Comparing the prediction accuracy of artificial neural networks and other statistical models for breast cancer survival

Harry B. Burke
Department of Medicine
New York Medical College
Valhalla, NY 10595

David B. Rosen
Department of Medicine
New York Medical College
Valhalla, NY 10595

Philip H. Goodman
Department of Medicine
University of Nevada School of Medicine
Reno, Nevada 89520

Abstract

The TNM staging system has been used since the early 1960's to predict breast cancer patient outcome. In an attempt to increase prognostic accuracy, many putative prognostic factors have been identified. Because the TNM stage model can not accommodate these new factors, the proliferation of factors in breast cancer has lead to clinical confusion. What is required is a new computerized prognostic system that can test putative prognostic factors and integrate the predictive factors with the TNM variables in order to increase prognostic accuracy. Using the area under the curve of the receiver operating characteristic, we compare the accuracy of the following predictive models in terms of five year breast cancer-specific survival: pTNM staging system, principal component analysis, classification and regression trees, logistic regression, cascade correlation neural network, conjugate gradient descent neural, probabilistic neural network, and backpropagation neural network. Several statistical models are significantly more ac-

curate than the TNM staging system. Logistic regression and the backpropagation neural network are the most accurate prediction models for predicting five year breast cancer-specific survival

1 INTRODUCTION

For over thirty years measuring cancer outcome has been based on the TNM staging system (tumor size, number of lymph nodes with metastatic disease, and distant metastases) (Beahr et. al., 1992). There are several problems with this model (Burke and Henson, 1993). First, it is not very accurate, for breast cancer it is 44% accurate. Second its accuracy can not be improved because predictive variables can not be added to the model. Third, it does not apply to all cancers. In this paper we compare computerized prediction models to determine if they can improve prognostic accuracy. Artificial neural networks (ANN) are a class of nonlinear regression and discrimination models. ANNs are being used in many areas of medicine, with several hundred articles published in the last year. Representative areas of research include anesthesiology (Westenskow et. al., 1992), radiology (Tourassi et. al., 1992), cardiology (Leong and Jabri, 1982), psychiatry (Palombo, 1992), and neurology (Gabor and Seyal, 1992). ANNs are being used in cancer research including image processing (Goldberg et. al., 1992) , analysis of laboratory data for breast cancer diagnosis (O Leary et. al., 1992), and the discovery of chemotherapeutic agents (Weinstein et. al., 1992). It should be pointed out that the analyses in this paper rely upon previously collected prognostic factors. These factors were selected for collection because they were significant in a generalized linear model such as the linear or logistic models. There is no predictive model that can improve upon linear or logistic prediction models when the predictor variables meet the assumptions of these models and there are no interactions. Therefore he objective of this paper is not to outperform linear or logistic models on these data. Rather, our objective is to show that, with variables selected by generalized linear models, artificial neural networks can perform as well as the best traditional models . There is no a priori reason to believe that future prognostic factors will be binary or linear, and that there will not be complex interactions between prognostic factors. A further objective of this paper is to demonstrate that artificial neural networks are likely to outperform the conventional models when there are unanticipated nonmonotonic factors or complex interactions.

2 METHODS

2.1 DATA

The Patient Care Evaluation (PCE) data set is collected by the Commission on Cancer of the American College of Surgeons (ACS). The ACS, in October 1992, requested cancer information from hospital tumor registries in the United States. The ACS asked for the first 25 cases of breast cancer seen at that institution in 1983, and it asked for follow up information on each of these 25 patients through the date of the request. These are only cases of first breast cancer. Follow-up information included known deaths. The PCE data set contains, at best, eight year follow-up.

We chose to use a five year survival end-point. This analysis is for death due to breast cancer, not all cause mortality.

For this analysis cases with missing data, and cases censored before five years, are not included so that the prediction models can be compared without putting any prediction model at a disadvantage. We randomly divided the data set into training, hold-out, and testing subsets of 3,100, 2,069, and 3,102 cases, respectively.

2.2 MODELS

The TMN stage model used in this analysis is the pathologic model (pTNM) based on the 1992 American Joint Committee on Cancer's Manual for the Staging of Cancer (Beahr et. al., 1992). The pathologic model relies upon pathologically determined tumor size and lymph nodes, this contrasts with clinical staging which relies upon the clinical examination to provide tumor size and lymph node information. To determine the overall accuracy of the TNM stage model we compared the model's prediction for each patient, where the individual patient's prediction is the fraction of all the patients in that stage who survive, to each patient's true outcome.

Principal components analysis, is a data reduction technique based on the linear combinations of predictor variables that minimizes the variance across patients (Jollie, 1982). The logistic regression analysis is performed in a stepwise manner, without interaction terms, using the statistical language S-PLUS (S-PLUS, 1992), with the continuous variable age modeled with a restricted cubic spline to avoid assuming linearity (Harrell et. al., 1988). Two types of Classification and Regression Tree (CART) (Breiman et. al., 1984) analyses are performed using S-PLUS. The first was a 9-node pruned tree (with 10-fold cross validation on the deviance), and the second was a shrunk tree with 13.7 effective nodes.

The multilayer perceptron neural network training in this paper is based on the maximum likelihood function unless otherwise stated, and backpropagation refers to gradient descent. Two neural networks that are not multilayer perceptrons are tested. They are the Fuzzy ARTMAP neural network (Carpenter et. al., 1991) and the probabilistic neural network (Specht, 1990).

2.3 ACCURACY

The measure of comparative accuracy is the area under the curve of the receiver operating characteristic (Az). Generally, the Az is a nonparametric measure of discrimination. Square error summarizes how close each patient's predicted value is to its true outcome. The Az measures the relative goodness of the set of predictions as a whole by comparing the predicted probability of each patient with that of all other patients. The computational approach to the Az that employs the trapezoidal approximation to the area under the receiver operating characteristic curve for binary outcomes was first reported by Bamber (Bamber, 1975), and later in the medical literature by Hanley (Hanley and McNeil, 1982). This was extended by Harrell (Harrell et. al., 1988) to continuous outcomes.

Table 1: PCE 1983 Breast Cancer Data: 5 Year Survival Prediction, 54 Variables.

PREDICTION MODEL	ACCURACY*	SPECIFICATIONS
pTNM Stages	.720	0,I,IIA,IIB,IIIA,IIIB,IV
Principal Components Analysis	.714	one scaling iteration
CART, pruned	.753	9 nodes
CART, shrunk	.762	13.7 nodes
Stepwise Logistic regression	.776	with cubic splines
Fuzzy ARTMAP ANN	.738	54-F2a, 128-1
Cascade correlation ANN	.761	54-21-1
Conjugate gradient descent ANN	.774	54-30-1
Probabilistic ANN	.777	bandwidth = 16s
Backpropagation ANN	.784	54-5-1

* The area under the curve of the receiver operating characteristic.

3 RESULTS

All results are based on the independent variable sample not used for training (i.e., the testing data set), and all analyses employ the same testing data set. Using the PCE breast cancer data set, we can assess the accuracy of several prediction models using the most powerful of the predictor variables available in the data set (See Table 1).

Principal components analysis is not expected to be a very accurate model; with one scaling iteration, its accuracy is .714. Two types of classification and regression trees (CART), pruned and shrunk, demonstrate accuracies of .753 and .762, respectively. Logistic regression with cubic splines for age has an accuracy of .776. In addition to the backpropagation neural network and the probabilistic neural network, three types of neural networks are tested. Fuzzy ARTMAP's accuracy is the poorest at .738. It was too computationally intensive to be a practical model. Cascade-correlation and conjugate gradient descent have the potential to do as well as backpropagation. The PNN accuracy is .777. The PNN has many interesting features, but it also has several drawbacks including its storage requirements. The backpropagation neural network's accuracy is .784.4.

4 DISCUSSION

For predicting five year breast cancer-specific survival, several computerized prediction models are more accurate than the TNM stage system, and artificial neural networks are as good as the best traditional statistical models.

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Learning with Product Units

Laurens R. Leerink
Australian Gilt Securities LTD
37-49 Pitt Street
NSW 2000, Australia
laurens@sedal.su.oz.au

C. Lee Giles
NEC Research Institute
4 Independence Way
Princeton, NJ 08540, USA
giles@research.nj.nec.com

Bill G. Horne
NEC Research Institute
4 Independence Way
Princeton, NJ 08540, USA
horne@research.nj.nec.com

Marwan A. Jabri
Department of Electrical Engineering
The University of Sydney
NSW 2006, Australia
marwan@sedal.su.oz.au

Abstract

Product units provide a method of automatically learning the higher-order input combinations required for efficient learning in neural networks. However, we show that problems are encountered when using backpropagation to train networks containing these units. This paper examines these problems, and proposes some atypical heuristics to improve learning. Using these heuristics a constructive method is introduced which solves well-researched problems with significantly less neurons than previously reported. Secondly, product units are implemented as candidate units in the Cascade Correlation (Fahlman & Lebiere, 1990) system. This resulted in smaller networks which trained faster than when using sigmoidal or Gaussian units.

1 Introduction

It is well-known that supplementing the inputs to a neural network with higher-order combinations of the inputs both increases the capacity of the network (Cover, 1965) and the the ability to learn geometrically invariant properties (Giles & Maxwell,

1987). However, there is a combinatorial explosion of higher order terms as the number of inputs to the network increases. Yet in order to implement a certain logical function, in most cases only a few of these higher order terms are required (Redding et al., 1993).

The product units (PUs) introduced by (Durbin & Rumelhart, 1989) attempt to make use of this fact. These networks have the advantage that, given an appropriate training algorithm, the units can automatically learn the higher order terms that are required to implement a specific logical function.

In these networks the hidden layer units compute the weighted product of the inputs, that is

$$\prod_{i=1}^{N} x_i^{w_i} \qquad \text{instead of} \qquad \sum_{i=1}^{N} x_i w_i \tag{1}$$

as in standard networks. An additional advantage of PUs is the increased information capacity of these units compared to standard summation networks. It is approximately $3N$ (Durbin & Rumelhart, 1989), compared to $2N$ for a single threshold logic function (Cover, 1965), where N is the number of inputs to the unit.

The larger capacity means that the same functions can be implemented by networks containing less units. This is important for certain applications such as speech recognition where the data bandwidth is high or if realtime implementations are desired.

When PUs are used to process Boolean inputs, best performance is obtained (Durbin & Rumelhart, 1989) by using inputs of $\{+1, -1\}$. If the imaginary component is ignored, with these inputs, the activation function is equivalent to a cosine summation function with $\{-1, +1\}$ inputs mapped $\{1, 0\}$ (Durbin & Rumelhart, 1989). In the remainder of this paper the terms *product unit (PU)* and *cos(ine) unit* will be used interchangeably as all the problems examined have Boolean inputs.

2 Learning with Product Units

As the basic mechanism of a PU is multiplicative instead of additive, one would expect that standard neural network training methods and procedures cannot be directly applied when training these networks. This is indeed the case. If a neural network simulation environment is available the basic functionality of a PU can be obtained by simply adding the *cos* function $cos(\pi * input)$ to the existing list of transfer functions. This assumes that Boolean mappings are being implemented and the appropriate $\{-1, +1\} \rightarrow \{1, 0\}$ mapping has been performed on the input vectors. However, if we then attempt to train a network on on the parity-6 problem shown in (Durbin & Rumelhart, 1989), it is found that the standard backpropagation (BP) algorithm simply does not work. We have found two main reasons for this.

The first is weight initialization. A typical first step in the backpropagation procedure is to initialize all weights to small random values. The main reason for this is to use the dynamic range of the sigmoid function and it's derivative. However, the dynamic range of a PU is unlimited. Initializing the weights to small random

values results in an input to the unit where the derivative is small. So apart from choosing small weights centered around $n\pi$ with $n = \pm 1, \pm 2, \ldots$ this is the worst possible choice. In our simulations weights were initialized randomly in the range $[-2, 2]$. In fact, learning seems insensitive to the size of the weights, as long as they are large enough.

The second problem is local minima. Previous reports have mentioned this problem, (Lapedes & Farber, 1987) commented that "using *sin*'s often leads to numerical problems, and nonglobal minima, whereas sigmoids seemed to avoid such problems". This comment summarizes our experience of training with PUs. For small problems (less than 3 inputs) backpropagation provides satisfactory training. However, when the number of inputs are increased beyond this number, even with the weight initialization in the correct range, training usually ends up in a local minima.

3 Training Algorithms

With these aspects in mind, the following training algorithms were evaluated: online and batch versions of Backpropagation (BP), Simulated Annealing (SA), a Random Search Algorithm (RSA) and combinations of these algorithms.

BP was used as a benchmark and for use in combination with the other algorithms. The Delta-Bar-Delta learning rate adaptation rule (Jacobs, 1988) was used along with the batch version of BP to accelerate convergence, with the parameters were set to $\theta = 0.35, \kappa = 0.05$ and $\phi = 0.90$. RSA is a global search method (i.e. the whole weight space is explored during training). Weights are randomly chosen from a predefined distribution, and replaced if this results in an error decrease. SA (Kirkpatrick et al., 1983) is a standard optimization method. The operation of SA is similar to RSA, with the difference that with a decreasing probability solutions are accepted which increase the training error. The combination of algorithms were chosen (BP & SA, BP & RSA) to combine the benefits of global and local search. Used in this manner, BP is used to find the local minima. If the training error at the minima is sufficiently low, training is terminated. Otherwise, the global method initializes the weights to another position in weight space from which local training can continue.

The BP-RSA combination requires further explanation. Several BP-(R)SA combinations were evaluated, but best performance was obtained using a fixed number of iterations of BP (in this case 120) along with one initial iteration of RSA. In this manner BP is used to move to the local minima, and if the training error is still above the desired level the RSA algorithm generates a new set of random weights from which BP can start again.

The algorithms were evaluated on two problems, the parity problem and learning all logical functions of 2 and 3 inputs. The infamous parity problem is (for the product unit at least) an appropriate task. As illustrated by (Durbin & Rumelhart, 1989), this problem can be solved by one product unit. The question is whether the training algorithms can find a solution. The target values are $\{-1, +1\}$, and the output is taken to be correct if it has the correct sign. The simulation results are shown in Table 1. It should be noted that one epoch of both SA and RSA involves

relaxing the network across the training set for every weight, so in computational terms their $\overline{n}_{epoch}$ values should be multiplied by a factor of $(N+1)$.

Parity N	Online BP		Batch BP		SA		RSA	
	n_{conv}	$\overline{n}_{epoch}$	n_{conv}	$\overline{n}_{epoch}$	n_{conv}	$\overline{n}_{epoch}$	n_{conv}	$\overline{n}_{epoch}$
6	10	30.4	7	34	10	12.6	10	15.2
8	8	101.3	2	700	10	52.8	10	45.4
10	6	203.3	0	-	10	99.9	10	74.1

Table 1: The parity N problem: The table shows n_{conv} the number of runs out of 10 that have converged and $\overline{n}_{epoch}$, the average number of training epochs required when training converged.

For the parity problem it is clear that local learning alone does not provide good convergence. For this problem, global search algorithms have the following advantages: (1) The search space is bounded (all weights are restricted to $[-2,+2]$) (2) The dimension of search space is low (maximum of 11 weights for the problems examined). (3) The fraction of the weight space which satisfies the parity problem relative to the total bounded weight space is high.

In a second set of simulations, one product unit was trained to calculate all $2^{(2^N)}$ logical functions of the N input variables. Unfortunately, this is only practical for $N \in \{2,3\}$. For $N=2$ there are only 16 functions, and a product unit has no problem learning all these functions rapidly with all four training algorithms. In comparison a single summation unit can learn 14 (not the XOR & XNOR functions). For N=3, a product unit is able to implement 208 of the 256 functions, while a single summation unit could only implement 104. The simulation results are displayed in Table 2.

Online BP		Batch BP		SA		RSA		BP-RSA	
$\overline{n}_{logic}$	$\overline{n}_{epoch}$	$\overline{n}_{logic}$	$\overline{n}_{epoch}$	$\overline{n}_{logic}$	$\overline{n}_{epoch}$	$\overline{n}_{logic}$	$\overline{n}_{epoch}$	$\overline{n}_{logic}$	$\overline{n}_{epoch}$
147.3	42.6	189.2	20.5	196.1	43.8	167.4	60.2	208	44.3

Table 2: Learning all logical functions of 3 inputs: The rows display $\overline{n}_{logic}$, the average number of logical functions implemented by a product unit and $\overline{n}_{epoch}$, the number of epochs required for convergence. Ten simulations were performed for each of the 256 logical functions, each for a maximum of 1,000 iterations.

4 Constructive Learning with Product Units

Selecting the optimal network architecture for a specific application is a nontrivial and time-consuming task, and several algorithms have been proposed to automate this process. These include pruning methods and growing algorithms. In this section a simple method is proposed for adding PUs to the hidden layer of a three layer network. The output layer contains a single sigmoidal unit.

Several constructive algorithms proceed by freezing a subset of the weights and limiting training to the newly added units. As mentioned earlier, for PUs a global

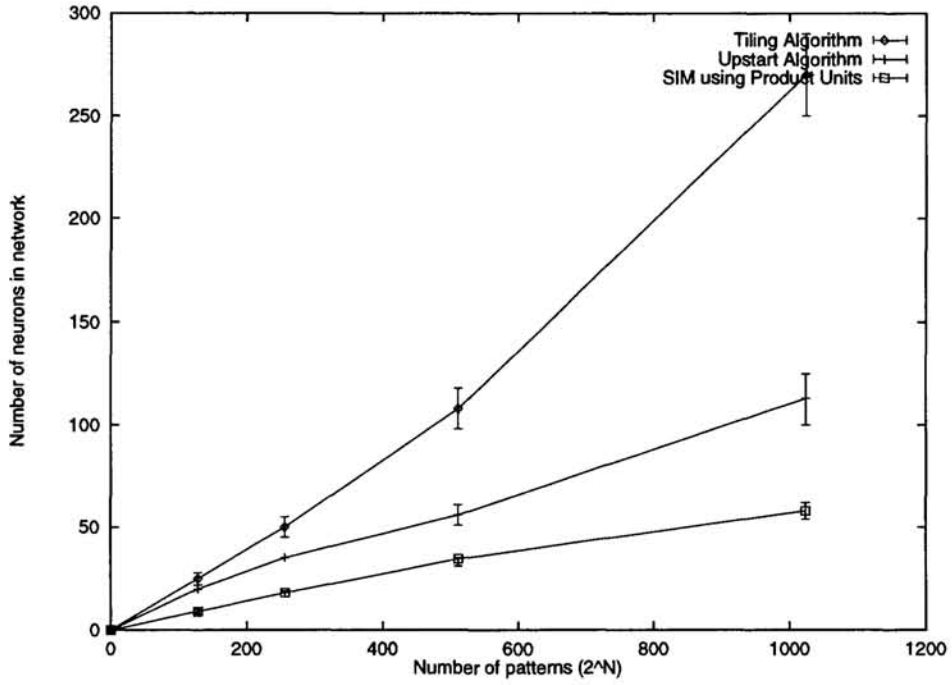

Figure 1: The number of units required for learning the random mapping problems by the 'Tiling', 'Upstart' and SIM algorithms.

search is required to solve the local-minima problems. Freezing a subset of the weights restricts the new solution to an affine subset of the existing weight space, often resulting in non-minimal networks (Ash, 1989). For this reason a simple incremental method (SIM) was implemented which retains the global search for all weights during the whole training process. The method used in our simulations is as follows:

- Train a network using the BP-RSA combination on a network with a specified minimum number of hidden PUs.
- If there is no convergence within a specified number of epochs, add a PU to the network. Reinitialize weights and continue training with the BP-RSA combination.
- Repeat process until a solution is found or the network has grown a predetermined maximum size.

The method of (Ash, 1989) was also evaluated, where neurons with small weights were added to a network according to certain criteria. The SIM performed better, possibly because of the global search performed by the RSA step.

The 'Upstart' (Frean, 1990) and 'Tiling' (Mézard & Nadal, 1989) constructive algorithms were chosen as benchmarks. A constructive PU network was trained on two problems described in these papers, namely the parity problem and the random mapping problem. In (Frean, 1990) it was reported that the Upstart

algorithm required N units for all parity N problems, and 1,000 training epochs were sufficient for all values of N except $N = 10$, which required 10,000. As seen earlier, one PU is able to perform any parity function, and SIM required an an average of 74.1 iterations for $N = 6, 8, 10$.

The random mapping problem is defined by assigning each of the 2^N patterns its target $\{-1, +1\}$ with 50% probability. This is a difficult problem, due to the absence of correlations and structure in the input. As in (Frean, 1990; Mézard & Nadal, 1989) the average of 25 runs were performed, each on a different training set. The number of units required by SIM is plotted in Figure 1. The values for the Tiling and Upstart algorithms are approximate and were obtained through inspection from a similar graph in (Frean, 1990).

5 Using Cosine Candidate Units in Cascade Correlation

Initially we wanted to compare the performance of SIM with the well-known 'cascade-correlation' (CC) algorithm of (Fahlman & Lebiere, 1990). However, the network architectures differ and a direct comparison between the number of units in the respective architectures does not reflect the efficiency of the algorithms. Instead, it was decided to integrate PUs into the CC system as candidate units.

For these simulations a public domain version of CC was used (White, 1993) which supports four different candidate types; the asymmetric sigmoid, symmetric sigmoid, variable sigmoid and gaussian units. Facilities exist for either constructing homogeneous networks by selecting one unit type, or training with a pool of different units allowing the construction of hybrid networks. It was thus relatively simple to add PU candidate units to the system. Table 3 displays the results when CC was trained on the random logic problem using three types of homogeneous candidate units.

N	CC Sigmoid		CC Gauss		CC PU	
	$\overline{n}_{units}$	$\overline{n}_{epochs}$	$\overline{n}_{units}$	$\overline{n}_{epochs}$	$\overline{n}_{units}$	$\overline{n}_{epochs}$
7	6.6	924.5	6.7	642.6	5.7	493.8
8	12.1	1630.9	11.5	1128.2	9.9	833.8
9	20.5	2738.3	18.4	1831.1	16.4	1481.8
10	32.9	4410.9	30.2	2967.6	26.6	2590.8

Table 3: Learning random logic functions of N inputs: The table shows $\overline{n}_{units}$, the average number of units required and $\overline{n}_{epochs}$, the average number of training epochs required for convergence of CC using sigmoidal, Gaussian and PU candidate units. Figures are based on 25 simulations.

In a separate experiment the performance of hybrid networks were re-evaluated on the same random logic problem. To enable a fair competition between candidate units of different types, the simulations were run with 40 candidate units, 8 of each type. The simulations were evaluated on 25 trails for each of the random mapping problems (7,8,9 and 10 inputs, a total of 1920 input vectors). In total 1460 hidden units were allocated, and in *all cases* PU candidate units were chosen above units of the 4 other types during the competitive stage. During this comparison all

parameters were set to default values, i.e. the weights of the PU candidate units were random numbers initialized in the range of $[-1, +1]$. As discussed earlier, this puts the PUs at a slight disadvantage as their optimum range is $[-2, +2]$.

6 Discussion

The BP-RSA combination is in effect equivalent to the 'local optimization with random restarts' process discussed by (Karmarkar & Karp, 1982), where the local optimization is this case is performed by the BP algorithm. They reported that for certain problems where the error surface was 'exceedingly mountainous', multiple random-start local optimization outperformed more sophisticated methods. We hypothesize that adding PUs to a network makes the error surface sufficiently mountainous so that a global search is required.

As expected, the higher separating capacity of the PU enables the construction of networks with less neurons than those produced by the Tiling and Upstart algorithms. The fact that SIM works this well is mainly a result of the error surface; the surface is so irregular that even training a network of fixed architecture is best done by reinitializing the weights if convergence does not occur within certain bounds. This again is in accordance with the results of (Karmarkar & Karp, 1982) discussed above.

When used in CC we hypothesize that there are three main reasons for the choice of PUs above any of the other types during the competitive learning phase. Firstly, the higher capacity (in a information capacity sense) of the PUs allows a better correlation with the error signal. Secondly, having N competing candidate units is equivalent to selecting the best of N random restarts, and performs the required global search. Thirdly, although the error surface of networks with PUs contains more local minima than when using standard transfer functions, the surface is locally smooth. This allows effective use of higher-order error derivatives, resulting in fast convergence by the quickprop algorithm.

In (Dawson & Schopflocher, 1992) it was shown that networks with Gaussian units train faster and require less units than networks with standard sigmoidal units. This is supported by our results shown in Table 3. However, for the problem examined, PUs outperform Gaussian units by approximately the same margin as Gaussian units outperform sigmoidal units. It should also be noted that these problems where not chosen for their suitability for PUs. In fact, if the problems are symmetric/regular the difference in performance is expected to increase.

7 Conclusion

Of the learning algorithms examined BP provides the fastest training, but is prone to nonglobal minima. On the other hand, global search methods are impractical for larger networks. For the problems examined, a combination of local and global search methods were found to perform best. Given a network containing PUs, there are some atypical heuristics that can be used: (a) correct weight initialization (b) reinitialization of the weights if convergence is not rapidly reached. In addition, the representational power of PUs have enabled us to solve standard problems

using significantly smaller networks than previously reported, using a very simple constructive method. When implemented in the CC architecture, for the problems examined PUs resulted in smaller networks which trained faster than other units. When included in a pool of competing candidate units, simulations showed that in all cases PU candidate units were preferred over candidate units of the other four types.

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