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一个基于自组织特征映射网络的混合神经网络结构*

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Hybrid Neural Network Architecture Based on Self-Organizing Feature Maps

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Abstract: An SOM(self-organizing feature maps)-based integrated network, namely ICBP-SOM, is constructed by applying the ICBP network model to the BP-SOM architecture. BP-SOM is a learning algorithm put forward by Ton Weijters, which aims to overcome some of the serious limitations of BP in generalizing knowledge from certain types of learning material. The motivation of presenting the integration is to employ BP-SOM good knowledge interpretation ability and the ICBP good generalization and adaptability to construct an ICBP-SOM, which processes favorable knowledge representation capability and competitive generalization performance. The experimental results on six benchmark data sets validate the feasibility and effectiveness of the integration.
Key words: neural network; circular back-propagation neural network (CBP); improved circular back-propagation neural network (ICBP); self-organizing feature maps (SOM); BP-SOM; classification

摘 要: 将ICBP网络模型引入BP-SOM(self-organizing feature maps)网络体系结构,并构建了一个基于SOM模型的集成型网络ICBP-SOM.BP-SOM是Ton Weijters提出的一种学习算法,它的目标是克服BP网络在特定类型的学习样本中存在的知识推广性方面的严重缺陷.提出此集成型网络的动机是,利用 BP-SOM 良好的知识解释能力和ICBP网络良好的推广性和自适应性构造一个ICBP-SOM模型,它具有良好的知识表示能力和极具竞争力的推广性能.在6个基准数据集上的实验结果验证了这一集成型网络的可行性和有效性.
关键词: 神经网络;圆型反向传播网络;改进的圆型反向传播网络;自组织特征映射;BP-SOM;分类
中图法分类号: TP183 **文献标识码**: A

1 Introduction

It is known that error back-propagation (EBP) learning algorithm[1] has its serious defects in generalizing knowledge from certain types of training material. Owing to such a case, Weijters developed BP-SOM model to

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partially overcome those defects[2]. The BP-SOM is a hybrid neural network architecture combining the EBP learning scheme used to train a multi-layered feedforward network (MFN), with the Self Organizing Mapping network[3] or SOM for short. The traditional MFN architecture is combined with SOMs: each hidden layer of the MFN is associated with one SOM. During training of the weights in the MFN, the corresponding SOM is trained on the hidden-unit activation patterns. After a number of training cycles of BP-SOM learning, each SOM develops self-organization to a certain extent, and then translates this self-organization into classification information. Weijters verified through experiments that the BP-SOM network and learning algorithm had a better generalization performance under the same training condition than the BP network.

Our ICBP (improved circular back-propagation) neural network was designed on the basis of CBP (circular back-propagation) network[4], its goal is to further boost CBP performance. With the original structure of CBP remaining unchanged, ICBP was constructed by adding an extra node with quadratic form to the original CBP inputs, while assigning fixed values (for instance, all 1 or all −1) to the weights connecting this extra node with all the hidden nodes. Compared with CBP, ICBP has the following virtues: (1) It has less adaptable weights but better generalization and adaptation; (2) ICBP has the characteristic of anisotropy; (3) the 2^{N_h} ICBP networks with different characteristics can be generated respectively from the 2^{N_h} combination of different assignments to the weights between the extra node and the hidden layer; (4) The BP learning algorithm can be adopted. Therefore, all the improvements made to BP can boost ICBP and CBP performances; (5) It is more general than CBP, and takes CBP as a special case. An interesting property of ICBP has been confirmed that although it may have less adaptable weights, it is better in generalization and adaptability than CBP[5−7].

The fact that ICBP can improve CBP has been confirmed in our previous work published in Ref.[6−8]. Here, we explain complementarily as follows: 1) ICBP comprises CBP in structure and in algebra expression; more importantly; 2) The number of ICBP weights is less than that of CBP ones, which implicitly indicates that ICBP can possess smaller complexity than CBP does. As a result, ICBP can generally have better generalization performance than CBP. Though the change made on CBP is natural, its structure is not only inherently kept unchanged but also not trivial in that we *skillfully* endow the connecting weights between the extra input node and all the hidden layer nodes with fixed values rather than variable weights to be optimized as in general BP networks. The purpose of doing so is to control the number of network weights, equivalently the complexity of the network, to achieve better generalization[6−8].

Despite demonstrating superiority of ICBP to BP, we find through experiments that it cannot solve highly nonlinear classification problem yet, such as Date-Calculation task, to a satisfactory degree. And we also observe by experiments that BP-SOM still can not effectively deal with the task satisfactorily, which inspire us to further improve both BP-SOM architecture and our ICBP network model jointly through integrating both. The effect of combining SOM with BP is that the hidden-unit activation patterns of instances associated with the same class tend to become increasingly similar to each other[2]. Therefore, we deduce intuitively that if SOM is combined with ICBP, then ICBP hidden-unit activation output of the same class will tend to become similar as well. The combination will be somehow natural and intuitive, because our ICBP has the similar structure to MFN. Desirably, ICBP-SOM will also inherit ICBP good performance in generalization and adaptability, which results in a further improvement to BP-SOM classification capability.

In this paper, we integrate our ICBP neural model with the classical SOM by simulating the way of Weijters combining MFN with SOM in order to further improve the performance of BP-SOM model. The work in this paper is the prophase of Ref.[8]. Compared to ICBP-KSOM model proposed in Ref.[8], ICBP-SOM model proposed in this paper has comparable and considerable performance. The goal of our algorithm is to combine supervised and unsupervised learning rather than just supervised learning alone to finally achieve the improvement the classification capability of our model against previous ones referenced in our paper, i.e. BP, BP-SOM, etc. Here unsupervised SOM is just used an assistant of supervised ICBP learning.

The rest of this paper is organized as follows: In Section 2, we introduce our ICBP network model. We combine our ICBP network model and SOM to obtain a general ICBP-SOM model in Section 3. Finally, Section 4 presents our experimental results of BP-SOM, SVM of linear, polynomial and RBF kernel, respectively, and the proposed ICBP-SOM model on six benchmark classification tasks. We execute 10-fold cross-validations in our experiments. Finally, our ICBP-SOM model is shown to improve classification and generalization performance over that of BP-SOM. However, on two data sets: DNA sequences and the glass identification task, SVM outperforms our ICBP-SOM model but its performances on the six data sets fluctuate violently, while ICBP-SOM is rather stable and favorable. So we draw conclusions in Section 5 that the new integrated architecture ICBP-SOM successfully expands the advantages of our ICBP network and boosts BP-SOM classification capability greatly.

2 ICBP Network

Figure 1 shows a three-layer ICBP network with entirely the same structure as CBP. It has N_O output nodes, N_h hidden nodes, d input nodes with respect to d dimensional input pattern. And it has an extra input node with the input being $x_{d+1}=\sum_{i=1}^{d}a_i^2x_i^2$, while in CBP $x_{d+1}=\sum_{i=1}^{d}x_i^2$ instead. Therefore when all a_i are taken equally as one, ICBP reduces to CBP. And furthermore, the way we treat those weights connecting the extra node to all the hidden nodes differ from each other: for ICBP $v_{j(d+1)}(j=1,\dots,N_h)$ take a common constant directly, while for the counterparts CBP they are adaptable parameters. Consequently, the discrepancy of the number of adaptable parameters for these two models is $|N_h-d|$. In general, the number of hidden nodes is larger than input nodes due to the proven conclusion that the forward multi-layer networks with sufficient hidden nodes number can approximate any continuous function to arbitrary precision[9]. Therefore, the adjustable parameters of ICBP are often less than those of CBP. However, we observe from practical experiments that, although ICBP has less adaptable weights, it is better in generalization and adaptability than CBP[5−7].

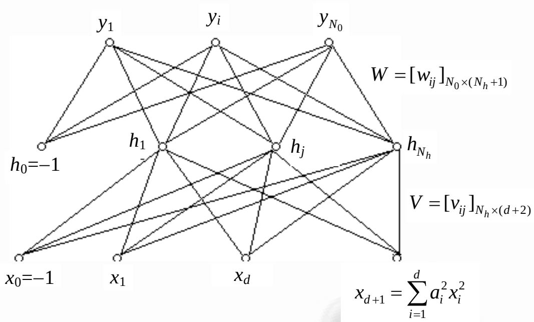

Fig.1 ICBP three-layer network model

For convenience, we list some notations which will be used later in this section.

$(x_0,x_1,\dots,x_d)$: ICBP network input.

x_{d+1}: the extra input as defined above.

V: the weight matrix between the input and hidden layer.

W: the weight matrix between the hidden and output layer.

$y_i=\sum_{j=0}^{N_h}w_{ij}h_j,\ i=1,\dots,N_o$: the i-th output of network.

$h_j=\sigma(r_j)=1/(1+e^{-r_j}),\ j=1,\dots,N_h$: the activation output of the j-th hidden node,

where r_j denotes the following sum of weighted inputs:

$$r_j(\vec{x},\vec{v})=\sum_{i=0}^{d}v_{ji}x_i+v_{j(d+1)}x_{d+1}=-v_{j0}+\sum_{i=1}^{d}(v_{ji}x_i+v_{j(d+1)}a_i^2x_i^2) \tag{1}$$

From Eq.(1), if we assign all $v_{j(d+1)}$ as +1, then ICBP extends the spherical activation fields of the neurons in the CBP hidden layer to quadratic hyper-ellipsoidal activation fields; if we set $v_{j(d+1)}$ as +1 or −1 alternatively, then the activation field of the neurons in the ICBP hidden layer is hyperboloid. Actually there exist 2^{N_h} different assignments of +1 or −1 to $v_{j(d+1)}(j=1,\ldots,N_h)$ and thus produce 2^{N_h} different ICBP network models. Therefore, we name our model as “**Improved** Circular Back-Propagation” network.

The sum-of-squares error function is defined as

$$E=\frac{1}{2}\sum_i (o_i-y_i)^2 \tag{2}$$

Adopting the known-as error back-propagation (EBP) learning algorithm (in fact, any other improved algorithms can be applied), the weight adjustment quantities between the output and hidden layers are easily derived as follows

$$\Delta w_{ij}(t)=-\eta\frac{\partial E_p}{\partial w_{ij}}=\eta[o_i(t)-y_i(t)]\cdot h_j(t)\ ,i=1,\ldots,N_o,j=0,\ldots,N_h \tag{3}$$

And the adjusting quantities in the weights between the hidden and input layers are

$$\Delta v_{jk}(t)=\eta\left[\sum_{l=1}^{N_o}(o_l(t)-y_l(t))w_{lj}\right]\cdot h_j(t)\cdot(1-h_j(t))x_k(t)\ ,j=1,\ldots,N_h,k=0,\ldots,d \tag{4}$$

Finally corresponding formula for Δa_k (k=1,…,d) are

$$\Delta a_k=2\eta\sum_{j=1}^{N_h}\left\{\sum_{i=1}^{N_o}\left[(o_i-y_i)w_{ij}\right]\cdot h_j(1-h_j)v_{j,d+1}\right\}\cdot a_k x_k^2\ ,k=1,\ldots,d \tag{5}$$

3 ICBP-SOM

3.1 ICBP-SOM architecture

Learning in ICBP-SOM is a cooperation between supervised learning in ICBP and unsupervised learning in SOM. The unsupervised dimension reduction and clustering on the SOM guide ICBP learning during the development of adequate hidden-layer representations on the MFN. The influence of the SOM causes clusters of hidden-layer representations associated with the same class, to become increasingly similar to each other. In this section we describe how the cooperation between ICBP and SOM is implemented. Figure 2 illustrates a ICBP-SOM network with d+1 input units, one hidden layer with N_h units, N_o output units, and one SOM. The size of the SOM is arbitrarily chosen to be 3×3. Each of the nine elements, denoted by E_i (i=1,…,9), contains an activation vector, denoted by V_{E_i}, of length N_h (equal to the number of hidden units), a class label, two class counters (equal to the number of output classes), and a reliability-value field[2,11].

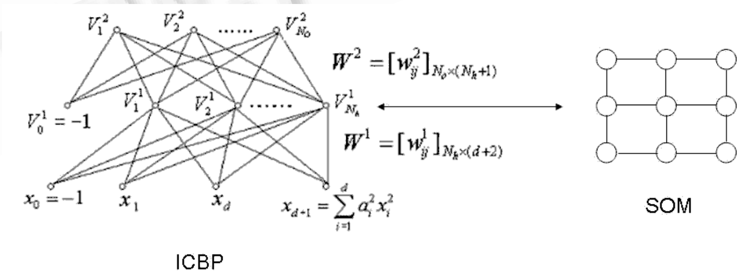

Fig.2 ICBP-SOM architecture

3.2 ICBP-SOM learning algorithm

We assume that ICBP-SOM, with l hidden layers and l associated SOM (l≥1), is trained on a classification task with two or more distinct output classes. Training of the ICBP and SOMs proceeds in parallel as follows: after feed-forward activation of an input instance, V_{hidden}, the activations of the units of each hidden layer of the ICBP part are used as learning vectors for the corresponding SOM. Each SOM is trained with Kohonen's SOM learning algorithm. After a number of training cycles, each SOM starts to develop topological order. Each SOM element is assigned an output-class label. The procedure for determining these labels is as follows: after each *n*th training cycle, all training instances are presented one by one to the ICBP. Each instance generates a pattern V_{hidden} on the hidden layer. The winning SOM unit E_i is the unit whose V_{E_i} has the smallest Euclidean distance to V_{hidden}. For each instance, the appropriate class counter of the winning unit is incremented by one. After all instances have been presented, the largest class counter of each unit defines its label. For example, let the ICBP-SOM be trained on a task which maps instances to either output class *A* or *B*. If a SOM element E_i is the best matching element to 4 activation vectors that map to class *A*, and to 2 activation vectors that map to class *B*, the class label of E_i is '*A*', with a reliability of 4/6=0.67.

For each training instance, the ICBP part of ICBP-SOM generates an error vector, V_{bp_error}, for the hidden units. The ICBP-SOM algorithm searches for the winning element E_i of those elements that are labeled with the same output class associated with the instance. It should be noted that this SOM element E_i may not be the overall best-matching element, since there may be another element labeled with an output class different from V_{hidden} that matches V_{hidden} better. In other words, the best-matching element labeled with the same class is searched for, and not the overall best matching SOM element. Taking the difference between the vectors V_{E_i} and V_{hidden} results in a SOM error vector V_{som_error}. If there is no SOM element labeled with the output class of V_{hidden}, all elements of V_{som_error} are set to zero. The error vector of a hidden unit *j*, referred to as $V_{icbp\_som\_error_j}$ is defined as

$$V_{ICBP-SOM-error_j}=\begin{cases}((1-\alpha)\times V_{ICBP-error_j})+(r\times\alpha\times V_{SOM-error_j}), \text{if } r>t\\ V_{ICBP-error_j}, \qquad \text{otherwise}\end{cases} \tag{6}$$

Here α denotes the influence of $V_{SOM\text{-}error}$ on the learning process (in our experiments typically set to 0.25). The parameter α determines the degree to which the V_{hidden} is trained to be more similar to V_{E_i}. The parameter *r* denotes the reliability of the winning SOM element E_i as described above; *t* is a *threshold* parameter, typically set to 0.95. The threshold parameter is used to prevent unreliable SOM elements to influence $V_{ICBP\text{-}SOM\text{-}error}$. During the last step of processing a training instance, the ICBP-SOM algorithm handles the $icbp\_som\_error_j$ of each hidden unit in the same way as ICBP uses the $icbp\_error_j$ in our previous proposed ICBP network.

Upon completion of learning, the SOMs become redundant, as they do not interact with the propagation of activation through the ICBP network[10,11].

3.3 Conceptual description of the ICBP-SOM learning algorithm

1. Initialize the ICBP and the corresponding SOMs. Initialize the class labels, the class counters, and the reliability field of all SOM elements to unlabeled, zero, and zero, respectively.
2. Train the ICBP during a fixed number of cycles (*m*). For each cycle do:
   For each training instance with its associated output class in the training set:
   - Compute the ICBP output via feed-forward activation through the ICBP. Collect for all hidden layers their V_{hidden}, and train the corresponding SOMs on these vectors using Kohonen's SOM learning algorithm[2].
   - Calculate $V_{ICBP\text{-}SOM\text{-}error}$ and update the ICBP weights according to the Eq.(6).

After each *n*-th training cycle (1≤*n*≤*m*), re-compute the class labels and reliability of all SOM elements by performing a class-labeling procedure as described in the text[2,11].

4 Experiment Results

4.1 Date calculation task

The date calculation task is the problem to classify dates (e.g., April 6, 1997) to the day of the week on which they fall. The dates used to train and test the four models were chosen from July 1, 1970 to April 1, 2004[2,10]. In order to compare our ICBP-SOM with BP-SOM and SVM[12−14], we applied them to the date calculation task respectively. We used 10-fold cross-validation, and the average classification error rates and error validated variations are given in Tables 1 and 2. From them we can see that the results of our ICBP-SOM significantly improve the classification accuracy and performance stability of BP-SOM and SVM.

4.2 12-Parity task

The 12-Parity task is the problem to determine whether a pattern of 12 0's and 1's contains an even number of 1's. The training set contained 1 000 different instances selected at random out of the 4 096 (2^{12}) possible patterns of length 12[2,10]. The 10-fold cross-validation results shown in Tables 1 and 2 again indicate better classification performances of our ICBP-SOM model compared to BP-SOM and SVM.

Table 1 Average classification errors on the test sets of date calculation, 12-Parity, gene detection, mushroom discrimination, breast cancer diagnosis, glass classification tasks using 10-fold cross-validation and utilizing BP-SOM, ICBP-SOM and SVM neural models in comparison

Neural models		BP-SOM			ICBP-SOM			SVM		
Experiments	Hidden nodes	15	20	40	15	20	40	Linear	Polynomial	RBF
Date calculation task		11.35	6.13	1.56	7.61	4.62	**0.53**	51.83	52.23	50.09
12-Parity task		2.63	2.23	2.89	**1.77**	1.9	2.29	30.33	33.86	31.05
Gene detection		10.67	10.43	9.88	3.76	3.28	2.99	1.51	2.24	**1.41**
Mushroom discrimination		6.31	6.29	6.71	5.59	**5.52**	6.49	12.61	11.75	13.55
Breast cancer diagnosis		2.99	2.78	2.79	2.55	**2.38**	2.62	3.77	3.70	3.89
Glass classification task		16.22	15.52	17.27	15.78	15.69	14.96	1.15	1.72	**1.05**

Table 2 Mean error rates and variations on the test sets of date calculation, 12-Parity, gene detection, mushroom discrimination, breast cancer diagnosis, glass classification tasks using 10-fold cross-validation and utilizing BP-SOM, ICBP-SOM and SVM neural models in comparison

Neural models	BP-SOM	ICBP-SOM	SVM
Date calculation task	1.56±4.05	**0.53**±0.22	50.09±0.21
12-Parity task	2.23±1.24	**1.77**±0.51	30.33±1.07
Gene detection	9.88±2.52	2.99±1.36	**1.41**±1.05
Mushroom discrimination	6.29±0.88	**5.52**±0.33	11.75±0.54
Breast cancer diagnosis	2.78±1.85	**2.38**±1.79	3.70±2.81
Glass classification task	15.52±4.29	14.96±4.17	**1.05**±2.12

4.3 Gene detection

The gene benchmark data set features 3 000 training instances and 190 test instances. The MFN or ICBP used in the experiments contained 120 input units and 3 output units (representing 'intron-exon boundary', 'exon-intron boundary', or 'neither')[2,10]. Tables 1 and 2 display the classification results of the two models, again indicating advantages of our ICBP-SOM network over BP-SOM. However, in this experiment, SVM obtains the best classification performance. Also, in the following Glass Classification Task, SVM again obtains the least classification error rate. Our explanation to these results is that SVM is surely an excellent and mature classification model in machine learning field. However, it performs rather poorly on Date Calculation Task, 12-Parity Task, Mushroom Discrimination Task and Breast Cancer Diagnosis Task. Therefore, SVM exhibitions seem extremely data sets dependent. Its simulation results fluctuate too frequently and largely. Comparatively, ICBP-SOM performs stable and achieves the best results in most of those data sets.

4.4 Mushroom discrimination task

The mushroom data set is composed of 8 000 training examples and 124 testing ones, of which 52% are edible[15]. From the average misclassification rate and validated error variations listed in Tables 1 and 2, we can see that our proposed ICBP-SOM outperforms BP-SOM and SVM. The best classification results achieved by ICBP-SOM boost that of BP-SOM by 0.77% and that of SVM by 6.23%.

4.5 The task of diagnosis of breast cancer

The total amount of Diagnosis of Breast Cancer examples are 699, and 599 of them are selected at random for training, with the remaining 100 ones for testing[15]. The 10-fold cross-validation simulation results are shown in Tables 1 and 2. From them we can see that, in most of the cases, ICBP-SOM model with 20 hidden nodes shows the best classification results. For example, in this task, ICBP-SOM with 20 hidden nodes outperforms BP-SOM with the same number ones by 0.4%, and surpasses SVM using Polynomial kernel function by 1.32%. Therefore, we might be able to conclude that a hidden layer of 20 hidden nodes is a rather good choice for BP-SOM and ICBP-SOM models.

4.6 Glass identification task

Presented in Tables 1 and 2 are the average misclassification rates and validated error variations on Glass Identification task[15] after 10-fold cross-validation simulations, and for each run the MFN and ICBP are trained by 1000 epochs. The results reflect that ICBP-SOM possesses better accuracy over BP-SOM by 0.56%, while SVM achieves the best accuracy and surpasses ICBP-SOM by 13.91%. As we noticed in the Gene Detection task, SVM classifier behaves too data dependent, while our ICBP-SOM represents smoothly and favorably.

4.7 Analysis for experimental results

In fact, from our experimental results shown in Tables 1 and 2, we find that our ICBP-SOM network outperforms BP-SOM and SVM on most of the classification tasks here. Concretely, our ICBP-SOM performs better in 4 out of 6 typical classification tasks. And it can be seen from Tables 1 and 2 that, in Date Calculation Task, the simulation experiment of the greatest disparity, ICBP-SOM improves the classification results of SVM by about 50%, implying that SVM seems not able also to effectively attack the same problem as the BP encounters. On the contrary, in Glass Classification task, for which SVM gets the best classification results. Such a fact is very natural in classification and regression, in fact, no learning algorithm can always be better in performance on all datasets unless it can make efficient use of the prior knowledge of problems under study.

5 Conclusions

Our ICBP network has an interesting property that it is better in generalization and adaptability than CBP due to that it possesses generally less adaptable weights, i.e., ICBP has lower VC dimension. However it also cannot solve those highly nonlinear pattern recognition problems just as BP and CBP to a satisfactory degree. Motivated by BP-SOM, we employ a combination of our previously-proposed ICBP model and SOM to further boost BP-SOM performance, and obtain two-fold benefits: performance improvements for ICBP network and BP-SOM. The experimental results on 6 benchmark classification tasks confirm the feasibility and effectiveness of our new integrated structure. Though so, in comparison to SVM, our ICBP-SOM has also a following limitation required to be overcome next that it lacks a sound theoretical basis of generalization as SVM, and thus does not have large margin property of SVM, so it might perform inferior to SVM on other specific tasks.

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