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Research Article

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Innovation capability prediction on complex pharmaceutical product based on algorithm compiled RBFNN with simulated annealing arithmetic

Chen Xu Sheng, Wang Xin and Wang Hong Qi

School of Management, Harbin University of Science and Technology, Harbin, Heilongjiang Province, China

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ABSTRACT

A new neural network in the field of innovation capability prediction arithmetic on complex pharmaceutical product based on RBFNN and simulated annealing arithmetic is discussed in detail. Radial basis function neural network (RBFNN) has been designed, and simulated annealing arithmetic is adopted in adjusting the network weights. MATLAB program is compiled here, innovation capability prediction analysis on 29 listed pharmaceutical companies have been done employing the algorithm. The experiments have shown that the arithmetic can efficiently approach the precision with 10^{-4} error, also the learning speed is quick and analysis results are ideal. Experiments have been done with other kind networks in comparison. Back-propagation (BP) learning algorithm network does not converge until 3500 iterative procedure, and exactness design RBFNN is time-consuming and has big error. The arithmetic based on RBFNN and simulated annealing arithmetic can keep the network away from the partial minimum.

Keywords: Innovation capability prediction, complex pharmaceutical product, Radial basis function neural network, simulated annealing arithmetic, Back-propagation learning algorithm network, Exactness design radial basis function neural network

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INTRODUCTION

Innovation of complex pharmaceutical product is the extension and expansion of the creative activity in enterprises; it includes the links of scale to new technology, unique service in the industry and a new enterprise business model etc [1]. Since innovation process is the result of interaction between enterprises, therefore, the collaboration between enterprises, the government regulation level, the financial environment and the active level of cooperation education of enterprise, university and scientific research organization (CEEUSRO) in the innovation process will have a certain influence on the innovative results. The innovation process shows different characteristics due to the impact of technological innovation, market demand and different drivers of the interaction between technology and market [2].

The formation of technology cooperation of the innovative division [3], shortening of industrialized time as well as achieving spread of common technology are the basis used to guarantee product quality and diversity in the process of complex product innovation [4]. The practice of manufacturing industry in recent years has shown that the penetration of information technology in different sections of research [5-7] and development (R&D) promoting the resources integration during the process of technology innovation [8]. The successful experience of the machinery industry in Germany has shown that parallel technology for development of complex products can improve innovation efficiency [9]. Besides, green manufacturing has become the basic requirements in equally important to improve product quality [10].

The exchanges and cooperation of the products, personnel and process of R&D between the enterprises, and the high profits generated by the innovative products have led to the spread of technology and management experience. Regarding to outsourcing production and knowledge management of business alliance, Gunasekaran has proposed

classification schemes of the knowledge management in manufacturing [11]. According to the empirical study of Science and Technology Park, Chien has built a nonlinear model for technological substitution and product decision [12]. For advanced manufacturing technology, the empirical results by Hottenstein have indicated that external consultants are the key factor to promote technology diffusion [13].

With the complex product innovation caused by central enterprises, development of industry will face the development obstacles such as unified technical standards, the formation of industrial labor division in the process of the industry growth, and the central enterprise itself is often with limited ability [14]. For developing countries, as the impact of the government makes regulation, implementing financial support and government procurement through industrial policy on product innovation is more evident [15]. In addition, the companies can take advantages of external resources through the contact with R&D institution, universities and intermediary organization, of which, the vertical cooperation is more favorable to the development of small and middle enterprises (SME) [16].

Capability of innovation of complex product in China is insufficient, this paper tries to give a prediction of innovation efficiency of complex pharmaceutical product and distinguish importance of different factor in process of innovations.

In the paper, a new arithmetic which RBFNN based on simulated annealing arithmetic is proposed. RBFNN is superiority to BP neural network on the aspect of approximating capability, classify capability and learning speed. Simultaneously, simulated annealing arithmetic has characteristic of global optimization which keep the network from getting into local minimum consequently.

EXPERIMENTAL SECTION

The radial basis function neural network is a kind of feed-forward three layers network. The general structure of the RBFNN is composed of input layer, hidden layer and output layer. Radial basis function adopts Gauss function which is defined as [17]

$$\boldsymbol{u}_j(\boldsymbol{X}) = \exp\left[-\frac{(\boldsymbol{X}-\boldsymbol{C}_j)^T(\boldsymbol{X}-\boldsymbol{C}_j)}{2\boldsymbol{\sigma}_j^2}\right] \quad \boldsymbol{j}=1,2,\cdots,\boldsymbol{N}_h \tag{1}$$

Where $\boldsymbol{u}_j(\boldsymbol{X})$ is output of the *j*th hidden node, $\boldsymbol{X}=(\boldsymbol{x}_1,\boldsymbol{x}_2,\cdots,\boldsymbol{x}_n)^T$ are input samples, $\boldsymbol{C}_j$ is center of Gauss function, $\boldsymbol{\sigma}_j$ is known as width parameter which control the radial effect scope of radial function and $\boldsymbol{N}_h$ represents number of hidden nodes.

The output of RBFNN is defined as [18]

$$\boldsymbol{y}_i(\boldsymbol{X}) = \sum_{j=1}^{N_h} \boldsymbol{w}_{ij}\boldsymbol{u}_j - \boldsymbol{\theta} = \boldsymbol{W}_i^T\boldsymbol{U} \qquad \boldsymbol{i}=1,2,\cdots,\boldsymbol{m} \tag{2}$$

Where W_i is the weights vector from hidden to output layer $W_i=(w_{i1},w_{i2},\cdots,w_{iN_h},-\theta)^T$, U denotes the output of hidden layer $U=(u_1,u_2,\cdots,u_{N_h},1)^T$ and θ is threshold vector.

To choose available radial basis function is important for neural network learning method in simulation. Here non-supervise learning method is adopted; hidden node center $\boldsymbol{C}_j$ and width $\boldsymbol{\sigma}_j$ are ascertained also. Among numerous clustering algorithms, seeking for center and width parameters, K-means algorithm is the most simple and effective method which is an unsupervised clustering method [19].

Simulated annealing (SA) is employed to adjust the weights in paper. Simulated annealing (SA) is a straightforward global optimization method used for combinatorial problems typically. This method was originated from the physical phenomenon of cooling metals where atoms move from a random state to a maximally organized state. The main parameter is the cooling schedule, which including an initial temperature, reducing temperature, controlling the duration at a given temperature and a terminal criterion. Solutions are altered via a move operator which usually transforms a solution to a neighboring one randomly.

The flow chart of RBFNN based on simulated annealing arithmetic is shown in Fig.1.

MATLAB program is compiled for the arithmetic in paper. Adjusting weight stage is described as follows:

① Initializing the original high temperature T, weights and threshold vector. Specify the initial weight values as system optimization solution W*. Specify sum squared error MSE which is obtained from the first network training as the minimum value MSE*. Specify network training target value ε and learning rate α, β for α>1，β>1 and α≠β. Choose suitable convergence criterion m, n and their maximal value M and N. Choose available temperature dropping strategy and step length accordingly.

②Sum squared error should be minimum value, target function is defined as

$$J = \frac{1}{N}\sum_{k=1}^{N}[\hat{y}(x_k) - y(x_k)]^2 \tag{3}$$

Where x_k are the input vectors. $\hat{y}(x_k)$ are the practical output vectors and $y(x_k)$ are the predicting output vectors of network. N is the samples number. Adjusting weights vector target is to make J approximately equal to ε.

③Dropping temperature by half step within a temperature range under original high temperature T. Adapting the weights according to $w' = w + \alpha\Delta w$, computing $\Delta J = J(w') - J(w)$, where Δw is a random increment. Here w is the former weight value and w' is the current weight value.

④Judging J, if $J < \varepsilon$, go to ⑨.

⑤Judging ΔJ, $\Delta J < 0$ means that error is reducing and training is successful. Specify w' in current training as W*and specify MSE as MSE*, set m=0.

⑥If $\Delta J \geq 0$, decide whether to specify w' in current training as W* according to probability function, where the probability function is given by

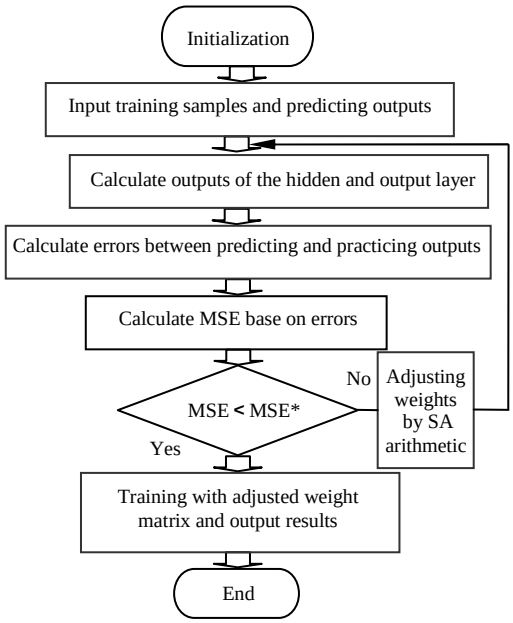
$$p = \exp(-\frac{\Delta J}{T_i}) \tag{4}$$

Where T_i is the current temperature value.

If w' is accepted to be W*, then weights $w' = w + \alpha\Delta w$, otherwise weights $w' = w - \beta\Delta w$. Set m=m+1.

⑦When m>M, if MSE is no longer reduced in training, then goes to ⑧, otherwise continue.

⑧Annealing: set T=λT, where λ is step length coefficient value in temperature dropping strategy. In the paper, λ=0.9. Repeat procedures from ③ to ⑥, if W* is reduced, n=0. Otherwise, n=n+1. When n>N, if MSE is no longer reduced, go to⑨. Otherwise, specify w' in current training as W*and specify MSE as MSE*, then continue.



⑨Export current W* and MSE*, stop.

Fig.1 Flow chart of RBFNN based on simulated annealing arithmetic

RESULTS AND DISCUSSION

RBFNN is established. It is a three layers neural network with five inputs and four outputs. Simulated annealing arithmetic methodology is used here to adjuste weights in network.

Input index is expressed as follow: input intensity of innovation fund in enterprise (X_1); input intensity of innovative

personnel in enterprise (X_2); ability of knowledge diffusion and absorption (X_3), financing environment of innovation (X_4), Innovation environment of science and technology (X_5).Output indicators include the level of industrial core technology (Y_1), intensity of technology innovation (Y_2), market quantity of new complex pharmaceutical product (Y_3), intensity of market development of complex pharmaceutical product (Y_4). The formulas are expressed as followed.

X_1= (experimental development on R&D + labor cost on R&D + equipment expenditure on R&D)/ gross enterprises output value;
X_2=researchers of full-time equivalent on R&D/ employed persons at the year-end of enterprises;
X_3=number of enterprises having R&D institutions / employed persons at the year-end of enterprises;
X_4=government funds on R&D + foreign funds on R&D + other funds on R&D (unit: ten thousand Yuan);
X_5=ratio of fund on R&D Projects of R&D Institutions by pharmaceutical enterprises;
Y_1= patent in force of R&D institutions in which the R&D institutions served + patent in force of pharmaceutical enterprises (piece);
Y_2= (invention patents of R&D institutions + invention patents of pharmaceutical enterprises)/ (patent application of R&D institutions + patent application of pharmaceutical enterprises);
Y_3= revenue from new complex pharmaceutical product (unit: ten thousand Yuan);
Y_4= revenue from new complex pharmaceutical product /revenue from principal business.
For the enterprises of complex pharmaceutical product, the research of the determinants of their innovation capability is conducted, based on the selected data of 29 listed companies in China. Research samples are listed in Tab 1.

Tab 1: Samples of pharmaceutical enterprises in China

No.	samples	No.	samples
1.	Zhejiang Medicine Co., Ltd.	16.	Renhe Pharmacy Co., Ltd.
2.	Zhejiang NHU Co., Ltd.	17.	Livzon Pharmaceutical Group Inc.
3.	Northeast Pharmaceutical Group Co., Ltd.	18.	Jiangsu Nhwa Pharmaceutical Co., Ltd.
4.	Zhejiang Hisun Pharmaceutical Co., Ltd.	19.	Wuhan National Pharmaceutical Technology Co., Ltd.
5.	North China Pharmaceutical Co., Ltd.	20.	Humanwell Healthcare (Group) Co., Ltd.
6.	Shanghai Fosun Pharmaceutical (Group) Co., Ltd.	21.	Shanghai Modern Pharmaceutical Co., Ltd.
7.	Joincare Pharmaceutical Group Industry Co., Ltd.	22.	Shenzhen Neptunus Bioengineering Co., Ltd.
8.	Harbin Pharmaceutical Group Co., Ltd.	23.	Harbin Pharm. Group Sanjing Pharmaceutical Shareholding Co., Ltd.
9.	Beijing Beilu Pharmaceutical Co., Ltd.	24.	Anhui Fengyuan Pharmaceutical Co., Ltd.
10.	Tianjin Chasesun Pharmaceutical Co., Ltd.	25.	Hualan Biological Engineering, Inc.
11.	Jiangsu Hengrui Medicine Co., Ltd.	26.	Beijing SL Pharmaceutical Co., Ltd.
12.	Shenzhen Salubris Pharmaceuticals Co., Ltd.	27.	Beijing Tiantan Biological Products Corporation Limited
13.	Chongqing Lummy Pharmaceutical Co., Ltd.	28.	Changchun High and New Technology Industry (Group) Inc.
14.	China Resources Sanjiu Medical and Pharmaceutical Co., Ltd.	29.	Shanghai Kehua Bioengineering Co., Ltd.
15.	China Meheco Co., Ltd.		

Expect innovation capability training results of pharmaceutical enterprises samples are listed in Tab 2.

Tab 2: Expect innovation capability training results of pharmaceutical enterprises samples

No.	1	2	3	4	5	6	7	8
Scores	47.3010	61.4008	27.1005	89.2002	62.5012	20.2013	0.0005	10.9015
No.	9	10	11	12	13	14	15	16
Scores	36.8003	19.1007	49.2008	45.7009	90.5011	6.8010	17.2000	16.9013
No.	17	18	19	20	21	22	23	24
Scores	17.5007	26.2006	0.0002	40.0004	23.8005	10.9009	0.2022	31.9018
No.	25	26	27	28	29			
Scores	10.9019	100.0002	27.6023	17.7019	0.0018			

Actual output innovation capability training results of pharmaceutical enterprises samples are listed in Tab 3.

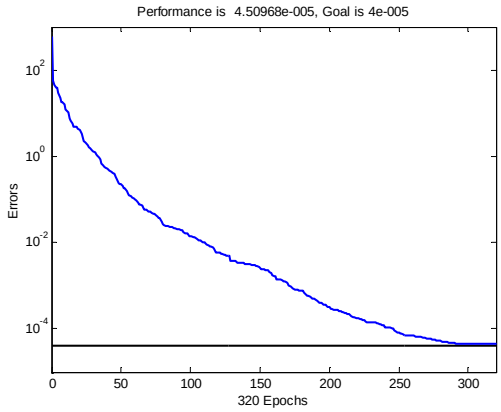
Tab 3: Actual output innovation capability training results of pharmaceutical enterprises samples

No.	1	2	3	4	5	6	7	8
Scores	47.3008	61.4005	27.1009	89.2006	62.5009	20.2015	0.0007	10.9012
No.	9	10	11	12	13	14	15	16
Scores	36.8007	19.1004	49.2005	45.7003	90.5008	6.8012	17.2001	16.9016
No.	17	18	19	20	21	22	23	24
Scores	17.5009	26.2008	0.0005	40.0006	23.8008	10.9011	0.202	31.9015
No.	25	26	27	28	29			
Scores	10.9016	100.0003	27.6012	17.7011	0.0027			

Employing the arithmetic and convergent RBF neural network based on simulated annealing algorithm to analysis innovation capability prediction on complex pharmaceutical product.

When RBF neural network based on simulated annealing algorithm has been convergent, input the total vectors, efficiency output value.
Here, ε is given by 10^{-4}, spread constant is specified as 0.668, the number of neurons identified as 255. Training analysis curve is shown in Fig.2, the network converges after iterating 320 times. It means that network learning speed is high. Error surface of output data is shown in Fig.3, we can see that errors are between -9×10^{-4}~9×10^{-4}, errors are very little.

Trainings have been done using other kinds of networks in comparison. Exactness design of radial basis function neural network, the network parameters is set as follows: network expansion constant is 1, neuron numbers are 25 and below, network training objectives (squares and error parameter) is 0, the errors are 10^{-4} orders of magnitude. Training analysis curve of exactness design RBFNN is Fig.4. If number of input data is large, neurons number is hugeness and training time is long. BP network does not converge until 3500 iterative procedures. Training analysis curve of BP network is Fig.5.



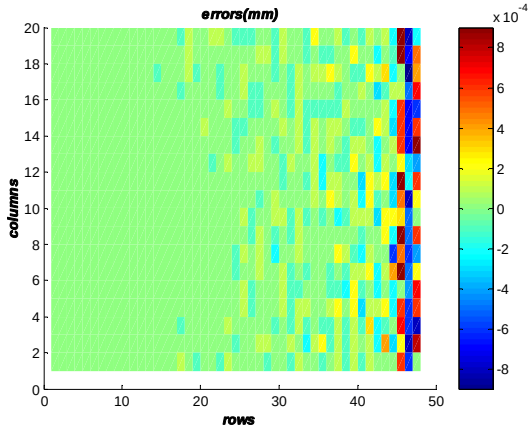
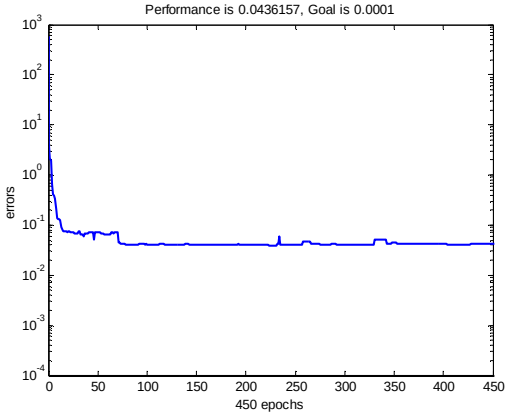


Fig.2 Training analysis curve of RBFNN based on simulated annealing algorithm **Fig.3 Error surface of output data**

Conclusion can be drawn that method proposed in this paper is preponderant.

BP learning algorithm and exactness design RBFNN neural network were employed in simulations here. BP network does not converge until 3500 iterative procedures. The exactness design RBFNN consumes exceeding 30 minutes when input data approaching 1200, at the same time RBFNN proposed in the paper consumes 214 seconds only.



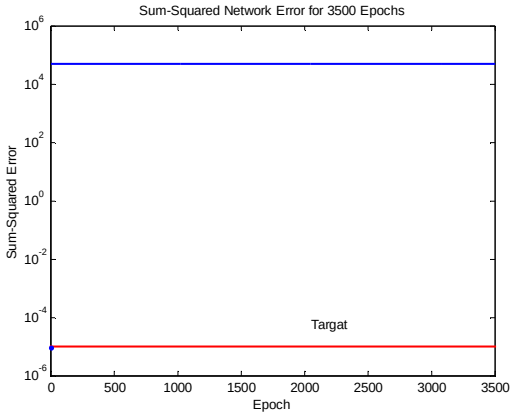


Fig.4 Training analysis curve of exactness design RBFNN **Fig.5 Training analysis curve of BP network**

CONCLUSION

A new neural network in the field of innovation capability prediction arithmetic on complex pharmaceutical product

based on RBFNN and simulated annealing arithmetic has been discussed in detail. Simulation in this research can lead to the following conclusions: The simulation results verify the method in paper is successful. Simulation shows that capability of the neural network in the paper is superior to BP learning algorithm and exactness design RBF neural network using same parameters.

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