determine the topological structure of BP neural network.
(3) Code BP neural network initial weights and threshold value by using the method of real

number code, randomize population size.
(4) Input training sample, calculate the error function value and evaluate the quality of individuals according to the fitness value sorted by the reciprocal of error square sum. Instead of small error, the fitness value is optimal, and vice versa.
(5) Select the optimal fitness as global optimization individual and parent population of the next generation.
(6) Adopt crossover and mutation operation to evolve current population and generate next population. Update the weights and threshold value of BP neural network with genetic operation.
(7) Loop to (4) until a criterion is met, which is the maximum number of iterations.
(8) Decode the global optimal individual and obtain weights and threshold value of BP neural network.

3. Simulations

In this paper, select 174 sets of sample data collected from the production of polyvinyl alcohol, and 120 sets as training sample for completing the training of soft-sensing model of VAC polymerization rate, others as testing sample for soft-sensing model.

To prove the effectiveness and feasibility of the proposed GA-BP network, we use simulations to compare the performance of the GA-BP network with the BP network. Simulations carry out with MATLAB and its toolbox GAOT. The parameters of GA algorithm are as follows: the maximum number of iterations $T_{\max}=200$; the number of population size $N=100$; mutation probability $P_m=0.2$.

The curve of fitness changing shows as Figure 3, it compares global optimal fitness value with the average value. And different optimization results of soft-sensing model of VAC polymerization rate based on GA-BP and BP network shows as Figure 4.

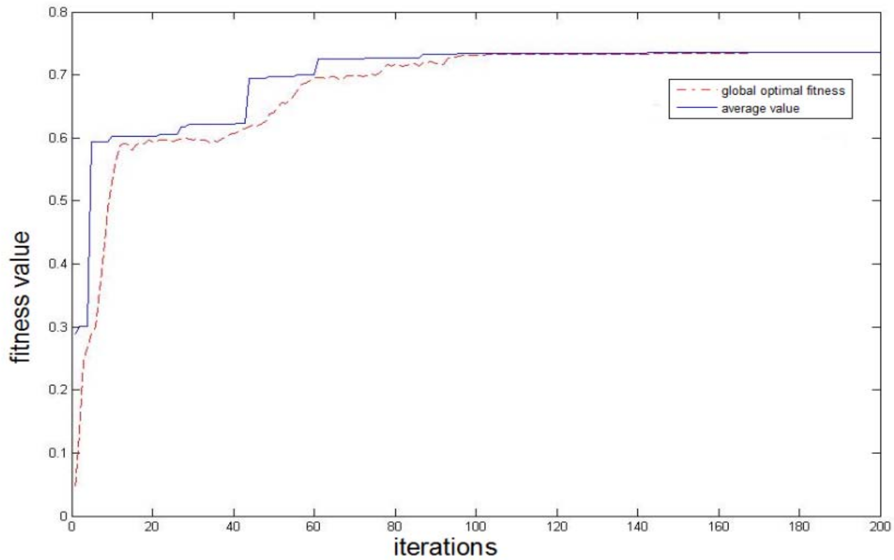

Figure 3. Curves of Fitness Changing

In Figure 3, the global optimal fitness value is superior to the average value and proves that the GA-BP algorithm is effective in searching the optimal individual. From the compared results in Figure 4, the relative error the GA-BP network obtained is stable in interval [-0.04, 0.04] and no abnormal fluctuations, while in BP network, the relative error changes violently and fluctuates greatly. The distribution of relative error the proposed method obtained is obviously better than that of BP network. It can help us realize the effectiveness of the sample data to obtain the VAC polymerization rate while with smaller relative error but higher accuracy.

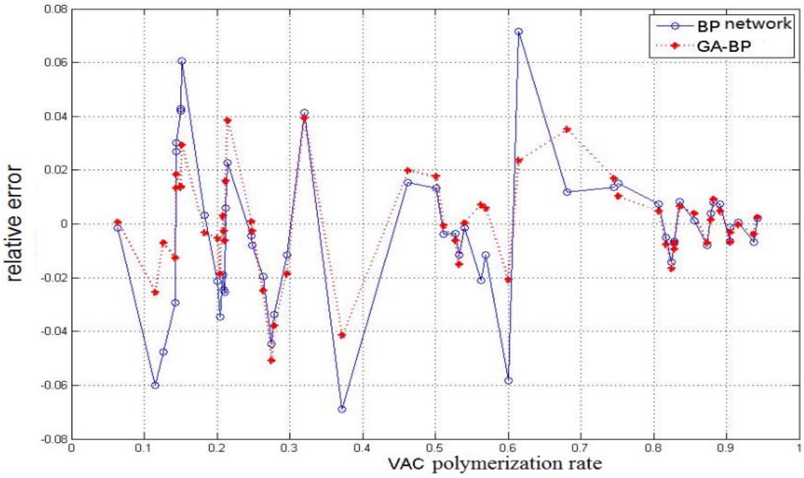

Figure 4. Relative Error of GA-BP Network and BP Network

4. Conclusion

In terms of the theoretical analysis and simulation results above, it proves that the GA-BP neural network owns the advantages combined genetic algorithm with BP neural network. It has high precision for network training. This new type of hybrid intelligence system is the essence of evolutionary computation and intelligent control technology, and modeling soft-sensing of VAC polymerization rate based on GA-BP neural network is feasible.

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