EXTENSIONS OF KALMAN RECURSIVE ESTIMATION THEORY TO RETROSPECTIVE UPDATING AND INTERPOLATION WITH APPLICATIONS TO INSTRUMENT CALIBRATION

by
C. ROGER GLASSEY
and
YOON C. CHOY

MASTER

OPERATIONS
RESEARCH
CENTER

P.O. 3684703

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

UNIVERSITY OF CALIFORNIA • BERKELEY

EXTENSIONS OF KALMAN RECURSIVE ESTIMATION THEORY TO RETROSPECTIVE
UPDATING AND INTERPOLATION WITH APPLICATIONS TO INSTRUMENT CALIBRATION

by

C. Roger Glassey
Department of Industrial Engineering
and Operations Research
University of California, Berkeley

and

Yoon C. Choy
Operations Research Center
University of California, Berkeley

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

SEPTEMBER 1977

ORC 77-25

This research was supported by the Lawrence Livermore Laboratory under Purchase Order No. 3684703 with the University of California. Reproduction in whole or in part is permitted for any purpose of the United States Government.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED *REA*

ABSTRACT

In this report, we consider the problem of estimation of a physical quantity from a set of measurements. We extend Kalman recursive estimation procedure in two ways. First, we explore how to use the latest observation to retrospectively update estimates of past system states. Second, we show how to apply the retrospective update idea to get interpolation estimates between the epochs of observations. We also show application of these ideas for instrument calibration in nuclear accountability systems.

TABLE OF CONTENTS

	Page
CHAPTER 0: INTRODUCTION AND SUMMARY	1
CHAPTER 1: REVIEW OF THE THEORY OF BEST LINEAR UNBIASED ESTIMATORS AND KALMAN RECURSIVE ESTIMATION	3
1.1 Best Linear Unbiased Estimators	3
1.2 Kalman Recursive Estimators	4
CHAPTER 2: APPLICATION OF RECURSIVE LINEAR ESTIMATION TO INSTRUMENT CALIBRATION	8
CHAPTER 3: RETROSPECTIVE UPDATE	13
CHAPTER 4: APPLICATION OF RETROSPECTIVE UPDATE TO INSTRUMENT CALIBRATION	15
CHAPTER 5: INTERPOLATION COMBINED WITH RETROSPECTIVE UPDATE	22
5.1 Update of Estimate at Observation Epochs	22
5.2 Interpolation	24
5.2.1 Interpolation When $n = m - 1$	25
5.2.2 Retrospective Update of Interpolation: $m > n + 1$	25
5.3 Summary	27
CHAPTER 6: INTERPOLATION AND RETROSPECTIVE UPDATE OF INSTRUMENT CALIBRATION	28
REFERENCES	37

EXTENSIONS OF KALMAN RECURSIVE ESTIMATION THEORY TO RETROSPECTIVE UPDATING AND INTERPOLATION WITH APPLICATIONS TO INSTRUMENT CALIBRATION

By

C. Roger Glassey and Yoon C. Choy

0. INTRODUCTION AND SUMMARY

In nuclear materials accountability systems, the requirements for precision and accuracy are quite stringent. It is therefore important to extract as much information as possible from the data that is collected by both process instrumentation and from laboratory analysis. When the data consists of a time series of correlated observations, the correlation structure can be utilized to improve the precision of estimates computed from the data.

One of the widely used techniques for making such computations is due to Kalman (see Reference [1] and [2]). This Kalman recursive estimation procedure is usually employed to estimate the state of the system of interest at the time of the most recent observation. In this report, we consider two extensions of this scheme. First, we explore how the latest observation can be used to retrospectively update estimates of past system states, thereby improving the precision of these estimates. Second, we consider situations in which it is desired to estimate the state of the system at times between the epochs of the observations. Finally, we show how to apply to retrospective update idea to these interpolation estimates.

All the estimators we consider are Best Linear Unbiased Estimators (BLUE) in the sense that the expected value of the estimator is the true value of the state; they are computed by linear transformations of the data; and they have minimum variance in the class of estimators having the first two

properties. The Kalman scheme recursively computes the BLUE of the system state and also the variance matrix of the estimator from the previous estimate, the previous variance matrix, and the latest observation. The properties of BLUE and the Kalman scheme are reviewed in Section 1.

The deviation of the retrospective update scheme is presented in Section 3 and the interpolation scheme, in Section 5.

There are many aspects of nuclear materials accountability to which these ideas could be applied. We have selected instrument calibration to illustrate our methods because the models are relatively simple, and because not much appears in the literature in the problem of designing a calibration strategy for an instrument to take advantage of the known (or suspected) way in which parameters drift over time.

The organization of this report is to illustrate each section of theory by applying it to the instrument calibration problem. Thus, Section 2 deals with the Kalman update of estimated calibration coefficients; Section 4 with retrospective update i.e., improving the estimate of last week's parameters based on this week's calibration results; Section 6 with interpolation i.e., how to estimate Wednesday's parameters based on calibrations performed on Monday and Friday. Section 6 also discusses circumstances under which retrospective update of coefficients is worthwhile, and suggests some general ideas about calibration strategies.

The example calculations show that the precision of estimated instrument calibration coefficients can be greatly increased by the use of the extensions to the Kalman updating scheme developed in this paper. Applications of these ideas to other areas of accountability systems may show similar potential improvements in precision.

1. REVIEW OF THE THEORY OF BEST LINEAR UNBIASED ESTIMATORS AND KALMAN RECURSIVE ESTIMATION

1.1 Best Linear Unbiased Estimators

Consider two jointly distributed vector valued random variables, X and Y with mean μ_x and μ_y respectively. We denote the variance-covariance matrix as

$$(1.1) \quad E\{(X - \mu_x)(Y - \mu_y)'\} = C\{X, Y\}$$

where E is the expectation operator and the prime symbol $'$ denotes a vector or matrix.* If $X \in R_m$ and $Y \in R_n^{**}$ then $C\{X, Y\}$ will be an $m \times n$ matrix. Clearly, $C\{Y, X\} = C\{X, Y\}'$, and the matrices $C\{X, X\}$ and $C\{Y, Y\}$ will be square and of order n .

Now suppose one observes the value of the vector X and desires to compute the $\hat{Y}$, Best Linear Unbiased Estimator (BLUE) of Y , given this observation. It is well known that

$$(1.2) \quad \hat{Y} = \mu_y + BZ$$

where $Z = X - \mu_x$ and B is given by

$$(1.3) \quad B = C\{Y, X\}C\{X, X\}^{-1}.$$

Define the residual vector $R = Y - \hat{Y}$. Then $C\{R, R\}$ may be computed from

$$(1.4) \quad C\{R, R\} = C\{Y, Y\} - C\{Y, X\}C\{X, X\}^{-1}C\{X, Y\}$$

$$(1.5) \quad C\{R, R\} = C\{Y, Y\} - BC\{X, Y\}.$$

* In this paper, all vectors are column vectors unless otherwise specified.

** R_m is a real m -dimensional vector space.

Finally, it is easy to show that

$$(1.6) \quad C\{R, Z\} = 0 .$$

1.2 Kalman Recursive Estimators

Now consider the discrete-time, dynamic system given by:

$$(1.7) \quad Y_{t+1} = AY_t + V_t$$

$$(1.8) \quad X_t = MY_t + W_t$$

where Y_t is the n -dimensional state vector of the system at time t , A is a known matrix of order n , called the state transition matrix, and V_t is a vector valued random variable. The m -vector X_t is observed at time t ; the $m \times n$ matrix M is known, and W_t is an m vector valued random variable. We assume that $E\{V_t\}$ and $E\{W_t\}$ are both zero vectors, and

$$(1.9a) \quad C\{V_t, V_s\} = \delta(t - s)C_v$$

$$(1.9b) \quad C\{W_t, W_s\} = \delta(t - s)C_w$$

$$(1.9c) \quad C\{V_t, W_s\} = 0 \text{ for all } t \text{ and } s$$

where the covariance matrices C_v and C_w are known and the delta function $\delta(t) = 1$ when $t = 0$ and is zero otherwise.

Thus the sequences V_t and W_t are mutually and temporally uncorrelated; V_t may be regarded as a random perturbation of the state vector, and W_t as representing measurement error.

Definitions:

$$\begin{aligned}\hat{Y}_{t|s} &= \text{BLUE of } Y_t \text{ given history of observations up to } X_s \\ \hat{X}_{t|s} &= \text{BLUE of } X_t \text{ given the same history. Note, when } s \geq t, \\ &\quad X_t \text{ has been observed so } \hat{X}_{t|s} = X_t \\ R_{t|s} &= Y_t - \hat{Y}_{t|s} \\ C[Z_t] &= E\{(X_t - \hat{X}_{t|t-1})(X_t - \hat{X}_{t|t-1})'\} \\ C[R_{t|s}] &= C\{R_{t|s}, R_{t|s}\}.\end{aligned}$$

The Kalman scheme (see Reference [1]) is a method of recursively computing $\hat{Y}_{t+1|t}$. Assume we have computed $\hat{Y}_{t|t-1}$, the BLUE of Y_t given the observation history up to X_{t-1} . Then we observe X_t and desire to update both our estimate of Y_t and, extrapolating one period into the future, compute the BLUE of Y_{t+1} . To obtain $\hat{Y}_{t|t}$, we use Equation (1.2) and (1.3). Since $\hat{Y}_{t|t-1}$ is the BLUE of Y_t , it is the conditional expectation of Y_t before X_t is observed; hence it plays the role of μ_y in (1.1). Similarly, $\hat{X}_{t|t-1}$ is the conditional expectation of X_t given the history to $t-1$ and substitutes for μ_x . Since X_t is linearly related to Y_t by (1.8), $\hat{X}_{t|t}$ is given by

$$(1.10) \quad \hat{X}_{t|t-1} = M\hat{Y}_{t|t-1}.$$

We also need the conditional variance matrix $C[Z_t]$, which can be computed from its definition as follows: subtract (1.10) from (1.8) and use the definition of $R_{t|t}$ to obtain

$$(1.11) \quad Z_t = X_t - \hat{X}_{t|t-1} = MR_{t|t-1} + W_t.$$

Hence, since $\hat{X}_{t|t-1}$ is the conditional expectation of X_t ,

$$(1.12) \quad \begin{aligned} C[Z_t] &= E\{(MR_{t|t-1} + W_t)(MR_{t|t-1} + W_t)'\} \\ &= MC[R_{t|t-1}]M' + C_w. \end{aligned}$$

In this computation, the cross product terms (covariance of $R_{t|t-1}$ with W_t) vanish because $R_{t|t-1}$ depends upon the V_t sequence and the W_k sequence for values of k less than t ; but W_t is uncorrelated with both. Similarly, we compute

$$(1.13) \quad C\{Z_t, R_{t|t-1}\} = E\{(MR_{t|t-1} + W_t)(R_{t|t-1})'\} = MC[R_{t|t-1}]$$

and, using (1.12),

$$(1.14) \quad B_{t|t} = C[R_{t|t-1}]M'(MC[R_{t|t-1}]M' + C_w)^{-1}.$$

After observing the measurement X_t , we can update our estimate of Y_t from

$$(1.15) \quad \hat{Y}_{t|t} = \hat{Y}_{t|t-1} + B_{t|t}(X_t - M\hat{Y}_{t|t-1})$$

which is an application of (1.1).

The variance matrix of $R_t|_t$ can be computed by applying (1.5) and using (1.13) to obtain:

$$(1.16) \quad C[R_t|_t] = C[R_t|_{t-1}] - B_t|_t MC[R_t|_{t-1}] .$$

To carry out the extrapolation, we use (1.7) to conclude that

$$(1.17a) \quad \hat{Y}_{t+1}|_t = A\hat{Y}_t|_t$$

and

$$R_{t+1}|_t = Y_{t+1} - \hat{Y}_{t+1}|_t = AY_t - A\hat{Y}_t|_t + V_t$$

$$(1.17b) \quad R_{t+1}|_t = AR_t|_t + V_t$$

$$(1.18) \quad C[R_{t+1}|_t] = AC[R_t|_t]A' + C_v .$$

Again, the covariance of $R_t|_t$ with V_t is zero because $R_t|_t$ depends only on V_{t-1} , W_t and older random variables which are uncorrelated with V_t .

Finally, we observe that, from Equation (1.6), $C\{R_t|_t, Z_t\} = 0$. Then, by direct substitution of Equation (1.7), (1.8), and (1.17a) into (1.15) and by using the definition of $R_t|_t$ we obtain

$$(1.19) \quad R_t|_t = (I - B_t|_t^M)AR_{t-1}|_{t-1} + (I - B_t|_t^M)V_{t-1} - B_t|_t W_t .$$

Hence, by induction,

$$(1.20) \quad C\{R_t|_t, Z_s\} = 0 \quad \text{for all } s \leq t .$$

Thus the residual at time t is uncorrelated with the history of the process preceeding t .

2. APPLICATION OF RECURSIVE LINEAR ESTIMATION TO INSTRUMENT CALIBRATION

One of the applications of recursive estimation to nuclear materials accountability is to the problem of laboratory instrument calibration. Since it is vital to obtain very precise estimates of concentration and isotopic composition of samples taken from the process stream, it is important to have the best possible estimates of instrument calibration for any fixed budget of time and effort. In principal, instruments can be calibrated to within the precision of preparation of laboratory standards, but in order to achieve this degree of precision it might be necessary to spend more time on the replication of calibration experiments than to the analysis of production samples. In this paper, we do not examine the question of how much effort should be spent on calibration experiments, but rather we develop methods of estimating calibration coefficients with the greatest precision possible from a fixed budget.

We consider only simple instruments that behave according to the following linear model:

$$(2.1) \quad s_t = a_t + b_t q_t + \epsilon_{0t}$$

where

s_t = output signal at time t

a_t = instrument "zero" parameter

b_t = instrument scale parameter

q_t = true value of physical quantity of interest

ϵ_{0t} = random measurement error.

We assume that the instrument parameters are subject to a random walk type of drift. The evolution of parameters over time is given by

$$(2.2) \quad a_{t+1} = a_t + \epsilon_{1t}$$

$$(2.3) \quad b_{t+1} = b_t + \epsilon_{2t}$$

where the random variables ϵ_{jt} have mean zero and are independent over time and between sequences, and have variance σ_j^2 , for $j = 0, 1, 2, \dots$

The dynamic behavior of these parameters is a simple case of Equation (1.7) in which the state vector Y_t has components a_t and b_t and the matrix A is the identity matrix of order 2. The matrix C_v is diagonal, containing the elements σ_1^2 and σ_2^2 on its diagonal.

Now suppose at time t we perform the following calibration experiment: two standard solutions are prepared with properties (concentrations for example) having the values q'_t and q''_t , which are known within a range of uncertainty that is much smaller than the standard deviation of the measurement error. We assume that the calibration experiment using the two solutions is performed so quickly that the parameter drift during the experiment is negligible. For example, t may be measured in days, while a calibration experiment may take less than an hour. In this case, the output signals obtained from the pair of standard solutions is given by Equation (2.1) which we write in matrix form as

$$(2.4) \quad \begin{bmatrix} s'_t \\ s''_t \end{bmatrix} = \begin{bmatrix} 1 & q'_t \\ 1 & q''_t \end{bmatrix} \begin{bmatrix} a_t \\ b_t \end{bmatrix} + \begin{bmatrix} \epsilon'_{0t} \\ \epsilon''_{0t} \end{bmatrix}.$$

Note that this equation is in the form of (1.8). In contrast to many applications of Kalman theory, in this case the matrix M in (1.8) is, in general, different each time the experiment is performed and is in fact determined by the choice of values of q'_t and q''_t .

The Kalman recursive estimation scheme shows how to make the best use of the history of calibration experiments together with the latest observations in estimating the current values of the calibration coefficients. In order to apply the results of Section 1, one must know of the relative magnitudes of the error and drift variances. These may be estimated by performing groups of calibration experiments widely separated in time and using analysis of variance techniques based on the within group and among group variances.

It happens that, for this particular model, the covariance matrix of the estimated coefficients converges, as long as q' and q'' are not identical, to a limiting matrix that is independent of the covariance matrix of the initial estimate. Table 1 shows the computed limiting covariance matrices for several cases. In these computations, we fix the measurement error variance, σ_w^2 , at 1. To examine the effect of increasing the range of the calibration, we fix q' at the value 1, and pick values of q'' to be 3, 10 or 100. We assume that both the intercept and slope coefficients are equally stable, that is that the two drift variances have the same value, σ_v^2 . We consider a relatively stable instrument, with $\sigma_v^2 = .001$, and less stable instruments with $\sigma_v^2 = .01$ and 0.1. Taking all combinations, we carry out the computations for nine cases.

$q'' \backslash \sigma_v^2$	.001	.01	.1
3	$\begin{bmatrix} .047 & -.016 \\ -.016 & .015 \end{bmatrix}$	$\begin{bmatrix} .15 & -.050 \\ -.050 & .045 \end{bmatrix}$	$\begin{bmatrix} .43 & -.15 \\ -.15 & .12 \end{bmatrix}$
10	$\begin{bmatrix} .035 & -.0035 \\ -.0035 & .0031 \end{bmatrix}$	$\begin{bmatrix} .11 & -.011 \\ -.011 & .0073 \end{bmatrix}$	$\begin{bmatrix} .31 & -.033 \\ -.033 & .013 \end{bmatrix}$
100	$\begin{bmatrix} .031 & -3.2 \times 10^{-4} \\ -3.2 \times 10^{-4} & .95 \times 10^{-4} \end{bmatrix}$	$\begin{bmatrix} .096 & -.97 \times 10^{-3} \\ -.97 \times 10^{-3} & 1.1 \times 10^{-4} \end{bmatrix}$	$\begin{bmatrix} .27 & -2.8 \times 10^{-3} \\ -2.8 \times 10^{-3} & 1.3 \times 10^{-4} \end{bmatrix}$

TABLE 1
LIMITING VARIANCE MATRIX OF INSTRUMENT PARAMETER ESTIMATORS

$$\sigma_w^2 = 1, M = \begin{bmatrix} 1 & 1 \\ 1 & q'' \end{bmatrix}$$

As can be seen from Table 1, increasing the baseline length reduces all elements in the variance matrix of the estimators for each instrument; the variance of the estimate of slope is reduced more than the variance of estimated intercept. If the instrument is known to be truly linear, the best choice of calibration values is at the extreme ends of the instrument operating range. In practice, of course, it is often desirable to check calibration at the midrange as well to test the hypothesis of linearity. Clearly, the less stable instrument has a larger variance of estimated calibration coefficients. As mentioned earlier, the variance of the estimated coefficients can be reduced by replicating the calibration experiment, which has the effect of reducing the variance of the measurement error σ_w^2 .

If both σ_w^2 and σ_v^2 are multiplied by the same scale factor, so is the variance matrix of the estimated coefficients. If, for example, $\sigma_v^2 = .001$ and $\sigma_w^2 = .1$ the ratio is .01, hence the variance matrix is obtained by multiplying the middle column of Table 1 by 0.1.

3. RETROSPECTIVE UPDATE

Observations obtained after time t may be used to improve our estimate of the system state at t . In this section, we consider t fixed and denote future epochs by $t+k$, where $k > 0$. Even though we are primarily interested in estimating Y_t , we continue to estimate Y_{t+k} for $k = 1, 2, \dots$ by the scheme described in Section 1. Suppose that the history of observations to time $t+k$ has been used to estimate both Y_t and Y_{t+k} , that is, both $\hat{Y}_{t|t+k}$ and $\hat{Y}_{t+k|t+k}$ have been computed. Then we observe the next output vector X_{t+1+1} and desire to update our estimate of Y_t .

As in Section 1, this estimate is updated by using

$$(3.1) \quad \hat{Y}_{t|t+k+1} = \hat{Y}_{t|t+k} + B_{t|t+k+1} Z_{t+k+1}$$

where B is computed, as in Equation (1.3), from

$$(3.2) \quad B_{t|t+k+1} = C\{R_{t|t+k}, Z_{t+k+1}\} C[Z_{t+k+1}]^{-1}$$

and the variance matrix of the residual of the updated estimator is obtained, as in Equation (1.5), from

$$(3.3) \quad C[R_{t|t+k+1}] = C[R_{t|t+k}] - B_{t|t+k+1} C[Z_{t+k+1}, R_{t|t+k}] .$$

In order to carry out these calculations, we need to compute the matrix $C[Z_{t+k+1}, R_{t|t+k}]$. Observe first that

$$(3.4) \quad Z_{t+k+1} = MAR_{t+k|t+k} + MV_{t+k} + W_{t+k+1} .$$

Since $R_{t|t+k}$ is a linear combination of the V_j sequence for $j < t+k$ and the W_j sequence for $j < t+k+1$, it is uncorrelated with V_{t+k} and W_{t+k+1} . Hence we have

$$(3.5) \quad C\{Z_{t+k+1}, R_{t|t+k}\} = \text{MAC}\{R_{t+k|t+k}, R_{t|t+k}\}.$$

Now notice that

$$(3.6) \quad R_{t|t+k} = R_{t|t} - \sum_{j=1}^k B_{t|t+j} Z_{t+j}.$$

Since $R_{t+k|t+k}$ is uncorrelated with Z_{t+j} for $j < k+1$ as shown by Equation (1.20), we have

$$(3.7) \quad C\{R_{t+k|t+k}, R_{t|t+k}\} = C\{R_{t+k|t+k}, R_{t|t}\}.$$

Finally we show how to update the term in the right of (3.7). Using Equation (1.19) to deduce the relationship between $R_{t+k|t+k}$ and $R_{t+k+1|t+k+1}$, we have

$$(3.8) \quad C\{R_{t+k+1|t+k+1}, R_{t|t}\} = (I - B_{t+k+1|t+k+1}^M) \text{AC}\{R_{t+k|t+k}, R_{t|t}\}.$$

In summary, Equations (3.1), (3.2), and (3.5) permits update of the estimate $\hat{Y}_{t|t+k}$. The variance of this estimator is updated recursively using (3.3), which also requires (3.5). This Equation, in turn, depends on (3.7) and the recursion of (3.8). The matrices $C[Z_{t+k+1}]$ in (3.2) and $B_{t+k+1|t+k+1}$ in (3.8) are obtained from the ordinary Kalman recursion of Section 1.

4. APPLICATION OF RETROSPECTIVE UPDATE TO INSTRUMENT CALIBRATION

In order to illustrate the use of the methods of the previous section, the instrument model of Section 2 has been studied in some detail. In these computations, we consider the four extreme cases of Table 1, that is, $\sigma_v^2 = .1$ and $.001$ and $q'' = 3$ and 100 . The covariance matrix $C[R_t | t+k]$ was computed for values of k ranging from 1 to 128, and the main diagonal elements plotted against k , with a logarithmic transformation of the k axis. Recall that the first component of the state vector in this model is a_t , the intercept of the calibration curve, and the second is the slope, b_t . The graphs of Figures 1-4 show the variances of estimates of these quantities.

It is clear from these plots that the maximum reduction in the variance of $\hat{b}_t$ is considerably less than for $\hat{a}_t$, particularly when q'' is set to 100 in the long base line case. In this case, no significant improvement is possible because each individual calibration experiment yields essentially all the information about the current value of slope, $\hat{b}_t$, that can be obtained. On the other hand, the variance of the estimate $\hat{a}_t$ can be reduced by about a third by future calibration experiments. We observe that when the instrument is unstable, that is σ_v^2 is large compared to σ_w^2 , the distant future contains little information about current values of the intercept a_t . The values of σ_a^2 declines to its limit fairly rapidly; after 8 periods have elapsed, further observations do not improve the estimate. By contrast, the more stable instrument shows a decline in σ_a^2 for 64 or 128 additional observations, but the initial decrease is not so rapid. After the first 8 additional observations, the variance has decreased by less than a third of the ultimate amount.

FIGURE 2

FIGURE 3

FIGURE 4

Table 2 shows the comparison between the variance matrices of the estimators before retrospective update and after. The first matrix in each block is copied from Table 1. The second is the result after improvements from retrospective updating become insignificant. The diagonal elements of each matrix are the variances of $\hat{a}$ and $\hat{b}$ respectively, and the off diagonal element is the covariance of $\hat{a}$ with $\hat{b}$.

We conclude from these examples that, for relatively unstable instruments, the retrospective update scheme may be an attractive way to improve the precision of estimated calibration coefficients since a few additional observations will yield significant variance reduction. However, if the instrument is relatively stable, many more additional calibration experiments must be performed to gain significant variance reduction. Furthermore, the variance of the estimated coefficients produced by the usual Kalman filter scheme is smaller for a more stable instrument, other things being equal, so the retrospective update of calibration coefficients may not be worthwhile in this case.

Since scaling all input variances by a constant multiplies the estimator variances by the same constant, as has been mentioned earlier, the stability of the instrument depends on the ratio of σ_w^2 to σ_v^2 rather than the absolute value of σ_w^2 . The effective value of σ_w^2 , the measurement error variance, can be reduced by replicating the experimental design and averaging the estimates is derived from each independent replicate. The result, of course, would be to reduce the variance of the retrospectively updated estimates. Since the ratio of σ_w^2 to σ_v^2 would be effectively reduced, so would relative stability. Consequently, the additional variance reduction obtained from retrospective updates will occur sooner, which would make the retrospective update scheme even more attractive.

$q'' \sigma_v^2$	.001	.1
3	$\begin{bmatrix} .047 & -.016 \\ -.016 & .015 \end{bmatrix}$ $\begin{bmatrix} .031 & -.011 \\ -.011 & .0091 \end{bmatrix}$	$\begin{bmatrix} .43 & -.15 \\ -.15 & .12 \end{bmatrix}$ $\begin{bmatrix} .24 & -.081 \\ -.081 & .074 \end{bmatrix}$
100	$\begin{bmatrix} .031 & -3.2 \times 10^{-4} \\ -3.2 \times 10^{-4} & .95 \times 10^{-4} \end{bmatrix}$ $\begin{bmatrix} .018 & 1.8 \times 10^{-4} \\ -1.8 \times 10^{-4} & .86 \times 10^{-4} \end{bmatrix}$	$\begin{bmatrix} .27 & -2.8 \times 10^{-3} \\ -2.8 \times 10^{-3} & 1.3 \times 10^{-4} \end{bmatrix}$ $\begin{bmatrix} .16 & -1.6 \times 10^{-3} \\ -1.6 \times 10^{-3} & 1.2 \times 10^{-4} \end{bmatrix}$

TABLE 2
COMPARISON BETWEEN LIMITING VARIANCE MATRIX AND
UPDATED VARIANCE MATRIX OF INSTRUMENT PARAMETER ESTIMATORS

$$\sigma_w^2 = 1, M = \begin{bmatrix} 1 & 1 \\ 1 & q \end{bmatrix}$$

5. INTERPOLATION COMBINED WITH RETROSPECTIVE UPDATE

In this section, we assume that observations are made at every k periods, that is when $t = mk$. All the observations obtained until epoch mk are used to find the best linear unbiased estimators of the system states at times $t = nk$, denoted $\hat{Y}_{nk|mk}$, for $n = 1, 2, \dots, m$. The same information is used to estimate the system states of the periods between observation epochs i.e., $\hat{Y}_{nk+l|mk}$, $l = 1, 2, \dots, k-1$; $n = 1, 2, \dots, m-1$.

The new observation vector $X_{(m+1)k}$ may be used to update our estimates $\hat{Y}_{nk+l|mk}$ i.e., to find the improved estimates $\hat{Y}_{nk+l|(m+1)k}$, $n = 1, 2, \dots, m$; $l = 1, 2, \dots, k$ and also the new estimates $\hat{Y}_{mk+l|(m+1)k}$, $l = 1, 2, \dots, k$, of the system state at times between the latest observation and the previous one.

5.1 Update of Estimate at Observation Epochs

The recursive estimation of system state at the observation epochs $t = mk$, $m = 1, 2, \dots$, accomplished by methods directly analogous to the basic Kalman recursion of Section 1.

Applying the linear dynamic relation Equation (1.7) k times recursively, we have

$$(5.1) \quad Y_{(m+1)k} = A^k Y_{mk} + V_{mk}^{*k}$$

where we define

$$V_{mk}^{*k} = A^{k-1} V_{mk} + A^{k-2} V_{mk+1} + \dots + V_{mk+k-1}$$

and hence

$$C[V^{*k}] = C\{V_{mk}^{*k}, V_{mk}^{*k}\} = \sum_{j=0}^{k-1} A^j C_v (A^j)'$$

thus,

$$(5.2) \quad \hat{Y}_{(m+1)k|mk} = A^k \hat{Y}_{mk|mk}.$$

We obtain from the above two equations, and the definition of the residual vector R ,

$$(5.3) \quad R_{(m+1)k|mk} = A^k R_{mk|mk} + V_{mk}^{*k}.$$

Now as in Section 1, we have

$$(5.4a) \quad Z_{(m+1)k} = X_{(m+1)k} - \hat{X}_{(m+1)k|mk}$$

$$(5.4b) \quad = M R_{(m+1)k|mk} + W_{(m+1)k}$$

$$(5.4c) \quad = M (A^k R_{mk|mk} + V_{mk}^{*k}) + W_{(m+1)k}.$$

The estimate of $Y_{(m+1)k}$ is updated from time mk by

$$(5.5) \quad \hat{Y}_{(m+1)k|(m+1)k} = A^k \hat{Y}_{mk|mk} + B_{(m+1)k|(m+1)k} Z_{(m+1)k}$$

where the matrix B is computed from

$$(5.6) \quad B_{(m+1)k|(m+1)k} = C[R_{(m+1)k|mk}] M' C[Z_{(m+1)k}]^{-1}.$$

The covariance matrices of the residual of the observation is computed using Equation (5.4b) from

$$(5.7) \quad C[Z_{(m+1)k}] = M C[R_{(m+1)k|mk}] M' + C_w.$$

The variance matrix of the updated state vector estimate is

$$(5.8) \quad C[R_{(m+1)k|mk}] = A^k C[R_{mk|mk}] (A^k)' + C[V^{*k}].$$

Notice that, in the procedure for computing $\hat{Y}_{(m+1)k|(m+1)k}$ we require the covariance matrix $C[R_{mk|mk}]$. We can compute this covariance matrix recursively from Equations (5.6), (5.7) and (5.8) in the usual way.

$$(5.9) \quad C[R_{(m+1)k|(m+1)k}] = C[R_{(m+1)k|mk}] - B_{(m+1)k|(m+1)k} \cdot C[Z_{(m+1)k}, R_{(m+1)k|mk}].$$

5.2 Interpolation

Next we show how to estimate the system states of the periods between observation epochs and compute the corresponding covariance matrix of residuals. To extrapolate from the latest observation into the future, we use the analog of Equation (5.1):

$$(5.10a) \quad \hat{Y}_{mk+l|mk} = A^l \hat{Y}_{mk|mk}, \quad l = 1, 2, \dots, k.$$

Interpolation and retrospective update are accomplished by:

$$(5.10b) \quad \hat{Y}_{nk+l|mk} = \hat{Y}_{nk+l|(m-1)k} + B_{nk+l|mk} Z_{mk}, \quad n = m-1, m-2, \dots$$

where

$$(5.10c) \quad B_{nk+l|mk} = C[R_{nk+l|(m-1)k}, Z_{mk}] C[Z_{mk}]^{-1}.$$

The matrix $C[Z_{mk}]^{-1}$ is obtained using the Equation (5.7). We show how to compute $C[R_{nk+l|(m-1)k}, Z_{mk}]$ by recursion on l first, then by recursion on m .

We focus our attention on the interval $t = nk, nk+1, \dots, nk+l, \dots, (n+1)k$, which includes the two observation epochs nk and $(n+1)k$. We consider first the interpolation between the latest two observation epochs, that is, the latest observation is X_{mk} where $m = n+1$. Then we show how to carry out the retrospective update computation as additional observations become available, that is when $m > n+1$.

5.2.1 Interpolation When $n = m - 1$

Consider $m = n + 1$. Since $R_{nk+l+1|nk} = AR_{nk+l|nk} + V_{nk+l}$, and using Equation (5.4c), we have the recursion on l :

$$(5.11a) \quad C\{R_{nk+l+1|nk}, Z_{(n+1)k}\} = AC\{R_{nk+l|nk}, Z_{(n+1)k}\} + C_v(A^{k-l})'M'$$

and the initialization:

$$(5.11b) \quad C\{R_{nk|nk}, Z_{(n+1)k}\} = C[R_{nk|nk}](A^k)'M'.$$

These matrices are used in Equation (5.10) to compute $\hat{Y}_{nk+l|(n+1)k}$.

5.2.2 Retrospective Update of Interpolation: $m > n + 1$

Now we consider subsequent observations when $m > n + 1$, i.e., $m = n + 2, n + 3, \dots$. Utilization of (5.10c) requires computation of $C\{R_{nk+l|(m-1)k}, Z_{mk}\}$. From the definition,

$$(5.12) \quad C\{R_{nk+l|(m-1)k}, Z_{mk}\} = E\{(Y_{nk+l} - \hat{Y}_{nk+l|(m-1)k})(Z_{mk})'\}.$$

Now notice that,

$$(5.13) \quad Y_{nk+l} = A^l Y_{nk} + V_{nk}^{*l}$$

and

$$(5.14) \quad \hat{Y}_{nk+l|(m-1)k} = \sum_{j=n+1}^{m-1} B_{nk+l|jk} Z_{jk} + A^l \hat{Y}_{nk|nk}$$

from recursive substitution in Equation (5.10b). By application of Equation (1.20),

$$(5.15) \quad C\{R_{nk|nk}, Z_{mk}\} = 0, \quad n = 1, 2, 3, \dots, m.$$

Expanding the Equation (5.12) using the results of (5.4), (5.13) and (5.14), setting to zero the cross product terms which are uncorrelated and utilizing (5.15), we obtain:

$$(5.16) \quad C\{R_{nk+l} | (m-1)k, Z_{mk}\} = MA^k \left[C\{R_{(m-1)k} | (m-1)k, R_{nk} | nk\} (A^L)^t + C\{R_{(m-1)k} | (m-1)k, V_{nk}^{*L}\} \right].$$

We derive the following recursive formulation to apply to Equation (5.16).

$$(5.17) \quad C\{R_{mk} | mk, R_{nk} | nk\} = \left(A^k - B_{mk} | mk MA^k \right) C\{R_{(m-1)k} | (m-1)k, R_{nk} | nk\},$$

$$m = n+1, n+2, \dots$$

$$(5.18a) \quad C\{R_{mk} | mk, V_{nk}^{*L}\} = \left(A^k - B_{mk} | mk MA^k \right) C\{R_{(m-1)k} | (m-1)k, V_{nk}^{*L}\},$$

$$(5.18b) \quad C\{R_{(n+1)k} | (n+1)k, V_{nk}^{*L}\} = (I - B_{(n+1)k} | (n+1)k) \left\{ A^{k-1} C_v(A^L)^t + \dots + A^{k-L} C_v \right\}.$$

Notice that the matrix B and $C\{R_{nk} | nk\}$ are known. Thus we use (5.17) and (5.18a) recursively with the initial equation (5.18b), then substitute to Equation (5.16) to compute the covariance matrix

$$C\{R_{nk+l} | (m-1)k, Z_{mk}\}, m = n+2, n+3, \dots$$

Finally we can compute the estimate using (5.10a) and (5.10b).

5.3 Summary

In practice, as each new observation, $X_{(m+1)k}$ is obtained, the current state is estimated, and then the retrospective updates of estimated states at earlier epochs are computed. The computation proceeds as follows:

- (1) Update $\hat{Y}_{(m+1)k|(m+1)k}$, $C[Z_{(m+1)k}]$ and $C[R_{(m+1)k}|m_k]$ using (5.5), (5.6), (5.7) and (5.8).
- (2) Compute the interpolation estimates $\hat{Y}_{mk+l|(m+1)k}$ from (5.10b), (5.10c), (5.11a) and (5.11b). These yields also $C[R_{nk+l}|m_k]$ and $Z_{(m+1)k}$, by recursion on l .
- (3) Update earlier interpolation estimates to compute $\hat{Y}_{nk+l|(m+1)k}$ by use of (5.10b), (5.10c) and applying (5.16) ~ (5.18b) for $n \leq m - 1$.

6. INTERPOLATION AND RETROSPECTIVE UPDATE OF INSTRUMENT CALIBRATION

The computing scheme of Section 5 can be illustrated by a simpler version of the instrument model discussed in Sections 2 and 4, in which we assume that only a single parameter need be estimated. For example, with some instruments, a background reading is routinely taken with every production sample to determine the instrument "zero", so only the scale parameter need be determined by calibration. In this section, we let σ_w^2 represent the variance of estimate of the current value of the instrument parameter as determined by a single calibration experiment. The variance of the parameter drift (per unit time) is σ_v^2 as before. In this case, of course, the instrument parameter and the observation resulting from a calibration experiment are scalar quantities.

We carry out the computations of Section 5 for instruments that are calibrated every 10 time units (days, for example). Two instruments are considered: a very stable instrument with $\sigma_v^2 = .001$, $\sigma_w^2 = 1$; and a less stable instrument with $\sigma_v^2 = .01$ and $\sigma_w^2 = .1$. As before, scaling both input variances by a constant will scale the estimator variance by the same factor; it is the ratio σ_v^2/σ_w^2 that determines relative stability.

The behavior of the more stable instrument is shown in Figure 5. The top line of the plot shows the variance of the estimator $Y_{nk+l|(n+1)k}$ as a function of l . We assume that calibration experiments are performed every 10 days at times $t = 10n$ and $t = 10n+10$. We have computed the variance of the interpolated calibration coefficient estimates for the points between these epochs. The plot shows that the variance of the interpolated estimates lies on the straight line between the variances of the estimators for the epochs of calibration, represented by $l = 0$ and $l = 10$. The variance of the estimate

FIGURE 5

at $t = 10n$ ($l = 0$) is less than the variance at the next calibration epoch, $t = 10n + 10$ ($l = 10$) because the later calibration has provided information for the retrospective update of the earlier estimate.

The next calibration experiment at $t = 10n + 20$ is used to update the estimated states at both $t = 10n$ and $t = 10n + 10$ and also the points between. The variances of these estimators fall on the line labeled " $m = n + 2$ ". Further retrospective updates of these estimators computed from calibrations performed at $t = 10n + 40$ and $10n + 80$ give rise to variances that lie on the plotted lines labeled $m = n + 4$ and $m = n + 8$.

The time behavior of the variances of the estimators at the calibration epochs and at the midpoint of the interpolation interval ($l = 5$) is shown on Figure 6. Here we observe the typical pattern of stable instruments, that is relatively small reduction in variance at first, but a continuing reduction as many additional observations become available. In this case, the variances of the estimates continue to decline out to the 16th additional data point at $t = 10n + 160$.

By contrast, the corresponding plot for the less stable instrument, shown in Figure 8, exhibits a large variance reduction resulting from the first new calibration at $t = 10n + 20$, and very small additional reductions. The variances of the estimated coefficients at all the interpolation points is shown in Figure 7. As with the stable instrument, the variances of the first interpolated estimates lie in the straight line between the observation epoch variances. However, the plot of variances resulting from the first retrospective update at $t = 10n + 20$ ($m = n + 2$) assumes a pronounced curvature.

FIGURE 6

The plots for $m = n + 4$ and $m = n + 8$ essentially coincide showing that more calibrations provide no additional information. The curvature of the lower plots shows that the calibration coefficients are known with greater precision at observation epochs than at the points between.

In comparing the plots of Figure 6 and 8, it is clear that the retrospective update of the interpolated estimates is much more attractive in the case of the less stable instrument because only one additional observation can result in substantial variance reductions (by factors as large as 2.5).

The theory of Section 5 can be used to examine some questions of calibration strategy. Suppose, for example, each calibration experiment costs a dollar, and the budget for calibration is a dollar a day. Is it better to calibrate daily or to perform 10 replicates every 10 days? To be concrete, let us consider an instrument characterized by $\sigma_v^2 = .01$ and $\sigma_w^2 = 1$. If this instrument is calibrated daily and the retrospective update scheme is used, the variance of the estimate of the instrument parameter as a function of the time lag is shown in Figure 9. Suppose that instead of the daily calibration, we replicate the calibration experiment 10 times every 10th day and treat the average of 10 estimates as a single observation. Independent replicates will reduce the variance of this observation to $\sigma_w^2 = .1$. Then the variance of the estimates derived from interpolation and retrospective update are shown in Figure 7 and 8. Since we have assumed that the cost of 10 replicates is 10 times the cost of the basic calibration experiment, both strategies have the same cost.

The question of which strategy is to be preferred is a little complicated. If we do no retrospective updating, the 10 day strategy produces estimates with variances ranging from .62 to 1.62, while the daily calibration

estimates have a variance of .95. Suppose that one retrospective update is done in the 10 day scheme. Then the estimates have variances shown in the middle line of Figure 7. Notice that these estimates range from 10 to 20 days old, the average age being 15 days. Now if we consult Figure 9, we see that estimates produced by daily scheme retrospectively updated for 15 days have a variance that is less than all but the first two points of the middle line of Figure 7. The variance ratios of the largest and smallest variances on that line to the 15 day point of Figure 9 are 1.2 and .9. Thus when the time lags involved in the retrospective update are comparable, the daily calibration scheme produces slightly more precise estimates than the 10 day scheme.

Under our assumption that each calibration experiment costs a dollar, it is slightly preferable to calibrate as often as the budget will allow rather than allowing more time to elapse and replicating the calibration experiments. However, if this assumption about costs fails to hold, a different conclusion follows. For example suppose the cost of two replicates performed sequentially is less than twice that of a single experiment. Then a fixed budget can be more effectively spent on less frequent replicated calibration experiments with retrospective updating of the interpolated estimates.

FIGURE 7

FIGURE 8

FIGURE 9

REFERENCES

- [1] Kalman, R. E., "A New Approach to Linear Filtering and Prediction Problems," Trans. ASME, J. Basic Eng., Vol. 82, pp. 35-44 (1960).
- [2] Kalman, R. E. and Bucy, "New Results in Linear Filtering and Prediction Theory," Trans. ASME, J. Basic Eng., Vol. 83, pp. 95-108, (1961).
- [3] Gelb, A., Applied Optimal Estimation, M.I.T. Press, Cambridge, Massachusetts, (1974).
- [4] Jaech, J. L., Statistical Methods in Nuclear Material Control, U.S. Atomic Energy Commission, (1973).
- [5] Kailath, T., "An Innovations Approach to Least-Squares Estimation - Part I: Linear Filtering in Additive White Noise," IEEE Trans. Aut. Con., Vol. AC-13, pp. 646-655, (December 1968).
- [6] Box, G. E. P., and G. M. Jenkins, Time Series Analysis: Forecasting and Control, Holden-Day, (1976).
- [7] Sorenson, H. W., "Kalman Filtering Techniques," Advances in Control Systems, Vol. 3, Academic Press, (1966).
- [8] Fagin, S. L., "Recursive Linear Regression Theory, Optimal Filter Theory and Error Analyses of Optimal Systems," 1964 IEEE Conv. Rec., pp. 216-240.

NOTICE

"This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately-owned rights."