Chapter 4

The Hidden Tree in Multilayer Network

Abstract – We develop a side direction process to assist the back propagation learning algorithm to resolve the premature saturation problem. To build this side process, we explore the idea of unfaithful representation which has been introduced in the tiling algorithm (M. Mezard, and J. P. Nadal, 1989). The algorithm may grow to an unpredictably large network for a given pattern set. This unfaithful representation is equivalent to the ambiguous binary representation. Binary numbers are used to represent the output binary vectors of hidden layers. More training patterns of different classes map to the same binary number; more patterns are misclassified. Besides, the presence of ambiguous binary representations is also an important pointer of when and where we should add a new hidden neuron to the multilayer perceptron. In this work, we explain the happening of ambiguous binary representation and develop a method to alleviate it. Using this method, both the number of ambiguous binary representations and the back propagation learning time are drastically reduced.

1. Introduction to the ambiguous binary representation

The back propagation (BP) algorithm is widely used for finding optimum weights of multilayer neural networks in many pattern recognition subjects (T. J. Sejnowski, and C. R. Rosenberg, 1986), (B. Widrow, and R. Winter, 1986). However, the critical problems of the algorithm are its slow learning speed and convergence to local minima (D. R. Hush, and B. G. Horne, 1993), (Y. Lee, S. H. Oh, and M. W. Kim, 1993). One of the major reasons of these problems is “ambiguous binary representation”. Binary numbers are used to represent the output binary vectors of hidden layers. More training patterns of different classes map to the same binary number; more patterns are misclassified. In this section, we illustrate the happening of

ambiguous binary representation.

To solve the problem, we should release the factors that cause them. In (Y. Lee, S. H. Oh, and M. W. Kim, 1993), it is proposed that "premature saturation" is one of the reasons of these problems. Premature saturation is a phenomenon that the error of the neural network stays significantly high constant for certain unpredicted period of time during learning. It is also stated that premature saturation could be avoided by setting the proper maximum value of initial weights. From our later discussion, we recommend to use the hyperplane grid or random boundaries for each layer as the initial weights to bound and discriminate all patterns as uniformly as possible. In our study premature saturation is the result of bad encoding of the pattern space. For example, the first hidden layer encodes the input pattern space to binary numbers (or binary vectors) of length *m*, where *m* is the number of neurons in the first hidden layer. Bad encoding causes the patterns of different classes map to the same binary number. We call this kind of binary numbers "ambiguous binary representations". Ambiguous binary representations do result in the premature saturation. Note that this encoding also preserves the input pattern neighbors in the neighborhood of Hamming tree for each layer.

One approach to the problem is using constructive algorithm: it begins with the smallest possible network and gradually increases the size if the error is kept above a level. The presence of ambiguous binary numbers is also an important pointer of when and where we should add a new hidden neuron to the MLP. By analyzing each individual ambiguous binary representation, we can constructively initialize the weights connected with the newly added neuron.

In the following we present simple cases to clearly illustrate the ambiguous binary representation problem. Consider a classification problem consisting in assigning training patterns of R^2 to 2 predetermined classes, i.e., class 0 and class 1. The training patterns of this classification problem are shown in Fig. 1. In Fig. 1(a), "x" represents patterns that belong to class 0. Assume that we already implement this classification using a three-layer neural network with 2 input units, 3 neurons in the first hidden layer, 3 neurons in the second hidden layer, 1 output neuron, and 3 bias units, as illustrated in Fig. 1(b). In this figure L_1, L_2, L_3 represent the first, second, third neuron in the first hidden layer and P_1, P_2, P_3 represent the first, second, third neuron in the second hidden layer and P'_1 is the output neuron.

Let the activation function used in this multilayer neural network be the hard-limited function. Then the function of every neuron is $F(X) = \{0 \text{ if } W \cdot X + w_0 < 0, 1 \text{ if } W \cdot X + w_0 > 0\}$, where X is the input vector, W is the weight vector of the hidden neuron or output neuron, and w_0 is the bias of the hidden neuron.

Now let's state the detailed function of the first hidden layer. Assume that Fig. 1

shows a perfect trained result of the BP learning algorithm. The three lines (or boundaries) shown in Fig. 1 are the lines corresponding to the three hidden neurons in the first hidden layer. The positive (F(X) > 0) and negative sides (F(X) < 0) of each line are also displayed. The function lines of the first, second, third neuron of the first hidden layer are { L_1 : -1.3 * x + 3 * y = 3.9, L_2 : x + 4 * y = -3, L_3 : 2.3 * x + y = 1.3}, where x and y are the inputs to the input layer. The coefficients of x and y are the trained weights of the neurons in the first hidden layer.

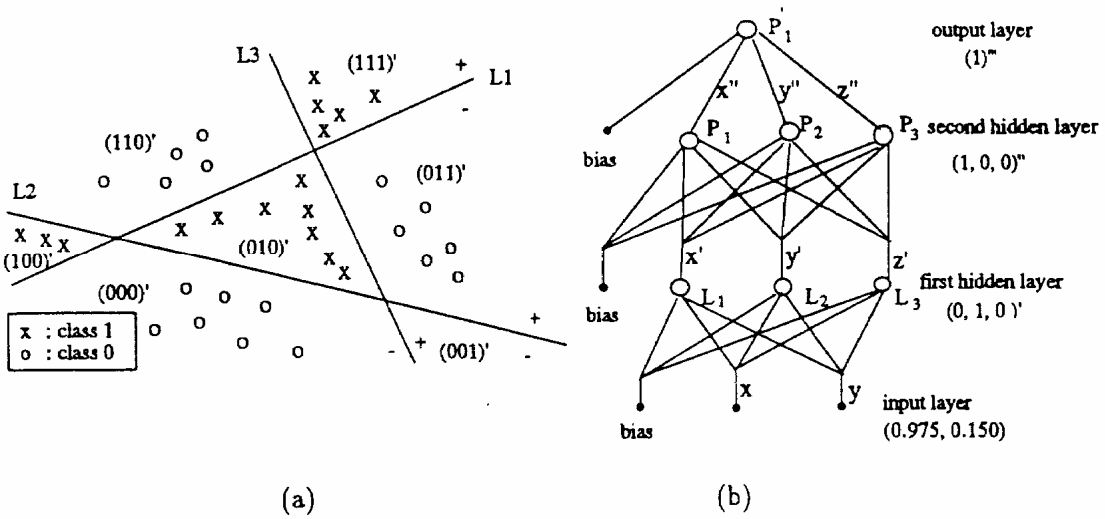


Fig. 1. The three-layer neural network and the discriminated regions of the first hidden layer.

The center region (polyhedral) in Fig. 1 lies on the negative part of L_1, positive part of L_2, and negative part of L_3. Thus this region is represented by the output binary vector (010)' of the first hidden layer. All of the seven binary representation regions discriminated by the first hidden layer shown in Fig. 1 are the finest *elementary building blocks* for all upper layers. All upper layers use the various combinations of these finest building blocks to achieve the classification performance. This means, when there exists a mixed class region in any of these seven elementary regions, such as the elementary region (011)' contains both types of patterns "x" and "o", the misclassification will persist with this ambiguous elementary region. This will cause difficulty in including it for all upper layers no matter how we tune the weights between the first hidden layer and the output layer.

Notice that in X, Y space the neighborhood regions also neighbor in X', Y', Z' cube. And the disconnected regions in X, Y space (like (011)' and (100)') also disconnected in X', Y', Z' cube. These two conditions are topology requirement manifold. For example, the binary vector for the center region is (010)' as in Fig. 1. These two connected neighborhood regions have a common boundary L_3 and have a

Hamming distance of only one bit neighbor in the 3-D cube. All connected neighborhood regions have an exactly one bit Hamming neighborhood distance. Far and unconnected regions may have maximum Hamming distance of all three bits and will not be neighbor in the 3-D cube. By the first hidden layer, the 2-class pattern topology in input space is easily converted to the Hamming topology in unit hypercube. In Hamming space, the neighborhood is counted in term of Hamming distance. Since these regions are finite and countable for the MLP, the hyperspace Hamming neighbors can be displayed by a Hamming tree structure with successive fans (T. J. Sejnowski, and C. R. Rosenberg, 1986). With this trained MLP, all output vectors of the first hidden layer can be presented as binary numbers of length of 3 (3 is the number of neurons in the first hidden layer). The total capacity of these binary representations is $2^3 = 8$. Note that there are seven representation regions can be allocated in this plane, see (G. Mirchandeni, and Wei Cao) for details. In most cases the number of representation regions is much less than the number of the training patterns when these patterns are cluster type. Thus monitoring the Hamming tree during BP learning is feasible in our processing.

Every training pattern map to one corner point of the cube as shown in Fig. 2. In general, the function H_1 of the first hidden layer is a mapping $H_1 : R^2 \rightarrow \{0, 1\}^3$, where 2 is the dimension of the input pattern space and 3 is the number of neurons in the first hidden layer.

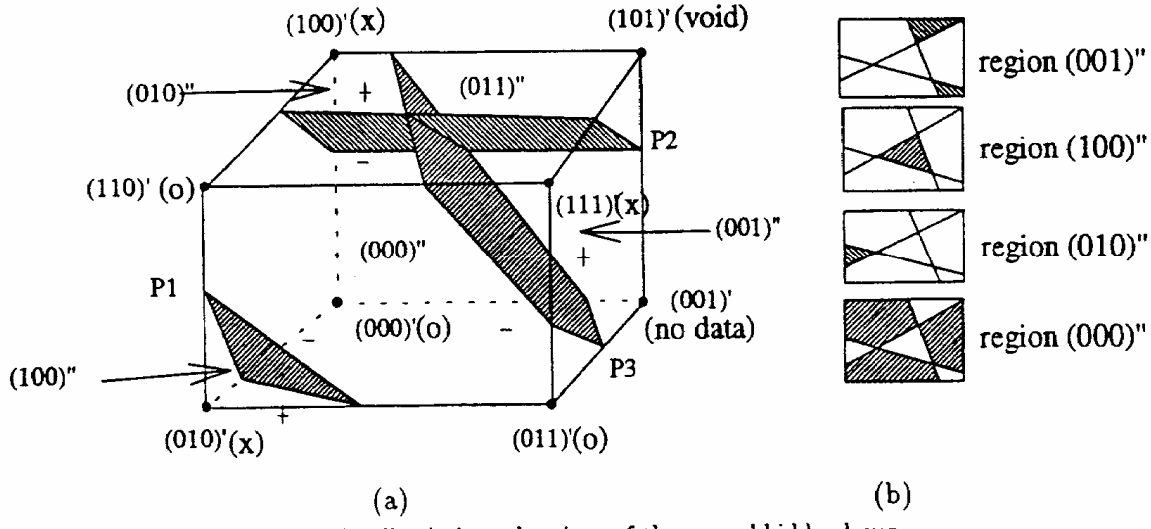


Fig. 2. The discriminated regions of the second hidden layer.

Once a button layer reaches homogenous, we train its all upper layers using the refined activation states next to this button layer, ex. use (x', y', z') to train P_1, P_2, P_3 and P_1', use (x", y", z") to train P_1' when the L_1, L_2, L_3 are all homogeneous borders.

Now let's state the function of the second hidden layer. The function H_2 of the second hidden layers is $H_2 : \{0, 1\}^3 \rightarrow \{0, 1\}^3$. That is, every neuron in the second hidden layer decides a plane to divide the unit cube of the first hidden layer. The plane (or boundary), P_1, corresponding to the first neuron in the second hidden layer is shown in Fig. 2. This neuron's output for (010)' is "1", all others are "0". Assume that the three planes shown in Fig. 2 corresponding to the three neurons in the second hidden layer are P_1, P_2, P_3. The plane functions of P_1, P_2, P_3 are {P_1: -0.9 * x' + 1.5 * y' - z' = 0.95, P_2: 2.5 * x' – 3.7 * y' + 0.37 * z' = 2.0, P_3: 2.5 * x' – 2 * y' + 4 * z' = 3.1}, where x' is the output value of the first neuron L_1, y' is the output value of the second neuron L_2, and z' are the output value of the third neuron L_3 in the first hidden layer. The coefficients of x', y', and z' are the trained weights. Then the training patterns which map to the binary number (010)' in the first hidden layer will cause the first neuron in the second hidden layer "ON". The training patterns which map to the binary vector (111)', (001)', and (101)' of the first hidden layer will cause the third neuron in the second hidden layer "ON".

Fig. 2 shows that the cube is divided into five regions by the three planes, P_1, P_2, and P_3. Each region is represented by an output binary vector of the second hidden layer. This means that each region is a combination of several finest element regions of the first hidden layer. The region (001)'' includes vertexes (111)' and (001)' which are tow element regions of the first hidden layer. The region (011)'' includes (101)'. The region (010)'' includes (100)'. We can see that the four regions in Fig. 2(b) which are discriminated by the second hidden layer are elementary building blocks of the output layers. This means that any ambiguous binary representation happened in this layer will cause misclassification in the output layer.

The outputs of the second hidden layer form a unit hypercube, too. The output neuron also decides a plane to divide this cube. This is shown in Fig. 3 and the plane function of the output neuron is {P_1': 5 * x'' + 6 * y'' + 6 * z'' = 3}, where x'' is the output value of the first neuron P_1, y'' is the output value of the second neuron P_2, and z'' is the output value of the third neuron P_3 in the second hidden layer. The coefficients of x'', y'', and z'' are the trained weights.

In each hidden layer, every binary number represents how many training patterns of class 0 map to it and how many training patterns of class 1 map to it. If there are only one kind of pattern of class 0 (or class 1) map to it, we say that this binary number's type is 0 (or 1) and homogenous. All binary representations in Fig. 1(a) are homogenous representations for the first hidden layer. If there are both patterns of class 0 and class 1 map to a same binary number, we say that its type is ambiguous or unfaithful (M. Mezard, and J. P. Nadal, 1989). As an example, the center region in Fig. 4(a) is in this situation, i.e., the binary number (010) of the first hidden layer is

ambiguous. The ambiguous binary number means that there are patterns belong to different classes map to the same output binary vector of the first hidden layer or any other hidden layer. If the region (010)' of the first hidden layer maps to output (0)''', the patterns of class 0 in this region are misclassified. This misclassification cannot be corrected or learned by training the all weights between the output layer and the first hidden layer. The region (001)'' shown in Fig. 4(b) is also an ambiguous region for the second hidden layer even when all regions of the first hidden layer are homogeneous. Fig 4(c) shows a compound case.

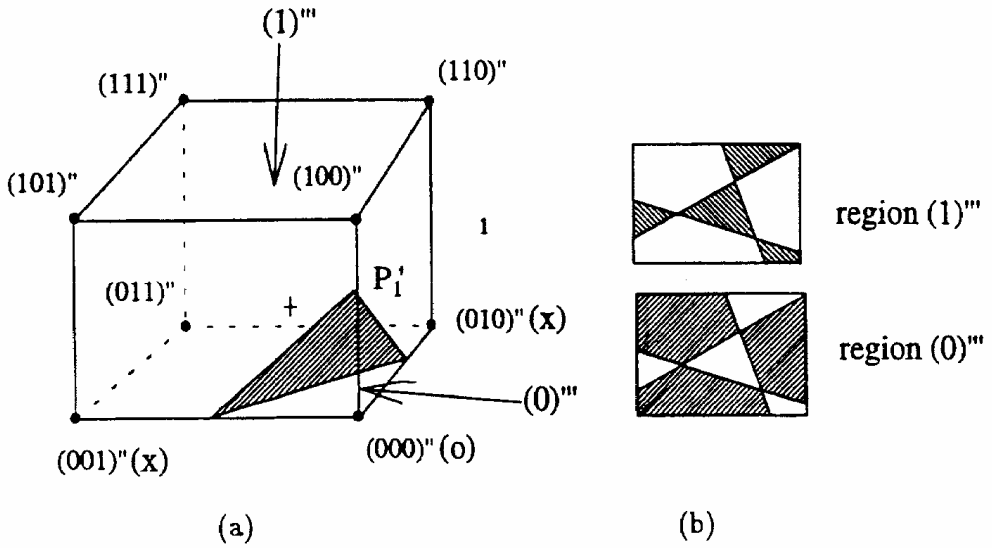


Fig. 3. The discriminated regions of the output neuron.

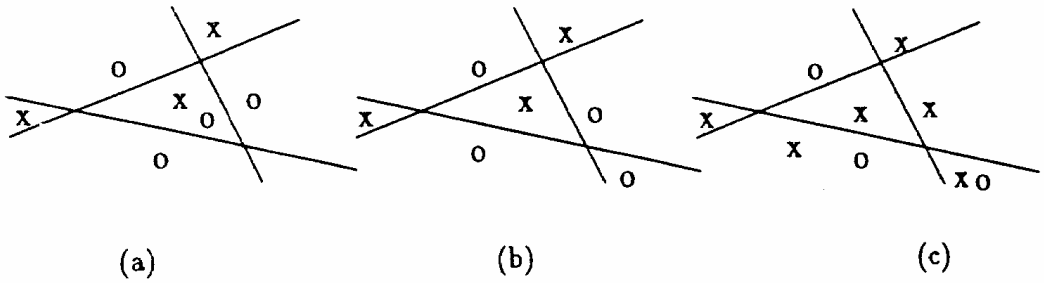


Fig. 4. Three types of different ambiguous representation.

The four elementary regions discriminated by the second hidden layer are sowing in the Fig. 2. All of the 4 binary representations are elementary building blocks of the upper output layer. In our case this means the output layer P' can discriminate patterns based on combinations of these 4 elementary regions. For example, when there are missed patterns in the region (001)'' shown in Fig. 4(b), the BP cannot converge by training the weights between the second hidden layer and the output layer.

The fact is that the patterns which cannot be discriminated in the first hidden

layer will mislead all upper layers' weights. This is because the binary represented regions of the lower layer are elementary building blocks of the regions of all its upper layers. This fact provides us the clue to improve the performance of the BP learning algorithm.

By monitoring the ambiguous binary representations for each hidden layer, we always can update the weights of the lowest hidden layer which contains any ambiguous region to improve the performance without turning the weights of all homogeneous layers below it. The learning starts from the most important first hidden layer which provides the finest elementary regions until all binary vectors of that layer represent homogeneous regions. Then we train the weights of the next upper layer and frozen all lower homogeneous layers' weights. An extra neuron is added to a hidden layer only when it fails to be homogeneous during the learning.

2. The argumented learning algorithm and simulation

Form Fig. 1, 2, and 3, each upper layer uses the successively combined discrete regions of its lower hidden layers to achieve the performance. The ambiguous regions in the lower layers can never be improved by adjusting the upper layers' weights. The ambiguous regions of the lower layers will confuse and mislead all its upper layers. According to the idea stated in the last section, to solve the ambiguous binary representation in the first hidden layer is more important than to solve the ambiguous binary representation in the second hidden layer. Thus we can solve the ambiguous binary representation problem by starting solving the ambiguous binary representation from the lowest first hidden layer.

Now let's consider how to solve the ambiguous binary representation in the first hidden layer. Initially we may train a multi-layer neural network by the formal BP learning algorithm (T. J. Sejnowski, and C. R. Rosenberg, 1986), (B. Widrow, and R. Winter, 1986). When no further improvement is seen in the level of error, we monitor the ambiguous binary representations of the first hidden layer (we check the presence of the ambiguous binary representations of the first hidden layer). If the error is small enough, we stop. Otherwise, only the lowest layer with ambiguous representations will be trained using the BP algorithm. If there exists stubborn ambiguous binary representations we add new neurons to the first hidden layer in an attempt to alleviate the number of ambiguous binary representations and include more pattern information flowing to the upper layers. To tackle this stubborn ambiguous binary representation problem, we first identify the regions and patterns belong to this ambiguous binary

numbers by calibrating the input pattern data. We then initialize the weights of the newly added neurons. This initialization is focused on adding new discriminative boundaries through each individual ambiguous region and keeping all other trained hyper boundaries.

The local training for each stubborn ambiguous region method is:

(1) Locate an ambiguous region (stubborn).
(2) Find the small set of patterns in this region.
(3) For each member of this set finding its pair (the closest pattern in the other pattern set).
(4) For each pair draw a bounding line pass the pair.
(5) Use this line as initialization for the new neuron that passes two kinds pattern data.
(6) Only these added neurons are trained during retrain and avoid that all patterns in this region are classified in the same side with one hyperplane.

Each ambiguous region can be analyzed individually. There are many methods for resolving different kinds of ambiguous regions (M. Mezard, and J. P. Nadal, 1989). We can also apply the method in (T. Denoeux, and R. Lengell, 1993) to any individual ambiguous region.

The learning starts from the first hidden layer and continues to the next upper layer until there exists no such ambiguous representation in any layer. Monitoring the ambiguous binary representation for each layer to help us understanding and improving the progress of the learning, is the introduced side process in this argumented learning algorithm. This will cost extra computations and memories. When the patterns are well cluster type, the memory size for use in memorizing the ambiguous representations is much less than the size of the total patterns. A Hamming tree can point the presence of ambiguous binary representations during the formal BP learning (T. J. Sejnowski, and C. R. Rosenberg, 1986). This tree is simple and clear for our purpose. The extra computations for obtaining this tree are on the order of the patterns with a well sorting algorithm. Fig. 5 shows the Hamming trees for several kinds of ambiguous regions as in Fig. 4. The ambiguous regions of the lower layers will propagate upwards along the tree to all linked regions of the upper layers. The presence of an ambiguous region in a layer may come from its own wrong combination of the homogeneous regions of the lower layer as in Fig. 4(b) and 5(b). It also may come from carrying on an ambiguous region of the lower layer as in Fig. 4(a) and 5(a). We can see the tree by reversing source flows spring to the tree root. Mixed source will flow to its following route but will not pollute any up stream.

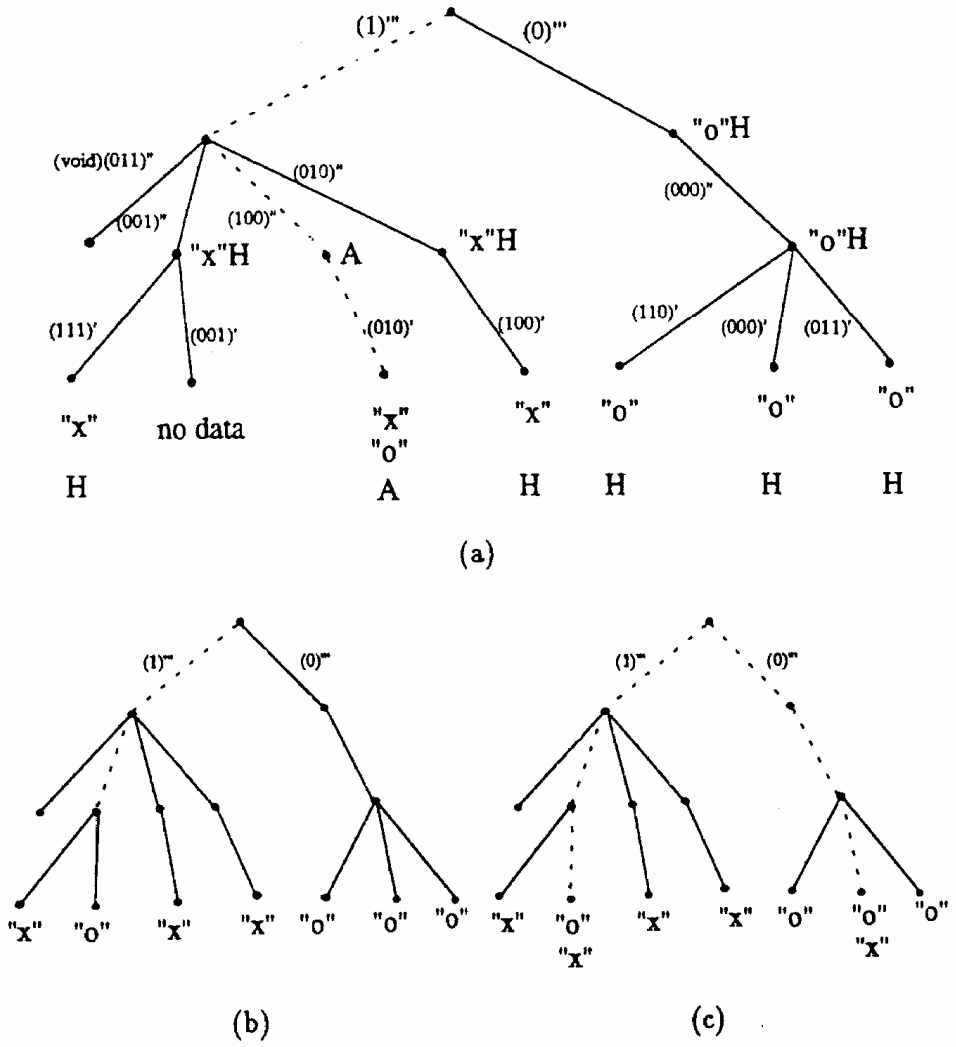


Fig. 5. The Hamming trees correspond to the cases in Fig. 4. Encoding input space (X-Y plane) or patterns into a tree structure.

For convenience, we may train a network by the formal BP algorithm and monitoring the occurrence of premature saturation (The error of the network is constantly high for a period of epoch). Once we detect its occurrence we trace the presence of the ambiguous binary representations and correct them as possible from the lowest ambiguous layer. The correction may be done by applying the formal BP to that layer and all its upper layers. Anew neuron is added only when a stubborn ambiguous representation cannot be resolved by the BP algorithm. The maximum number of hidden neurons follows the discussion in (G. Mirchandeni, and Wei Cao).

Fig. 6 shows the simulation result for a two-spirals problem. We can see that the argumented method is significantly better than the formal BP algorithm. The problem has 419(209+210) patterns which form the two spirals. The network has two hidden

layers with 5 neurons in the first hidden layer and 25 neurons in the second hidden layer. Fig. 7 shows the total amount of patterns belongs to the ambiguous regions in each hidden layer during training. Using the formal BP algorithm and the argumented BP algorithm respectively. Both trainings start with small random weights.

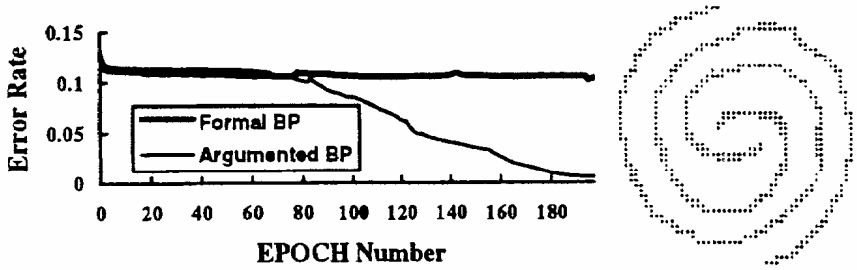


Fig. 6. The simulation result for this two-spirals' problem.

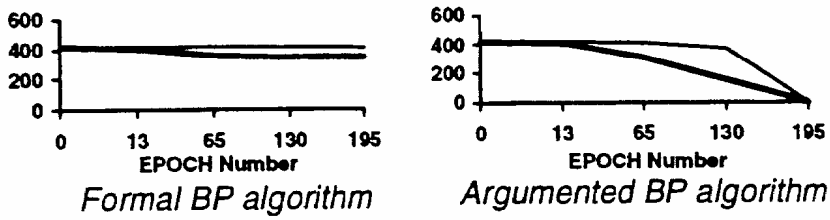


Fig. 7. Total amount of patterns belongs to the ambiguous regions in each layer. The thin line is for the second hidden layer, the thick line is for the first hidden layer.

3. Discussions and conclusions

In this work, the ambiguous binary representation problem in the multilayer perceptron is discussed. It is one of the major reasons for the learning problem of the formal BP method. We propose an argumented method to alleviate the ambiguous binary representation. Simulation results show that this argumented method can drastically reduce the learning time for many kinds of extremely difficult classification problems.

In many other works people initialize multi-layer neural networks with small random weights. According to the idea that the finest binary regions of the first hidden layer which provide very discriminative pattern information to all the upper layers and ease the learning for those layers, we would suggest to initialize the weights with regular or random discriminative boundaries which evenly spread over the pattern ranges in each layer. For each second or higher hidden layer, these boundaries would

divide the unit hypercube evenly. These boundaries will meet the suggested initialization method in (Y. Lee, S. H. Oh, and M. W. Kim, 1993). Using small random weights as initial weights, the ambiguous binary representation problem is much severe. This is because most discriminative regions may concentrate near the origin in the beginning of the learning and they progress slowly to cover the wide ranges of patterns. This will cause insufficient pattern information flowing to the upper layers to afford the beginning learning informal BP learning.

Since the formal BP learning algorithm uses the error of the whole network as its all updating information, any local ambiguous region cannot be accurately corrected by using this error only. The BP algorithm will even revise all layers when lowest layers are all homogeneous. This makes no sense. Since we can locate ambiguous regions accurately, we can save computations, speed the learning, improve the performance in the argumented method.

Addendum

The neural networks, which had been trained completely, may have redundant neurons. The existence of those neurons doesn’t affect the training result. We can remove those neurons to save computing time and reduce the complexity of the whole network. Those redundant neurons have three types.

(1) Idle neuron (void neuron): unchanged sign for all training patterns.

(2) Neuron has same sign (or reversed sign) as any other neuron.

(3) Homogeneity unchanged when we suppress this neuron.

The above three type neurons can be detected by a simple method: For each neuron in the network, remove it. If cause ambiguous situation, put it back. Otherwise, this neuron is redundant.

On the other hand, when we remove a neuron will cause most homogeneous regions becoming inhomogeneous (ambiguous) region; this neuron is the most significant neuron in its layer.

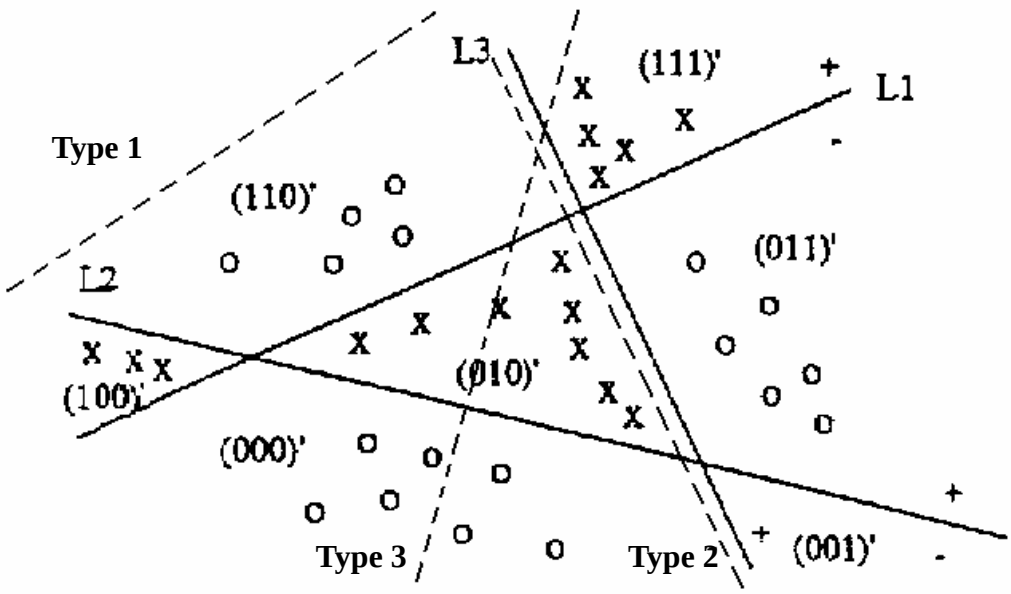
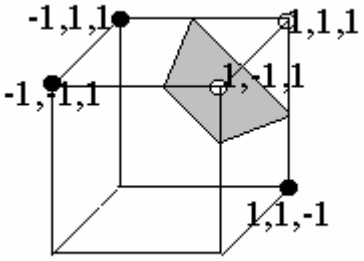


Fig. 8. The three types of redundant neurons.

We can remove the redundant neurons. Can we also remove the redundant synaptic connections (weights)? Consider the following neuron.



Input data:

○: (1, 1, 1), (1, -1, 1)

●: (-1, 1, 1), (-1, -1, 1), (1, 1, -1)

Training result:

W = (-10.5420, 3.4399, -7.1210)

Bias = 6.6073

Observe the distribution of input data on the cube. We find that the cube can map to a 2D plane and doesn't affect the classification.

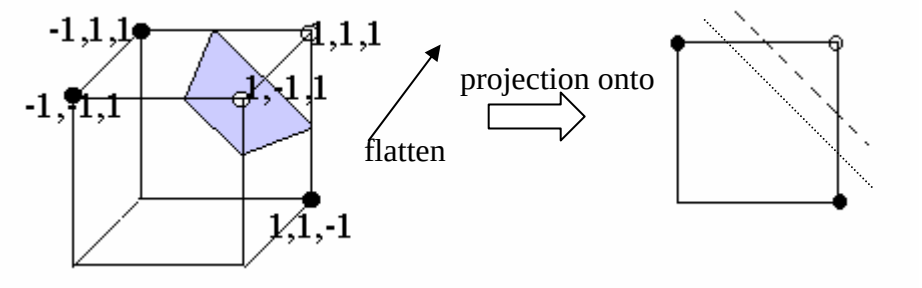
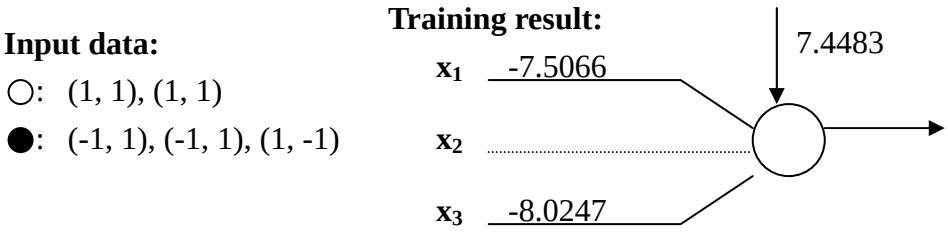


Fig. 9. The mapping from 3D cube to 2D plane.

So we can remove the second synaptic connection and retrain the neuron using 2 dimension input data. (If the neuron uses hard limit transfer function, we don't need to retrain the neuron.)



We can find the redundant synaptic connection by the method similar to find the redundant neurons. For each dimension of input data, remove it. If cause different dichotomy of this neuron, put it back. Otherwise, the corresponding synaptic connections are redundant. Then we remove the maximum removable synaptic connections.

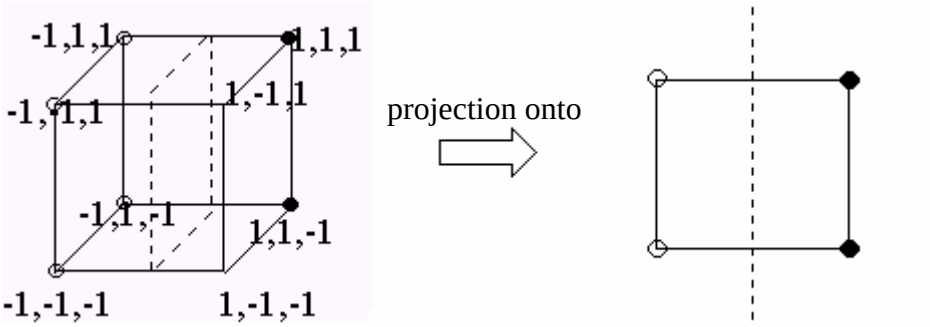


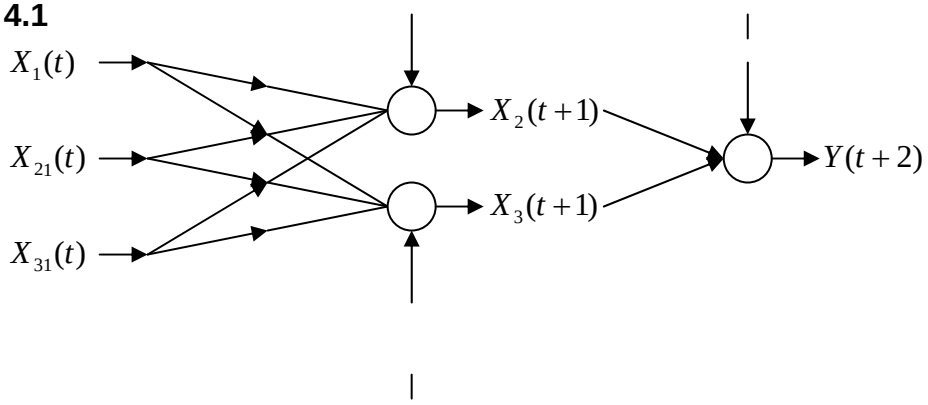
Fig. 10. An other example of mapping from 3D cube to 2D plane.

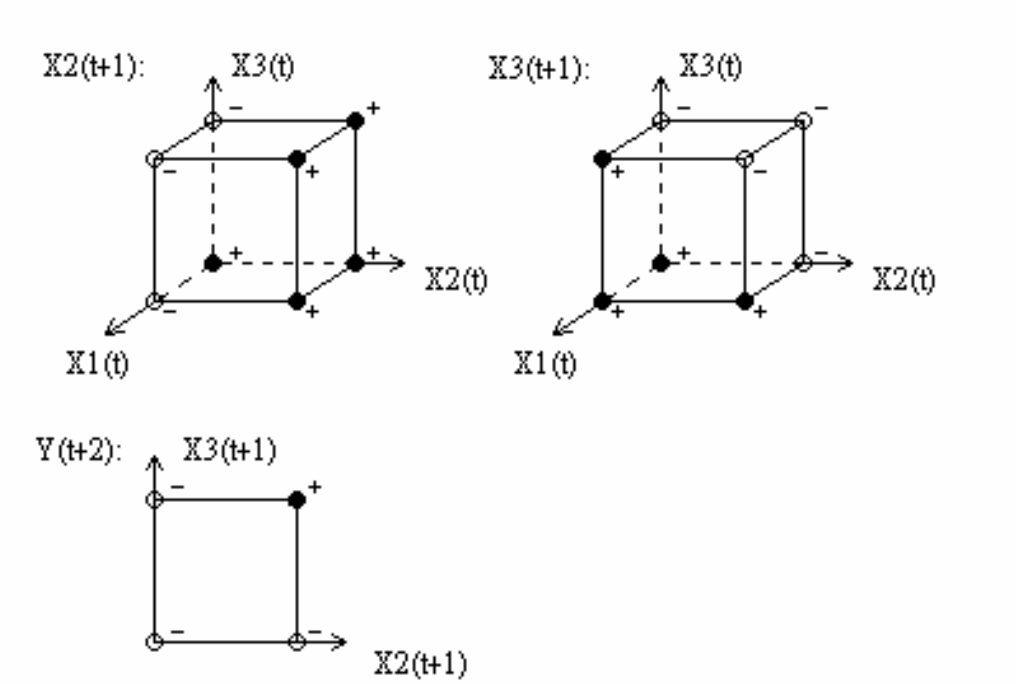
For each neuron in the network that had been trained completely, we remove the redundant synaptic connections and retrain the neuron. We will get a quiet compressed neural network finally.

We also can build a compressed network before training by observing the input patterns. Removing the synaptic connections is the same as reducing the dimensions of input pattern. That will save a lot of training time.

Exercise

4.1





Discuss and analyze the above Elman network on the sequence $x_1(t)$, t = 1, 2, … and y(t), t = 1, 2, 3, …..