Implementation of SEEK-FIND algorithm for diagnosis and prediction of pollution states

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Abstract

In order to enhance the estimation rate of the SEEK(Switching mode Enhanced Extended Kalman) algorithm an artificial neural network is embedded within the SEEK algorithm. The SEEK-FIND(SEEK For Initialisation of Neural Descriptor) algorithm is efficient to estimate state variables in multi-modal nonlinear systems such as contaminant dispersion processes. When a nonlinear system has regularities and irregularities such as bifurcation the neural network is applied to estimate the regular states after leaning by using the state variable estimated from the SEEK filter as teacher signals. The SEEK filter takes over again when the system shows irregularities. The SEEK filter and the neural network are automatically switched by monitoring the maximum estimation error. The numerical demonstrations indicate the state variables are accurately estimated and the estimation speed is enhanced in the SEEK-FIND algorithm.

1 Introduction

The SEEK(Switching mode Enhanced Extended Kalman) algorithm[1,2] has been developed so as to maximise the convergence rate of the estimation error covariance matrix by selecting the optimal observation matrix. The SEEK algorithm has been proved to achieve the excellent performance in estimating the state variables even in complicated chaotic systems such as a Lorenz system with a switched parameter[2]. However, the algorithm seems to be redundant in the case where the system is in a regular state, or the state variables take no abrupt change as can be seen in the switched Lorenz system[2]. Frequent switching of the observation matrix is inefficient in estimating regular state variables for saving the estimation time.

The SEEK-FIND(SEEK For Initialisation of Neural Descriptor) algorithm is inspired by the idea that the calculation time for the estimation of state variables is decreased when an artificial neural network is incorporated and applied to estimate the state variables in a regular state. The SEEK filter is applied to initialise and optimise the neural network and to take over it again when the maximum estimation error crosses over a desired value in an irregular state. We sometimes come across irregularities in estimating pollution state variables. For example, the parameters involved in a state equation describing a pollution state have to be abruptly varied due to environmental irregularities.

The combination of the extended Kalman filter and a neural network recently appears not only in the system estimation but also in the modification of the leaning algorithm of the neural network. Simutis, Havlik & Luebbert[3] have estimated the states of a biotechnical process using the fuzzy aided extended Kalman filter and neural networks. Watanabe, Fukuda & Tzafestas[4], Iiguni, Sakai & Tkumaru[5], Ishida et. al.[6], Puskorius & Feldkamp[7] and Ruck et. al.[8] have proposed Kalman filter assisted leaning algorithms for neural networks to enhance the learning speed instead of the error back propagation algorithm.

In this paper, the structure of the SEEK-FIND algorithm is explained in the second section. Then the SEEK-FIND algorithm is implemented and applied to estimate the state variables in the parameter-fixed Lorenz system and the parameter-switched Lorenz system in the third section. The concluding remarks are summarised in the final section.

2 SEEK-FIND algorithm

The SEEK algorithm was inspired by the motive of enhancing the convergence rate of the estimation error covariance matrix by optimally selecting the observation matrix. However, it takes longer time to estimate state variables because the optimisation has to be carried out in each time step. We discuss here on a system described by a nonlinear state equation accompanied with a linear observation equation, which are generally written as

$$\dot{x}(t) = f[x(t)] + g[x(t)]w(t) \tag{1}$$

$$y(t) = H(t)x(t) + v(t) \tag{2}$$

where $x(t)$ is the n-th order state vector at time t, $y(t)$ is the observation vector, f and g are the nonlinear functions of $x(t)$, $H(t)$ is the observation matrix, $w(t)$ is the system Gaussian white noise with the covariance matrix of Q and $v(t)$ is the observation Gaussian white noise which is independent of the system noise and has the covariance matrix of R.

In the SEEK algorithm the switching mode observation matrix is defined by

$$H(t) = \mathrm{diag}[\mu_1, \mu_2(1-\mu_1), \cdots, \mu_{n-1}\prod_{i=1}^{n-2}(1-\mu_i), \prod_{i=1}^{n-1}(1-\mu_i)] \tag{3}$$

and the parameters are decided so as to maximise the convergence rate of the error covariance matrix given by

$$\dot{P} = FP + PF^T + GQG^T - PH^TR^{-1}HP \tag{4}$$

where P is the error covariance matrix, F is the Jacobian matrix derived from the nonlinear state equation (1) for which the current estimates are substituted, G is the current driving matrix and the superscript T denotes the transpose of the matrix.

Thus the current objective function is derived from taking into account the Jacobian matrix of Equation (4) [2] and given by

$$J = \mathrm{abs} < \sum_{i=1}^{n} a_{ii} - \{\mu_1^2 \hat{P}_{11} + \mu_2^2 \hat{P}_{22}(1-\mu_1)^2 + \cdots + \mu_{n-1}^2 \hat{P}_{(n-1)(n-1)} \prod_{i=1}^{n-2}(1-\mu_i)^2 + \hat{P}_{nn}\prod_{i=1}^{n-1}(1-\mu_i)^2\}] > \tag{5}$$

where $a_{ii}(i = 1,\cdots,n)$ is the diagonal component of the matrix F, $\hat{P}_{ii}$ denotes the estimate of the diagonal component of the error covariance matrix. The conjugate gradient algorithm proposed by Fletcher & Powell[9] is applied to maximise Equation (5) in the SEEK algorithm.

In order to reduce the switching frequency for the observation matrix and enhance the estimation speed we propose the SEEK-FIND algorithm. The leaning algorithm is illustrated in Figure 1. The SEEK filter produces state estimates using an optimal observation. The current observation and one step delayed estimates are utilised as the input signals, whilst the current estimates from the SEEK filter are regarded as the teacher signals to the neural network. The error between the teacher signal and the output of the neural network is back-propagated and the link weight matrices between layers are decided so as to minimise the estimation error. The SEEK filter and the neural network work parallel in the training stage.

The estimation algorithm for the neural network is illustrated in Figure 2. The SEEK filter is switched off after the neural network has completed leaning. Then the trained neural network works to estimate state variables using a current observation and the one step delayed outputs as the input signals. The SEEK filter is switched on and the leaning of the neural network starts again when the trajectory of an estimate goes on a wrong way compared with an observation. The training and estimation stages are automatically switched in the SEEK-FIND algorithm by monitoring the estimation error, which makes the overall estimation time shorter.

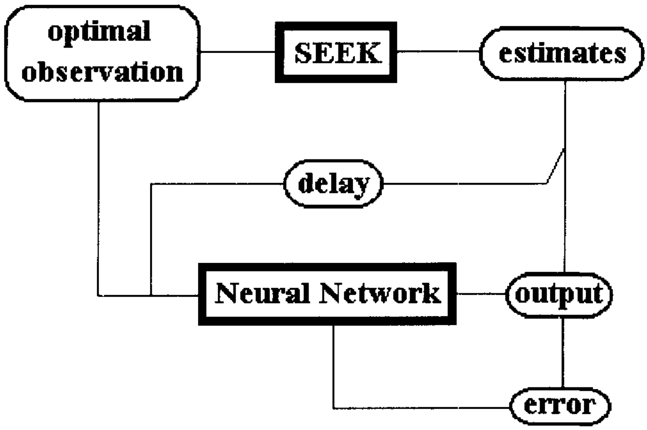

Figure 1: Learning algorithm for the neural network in the SEEK-FIND algorithm

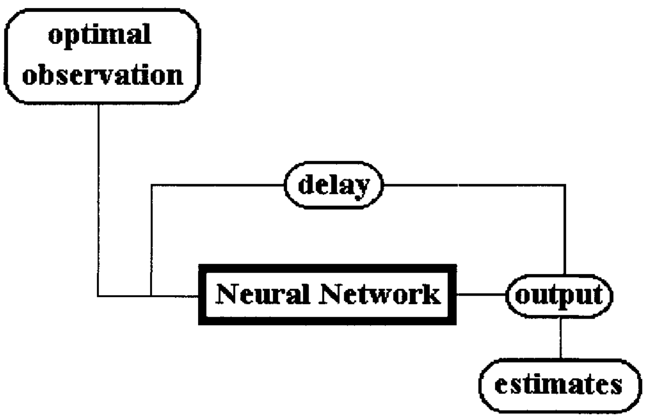

Figure 2: Estimation algorithm for the trained neural network in the SEEK-FIND algorithm

3 Application of the SEEK-FIND algorithm

As a model illustration here, we offer the following Lorenz equation[10] with superimposed Gaussian white noise;

$$\begin{bmatrix} \dot{x}(t) \\ \dot{y}(t) \\ \dot{z}(t) \end{bmatrix} = \begin{bmatrix} -\sigma & \sigma & 0 \\ r & -1 & -x \\ y & 0 & -b \end{bmatrix} \begin{bmatrix} x(t) \\ y(t) \\ z(t) \end{bmatrix} + \begin{bmatrix} g_{11} & \cdots & g_{1m} \\ g_{21} & \cdots & g_{2m} \\ g_{31} & \cdots & g_{3m} \end{bmatrix} \begin{bmatrix} w_1(t) \\ w_2(t) \\ w_3(t) \end{bmatrix} \tag{6}$$

where the Lorenz parameters σ, r and b are positive definites, m is the order of the system noise, g_{jk} denotes the jk-th component of the driving matrix. We have focused attention on the parameter sets $\sigma=10$, $b=8/3$, $r=28$ and 112 when the strange attractors are activated[11], namely $r=28$ is selected in the parameter-fixed system and the parameter r is switched between 28 and 112 in the parameter-switched system.

The structure of the neural network embedded within the SEEK-FIND algorithm is illustrated in Figure 3.

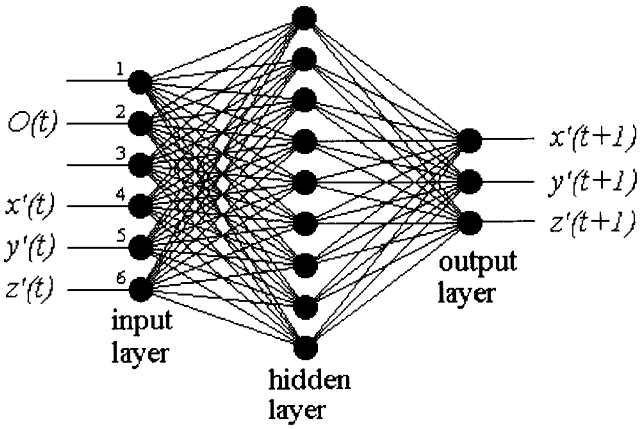

Figure 3: Neural network embedded within the SEEK-FIND algorithm

The numbers of the neurones are 6 in the input layer, 9 in the hidden layer and 3 in the output layer. The optimal observation $O(t)$ is taken into the No.1 input neurone when $O(t)$ is related to $x(t)$ and the No.2 and No.3 input neurones are not excited. The $y(t)$-related $O(t)$ is taken into the No.2 neurone, whilst the $z(t)$-related $O(t)$ excites the No.3 neurone. One step delayed estimates $x'(t)$, $y'(t)$ and $z'(t)$ are taken into the No.4, No.5 and No.6 neurones, respectively.

The link weight matrix between the input layer and the hidden layer or between the hidden layer and the output layer is optimised by the conventional error back-propagation method[12]. The leaning speed is enhanced by using the adaptive momentum algorithm[13]. The training of the neural network is completed for the Lorenz system with the parameter of r=28 when the sum of the squared errors is lower than a desired value. Then the neural network operates to produce the estimates $x'(t+1)$, $y'(t+1)$ and $z'(t+1)$ until the maximum estimation error crosses over a desired value. For example, leaning starts again when the system with r=28 is switched to the system with r=112.

The performance of the SEEK-FIND algorithm applied to the Lorenz system with the parameter of r=28 is shown in Figure 4.

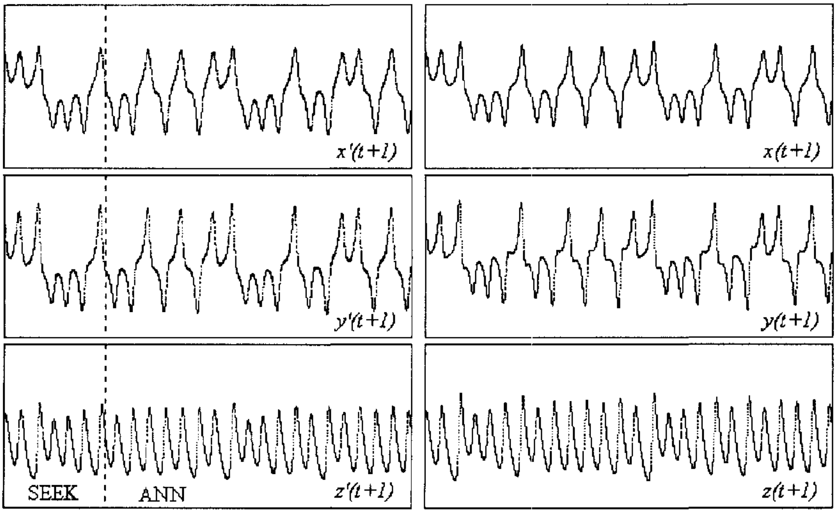

Figure 4: Estimation of the parameter-fixed Lorenz system by the SEEK-FIND algorithm

Left-hand three illustrations show the behaviour of the estimates $x'(t+1)$, $y'(t+1)$, $z'(t+1)$ described as the time series, whilst right-hand three illustrations correspond to the theoretical trajectories derived from the initial conditions of $x(0)$=5, $y(0)$=10 and $z(0)$=20. As can be seen, three state variables are estimated well after leaning assisted by the SEEK filter and the SEEK filter is smoothly switched to the neural network at the time marked by the vertical broken line. The estimation speed is enhanced by twelve times in the SEEK-FIND algorithm compared with the SEEK algorithm.

The state variables in the parameter-switched Lorenz system have been estimated by using the SEEK-FIND algorithm. The estimation results are shown in Figure 5 and Figure 6 as the time series, in which the parameter is switched once from r=28 to r=112. The SEEK filter takes over the neural network just after the system is switched and the neural network is initialised and trained by using the estimates derived from the SEEK filter. The SEEK filter is replaced by the trained neural network when the sum of the squared estimation errors becomes lower than a desired value. As can be seen from Figure 5, the SEEK filter returns the accurate estimates in the switched system after short term locking-on.

In Figure 6 the left-hand illustrations show the state estimates from the SEEK filter and the trained neural network, which are compared with the theoretically derived state variables as shown in the right-hand illustrations. The time scale is elongated by two times in Figure 6 compared with Figure 4. The

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trained neural network also returns the accurate estimates in the switched system as can be seen from Figure 6.

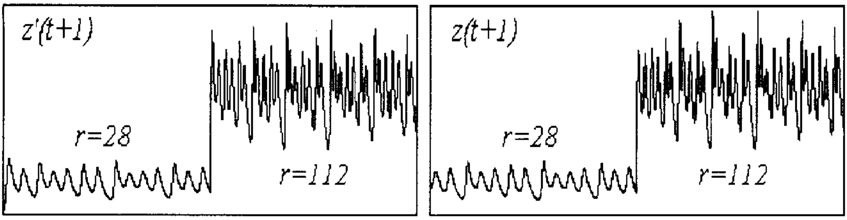

Figure 5: Estimation of the parameter-switched Lorenz system by the SEEK filter

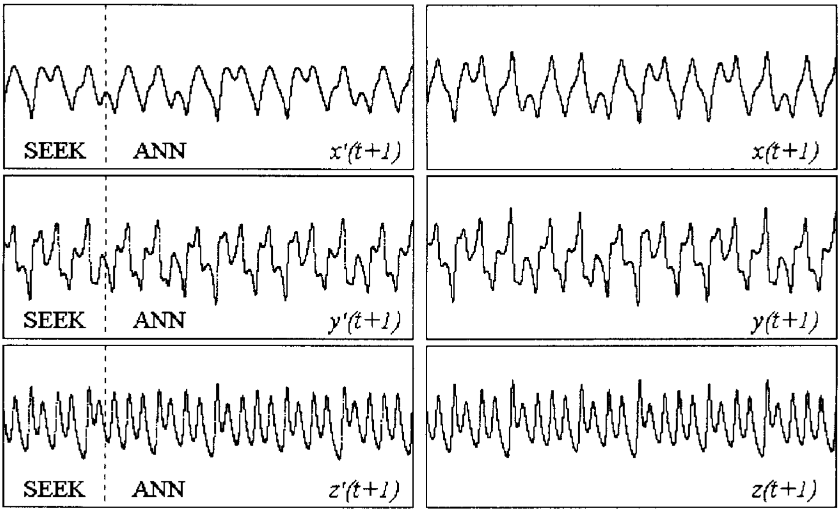

Figure 6: Estimation of the Lorenz system with r=112 by the SEEK-FIND algorithm

The neural network needs longer leaning period in the Lorenz system with r=112 because the frequency of the state variation is much higher than that in the system with r=28. Consequently, the SEEK-FIND algorithm has to be applied to the switching system in which the switching interval is much longer than the learning time in the neural network.

4 Conclusion

In order to enhance the calculation time in estimating nonlinear state variables the SEEK-FIND algorithm is proposed, in which a neural network is embedded to replace the SEEK filter in a regular state. The neural network is trained by an optimal observation and one step delayed estimates from the

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SEEK filter. The SEEK filter takes over the neural network when the estimation error crosses over a desired value, as realised in switched-parameter systems and systems with bifurcation. As a model demonstration here, the SEEK-FIND algorithm is applied to estimate the state variables not only in the parameter-fixed Lorenz system but also in the switched-parameter Lorenz system. The simulation indicates the SEEK-FIND algorithm returns accurate estimates and the estimation speed is enhanced by twelve times. We regard this demonstration as a convincing evidence of the capability of our SEEK-FIND algorithm as an accurate estimator of the state variables even for multi-modal strongly nonlinear systems as realised in contaminant transport processes.

References

1. Nonaka, M. & Thomas, N. H. Kalman filter method for statistical modelling of contaminant Transport: An outline of the methodology, in *Proc of the Sixth Int Conference on Stochastic Hydraulics,* Taipei, pp. 647-654, 1992.
2. Nonaka, M. & Thomas, N. H. An enhanced methodology for diagnosing and predicting air pollution states, in *Computer Simulation, Air Pollution II* Vol. 1 (ed J.M. Baldasano, C.A. Brebbia, H. Power & P. Zannetti), pp. 105-112, Computational Mechanics Publ., 1994.
3. Simutis, R., Havlik, I. & Luebbert, A. Process state estimation and prediction in a production-scale beer fermentation using fuzzy aided extended Kalman filter and neural networks, *IFAC Symposium Series No. 10*, pp. 95-100, Pergamon Press, 1992.
4. Watanabe, K., Fukuda, T. & Tzafestas, S. G. Learning algorithm of layered neural networks via extended Kalman filters, *Int J Systems Science*, **22**, 4, 1991, 753-768.
5. Iiguni, Y., Sakai, H. & Tokumaru, H. A real-time leaning algorithm for a multilayered neural network based on the extended Kalman filter, *IEEE Trans Signal Process*, **40**, 4, 1992, 959-966.
6. Ishida, R. et. al. Superquick neuron training by extended Kalman filter(2nd Report), *Nippon Kikaigakkai Ronbunshu C*, **59**, 564, 1993, 2312-2317.
7. Pukorius, G. & Feldkamp, L. A. Neurocontrol of nonlinear dynamical systems with Kalman filter trained recurrent networks, *IEEE Trans Neural Network,* **5**, 2, 1994, 279-297.
8. Ruck, D. W. et. al. Comparative analysis of backpropagation and the extended Kalman filter for training multilayer perceptrons, *IEEEPAMI*, **14**, 1992, 686-691.
9. Fletcher, R. & Powell, M. J. D. A rapidly convergent descent method for minimization, *Comput J*, **6**, 1963/1964, 163-168.
10. Lorenz, E. N. Deterministic nonperiodic flow, *J Atmos Sci*, **20**, 1963, 130-141.
11. Sparrow, C. *The Lorenz Equations : Bifurcation, Chaos and Strange Attractors*, Springer-Verlag, New York, 1982.
12. Rumelhart, D. E., Hinton, G. E. & Williams, R. J. Learning internal representations by error propagation, *Parallel Distributed Processing*, pp. 318-362, MIT Press, 1986.
13. Qiu, G., Varley, M. R. & Terrell, T. J. Accelerated training of backpropagation networks by using adaptive momentum step, *Electron Lett*, **28**, 4, 1992, 377-379.