Smoothing of Chemical Analysis Data by Neural Networks

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We applied neural networks to the smoothing of chemical data. The input data corresponding to the spectra of X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES) were prepared by adding the noise to the original signals, which consist of one peak or two peaks with a Gaussian distribution. The results of smoothing by neural networks were compared with those by the previous methods, that is, a polynomial approximation method or a spline method. From the results, we found that the signal curve was able to be reproduced, even if 200% noise was included in the input pattern. Therefore, the neural network is thought to be effective in smoothing the chemical data including noise.

1. INTRODUCTION

In general, the spectra observed with various chemical analysis methods such as X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES) included the noise, which is caused by the performance of experimental instruments. In order to analyze the spectra, it is necessary to remove a background from the spectra and to smooth the chemical data. Especially, the smoothing of chemical data has been carried out by a spline method, a polynomial approximation method and a method of least squares up to date. However, there are many problems when above methods are used for real chemical data. One of them is to determine many optimum parameters for the smoothing of chemical data, which has been searched by trial and error. The optimum parameters directly affect the results of smoothing.

Neural networks are applied to various fields. The typical neural network with unsupervised learning or competitive learning is self-organizing maps (SOM)[1,2,3,4,5], whereas the typical neural network with a supervised learning is a back-propagation method (BP) [6,7,8,9].

Recently, the neural networks begun to be applied to the analysis of chemical data. We previously reported that the neural networks with SOM and BP method were useful in analyzing XPS and AES data quantitatively without determining the number and the shape of XPS or AES peaks[10,11]. In addition, we reported that XPS and AES spectra were able to be classified by the neural networks without any pre-processing of chemical data in order to identify the chemical species[11,12]. However, the performance of neural networks for the smoothing of chemical data is not clarified significantly.

In this study, we applied neural networks to the smoothing of chemical data, for example, XPS and AES spectra. Here, two BP neural networks were used for smoothing of chemical data.

2. EXPERIMENTAL

We used three-layered neural network of BP1 with input layer (1 unit), hidden layer (10 units) and output layer (1 unit) as shown in Fig.1. The learning algorithm was a Back Propagation (BP) method. Here, the input data is the Y-value for the X-value on the signal curve. In the neural network learning coefficient and momentum factor in BP1 networks were 0.8 and 0.9, respectively.

The input patterns for learning and testing were prepared by adding the noise to the original signal curves, which consist of one peak or two peaks with a Gaussian distribution. X% noise of the average of Y-values over the signal curve was added to the signal curves. The

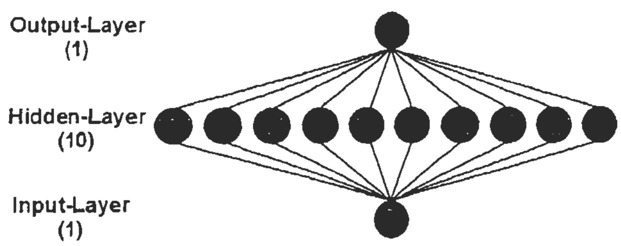

Fig.1 Structure of BP1 neural network

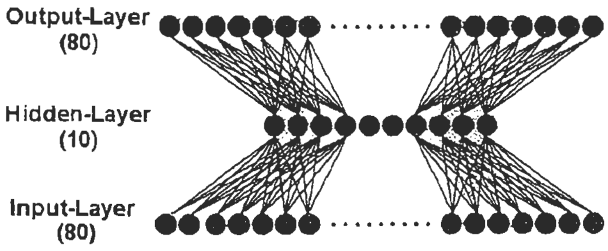

Fig.2 Structure of BP2 neural network

experimental results were obtained for the noise range from X=0 to 300%. When the curves of signal + X% noise were used as an input pattern, we investigated whether the signal curve can be reproduced after learning. The curve of the signal + X% noise was prepared as input patterns. Since we know the solution for input patterns, we can exactly estimate the performance of neural networks for the smoothing of input patterns.

Fig.2 shows the three-layered neural network of BP2 with input layer (80 units), hidden layer (10 units) and output layer (80 units). The learning algorithm was a BP method. In the neural network learning coefficient and momentum factor in BP2 networks were 0.8 and 0.9, respectively.

3. RESULTS and DISCUSSION

Fig.3 shows the curves of signal, signal + 300% noise and the calculated results. The signal + 300% noise was prepared by adding 300% noise to the signal curve, which consists of one peak with a Gaussian distribution. The result was obtained with the BP1 neural network (after learning). After learning iterations of 10,000, the curve of signal + 300% noise became smooth, which was nearly equal to the curve of signal. The result calculated by a sixth polynomial approximation method, was nearly equal to the result after learning. However, the result at about X=0 and X=1.0 was very different from the signal curve and the result after learning with the BP1 neural network.

Although the figure are not shown, the results after learning tend to approach to the signal curve with increasing learning iterations. In addition, the result of BP1 neural network may be improved and modified by using an optimum network structure.

Fig.4 shows the curves of signal, signal + 200% noise and the calculated results. The signal + 200% noise was prepared by adding 200% noise to the signal curve, which consists of two peaks with a Gaussian distribution. After 50,000 learning iterations, the result was nearly

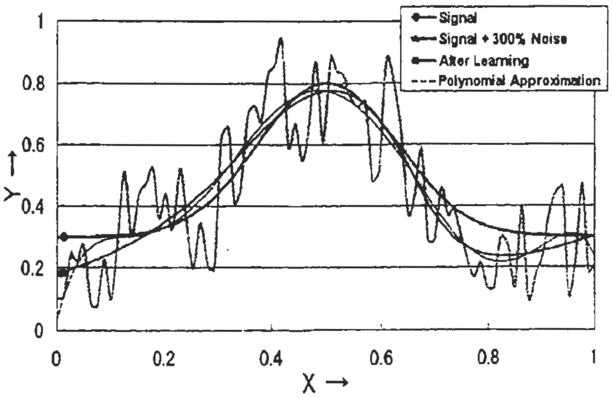

Fig.3 Result by a BP1 neural network
-one peak-

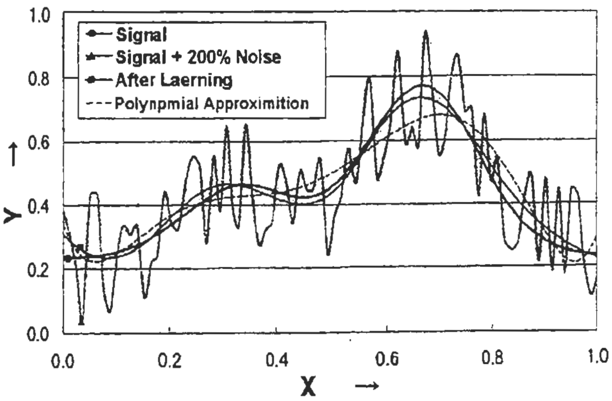

Fig.4 . Results by a BP1 neural network
-two peaks-

equal to the signal curve except X=0, whereas the result obtained by the sixth polynomial approximation method was different from the signal curve. This indicates that the signal curve was able to be reproduced by using the neural network of BP1, even if 200% noise was included in the signal curve. Therefore, the neural network of BP1 after learning can reproduce the signal curve better than the sixth polynomial approximation method.

Fig.5 shows the square error of the BP1 neural

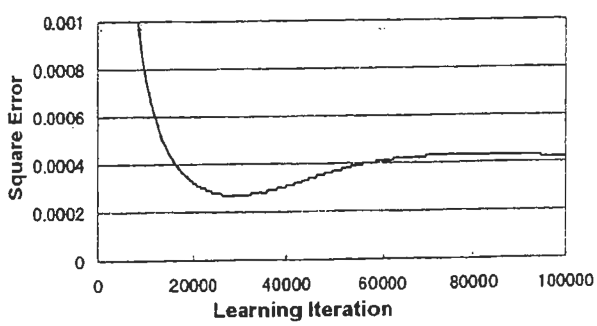

Fig.5 Square error as a function of learning iteration

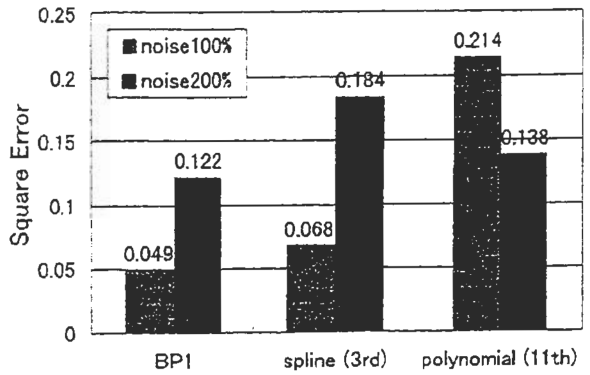

Fig.6 Square errors by various methods of a BP1 neural network, a 3rd spline method and a 11th polynomial approximation method.

network as a function of learning iteration. The square error begins to decrease with increasing learning iteration. Then, the square error became minimum at about 30,000 learning iterations, and again increased with learning iterations. Finally, the square error of BP1 neural network was saturated at about 60,000 learning iterations.

Although the figures were not shown, the smoothing of the signal + 200% noise curve was also carried out with a third spline method and an eleventh polynomial approximation method. The result obtained eleventh polynomial approximation method was nearly equal to that with the BP1 neural network except both edges, where the BP1 neural network was better than the eleventh polynomial approximation method. The result obtained with the third spline method was nearly equal to that with the BP1 neural network except about a high peak, where the BP1 neural network was better than the third spline method. We calculated the square error of the results obtained with the BP1 neural network, the third spline method and the eleventh polynomial approximation method for the original signal curve.

Fig.6 shows the square error of the results for the input signal curve. The results were calculated with the neural network of BP1, the third spline method and the eleventh polynomial approximation method. The square errors obtained with BP1 neural network and the third spline method were less than that with the eleventh polynomial approximation method for the curve of signal + 100% noise. For the input data of signal + 200% noise, the square error obtained with the BP1 neural network was less than that of the eleventh polynomial approximation, and it was less than that of the third spline method. From the results, we found that the smoothing of the BP1 neural network

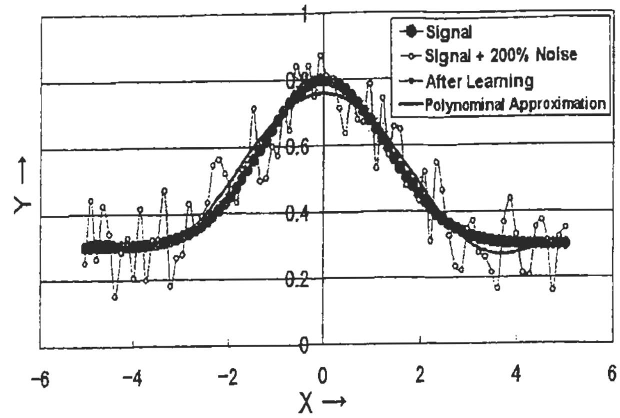

Fig.7 Results by a BP2 neural network -one peak-

was better than those of the third spline method and the eleventh polynomial approximation method for the input patterns of the signal + 100% and the signal + 200% noise.

Fig.7 shows the curves of signal, signal + 200% noise and the calculated results. The signal + 200% noise was prepared by adding 200% noise to the signal curve, which consists of one peak with a Gaussian distribution. The result obtained with the BP2 neural network was approximately equal to the signal curve. This indicated that the signal curve was able to be reproduced by using the neural network of BP2, even if 200% noise was contained in the input pattern. However, the result obtained with the sixth polynomial approximation method was worse than that of the BP2 neural network. Although the BP2 neural network is able to reproduce the signal curve, the network has to learn true data.

4. CONCLUSION

We applied neural networks of BP1 and BP2 to the smoothing of chemical data, which were prepared by adding noise to the peaks with a Gaussian distribution. The neural network of BP1 is effective in smoothing the chemical data including noise, when the shape of the curve is unknown. In addition, the neural network of BP2 is effectively used for smoothing of the data, when the original shape and function of the curve is previously known. Therefore, the neural networks are thought to be effective in smoothing the chemical data including much noise.

5. References

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