

Detection of abrupt changes in water quality time series by the adaptive Kalman filter

AKIRA KAWAMURA, KENJI JINNO, TOSHIHIKO UEDA
& REYNALDO REAL MEDINA

*Department of Civil Engineering Hydraulics and
Soil Mechanics, Faculty of Engineering,
Kyushu University, 6-10-1 Hakozaki,
Higashi-ku, Fukuoka 812, Japan*

ABSTRACT The adaptive Kalman filter (AKF) is derived for both unknown abrupt change and observed variables being vectors. It is proposed for detecting abrupt changes in the characteristic pattern of water quality indicator time series. A new and simple method is proposed for on-line detection of the time of occurrence of abrupt change. The algorithm of the derived AKF is presented, incorporating this method. To show its effectiveness, adaptability and ability to detect changes, the derived AKF is applied to a synthetically generated water quality indicator time sequence, which is represented by a periodic function having many frequency components whose amplitudes may change abruptly and randomly at unknown points in the sequence. The results show that AKF detects exactly the time of occurrence of abrupt change and estimates precisely its magnitude, thereby obtaining very accurate predictions of the water quality indicator after the detection of abrupt change.

NOTATION

$A_i B_i$	periodic coefficients
$Cov [\]$	covariance operator
$E [\]$	expectation operator
f_i	frequency component
G	unknown ($n \times 1$) abrupt change vector
H	known ($m \times n$) observation matrix
I	($n \times n$) identity matrix
j	present time step
K	($n \times m$) Kalman gain matrix
k	time step
l	innovation cumulative number
n	number of system parameters
P	($n \times n$) estimation error covariance matrix
q	number of significant frequency components
S	data window
U	known ($p \times p$) covariance matrix of u
u	independent, zero mean, white Gaussian ($p \times 1$) system noise vector

W	known (m x m) covariance matrix of w
w	independent, zero mean, white Gaussian (m x 1) observation noise vector
x	(n x 1) system state vector
y	(m x 1) observation vector (m ≤ n); observed (synthetically generated) value of the water quality indicator
Γ	known (n x p) system matrix
$\delta_{k\theta}$	Kronecker's delta ($\delta_{k\theta} = 1$ if $k=\theta$ and $\delta_{k\theta} = 0$ if $k \neq \theta$)
η	threshold value
θ	unknown time step when abrupt change occurred
$\hat{\theta}$	maximum likelihood estimate of time step θ
Λ	likelihood ratio
Λ_g	generalized likelihood ratio
v	(m x 1) innovation (step 1 prediction residual) vector
ϕ^*	abnormality detection index
D	equal by definition
	determinant of a matrix

INTRODUCTION

The problem considered in this paper is the detection of abrupt changes in water quality time series. These abrupt changes may be due to many reasons, e.g., sudden disposal of a pollutant during the monitoring of a body of water for various water quality indicators. Because of the difficulty in predicting these abrupt changes beforehand, a need arises for ways to detect at once the time at which they occurred and to quantitatively estimate their magnitudes, which are indispensable information in taking countermeasures against their undesirable effects.

This problem is treated as a system identification problem involving detection of abrupt changes in the system dynamics. However, the detection of abrupt changes is designed specifically to identify the point in time when the characteristic pattern of a water quality was terminated by a rather sharp transition to another period with a different characteristic pattern.

The adaptive Kalman filter (AKF) (Ueda et al. 1984) is used to detect the presence of these kinds of abrupt changes by treating them as abrupt changes in the system state variables and to estimate on-line their time of occurrence and magnitude. Also AKF makes it possible for the state variables to adjust at once to the new system.

AKF follows the work of Willsky & Jones (1976), and it has been applied to hydrological problems by Kitanidis & Bras (1980) and Kawamura et al. (1985). However, the AKF, derived and considered in the present paper, is for the case of both the unknown abrupt change and the observed variables being **vectors**.

The present paper proposes a new and simple method, which is incorporated in the derivation of the AKF for the above mentioned case, for on-line detection of the time of occurrence of abrupt change. Specifically, this paper aims to show the inherent characteristics of the AKF, such as adaptability, ability to detect abrupt changes, etc., and to demonstrate its effectiveness by the

very accurate predictions of the water quality indicator after the detection of abrupt changes. This is accomplished by applying AKF to a synthetically generated water quality indicator time sequence, which is represented by a periodic function having many frequency components whose amplitudes may change abruptly and randomly at an unknown time.

ADAPTIVE KALMAN FILTER

The AKF formulation considers the following system and observation equations.

$$x(k+1) = \Phi(k)x(k) + \Gamma(k)u(k) + \delta_{k\theta} G(k) \quad (1)$$

$$y(k) = H(k)x(k) + w(k) \quad (2)$$

Here, system equation (1) is composed of the system equation for the ordinary Kalman filter (OKF) and the term $\delta_{k\theta}G(k)$ for the magnitude of abrupt change in the state variables.

The AKF detects whether an abrupt change in the system parameters occurs or not by evaluating the innovations (step-one prediction residuals) sequence using generalized likelihood ratio test. When such abrupt change is detected, its time of occurrence and magnitude are estimated quantitatively, and the state variables are appropriately corrected according to the magnitude of this abrupt change.

Equation (1) can be split up into two hypotheses: hypothesis H_0 is the assumption that no abrupt change has occurred, and hypothesis H_1 is that an abrupt change occurred at time $k=\theta$. Under hypothesis H_0 , equation (1) is reduced to OKF formulation.

Since the system is linear, the innovation at time step $\theta+i$, $v_{old}(\theta+i)$, resulting from OKF calculation under hypothesis H_1 , can be divided into two terms:

$$v_{old}(\theta+i) = v_0(\theta+i) + A(\theta, \theta+i)G(\theta) \quad (3)$$

where

$$A(\theta, \theta+i) \triangleq H(\theta+i)\Psi(\theta, \theta+i) \quad (m \times n \text{ matrix}) \quad (4)$$

$$\Psi(\theta, \theta+i) \triangleq \begin{cases} \Phi(\theta+i-1)[I-K(\theta+i-1)H(\theta+i-1)]\Psi(\theta, \theta+i-1) & (\text{if } i \geq 1) \\ I & (\text{if } i=1) \\ 0 & (\text{if } i \leq 0) \end{cases} \quad (n \times n \text{ matrix}) \quad (5)$$

The term $v_0(\theta+i)$ in equation (3) is the innovation vector under hypothesis H_0 and is neither influenced by the time of occurrence of the abrupt change, θ , nor its magnitude, $G(\theta)$; the second term is the one caused by abrupt change. Expectation and covariance of the innovation vectors under each hypothesis are as follows:

$$E[v_0(\theta+i)] = 0 \quad (6)$$

$$E[v_{old}(\theta+i)] = A(\theta, \theta+i)G(\theta) \quad (7)$$

$$\begin{aligned}
 V(\theta+i) &\triangleq \text{Cov}[v_{\theta}(\theta+i)] = \text{Cov}[v(\theta+i)] \\
 &= H(\theta+i)P_{\theta}(\theta+i | \theta+i-1)H^T(\theta+i) + W(\theta+i) \tag{8}
 \end{aligned}$$

where $P_{\theta}(\theta+i | \theta+i-1)$ is P at time $\theta+i$, given observations up to time step $\theta+i-1$, and is calculated by OKF under hypothesis H_0 .

Since $v(\theta+i)$ is given as a linear function of the normally distributed stochastic sequence $u(k)$ and $w(k)$ and the initial state of the system $x(0)$, the innovation should also be normally distributed under both hypotheses. Therefore, under hypothesis H_0 , as $v(\theta+i)$ ($i=1,2,\dots,l$) are mutually independent, the joint probability density function for a series of innovation vectors (of number l), $v(\theta+1), v(\theta+2), \dots, v(\theta+l)$, with the mean and covariance given respectively by equations (6) and (8) is

$$\begin{aligned}
 &p(v(\theta+1), \dots, v(\theta+l) | H_0) \\
 &= \prod_{i=1}^l \frac{1}{(2\pi)^{m/2} |V(\theta+i)|^{1/2}} \exp\{-\frac{1}{2}v^T(\theta+i)V^{-1}(\theta+i)v(\theta+i)\} \tag{9}
 \end{aligned}$$

Similarly, under hypothesis H_1 , the joint probability density function is

$$\begin{aligned}
 &p(v(\theta+1), \dots, v(\theta+l) | H_1) \\
 &= \prod_{i=1}^l \frac{1}{(2\pi)^{m/2} |V(\theta+i)|^{1/2}} \exp\{-\frac{1}{2}[v(\theta+i) - A(\theta, \theta+i)G(\theta)]^T \\
 &\quad V^{-1}(\theta+i)[v(\theta+i) - A(\theta, \theta+i)G(\theta)]\} \tag{10}
 \end{aligned}$$

with the mean and covariance given by equations (7) and (8) respectively.

The likelihood ratio $\Lambda(\theta, G(\theta), l)$ is defined as the ratio of equation (9) to equation (10) and is given as

$$\begin{aligned}
 \Lambda(\theta, G(\theta), l) &\triangleq \frac{p(v(\theta+1), \dots, v(\theta+l) | H_1)}{p(v(\theta+1), \dots, v(\theta+l) | H_0)} \\
 &= \exp[\phi^T(\theta, l)G(\theta) - (1/2)G^T(\theta)\mu(\theta, l)G(\theta)] \tag{11}
 \end{aligned}$$

where

$$\phi(\theta, l) \triangleq \sum_{i=1}^l A^T(\theta, \theta+i)V^{-1}(\theta+i)v(\theta+i) \tag{12}$$

$$\mu(\theta, l) \triangleq \sum_{i=1}^l A^T(\theta, \theta+i)V^{-1}(\theta+i)A(\theta, \theta+i) \tag{13}$$

$\phi(\theta, l)$ is a $(nx1)$ vector and $\mu(\theta, l)$ is a (nxn) positive definite matrix. Maximum likelihood estimate $\hat{G}(\theta)$ of $G(\theta)$ is given by taking the logarithm of equation (11), differentiating and setting the result equal to zero:

$$\hat{G}(\theta) = \mu^{-1}(\theta, l)\phi(\theta, l) \tag{14}$$

Notice that $G(\theta)$ is a $(n \times 1)$ vector which is normal with mean $\hat{G}(\theta) = \mu^{-1}(\theta, 1)\phi(\theta, 1)$ and covariance $\mu^{-1}(\theta, 1)$ (Ueda *et al.* 1984). Since the likelihood ratio $\Lambda(\theta, G(\theta), 1)$ is a function of $G(\theta)$, replacing $G(\theta)$ with $\hat{G}(\theta)$ in equation (14), the result is called a generalized likelihood ratio (GLR). The GLR $\Lambda_g(\theta, 1)$ is calculated as follows:

$$\Lambda_g(\theta, 1) \ni \Lambda(\theta, \hat{G}(\theta), 1) = \exp\left[\frac{1}{2}\phi^T(\theta, 1)\mu^{-1}(\theta, 1)\phi(\theta, 1)\right] \quad (15)$$

If $\Lambda_g(\theta, 1)$ (in equation (15)) is greater than a threshold value, hypothesis H_1 is accepted, otherwise, hypothesis H_0 is accepted; this is called generalized likelihood ratio test (GLRT). This GLRT is equivalent to comparing the value of $\phi_*(\theta, 1)$, defined by equation (16) which is the transformation of equation (15), with a threshold η .

$$\phi_*(\theta, 1) \ni [2\ln\Lambda_g(\theta, 1)]^{0.5} = [\phi^T(\theta, 1)\mu^{-1}(\theta, 1)\phi(\theta, 1)]^{0.5} \quad (\text{scalar}) \quad (16)$$

That is, one detects whether an abrupt change exists or not by

$$\phi_*(\theta, 1) \begin{matrix} \geq \\ < \end{matrix} \begin{matrix} H_1 \\ H_0 \end{matrix} \eta \quad (17)$$

Hereinafter we refer to $\phi_*(\theta, 1)$ as the abnormality detection index.

The matrix $\mu(\theta, 1)$ defined by equation (13) must be full rank to ensure the calculation of its inverse for the estimation of $G(\theta)$ and $\phi_*(\theta, 1)$, and the number of cumulative data needed to make it full rank is l_{\min} . The time step k at which $\Lambda_g(k, 1)$ is maximum gives the maximum likelihood estimate $\hat{\theta}$, i.e.,

$$\hat{\theta} = [k \mid \max \Lambda_g(k, 1)] = [k \mid \max \phi_*(k, 1)] \quad (18)$$

The value $\hat{\theta}$ is used to estimate $G(\theta)$ through equation (14) and to perform the GLRT through equation (17).

When the GLRT accepts that hypothesis H_1 is true at time step $\theta+i$, the state variables must be corrected at that time step to let the filter adjust to the new system. Hence, given the $\hat{G}(\theta)$, the compensated estimate of the state vector and its compensated error covariance matrix are

$$\hat{x}_{\text{new}}(\theta+i \mid \theta+i) = \hat{x}_{\text{old}}(\theta+i \mid \theta+i) + \Delta(\theta, \theta+i)\hat{G}(\theta) \quad (19)$$

$$P_{\text{new}}(\theta+i \mid \theta+i) = P_{\text{old}}(\theta+i \mid \theta+i) + \Delta(\theta, \theta+i)\mu^{-1}(\theta, 1)\Delta^T(\theta, \theta+i) \quad (20)$$

where

$$\Delta(\theta, \theta+i) \ni [I - K(\theta+i)H(\theta+i)] \Psi(\theta, \theta+i) \quad (m \times n \text{ matrix}) \quad (21)$$

Here $\hat{x}_{\text{old}}(\theta+i \mid \theta+i)$ and $P_{\text{old}}(\theta+i \mid \theta+i)$ are the estimate of $x(\theta+i)$ and its error covariance matrix, respectively, prior to compensation and are calculated recursively by OKF.

DETECTION OF TIME OF OCCURRENCE OF ABRUPT CHANGE

Fig.1(a) shows a plot of the innovations v sequence. In this figure, k represents the time step at which ϕ_* is desired and calculated at the present time step j .

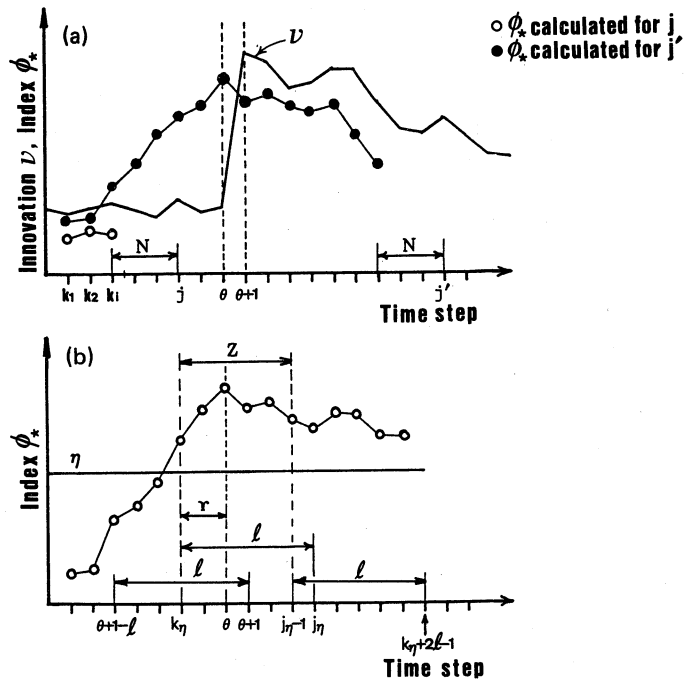


FIG.1 Estimation of the time of occurrence of an abrupt change.

The maximum likelihood estimate $\hat{\theta}$ is given by equation (18), which means that $\hat{\theta}$ is the time step k when $\phi_*(k, l)$ is maximum. The estimation of $\hat{\theta}$ through this equation is done most likely by calculating a sequence of ϕ_* for every forward move (step-by-step) of j . Here, the range of the sequence is from k_1 to $k_i = j - N$ ($N \geq l_{\min}$). In each dequence, $\phi_*(k_1, l)$ is calculated through equation (16) using v from k_1+1 to j , $\phi_*(k_2, l)$ using v from $k_1+2 = k_2+1$ to j , and so on. Note that two sequences of ϕ_* are plotted in Fig.1(a): one, shown by white small circles, is for the indicated j and the other one, shown by small black circles, is for an assumed present time step j' after θ . The other approach, which is used commonly, limits the calculations of ϕ_* to within a finite data window S , given as $j-s_2 \leq k_1 \leq j-s_1$ ($s_2-s_1 = S > 0, s_1 \geq l_{\min}$), for every advance of j . In both approaches, the maximum ϕ_* is determined from a large number of sequences of $\phi_*(k, l)$; both approaches are indeed a computational burden. Also they require l to vary correspondingly with k .

In the present paper, we propose a method for estimating $\hat{\theta}$ where l is made constant. In this method, only one magnitude of ϕ_* is calculated for every forward move of j ; thus, only one sequence of ϕ_* is needed to determine the maximum ϕ_* . However it should be noted that taking a constant value of l is valid since ϕ_* defined by equation (16), which is based on equation (11), does not change

statistically for any value of l (Ueda *et al.*, 1984).

As shown in Fig.1(b), k_η is the time step at which the magnitude of ϕ_* , calculated at the present time step j_η , is above η for the first time. The proposed method estimates θ by searching for the maximum ϕ_* in the range from k_η to $j_\eta-1$ (i.e., the range z $\{l-1$ time-steps $\}$ in the same figure), and its time of occurrence in this range is regarded as $\hat{\theta}$. This is because the abrupt change is detected through ϕ_* at k_η from the innovations in the range from $k_{\eta+1}$ to j_η . The search is done as follows (refer to Fig.1(b)). The ϕ_* at $k_{\eta+1}$ is calculated at the next $j(=j_\eta+1)$, denoted as ϕ_{*now} and compared with ϕ_{*max} at k_η . The larger ϕ_* is kept and denoted as ϕ_{*max} . Similarly the ϕ_* at $k_{\eta+2}$ is calculated at the next $j(=j_\eta+2)$, denoted as ϕ_{*now} and compared with ϕ_{*max} , and the larger one is retained as the new ϕ_{*max} . This procedure continues until all the ϕ_* within the time-range z are evaluated, i.e., at every advance of j . Thus the time of occurrence of abrupt change is determined precisely through ϕ_{*max} at time step $j_\eta-1=k_{\eta+1}-1$. However, it is actually decided at the present time step $j_\eta-1+1(=k_{\eta+2}-1)$. On the other hand, if k_η is r time-steps ($0 \leq r \leq l-1$) before the abrupt change occurs, i.e., $k_\eta = \theta - r$, then the time of occurrence of abrupt change is judged at $\theta + 2l - 1 - r$.

To decide the time of occurrence of abrupt change quicker, a choice of a smaller value of l will be better. However, l must be greater than or equal to l_{min} . In addition if l is too small, ϕ_* will be influenced very much by noise such that the time of occurrence of maximum ϕ_* may not correspond to $\hat{\theta}$. Hence, these considerations will dictate the choice of l .

The proposed method (or algorithm) requires much less computing effort compared with the two approaches mentioned above and is suitable for on-line calculation. The flow chart of the proposed algorithm is presented in Fig.2.

NUMERICAL SIMULATION STUDY

To evaluate the performance of the proposed method, we used a synthetically generated time sequence, which is represented by a periodic function with multiple periodic components, incorporating an abrupt change. The use of periodic function is common in characterizing the annual, seasonal and diurnal variations of water quality data (see Steele, 1985). For the present paper, we considered the following periodic function.

$$y(k) = \sum_{i=1}^q (A_i \sin 2\pi f_i k + B_i \cos 2\pi f_i k) + w(k) \quad (22)$$

In this simulation study, we assumed for the stochastic component $w(k)$ a Gaussian random sequence with zero as mean and 0.25 as standard deviation, set $q=5$ and gave the values of the periodic components and the state variables (A_i and B_i) before and after the occurrence of abrupt change at $k=72$ as shown in Table 1. In this table, the magnitude of abrupt change $G(\theta)$ is the difference of the given values of the state variables before and after the occurrence of abrupt of change. Here, the synthetically generated time sequence consisted of 180 data.

Now we consider the problem of identifying the parameters A_i and

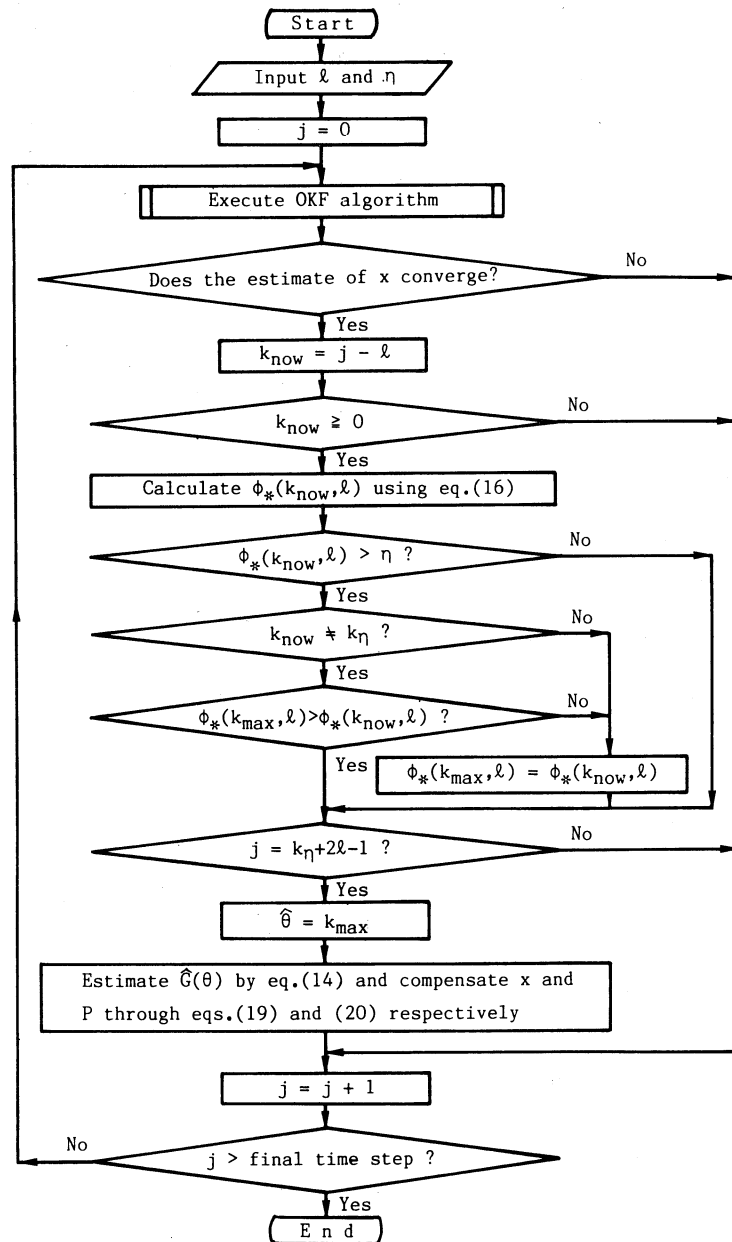


FIG.2 The algorithm of the proposed AKF.

B_i which may change abruptly and randomly at an unknown time and of predicting the values of the water quality indicator at future time leads by Kalman filter. These problems correspond to the case of the Kalman filter where the observation vector's dimension $m=1$ (i.e., $y(k)$ is scalar), $n=10$, $x(k)=[A_i B_i \dots A_q B_q]^T$, $\Phi(k)=I$ and $H(k)=[1 \sin 2\pi f_1 k \cos 2\pi f_1 k \dots \sin 2\pi f_q k \cos 2\pi f_q k]$.

The following initial conditions, which are required for the recursive applications of the Kalman filter algorithm, were used in the simulation study: $x(0|0)$ was given as shown in the third column of Table 1; the diagonal elements of $P(0|0)$ were all taken as 5.0 and off-diagonal as 1.0; $U=0$; and $W=0.25^2$. With these initial values, both OKF and AKF were executed, yielding the parameter estimates at

TABLE 1 Constants for data generation

f_i	Parameter	$1 \leq k \leq 72$	$73 \leq k \leq 180$	$G(\theta)$
1/36	A_1	-0.7	0.5	1.2
	B_1	-2.5	1.0	3.5
1/18	A_2	0.0	-0.6	-0.6
	B_2	0.0	-2.5	-2.5
1/9	A_3	0.0	0.0	0.0
	B_3	1.2	0.0	-1.2
1/7	A_4	-0.6	0.0	0.6
	B_4	-1.1	0.0	1.1
1/6	A_5	0.6	-0.5	-1.1
	B_5	0.6	-1.0	-1.6

each time step as plotted in Fig.3. (In this figure, plotting is done at every three time-steps). In executing AKF, $l=15$ and $\eta=7.0$. Figs.4 and 5 show respectively the step-one predictions series and innovations (step-one prediction residuals) sequence, and Fig.6 illustrates the plot of $\phi_*(k,l)$.

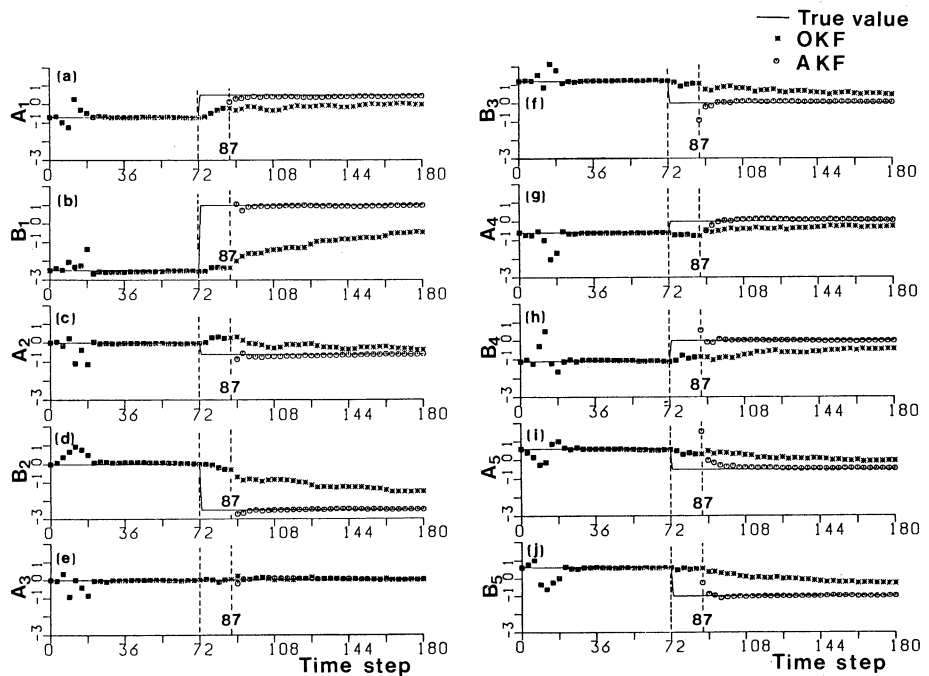


FIG.3 System parameters A_i and B_i identified by OKF and AKF.

DISCUSSION

As shown in Fig.3, the OKF cannot track the abrupt change immediately, resulting in large errors in the estimates of the amplitudes A_i and B_i . Consequently, large errors in the predictions

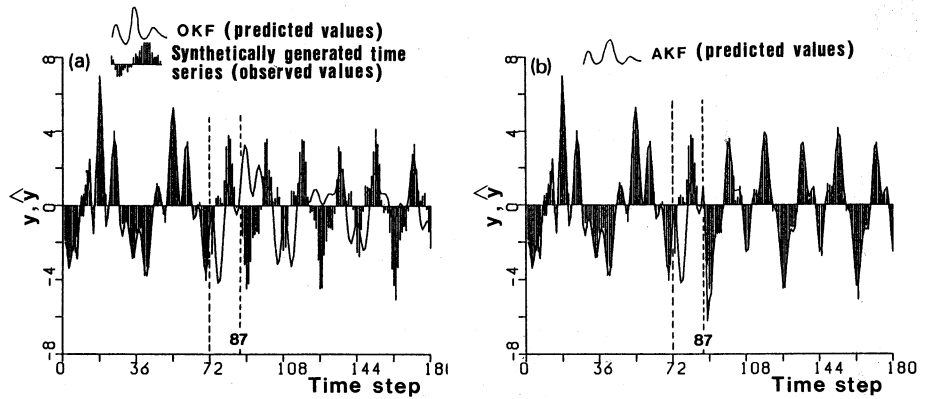


FIG.4 One-step ahead predicted values by (a) OKF and (b) AKF.

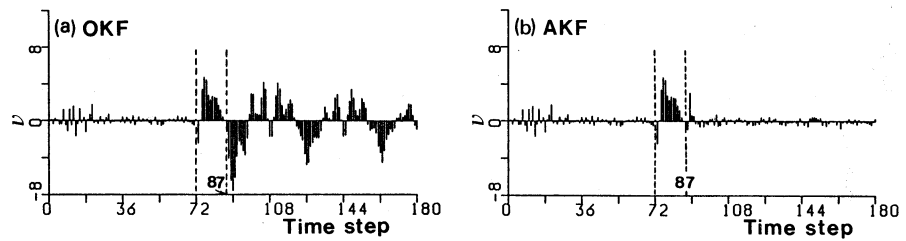


FIG.5 Innovations sequence by (a) OKF and (b) AKF.

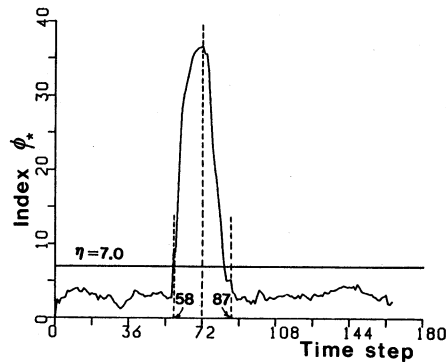


FIG.6 Time series plot of the abnormality detection index ϕ_* by AKF for $l=1.5$.

of the variable $y(k)$ develop after the occurrence of abrupt change, as illustrated in Figs.4(a) and 5(a).

Fig.6 shows that ϕ_* is over η for the first time at time step 58; hence, $k_\eta=58$. Thus Θ exists in the range from $k_\eta=58$ to $k_{\eta+1}-1=72$. As shown in the same figure, $k=72$ is identified as the time of occurrence of maximum ϕ_* in this range and is therefore judged as the time of occurrence of abrupt change. At $k=87$, which is the present time step j when maximum ϕ_* is identified, the state variables (A_i, B_i) and their error covariance are corrected through equations (19) and (20). However \hat{x}_{new} may not correspond to their true or new parameters at the start of compensation

(at $k=87$) because errors are contained in $\hat{G}(\theta)$. This can be seen in Fig.3 as an absence of plot of the parameter estimate at $k=87$; actually the value of the parameter estimate at this k is over the range of the ordinate. The same figure illustrates that this overcorrection (known as overshooting) is damped immediately after $k=87$ by the calculated \hat{x}_{new} and P_{new} . As demonstrated in Fig.3 the given changes at $k=72$, which are shown in Table 1, such as phase shift, no change in amplitude, appearance and disappearance of one component, and changes in amplitudes of components that are very near to each other ($1/7$ and $1/6$ frequency components) are all detected correctly. This results in the behaviour of the AKF predictions following that of the generated time sequence and in the prediction residuals being effectively small. These results are illustrated (after $k=87$) in Figs.4(b) & 5(b). It is interesting to note that predictions are also accurate even in the short period (right after $k=87$) where the estimates of the parameters overshoot. This is because these 'overshooting' estimates are combined and balanced out through equation (22), resulting in the predictions of $y(k)$ close to the observed (generated) values. However, overshooting can be suppressed if l takes a larger value. In Fig.6, the ϕ_* -curve decreases quickly after $k=72$ since smaller innovations and larger covariance (P_{new}) were considered.

On the other hand, the practical setting of η should be done by first providing adequate values for U , W and l , then calculating several ϕ_* -values from data that are taken under normal condition, and finally setting η above the plot of these ϕ_* -values.

In this simulation study, the number of calculations is decreased remarkably when the dimension n is larger. However, see Kawamura *et al.* (1984) for the other characteristics of the AKF.

In addition, AKF includes OKF and is equivalent to OKF when no abrupt change in the state variables occurred. Hence AKF can be applied to any problems where OKF is applicable. Furthermore it has even wider range of applications than OKF since it has the added capability to detect abrupt changes.

The proposed method is also effective when the occurrence of abrupt change is difficult to predict beforehand. In this case, however, the biggest problem lies on how to formulate the system and observation equations in order that the actual phenomenon can be suited for AKF implementation.

CONCLUSIONS

In this paper, we have considered a case of the AKF where both abrupt change and observed variables being vectors and have shown that AKF can make its predicted values follow quickly the observed values after the abrupt change is detected. Also we have simplified the algorithm to detect the time of occurrence of abrupt change and have proposed this simplified one as a new and more practical detection method, excellent for on-line calculation. We have described in detail this new algorithm and have shown its usefulness.

Next we have generated synthetically a time sequence, which is

represented by a periodic function, incorporating an abrupt change. As shown by the results, the proposed method has identified precisely the time of occurrence and magnitude of abrupt change and has made the parameters adapt to the new parameters much faster than OKF, resulting in accurate predictions. Therefore, we have verified the adaptability, effectiveness and ability to detect abrupt change of the proposed AKF algorithm.

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