

Modeling chemical processes using multiresolution representation neural networks

K. Yoda

*Production Engineering Administration, Asahi Chemical Industry Co. Ltd.,
2-1, Samejima, Fuji-city, Shizuoka-pref., 416 Japan, E-mail:
yoda@asahi-kasei.co.jp*

and

T. Furuya

*Toho University, Faculty of Science, Department of Information Science, Miyama
2-2-1, Funabashi-city, Japan, E-mail: furuya@toho-u.ac.jp*

1. Introduction

This chapter discusses neural networks that use multiresolution representation signals as their input, and the use of those neural networks for modeling nonlinear chemical systems. Decomposing an original signal into a multiresolution representation enables its analysis at different resolutions. By using a multiresolution representation as its input, neural networks can substantially expand the time range of a signal. According to the wavelet theory, these decomposition signals can be used to easily reconstruct an original signal, and certain types of feedforward neural networks can learn this reconstruction. We have studied the modeling with this type of neural network for a nonlinear system with a highly underdamped system and a continuous polymerization reactor.

In chemical engineering, feedforward neural networks have proven to be the most popular tool for modeling and control problems. The use of neural networks for modeling is more effective than traditional methods such as the ARMA model [1, 2].

However, in a real chemical process, the input/output signals include noise and disturbance. This may impose unknown parameters such as time constants, delay times and so on. In addition, the sampling rate and time may be less than ideal. In such situations, when a neural network is used for modeling, that input layer needs a large number of input nodes to enable it to gain sufficient information about the target plant. But, by increasing the number of nodes, the learning time becomes long and the process is more difficult.

Using a multiresolution representation as the input for a neural network, the above problems can be avoided.

Multiresolution representations are a highly effective means of analyzing the information content of chemical plant signals. Multiresolution decomposition enables us to perform scale-invariant interpretation of the signal. At different resolutions, the details of a signal generally characterize different physical phenomena. For a coarse resolution, these details correspond to the trend of the system. On the other hand, at a fine resolution, they may correspond to noise or local phenomena in time.

Using multiresolution representations as input can substantially expand the time range of a signal.

2. Multiresolution representation

The concept of multiresolution representation of functions was introduced by Mallat [3]. This provides a powerful framework to enable the understanding of wavelet decomposition. The basic idea of this process is one of successive approximation, together with “added detail”, as one goes from one approximation to the next finer one. Assume we have a ladder of spaces such that:

$$\cdots \subset V_2 \subset V_1 \subset V_0 \subset V_{-1} \subset V_{-2} \cdots \quad (1)$$

with the property such that if $f(x) \in V_i$ then $f(2x) \in V_{i-1}$. V_{i-1} is a lower resolution sub-space than V_i . Call W_i the orthogonal complement of V_i in V_{i-1} .

$$V_{i-1} = V_i \oplus W_i \quad (2)$$

Thus, W_i contains the “detail” necessary to go from V_i to V_{i-1} . Iteration (2) gives

$$V_{i-1} = W_i \oplus W_{i+1} \oplus W_{i+2} \cdots \quad (3)$$

That is, a given resolution can be attained by summing the added details.

Given an original sequence f_0 , $n \in Z$, we can derive a lower resolution signal by low pass filtering with a halfband low pass filter having an impulse response $g(n)$.

$$f_1(n) = \sum_{k=-\infty}^{+\infty} g(k)f_0(n-k) \quad (4)$$

which is $f_0(n) \in V_0$, $f_1(n) \in V_1$. From (2),

$$d_1(n) = f_0(n) - f_1(n), d_1(n) \in W_1 \quad (5)$$

$d_1(n)$ contains the detail needed to go from $f_1(n)$ to $f_0(n)$. See Figure 1.

3. Modeling using neural networks

For simple neural networks used for modeling, the initial input is a moving window of time series data. Then, the next time step value for the system is estimated. See Figure 2. The window size corresponds to a time range and is usually fixed.

When using multiresolution representations as the input, the data input to the neural network is the value of each decomposed signal at time t . Figure 3 shows multiresolution representation neural network (MRR neural network).

4. Examples

We consider two examples to illustrate the use of MRR neural networks. The first example is a highly underdamped system and the second one is a continuous polymerization reactor.

4.1. Example 1: An underdamped system with a delay

The process used in this illustrative example was drawn from the article by Tulleken [4]. It is a highly underdamped system defined by the following transfer function:

$$G(s) = \frac{1}{2s^2 + 0.4s + 1} \quad (6)$$

In addition, a four-unit time step delay and white noise was added to this transfer function.

The plant neural models were trained using data sets consisting of 450 input-output pairs. The training data sets were obtained by randomly varying the input to the plant within the range of $[-2, +2]$. See Figure 4.

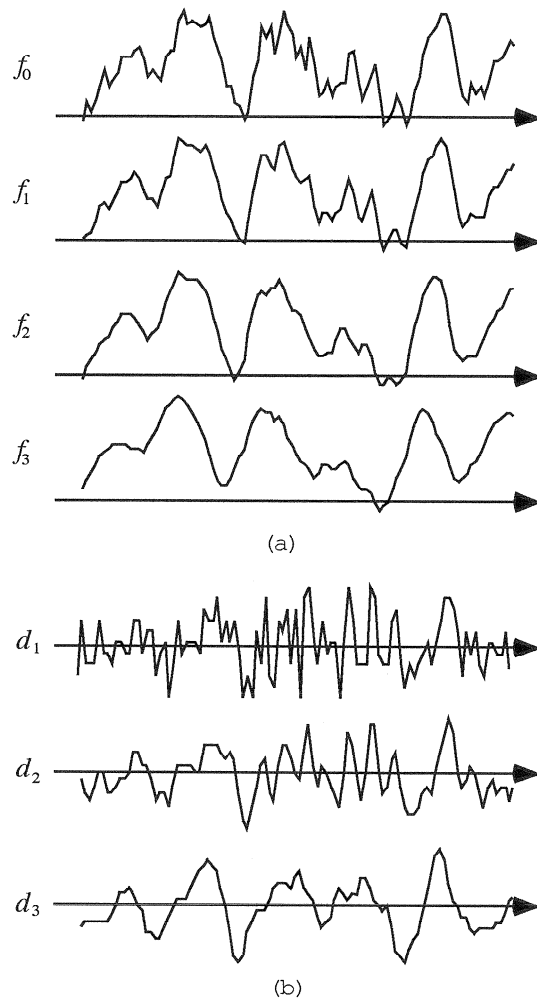


Figure 1. (a) Multiresolution approximation. f_0 is an original signal. f_1, f_2, f_3 are the approximations of function f_0 at each of resolutions $1/2, 1/4$ and $1/8$. (b) Multiresolution representations. d_1, d_2, d_3 are the details at each of resolutions $1/2, 1/4$ and $1/8$.

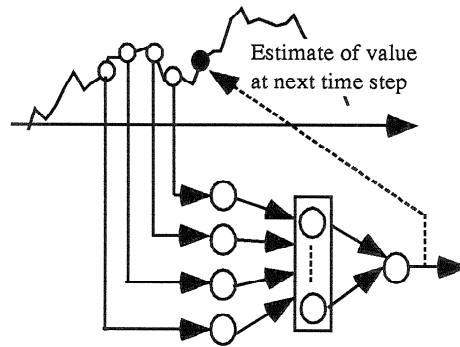


Figure 2. Simple neural network.

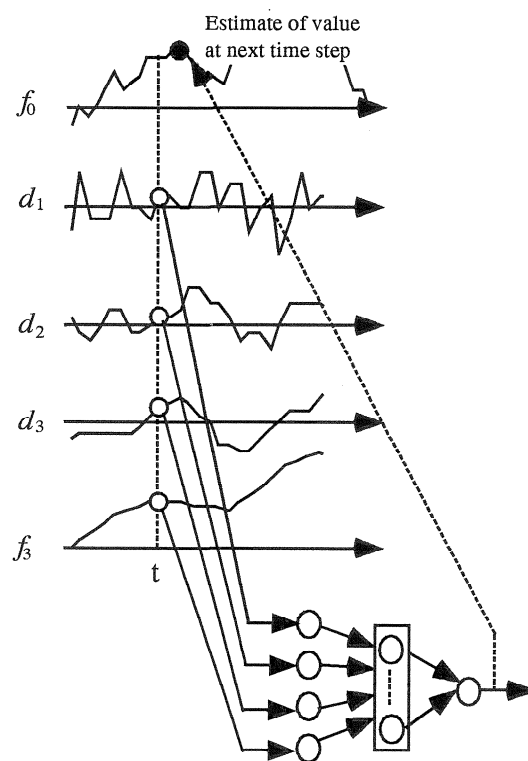


Figure 3. MRR neural network.

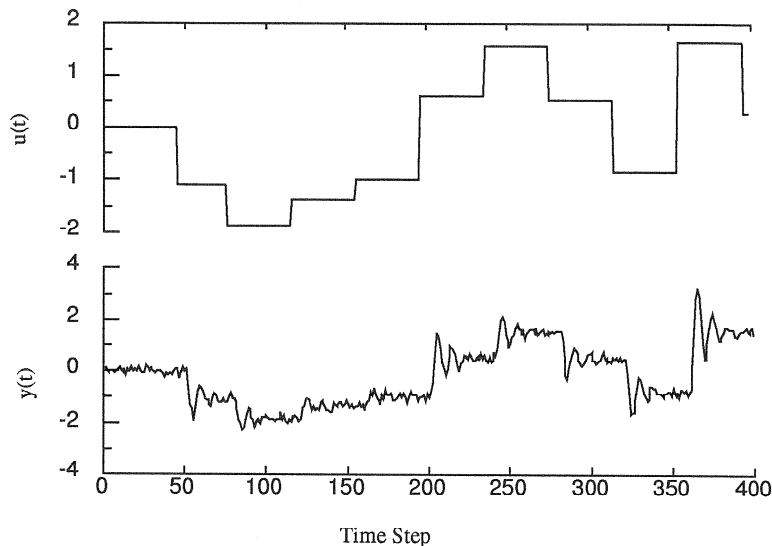


Figure 4. Training Data.

For simple neural networks, the next time step value is estimated from the four previous output values, three previous inputs and a next time step input value. For multiresolution representation (MRR) neural networks, the value for the next time step is estimated from the four output values at four different resolutions, as well as the four input values at those same four resolutions.

After the neural network was trained by backpropagation, the performance of the neural network was evaluated by using unknown input data. Figure 5 shows the step response. It can be seen that the simple neural networks failed to learn the delay time. The MRR neural networks, however, were able to learn the delay and learn the model more accurately.

4.2. Example 2: Methyl methacrylate polymerization

The second example concerns the CSTR described by Daoutidis [5] shown in Figure 6 where the free-radical polymerization of methyl methacrylate (MMA) takes place, with azo-bis-isobutyronitrile (AIBN) as the initiator and toluene as the solvent. The reaction is exothermic, hence a cooling jacket is provided to remove the heat.

The input to the neural networks is the volumetric flow rate of the cooling water. The output is the reactor temperature.

The learning data sets are contained in 950 input-output pairs. The training data is shown in Figure 7. In the same way as in example 1, after training

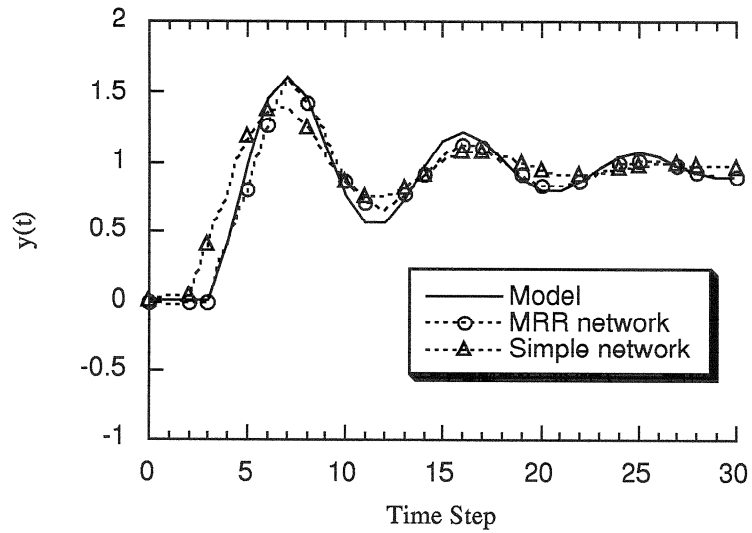


Figure 5. Step Response.

the neural networks, the simple neural networks and MRR neural networks are evaluated on the basis of their unknown step response. The results are shown in Figure 8. The results of this example are similar those in example 1. The simple neural networks did not learn the delay time. The MRR neural networks, however, learned the delay time, and also learned the model more accurately.

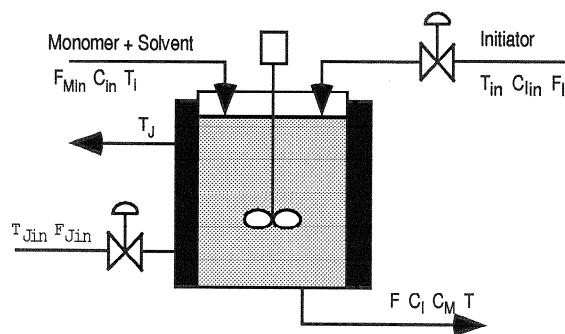


Figure 6. Simulated continuous polymerization reactor.

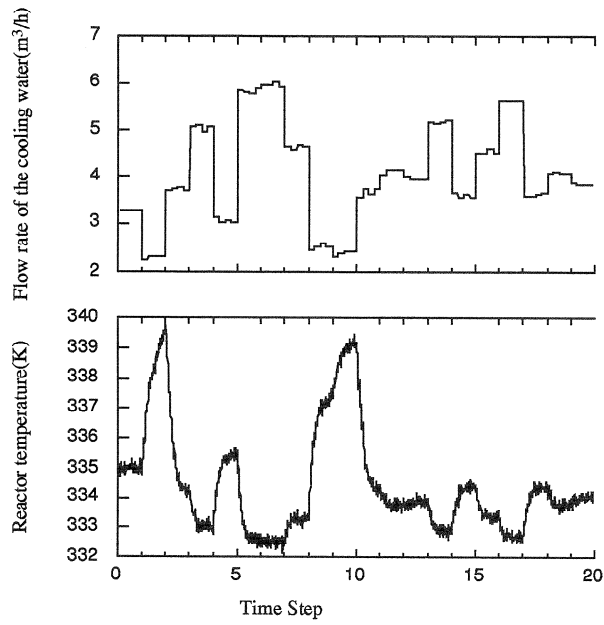


Figure 7. Training Data.

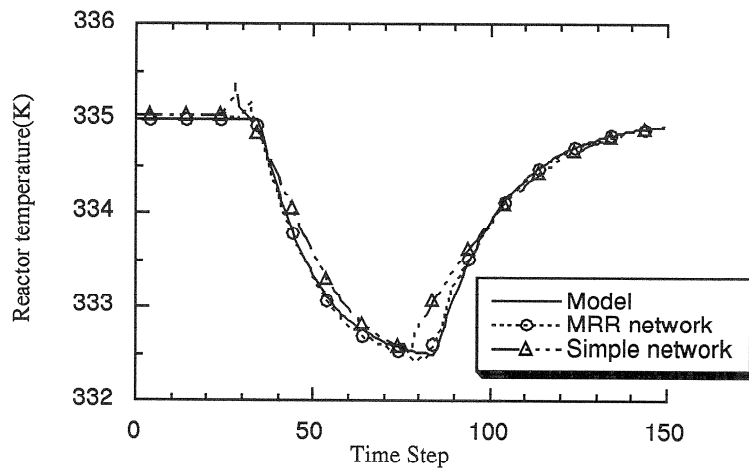


Figure 8. Step Response.

5. Conclusion

This chapter has discussed neural networks that use multiresolution representation signals as their input and the use of those neural networks for modeling nonlinear chemical systems. Modeling ability is compared for simple neural networks and MRR neural networks. The MRR neural networks can both learn the model more accurately, and also learn the delay.

References

- [1] N. V. Bhat, P. A. Minderman, T. McAvoy, and N. S. Wang (1990), "Modeling Chemical Process Systems via Neural Computation", *IEEE Control Systems Magazine*, Vol. 10, pp. 24-25
- [2] J. F. Pollard, M. R. Broussard, D. B. Garrison and K. Y. San (1992), "Process identification using neural networks", *Computer chem Engng*, Vol. 16, No. 4, pp. 253-270
- [3] S. G. Mallat (1989), "A Theory for Multiresolution Signal Decomposition: The Wavelet Representation", *IEEE Trans.on Pattern Analysis and Machine Intelligence*, Vol. 11, No. 7
- [4] Tulleken, H. (1990), "Generalized Binary Noise Test-Signal Concept for Improved Identification — Experiment Design", *Automatica*, 26, 1, pp. 37-49
- [5] P. Daoutidis, M. Soroush and C. Kravaris (1990), "Feedforward/Feedback Control of Multivariable Nonlinear Processes", *AIChE Journal*, Vol. 36, No. 10, pp. 1471-1484