

Prediction of coal ash fusion temperature using constructive-pruning hybrid method for RBF networks

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Abstract: A constructive-pruning hybrid method (CPHM) for radial basis function (RBF) networks is proposed to improve the prediction accuracy of ash fusion temperatures (AFT). The CPHM incorporates the advantages of the construction algorithm and the pruning algorithm of neural networks, and the training process of the CPHM is divided into two stages: rough tuning and fine tuning. In rough tuning, new hidden units are added to the current network until some performance index is satisfied. In fine tuning, the network structure and the model parameters are further adjusted. And, based on components of coal ash, a model using the CPHM is established to predict the AFT. The results show that the CPHM prediction model is characterized by its high precision, compact network structure, as well as strong generalization ability and robustness.

Key words: radial basis function (RBF) networks; function approximation; ash fusion temperature

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The AFT of coal directly relates to the thermal efficiency of steam boilers in coal-fired power stations^[1]. Romero et al.^[2-4] reported the fusibility of the ash as a function of the content of the eight principal oxides frequently found in coal ash, i. e., SiO₂, Al₂O₃, Fe₂O₃, CaO, MgO, TiO₂, K₂O and Na₂O. And until now, many relational expressions about the AFT have been developed with a number of parameters which involve one or more chemical constituents of the coal ash. The regression formula is one of the widely used methods while there are less mature schemes. However, in many cases, more optimal results are obtained by neural networks^[5].

Amoudi et al.^[6-7] reported comparisons of back propagation (BP) and RBF neural networks and proved that RBF networks perform better than MLP networks using the BP algorithm in model building, prediction accuracy and network simplicity.

However, practical model performance of RBF networks heavily depends on the network structure. In general, minimal networks that satisfy training accuracy are preferred to ensure the generalization performance. In this paper, we propose a CPHM for designing RBF nets and apply it to establish a prediction model of the AFT. The CPHM com-

bines the advantages of ROLS^[8], RAN^[9], and regularization^[10], so the number and position of unit centers of the RBF net are both adapted in learning. The learning process of the CPHM can be divided into two stages: rough tuning and fine tuning. In rough tuning, hidden units are added to the current network using RAN until some performance index is met. In fine tuning, the fat of the network is pruned using regularization. In experiments, we show that RBF networks obtained with the CPHM not only generalize well, but also maintain satisfactory performance even when the training set is changed. And the prediction model of the AFT works well.

1 Structure Definition

Considering an RBF net with N inputs, M hidden units, one output, and Gaussian radial basis functions (see Fig 1), the overall input-output transfer function of the network can be defined as

$$f(\mathbf{x}) = \sum_{i=1}^M w_i \varphi_{c_i}(\mathbf{x}) + b \quad (1)$$

where $\mathbf{x} \in \mathbf{R}^n$ and $f(\mathbf{x}) \in \mathbf{R}$ are the input and output of the network, w_i denotes the weight from the i -th hidden unit to the output node, and b is the bias term. $\varphi_{c_i}(\mathbf{x}) = e^{-\|\mathbf{x}-\mathbf{c}_i\|/r_i}$ is the response of hidden units, where $\mathbf{c}_i \in \mathbf{R}^n$ is unit centers, r_i is the spread of the i -th radial basis function.

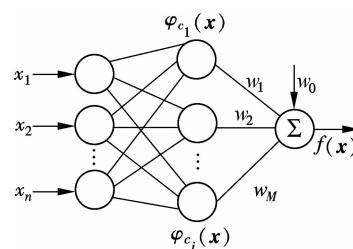


Fig. 1 Structure of RBF net

The N observations of the net are $T = \{(\mathbf{X}_i, y_i) \mid i = 1, 2, \dots, N\}$. We use $\mathbf{X} = [\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_N]$ to denote observation input matrix, and the teacher signal is $\mathbf{Y} = [y_1, y_2, \dots, y_N]^T$. Thus, the output of the RBF net is

$$f(\mathbf{X}) = \mathbf{P}_M \mathbf{W} + \mathbf{B} = \sum_{i=1}^M w_i \mathbf{p}_i + \mathbf{B} \quad (2)$$

where $\mathbf{W} = [w_1, w_2, \dots, w_M]^T$ is the output weight vector, $\mathbf{P}_M = [\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_M]$, $\mathbf{p}_i = [\varphi_{c_i}(\mathbf{X}_1), \varphi_{c_i}(\mathbf{X}_2), \dots, \varphi_{c_i}(\mathbf{X}_N)]^T$; and \mathbf{B} is the bias vector. Generally, there is a deviation \mathbf{e} between $f(\mathbf{X})$ and \mathbf{Y} ,

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$$Y = f(X) + e = P_M W + B + e = \bar{P}_M \bar{W} + e \quad (3)$$

where $\bar{P}_M = [p_1, p_2, \dots, p_M, \mathbf{1}_N]$, $\mathbf{1}_N$ is an N -dimensional column vector with all its elements equal to 1, and $\bar{W} = [w_1, w_2, \dots, w_M, b]^T$.

2 Constructive-Pruning Hybrid Method

The training process of the CPHM is divided into two stages: rough tuning and fine tuning. In rough tuning, we add new hidden units to the current network. In fine tuning, we further use regularization to adjust the network structure and model parameters including unit number, unit centers, and output weights.

2.1 Rough tuning

The crux of rough tuning is how to select a new hidden unit and when to terminate this process.

If the current RBF net with M hidden units cannot approximate the target function well, we add new hidden units to the RBF net. Consider adding one unit each time. Since we have no prior knowledge about the target function, we select the center of the new hidden unit among sample inputs, and then adjust it to an appropriate position.

From Eq. (3), if we consider Y as a vector with dimension N , then Y is a linear combination of p_i 's and $\mathbf{1}_N$. Then $\{p_1, p_2, \dots, p_M, \mathbf{1}_N\}$ forms a basis in an N -dimensional vector space.

The cost function with Gaussian regularization is

$$E = (Y - \bar{P}_M \bar{W})^T (Y - \bar{P}_M \bar{W}) + \lambda \bar{W}^T \bar{W} \quad (4)$$

where λ is the regular. Let $\partial E / \partial \bar{W} = 0$, we obtain the minimum value of Eq. (4),

$$E_M = Y^T [I_N - \bar{P}_M (\bar{P}_M^T \bar{P}_M + \lambda I_M)^{-1} \bar{P}_M^T] Y \quad (5)$$

Suppose that the newly selected unit center is X_i . Let $s_i = [\Phi_{c_i}(X_1), \Phi_{c_i}(X_2), \dots, \Phi_{c_i}(X_N)]^T$, $S = [s_1, s_2, \dots, s_N]$, and $\bar{P}_{M+1} = [\bar{P}_M \ s_i]$. Thus, we should select s_j that satisfies

$$E_{M+1}(s_j) = \min\{E_{M+1}(s_i), i = 1, 2, \dots, N\} \quad (6)$$

The first unit center is selected as the sample input X_i such that the relative s_j has the maximum projection on Y . That is

$$E_1(X_i) = \max\{Y^T s_j, j = 1, 2, \dots, N\} \quad (7)$$

As we know, the condition number of a matrix indicates its illness, so we can use the condition number of $\bar{P}_{M+1}^T \bar{P}_{M+1}$ to decide when to stop rough tuning. Concretely, when the following equation is satisfied, we stop rough tuning.

$$C(\bar{P}_{M+1}^T \bar{P}_{M+1}) > C_{\max} \quad (8)$$

where $C(A) = \|A\| \|A^{-1}\|$ is the condition number of matrix A , $\|A\|$ is the Frobenius distance. C_{\max} should be selected *a priori*. Empirically, it should not be greater than 10^6 , because most simulation software such as Matlab will give warning if C_{\max} is greater than 10^6 .

2.2 Fine tuning

Fine tuning includes the tuning of unit centers and the

output weights, and the pruning of redundant units.

Considering that the RBF net has a "local" property, we use those observations whose inputs are near the new unit center to tune its position. If c_i is the new unit center and r_i is its spread, then the teacher samples are

$$A_i = \{(X_j, y_j) \mid \|X_j - c_i\| < \kappa r_i \quad j = 1, 2, \dots, N\} \quad (9)$$

where κ denotes the overlap coefficient. The greater κ is, the more teacher samples are selected.

We use the least mean square algorithm to adjust the unit center, and then the modification to c_i is

$$\Delta c_i(X_j, y_j) = 4 \frac{\eta}{r_i} (X_j - c_i) \phi_{c_i}(X_j) (y_j - f(X_j)) w_i \quad (10)$$

where η is the learning rate.

Each time we adjust the unit centers, and we should also adjust the output weights and bias. In fact, when all the unit centers are fixed, we can obtain the optimal output weights by minimizing Eq. (4). So we obtain

$$[w_1, w_2, \dots, w_M, b]^T = \bar{W}_M \quad (11)$$

In the CPHM, the cost function has a pruning property, some redundant output weights may decay to zeros during fine tuning. Thus, the corresponding hidden units can be deleted. For convenience, if the output weight w_i meets the following condition the corresponding hidden unit can be pruned.

$$\text{abs}(w_i) < w_{\min} \quad (12)$$

where w_{\min} is the threshold weight. Besides, we use the rules proposed by Weigend^[11] to adjust λ by introducing the following errors and checking their relationships during learning.

3 Test of CPHM on Function Approximation Problem

Considering the approximation of the following polynomial function,

$$y(x) = \sin(3(x + 0.8)^2)$$

where $x \in \mathbf{R}$. The training set is generated as follows: The size is $N = 100$, with sample inputs x_i uniformly generated from $[1, 1]$ and sample outputs $y(x_i) + e_i$. Here e_i is a Gaussian noise with mean 0, variance 0.5.

Fig. 2(a) shows a typical training set, and Figs. 2(b), (c) and (d) show the results fitted by RAN, ROLS and CPHM, respectively. In Fig. 2, RAN generates 6 hidden units, with $\delta_{\max} = 1.6$, $\delta_{\min} = 0.3$, $\gamma = 0.977$, $\kappa = 0.87$, $\eta = 0.05$, and the learning epoch is 400; ROLS generates 25 hidden units, with parameters $\gamma = 0.2$ and $\lambda = 0.006$.

Comparatively, the CPHM generates 17 hidden units with the following parameters: $\gamma = 0.2$, $\kappa = 1$, $\lambda = 0.006$, $\Delta\lambda = 0.003$, $\mu = 0.95$, $\rho = 0.95$, $\eta = 10^{-4}$, $C_{\max} = 10^6$ and $w_{\min} = 0.1$. The target error is set to zero, and the learning epoch is 200.

Fig. 3 shows the history of training error, regular λ and the number of hidden units in the CPHM. In rough tuning,

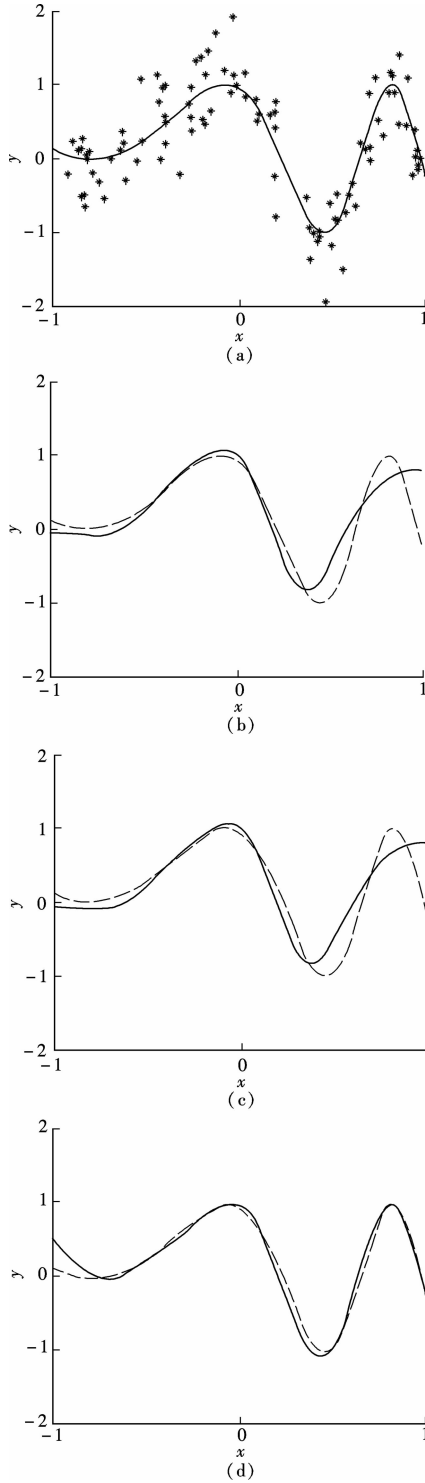


Fig. 2 Training set and fitting curves of RAN, ROLS, and CPHM. (a) Target function and one example of the training sets; (b) Fitted by RAN; (c) Fitted by ROLS; (d) Fitted by CPHM

training error decreases rapidly with the increase in hidden units. When the number of hidden units reaches 24, the network reaches its condition number threshold, and rough tuning stops, and fine tuning begins. During fine tuning, the training error fluctuates slightly, but the hidden unit number decreases as λ increases. At the 71th epoch, the hidden unit number is 18. After that, this number remains unchanged although λ increases. This indicates that the fine tuning is able to adjust weights and simplify the network without in-

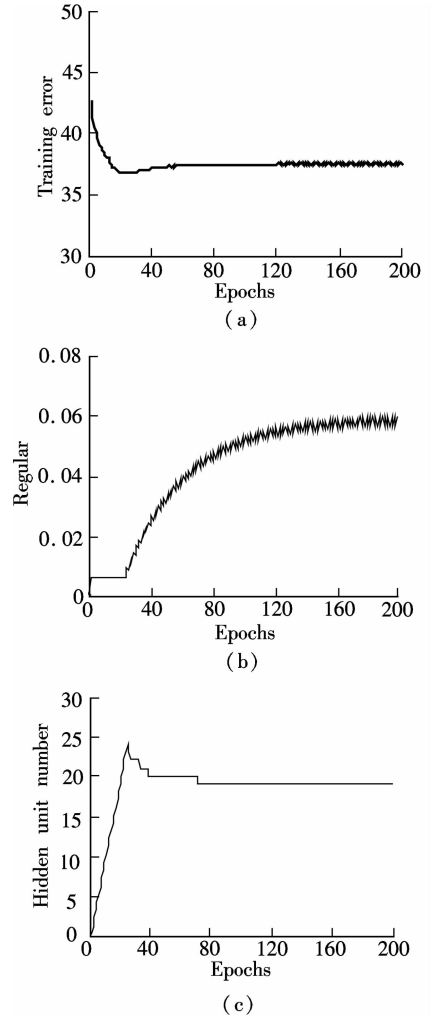


Fig. 3 History of training error, λ and number of hidden units. (a) Training error; (b) λ ; (c) Hidden unit number

creasing the training error.

To further compare the performance of the three methods, we give plots of data error vs. fitting error for 100 training

sets (see Fig. 4). Data error is defined as $\sqrt{\frac{1}{N} \sum_{i=1}^N e_i^2}$, and

fitting error is $\sqrt{\frac{1}{100} \sum_{i=1}^{100} (G(\tilde{x}_i) - f(\tilde{x}_i))^2}$, which can be denoted as a generalization error of the RBF net. In Fig. 4, each data set corresponds to a point, and each data error is near 0.5, which is the variance of the noise.

Tab. 1 shows major performance of the RBF nets obtained by three methods on 100 and 40 different data sets. All the parameters are well chosen to obtain optimal performance.

From Fig. 4 and Tab. 1, we can find that although networks obtained by RAN have the compact structure, they do

Tab. 1 Comparison of RBF nets obtained by three methods

Items	100 data sets			40 data sets	
	RAN	ROLS	CPHM	ROLS	CPHM
Averaged hidden units	8.35	21.6	16.1	27.5	18.6
Variance of hidden units	1.037	5.471	8.628	16.47	18.64
Averaged data error	0.496	0.499	0.501	0.496	0.489
Averaged fit error	0.265	0.172	0.157	0.327	0.231
Variance of fit error	0.008	0.001	0.001	0.016	0.003

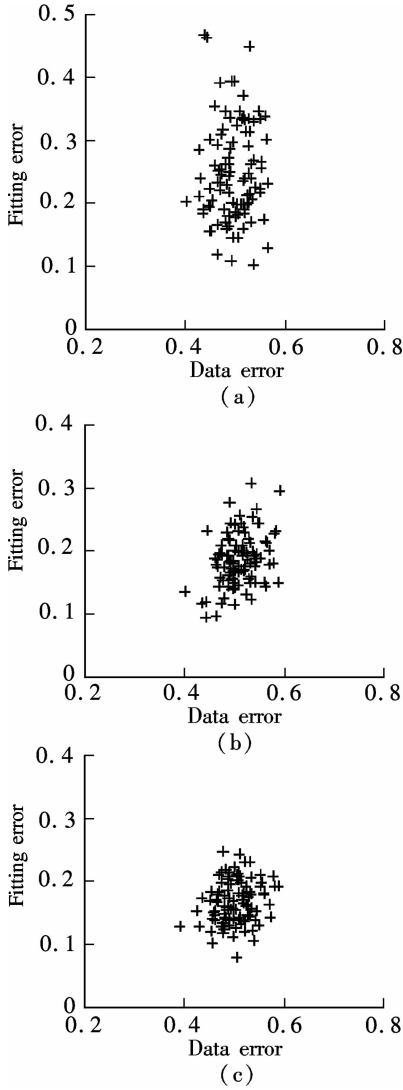


Fig. 4 Data-fitting error plot of three methods when using 100 training samples. (a) RAN; (b) ROLS; (c) CPHM

not generalize so well as networks obtained by the CPHM and ROLS. In our simulation with RAN, we try to decrease δ_{\min} and γ , but the results become worse with dramatically increased hidden units and fitting error. Comparatively, RBF nets designed with the CPHM have both compact structure and low testing error, indicating that fine tuning of the CPHM not only has the simplified network structure, but also increases its generalization ability. When we use 100 samples in each data set, the testing error of the RBF nets obtained by ROLS is comparable to that of the CPHM, indicating that rough tuning of the CPHM is efficient. The variance of the fitting error of the CPHM is smaller than that of ROLS, indicating that fine tuning can increase generalization ability of RBF nets and robustness on different data sets.

In the above simulation, we use 100 samples in each data set. In this case, the bias between the original unit centers and their optimal values after fine tuning is small, so the fine tuning does not improve generalization so much. In the next experiment, we use 40 samples in each data set, and the results are shown in Tab. 1. It is obvious that the testing error of the CPHM is much lower than that of ROLS, which

indicates that the CPHM performs better than ROLS when the size of the training set is small. The fitting error of the CPHM remains at 0.003, indicating that the CPHM maintains good robustness even when the data set is changed.

4 Prediction of Fusion Temperature of Coal Ash

A RBF net with eight inputs and one output is used to predict the fusion temperature of mixed coal, the eight inputs are the ingredients of the oxides SiO_2 , Al_2O_3 , Fe_2O_3 , CaO , MgO , TiO_2 , K_2O and Na_2O , and the output is the fusion temperature. 155 samples are used for training, and 50 other samples are used for testing. All the samples are obtained by using chemical analysis in the field, and all the samples are normalized in the range of $[0, 1]$.

The CPHM and RAN are used to design RBF nets. In the CPHM, the epoch is 145, spread constant $\gamma = 0.88$, $\lambda = 0.006$, $C_{\max} = 10^6$, $\Delta\lambda = 0.0002$, $\mu = 0.95$, the target error is set to zero, the learning rate $\eta = 10^{-8}$, and the threshold weight for pruning is $\omega_{\min} = 0.1$. In RAN, $\delta_{\max} = 2.6$, $\delta_{\min} = 0.8$, learning rate $\eta = 0.01$, $e_{\min} = 60$, and the epoch is 165.

Tab. 2 shows the results of two methods. Fig. 5 plots predicted fusion temperature vs. measured fusion temperature on testing samples and training samples. In Fig. 5, “+” is for testing samples, “*” is for training samples, and the diagonal line indicates that the measured fusion temperature

Tab. 2 Comparison of RBF nets obtained by CPHM and RAN methods

Method	Training error/ 10^5	Testing error/ 10^5	Hidden units
RAN	5.541	1.748	10
CPHM	4.604	1.436	4

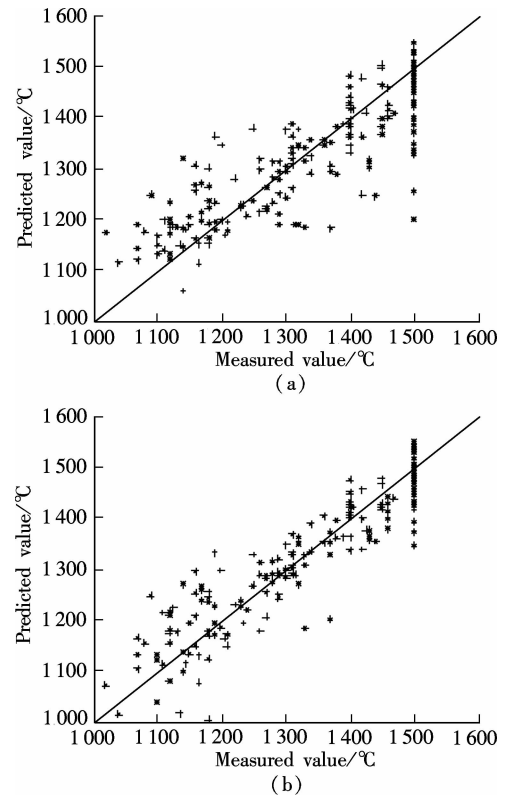


Fig. 5 Test fusion temperature of RBF nets obtained by CPHM and RAN. (a) RAN; (b) CPHM

is equal to the predicted fusion temperature.

Compared with RAN, we can find from Tab. 2 and Fig. 5 that the RBF net obtained with the CPHM has not only small training and testing errors, but also a more compact network structure.

5 Conclusion

In this paper, an RBF model is developed for the prediction of the ash fusion temperature from ash composition using the constructive-pruning hybrid method. And the trained model can always achieve much better results than traditional RAN and ROLS nets. With the CPHM, we adjust both the network structure parameters and the model parameters in learning. Tests show that networks designed with the CPHM have both compact structure and better generalization ability. And, the CPHM method maintains good performance even when training set is changed. That is to say, designed networks have a low variance of fitting error with different training data sets.

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基于构造-剪枝混合优化 RBF 网络的煤灰熔点预测方法

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摘要:为提高煤灰熔点的预测精度,提出了一种基于构造-剪枝混合优化 RBF 网络的煤灰熔点预测方法.该方法融合了神经网络构造算法和剪枝算法的优点,分为“粗调”和“精调”2个阶段.粗调阶段动态增加隐节点数目直至满足相应的停止准则;精调阶段对粗调得到的 RBF 网络的结构和参数作进一步调整.基于煤灰的化学组成成分建立相应的构造-剪枝混合优化 RBF 网络预测煤灰熔点.预测结果表明:所建模型在具有较高精度的同时,具有较小的结构、较好的泛化能力和较强的鲁棒性.

关键词:RBF 网络;函数逼近;煤灰熔点

中图分类号:TQ520.62