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USE OF STATE ESTIMATION TECHNIQUES IN WATER RESOURCE SYSTEM MODELING[1]

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ABSTRACT: A relatively straightforward illustration of the potential uses of State Estimation techniques in water resources modeling is given. Background theory for Linear and Extended Kalman Filters is given; application of the filter techniques to modeling BOD and oxygen deficit in a stream illustrates the importance of model conceptualization, model completeness, uncertainty in model dynamics and incorporation of measurements and measurement errors. Potential applications of state estimation techniques to measurement system design; model building, assessment and calibration; and data extension are explored.
(KEY TERMS: State Estimation; water quality modeling; measurement system design; uncertainty analysis.)

INTRODUCTION

The last fifteen years have seen substantial breakthroughs in the field of State Estimation. Most of the pioneering work in this field, beginning with the classic papers of Kalman (1960), Kalman and Bucy (1961), and Kalman (1963) saw application to navigation problems. The typical navigation problem, briefly, is to obtain real time estimates of the trajectory of a vehicle given noisy (imprecise) observations of position and a model of the dynamics of the trajectory. It has only been in the last several years that applications of the theory have been proposed in the field of water resources research, although many of the problems faced by researchers and practitioners in this field may be approached using state estimation techniques.

Most of the state estimation literature presupposes some familiarity with stochastic calculus and deterministic control theory. Lack of this familiarity has resulted in difficulty on the part of workers in the water resources field to appreciate the potential of state estimation techniques. This is the classical problem of not being able to see the forest for the trees. It is the purpose of this paper, therefore, to explain the theory in a manner understandable to a person without the background assumed in the existing literature and to suggest applications to water resource problems.

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BACKGROUND

State estimation is a term loosely used to classify methods which combine a knowledge of the dynamics of evolution of a vector of state variables with a measurement of a function of some or all of the state variables to yield an estimate of the actual value of the state vector. Usually both the dynamical (theoretical or modeled) estimate of state and the measurement estimate are not exact. Thus, both theoretical estimates and measurements contain noise terms. These fundamental relationships may be described as:

$$\frac{d\underline{X}}{dt} = \underline{f}(\underline{X},t) + \mathbf{G}(t)\,\underline{W}(t) \tag{1}$$

$$\underline{Y}(t) = \underline{h}(\underline{X},t) + \underline{V}(t) \tag{2}$$

Here, and throughout this paper, the underbar notation ("$\underline{A}$") denotes a (column) vector, and the boldface notation ("**B**") denotes matrices, and

$\underline{X}$ = vector of state variables (dimension n x 1)
$\underline{f}$ = driving function of differential equation of state (n x 1)
$\mathbf{G}(t)$ = system noise coefficient matrix (n x r)
$\underline{W}(t)$ = vector of system noise (r x 1)
$\underline{Y}(t)$ = vector of measured variables (m x 1)
$\underline{h}$ = measurement function (m x 1)
$\underline{V}(t)$ = vector of measurement noise (m x 1)

The system noise vector and the measurement noise vectors have, by definition, the covariance matrices $\mathbf{Q}(t) = E[\underline{W}(t)\ \underline{W}^T(t)]$; $\mathbf{R}(t) = E\ [\underline{V}(t)\ \underline{V}^T(t)]$ where the notation $E(\cdot)$ indicates the mathematical expectation. **Q** and **R** are referred to hereafter as the system and measurement noise covariance matrices, respectively.

Frequently, in water resources systems, the measurement function $\underline{h}$ is linear, i.e., $\underline{h}(\underline{X},t) = \mathbf{H}(t)\underline{X}$. An example of a nonlinear measurement system is the estimation of stream discharge using a measurement of stream stage. The more common linear relationship is illustrated by measurements taken of dissolved oxygen when the state variable is also dissolved oxygen. The system driving function $\underline{f}$ is, however, often nonlinear. Hence, in water resource applications we are typically faced with a "nonlinear dynamics-linear measurement" state estimation problem.

Equations 1 and 2 describe the general state estimation problem. The problem may be further categorized by the relationship between times of measurements and times at which estimation is desired. If an estimate of the state vector, $\underline{X}$, at time t is desired based on measurements up to time t, the problem is termed the **filtering problem.** If an estimate of the state vector $\underline{X}$ at time $t' < t$ is desired, based on measurements up to time t, the problem is termed the **smoothing problem.** If an estimate of $\underline{X}$ at time $t' > t$ is desired based on measurements to time t the problem is termed the **prediction problem.** Principle interest in this paper is in the filtering and prediction problems.

AN EXAMPLE

To illustrate the concept of state estimation, the simplified Streeter-Phelps equations may be modeled using the framework of equations 1 and 2. The simplified equations, considering only BOD decay and reaeration are:

$$\frac{dB}{dt} = -K_1 B \quad (3)$$

$$\frac{dD}{dt} = -K_2 D + K_1 B \quad (4)$$

Where D is oxygen deficit (OD), B is BOD remaining at time t, K_1 is the BOD decay coefficient, and K_2 is the reaeration coefficient.

If we take a state vector $\underline{X}$ having two elements $X_1 = B$ and $X_2 = D$, equations 3 and 4 can be rewritten in the form of equation 1 as

$$\frac{d}{dt}\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} -K_1 X_1 \\ K_1 X_1 - K_2 X_2 \end{bmatrix} + \begin{bmatrix} W_1 \\ W_2 \end{bmatrix} \quad (5)$$

where the system noise coefficient matrix is taken to be $\mathbf{G}(t) = \left[\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right]$. If only OD ($X_2$) is measured, equation 2 becomes

$$\underline{Y} = [\,0\;1\,]\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} + [\,V_2\,] \quad (6)$$

DERIVATION OF THE MINIMUM MEAN SQUARE ERROR LINEAR FILTER

Equations 1 and 2 provide the basis for two independent estimates of the system state $\underline{X}$ if the system and measurement noise are uncorrelated, i.e., $E[\underline{W}(t)\underline{V}(s)] = 0, \forall t,s$. Justification for an assumption of independence of system noise (modeling error) and measurement noise is that the system driving function $\underline{f}$ is usually derived from data sets different from that containing the measurements used in equation 2.

The filter we desire is no more than a "recipe" for combining these two independent estimates of $\underline{X}$. A mathematically rigorous filter derivation requires a background in stochastic calculus. A less rigorous, but more intuitive derivation has been presented by Barham and Humphries (1970) and is summarized here because of the insight it yields.

We consider first the case for a single dimension. Given two independent estimates A_1 and A_2 of a quantity X with corresponding variances V_1 and V_2, we desire a linear combination of A_1 and A_2 giving the minimum variance estimate, $\hat{X}$, of X. Taking $0 \leqslant c \leqslant 1$, let

$$X = (1 - c)\, A_1 + cA_2 \quad (7a)$$

then

$$E(\hat{X}) = (1 - c)\,E(A_1) + cE(A_2)$$

and

$$\begin{aligned} \text{Var}\,(\hat{X}) &= E(X - E(X))^2 \\ &= (1-c)^2\,E[(A_1 - E[A_1])^2\,] \;+\; c^2 E\,[A_2])^2\,] \\ &= (1-c)^2\,V_1 + c^2 V_2 \end{aligned}$$

hence, minimizing Var $(\hat{X})$ with respect to c,

$$\frac{\partial\,\text{Var}\,(\hat{X})}{\partial c} = -2(1-c)V_1 + 2cV_2 = 0$$

Thus c*, the minimum variance estimate of c becomes

$$c^* = \frac{V_1}{V_1 + V_2}$$

Therefore equation 7a becomes

$$X = A_1 - c^*(A_1 - A_2) \tag{7b}$$

and the minimum variance is

$$V^* = V_1\,(1 - c^*) \tag{8}$$

If we let $A_1 = X_1$ be the **model estimate** of X, and $A_2 = Y$ be the **measurement** of X,

$$\hat{X} = X_1 - c^*(X_1 - Y) \tag{7c}$$

The extension to multiple dimensions requires matrix algebra and is slightly more complex than the case for a single dimension. The development is not presented here because of space limitations. The only conceptual difference, however, is that the two estimates $\underline{A}_1$ (modeled) and $\underline{A}_2$ (measured) of $\underline{X}$ may not be of the same dimension, for instance, not all the state variables may be measured. The result for a state vector of arbitrary dimension is:

$$\hat{\underline{X}} = \underline{X}_1 - K(M\underline{X}_1 - \underline{Y}) \tag{9}$$

where

$$\mathbf{K} = \mathbf{P'M}^T\ (\mathbf{MP'M}^T + \mathbf{R})^{-1} \tag{10}$$

and

$$\mathbf{P^*} = \mathbf{P'} - \mathbf{KMP'} \tag{11}$$

Here **M** is a measurement matrix which describes the elements of the state vector which are measured, i.e., $\underline{Y} \sim \mathbf{M}\underline{X}$; **P′** is the conditional value of the state covariance matrix **P** before the measurement $\underline{Y}$ is taken, **P*** is the value of **P** after the measurement, and **K** is the gain matrix analogous to the weighting factor "c" for the single dimensional case. It should be emphasized that P is the value of the state covariance matrix conditioned on the best estimate $\hat{\underline{X}}$ of $\underline{X}$, $\mathbf{P} = E(\underline{X} - \hat{\underline{X}})(\underline{X} - \hat{\underline{X}})^T$ and is not to be confused with the system error covariance matrix $\underline{Q}$. The state covariance matrix **P** is computed by the filter whereas the system error covariance **Q** must be estimated *a priori.*

The measurement matrix **M** cannot be chosen freely; a condition known as **observability** must be satisfied. A conceptual definition of observability is that, given the sequence of measurements $\underline{Y}(t)$, $t \leq t_o$, the behavior of the state $\underline{X}(t)$ can be inferred for all $0 \leq t \leq t_o$. Observability conditions are not always straightforward to establish. They will normally be satisfied, however, if measurements are taken of all state variables not highly interdependent with any other measured variable. In the case of the DO-BOD model, for instance, measurement of either DO or BOD will satisfy observability as DO and BOD are substantially interdependent in the model dynamics.

No assumptions concerning the form of the system equations have been made thus far, i.e., we have not specified how the model estimate $\underline{A}_1$ or $\hat{\underline{X}}$ is to be made. The minimum mean square error (MMSE) filter provides the mechanism for combining predictions and measurements. We first consider the case where system dynamics are linear.

KALMAN FILTER ALGORITHM

The Kalman filter is that derived in the original work by Kalman (1960). It is applicable for the case of a linear system with linear measurements, and for this reason, is also known as the **linear filter**. The equations of state and measurement are:

$$\frac{d\underline{X}}{dt} = \mathbf{F}(t)\underline{X} + \mathbf{G}(t)\underline{W}(t) \tag{12}$$

$$\underline{Y}(t) = \mathbf{H}(t)\underline{X} + \underline{V}(t) \tag{13}$$

If we define the $\underline{X}(k + 1|k)$ to be an estimate of $\underline{X}$ at discrete time increment $k + 1$, conditioned by an estimate at time period k, the solution is: (a) prior to taking measurement $\underline{Y}(k + 1)$

$$\underline{X}(k + 1|k) = \phi(k + 1, k)\,\underline{X}(k|k) \tag{14}$$

$$P(k+1|k) = \phi(k+1,k)\,P(k|k)\,\phi^T(k+1,k) + G(k)\,Q(k+1)\,G^T(k) \quad (15)$$

$$K(k+1) = P(k+1|k)\,M^T(k+1)\,[\,M(k+1)\,P(k+1|k)\,M^T(k+1) + R(k+1)\,]^{-1} \quad (16)$$

(b) after taking measurement $\underline{Y}(k+1)$

$$\hat{\underline{X}}(k+1|k+1) = \hat{\underline{X}}(k+1|k) + K(k+1)\,[\,\underline{Y}(k+1) - M(k-1)\,\underline{X}(k+1|k)\,] \quad (17)$$

$$P(k+1|k+1) = [\,I_n - K(k+1)\,M(k+1)\,]\,P(k+1|k) \quad (18)$$

where $\phi(t)$ is the solution to

$$\frac{d\phi(t,t_o)}{dt} = F(t)\phi(t,t_o)$$

with initial condition $\phi(t,t)|_{t=t_o} = I_n$, the n x n identity matrix (19)

The matrix **P** is the state covariance matrix given in general by

$$P(i|j) = E\,[\,(\hat{\underline{X}}(i|j) - \underline{X}_i)\,(\hat{\underline{X}}(i|j) - \underline{X}_i)^T\,] \quad (20)$$

The filter is implemented beginning at time step 0 by solving equation 19 for $\phi(1|0)$. Equations 14-18 are then solved sequentially, ultimately yielding $P(1|1)$ and $\hat{\underline{X}}(1|1)$. The process may then be repeated. The initial values $P(0|0)$ and $\hat{\underline{X}}(0|0)$ must be chosen *a priori*. In general, a very large initial estimate of $P(0|0)$ is equivalent to assuming no *a priori* knowledge and gives the *a priori* estimate $\hat{\underline{X}}(0|0)$ virtually no weight in the first filter equation $\hat{\underline{X}}(1|1)$.

The Kalman filter approach can be illustrated by considering the Streeter-Phelps equations in linear form, i.e., K_1 and K_2 are constant. For the Streeter-Phelps model with constant K_1 and K_2, equation 19 becomes:

$$\frac{d\phi(t)}{dt} = \begin{bmatrix} -k_1 & 0 \\ k_1 & -k_2 \end{bmatrix} \phi(t) \quad (21)$$

The solution to equation 21 is

$$\phi(t) = \begin{bmatrix} e^{-k_1(t-t_o)} & 0 \\ \frac{k_1}{k_2-k_1}\left\{e^{-k_1(t-t_o)} - e^{-k_2(t-t_o)}\right\} & e^{-k_2(t-t_o)} \end{bmatrix} \quad (22)$$

Equation 22 is readily recognized as the integrated form of the simplified Streeter-Phelps equations in matrix notation.

Table 1 summarizes the filter defined by equations 14-19 and the origin of each of the terms. The measurement error covariance matrix **M** is usually available from experience in the form of expected errors in analytic methods. As an example, laboratory errors in DO and BOD measurements are usually from experience or literature values can be used, for instance, American Public Health Association (1971). In the measurement error covariance matrix **R** the off-diagonal elements are taken to be zero unless some knowledge of measurement error correlation is available. Initially, the system error covariance matrix **Q** is taken as zero. This may be adjusted if divergence, discussed later, is encountered.

NONLINEAR PROBLEMS

The Kalman filter is of limited use since system models of the type used in water resource applications are often nonlinear. The most straightforward approach to this problem is the extended (linearized) Kalman filter. This filter requires the choice of a

TABLE 1. Initial Values and Updating Procedures for Vectors and Matrices of Equations 14 through 18.

Vector or Matrix	Initial Value	Updating Procedure
State Vector $\hat{\underline{X}}(k\|k)$	$\hat{\underline{X}}(0\|0)$ *a priori* estimate	equation 17
State Vector $\hat{\underline{X}}(k+1\|k)$ before measurement taken		equation 14
Driving Function $\phi(k+1, k)$		equation 19 $t = k + 1; t_o = k$
System Covariance Matrix P (k|k)	P (0|0) *a priori* estimate	equation 20
Noise Coefficient Matrix G(k)	Take as zero unless divergence problems occur	See section on divergence
System Noise Covariance Matrix Q(k + 1)	$E[\underline{W}(1)\,\underline{W}(1)^T]$	$E[\underline{W}(k+1)\,\underline{W}(k+1)^T]$ Unknown but fixed by system dynamics
Measurement Noise Covariance Matrix R(k + 1)	$E[\underline{V}(1)\,\underline{V}(1)^T]$	$E[\underline{V}(k+1)\,\underline{V}(k+1)^T]$ Known from quality of measurements
Measurement Matrix M(k + 1)		Refined by choice of state variable to be measured at time k + 1

nominal trajectory about which equation 1 is linearized. The measurement equation, equation 2, is assumed in this derivation to be in the linear form of equation 13. This assumption is usually valid in water resource applications; if nonlinear measurements are encountered the measurement equation may be linearized as well. The linearization of equation 1 takes the form of a first order approximation to the Taylor Series expansion of $\underline{f}$:

$$\underline{f}(\underline{X},t) = \underline{f}(\underline{X}^*,t) + F(\underline{X}^*,t)(\underline{X} - \underline{X}^*) \tag{23a}$$

where $\underline{X}^*$ is the nominal trajectory, and

$$F(X^*, t) = f_{ij} = \left[\frac{\partial fi}{\partial xj} \right]$$

where f_i is the ith component of the system driving vector $\underline{f}$ (equation 1) and x_j is the jth component of the state vector $\underline{X}$.

Equation 23 may be rewritten:

$$\underline{f}(\underline{X},t) - \underline{f}(\underline{X}^*,t) = \delta \underline{f}(\underline{X},t) = F(\underline{X}^*,t)\, \delta \underline{X} \tag{23b}$$

where $\delta \underline{X} = \underline{X} - \underline{X}^*$, the difference between the true and nominal values of $\underline{X}$. If one takes the dynamics of the nominal trajectory as being exact,

$$\frac{d\underline{X}^*}{dt} = \underline{f}(\underline{X}^*, t) \tag{24}$$

Subtraction of equation 24 from equation 1 and substitution of approximation 23b yields,

$$\frac{d\underline{X}}{dt} - \frac{d\underline{X}^*}{dt} = F(\underline{X}^*,t)(\underline{X} - \underline{X}^*) + G(t)\underline{W}(t) \tag{25a}$$

or, recalling that $\delta \underline{X} = \underline{X} - \underline{X}^*$,

$$\frac{d(\delta \underline{X})}{dt} = F(\underline{X}^*,t)(\delta \underline{X}) + G(t)\underline{W}(t) \tag{25b}$$

Equation 25b is used to solve for $\phi(t)$:

$$\frac{d\phi(t)}{dt} = F(\underline{X}^*,t)\,\phi(t) \tag{26}$$

The value of $\phi(t)$ determined from equation 26 is used in the extended Kalman filter algorithm. We now solve the nonlinear equation

$$\frac{d\hat{\underline{X}}(t|k)}{dt} = \underline{f}(\underline{X}^*,t), \qquad k \leqslant t \leqslant k+1 \tag{27}$$

directly for $\hat{\underline{X}}(k+1|k)$ based on the initial condition $\hat{\underline{X}}(t|k)|_{t=k} = \hat{\underline{X}}(k|k)$. The extended Kalman filter algorithm uses equations 14 and 19 with equation 14 replaced by equation 27 and equation 19 replaced by equation 26 in exactly the same manner as the linear filter. An example application requiring use of the nonlinear filter follows.

We again consider the simplified Streeter-Phelps equations. If the reaeration and BOD decay coefficients K_2 and K_1 are taken as constant, the linear filter may be implemented. Figures 1 and 2 show the results if the initial values are taken identical to those of Burges and Lettenmaier (1975). The filtered trajectories follow closely the true trajectory. The uncertainties in both BOD and DO, conditional on a single initial measurement, decay, however, in contrast to both the first-order and Monte Carlo results of Burges and Lettenmaier (1975), as shown in curves 1 and 2 of figure 3. This results from the dynamics of the constants being ignored.

If parameter uncertainty is included, i.e., if we consider the "constants" K_1 and K_2 to be random variables the problem is seen to be (equation 5) nonlinear and may be solved using an extended Kalman filter. In order to include uncertainty in stream velocity a downstream spatial coordinate y, rather than time t must be taken as the independent variable. The transformation made is $\frac{dx}{dy} = \frac{1}{U}\frac{dx}{dt}$, where U, the stream velocity, is taken to be a random variate with constant dynamics $\frac{dU}{dy} = 0$. For convenience let $X_1 = B$; $X_2 = D$; $X_3 = K_1$; $X_4 = K_2$; $X_5 = U$. Hence the (nonlinear) state equation is:

$$\frac{d}{dy}\begin{bmatrix} X_1 & -X_3X_1/X_5 \\ X_2 & (X_3X_1 - X_4X_2)/X_5 \\ X_3 & 0 \\ X_4 & 0 \\ X_5 & 0 \end{bmatrix} \tag{28}$$

and

$$F(\underline{X}^*,y) = \begin{bmatrix} \frac{-X_3}{X_5} & 0 & \frac{-X_1}{X_5} & 0 & \frac{X_3X_1}{X_5^2} \\ \frac{X_3}{X_5} & \frac{-X_4}{X_5} & \frac{X_1}{X_5} & \frac{-X_2}{X_5} & \frac{X_4X_2 - X_3X_1}{X_5^2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{29}$$

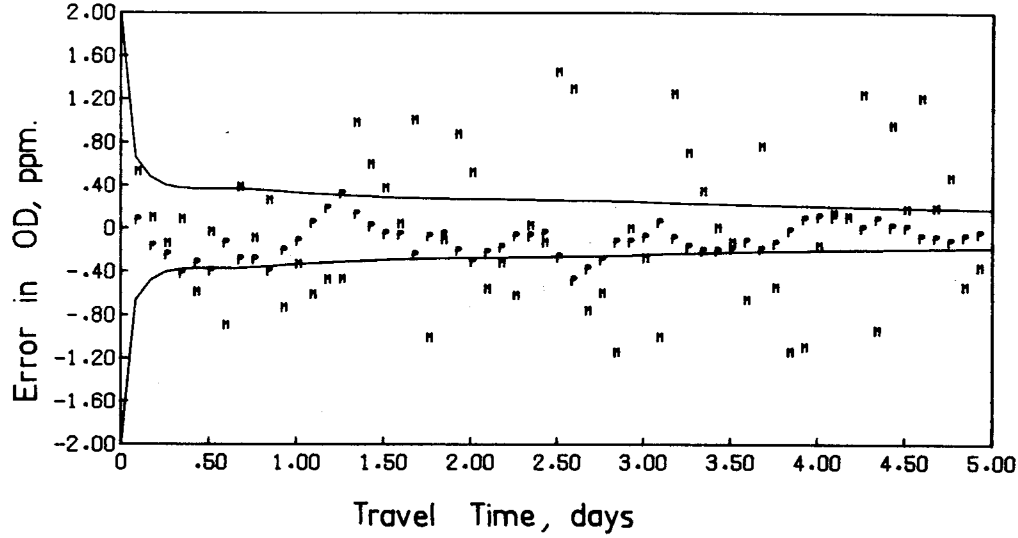

Figure 1. Predicted, Actual and Measurement Errors in OD for a Linear Kalman Filter.

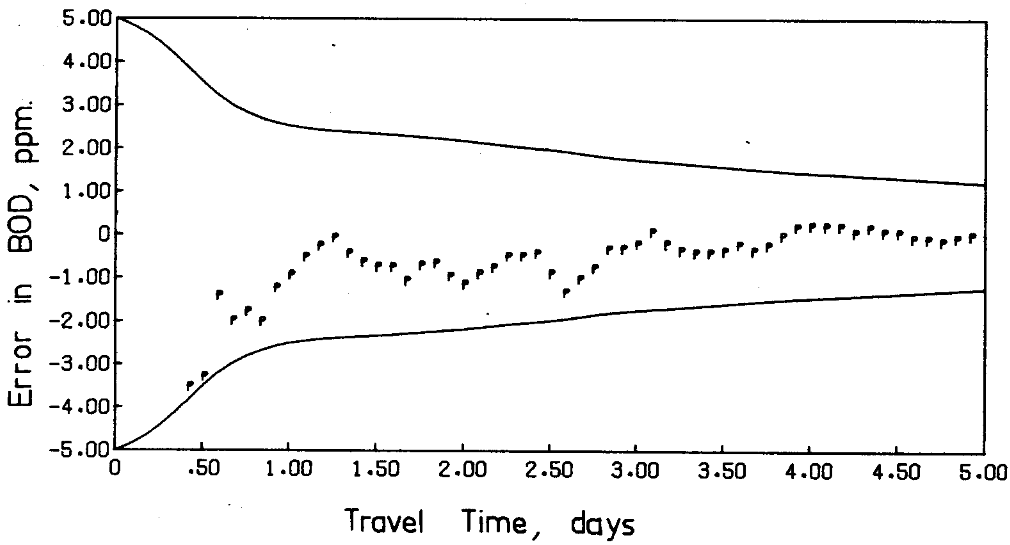

Figure 2. Predicted and Actual Errors in BOD for a Linear Kalman Filter.

A numerical solution for $\phi(Y)$ using (26) is performed, and equations 27, 15-18 are iterated. For the same initial conditions and error covariance matrices as figures 1 and 2 the error trajectories of figures 4 and 5 are now followed. Results show substantially different dynamics of the error covariance matrices, resulting from inclusion of

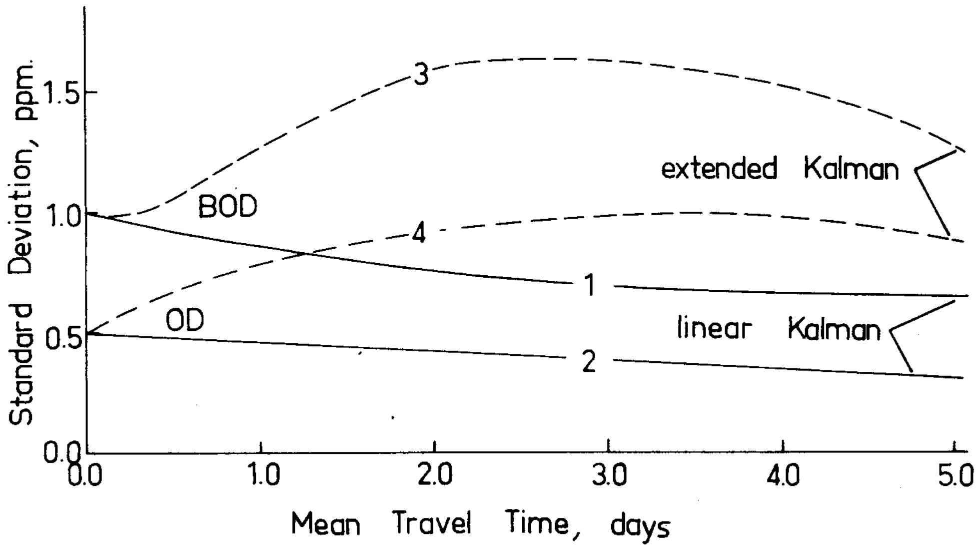

Figure 3. Predicted Errors in BOD and OD, Conditioned upon Initial Measurements, for Linear and Extended Kalman Filter Models of a BOD-OD System.

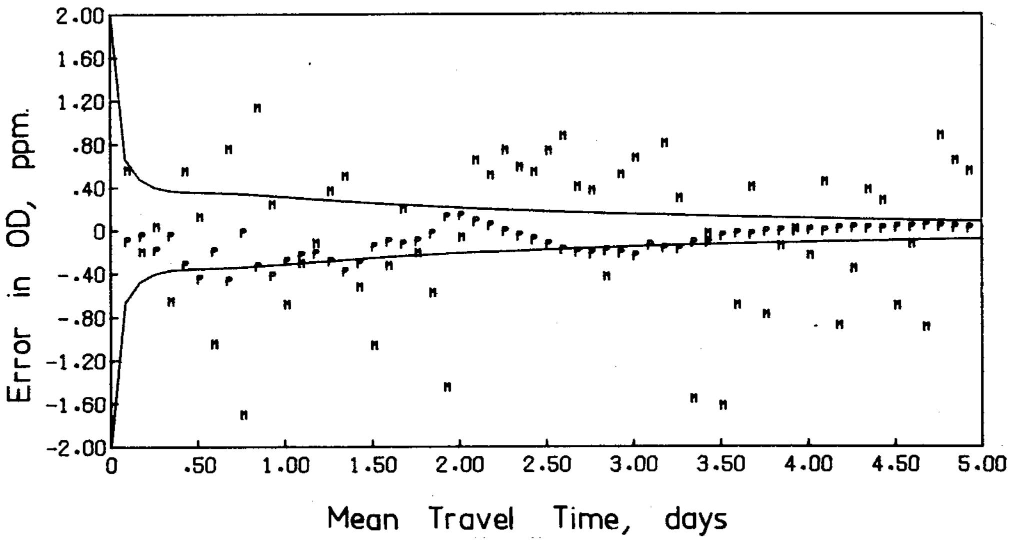

Figure 4. Predicted, Actual, and Measurement Errors in OD for an Extended Kalman Filter.

uncertainty in steam velocity, K_1 and K_2. These results are, however, more realistic as uncertainty in these parameters cannot normally be ignored.

Curves 3 and 4 of figure 3 show the predicted trajectories, conditioned only on an initial measurement, for the extended Kalman Filter model of BOD and OD. The dashed

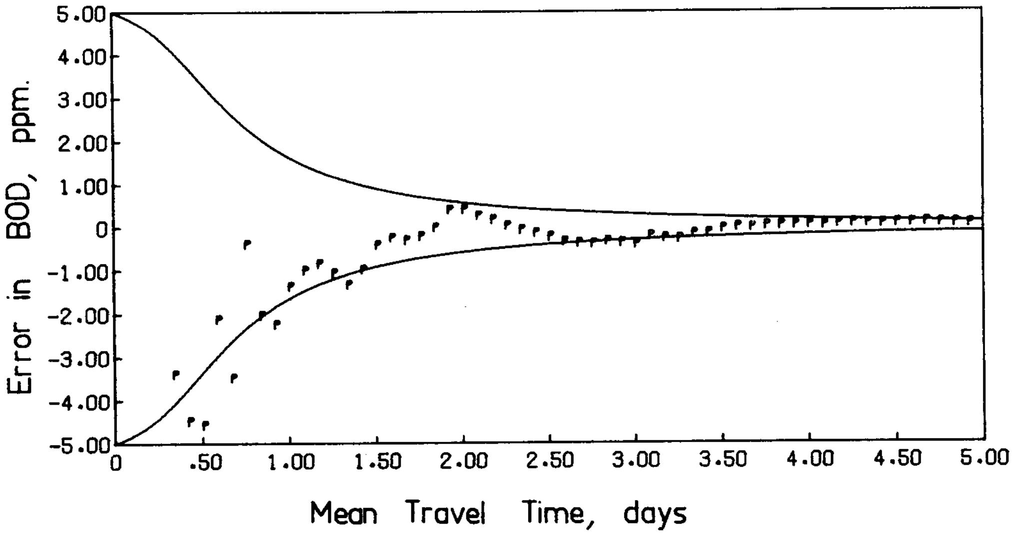

Figure 5. Predicted and Actual Errors in BOD for an Extended Kalman Filter.

trajectories shown (curves 3 and 4) are similar to those given by Burges and Lettenmaier (1975) and closely represent uncertainty propagation to be expected. The trajectories that result from assumptions of constant coefficients (linear Kalman filter model) are shown as solid lines (curves 1 and 2) in figure 3. Use of constant coefficients implies decaying uncertainty with time for BOD and OD which can lead to erroneous interpretations of sampling needs. The importance of including uncertainty in travel time and the coefficients K_1 and K_2 as examined by Burges and Lettenmaier (1975) and modeled in figure 3 via the extended Kalman filter is readily apparent.

The extended Kalman filter is only one of many possible approaches to nonlinear problems, almost all of which require some approximation to equation 1, normally a Taylor series expansion. This expansion requires the choice of a nominal trajectory about which the expansion proceeds. This choice of nominal trajectory is a very important one. In general, performance is improved by using an expansion about the filtered state estimate, rather than an *a priori* nominal trajectory. Higher order expansions usually lead to some improvement in performance (Schwartz and Stear 1968) although this improvement is often not substantial and may not warrant the increased computational load. Throughout the remainder of this work the extended Kalman filter with linearization about the filtered state estimates has been used.

DIVERGENCE

A problem frequently encountered in filter applications is that of divergence. The applications thus far have assumed the system noise covariance matrix, Q(t), to be zero; only measurement noise has been considered. However, the models used in almost all applications and particularly in water resource applications can only be conceptualizations of a real process and normally incorporate substantial simplifications. The choice of a zero **Q** (or **G**) matrix implies, however, exact knowledge of the dynamics. Consequently, the conditional error covariance matrix $\mathbf{P}(k+1|k)$ ultimately decays with each measurement. Investigation of equations 16 and 17 shows that a small covariance matrix ultimately leads to the filter "ignoring" new measurements and relying almost entirely on the a priori predictions $\hat{\underline{X}}(k+1|k)$. Hence, the filtered estimate can diverge from the true values. The divergence problem may be illustrated by generating the measured values of the DO-BOD system from a model containing terms for BOD settling and BOD supply from nonpoint runoff:

$$\frac{dB}{dt} = -(K_1 + K_3)B + \theta \tag{30}$$

$$\frac{dD}{dt} = K_1 B - K_2 D \tag{31}$$

where K_3 = BOD settling constant, θ = BOD nonpoint source supply rate. Figure 6 shows predicted and actual errors in BOD for the extended Kalman filter with initial conditions and measurement error identical to that used earlier. The measurements are generated from the model of equations 30 and 31. The response shows that the filter cannot follow the true BOD trajectory.

Correction for divergence requires estimation of an appropriate system error covariance matrix **Q**. The **Q** matrix is used as a catchall to correct for errors caused by linearization of nonlinear dynamics, neglected parameters in the dynamical model, etc. In general, a **Q** matrix with elements that are too small causes divergence, whereas if the

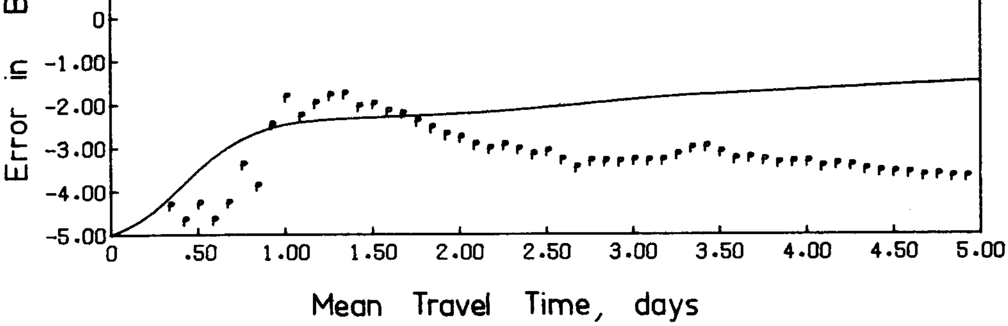

Figure 6. Predicted and Actual Errors in BOD for an Extended Kalman Filter Model of a BOD-OD System where Sedimentation and Non-Point Source Terms are Significant but are Neglected in the Model Dynamics.

magnitude is too large the filtered estimates will follow the measured estimates too closely, resulting in the filtered estimate being essentially the measured value. One approach to estimation of **Q** is trial and error. The **G** matrix is initially assumed to be the n x n identify matrix $\mathbf{I}_n$. This is the approach used here. Figure 7 shows the estimated normalized error contours for the filter model as a function of Q_{11} and Q_{22} where all other elements of the system noise matrix are taken as zero. Here the mean square error used is:

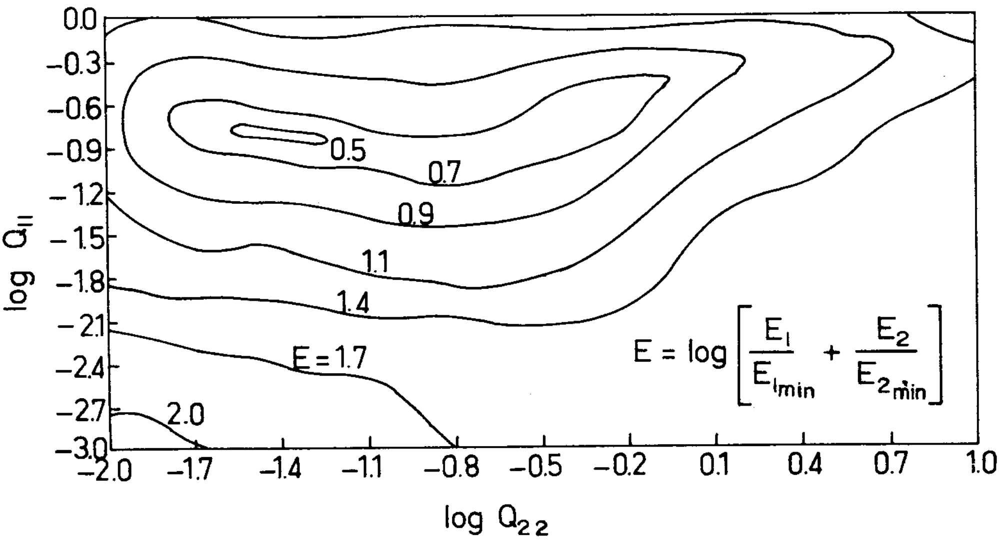

Figure 7. Estimated Bivariate Contours of the Rescaled Mean Square Error for a BOD-OD System where Sedimentation and Non-Point Source Terms are Significant but have been Neglected in the Model Dynamics.

$$MSE = \frac{2}{n} \sum_{i = [n/2] + 1}^{n} (y_i - X_i)^2 \tag{32}$$

and the normalized error is $E = \frac{E_1}{E_{1min}} + \frac{E_2}{E_{2min}}$ with E_1 and E_2 the mean square error in OD and BOD, respectively; where [j] is defined as "the greatest integer less than j."

For illustrative purposes, performance has been measured using the true mean square error. In a real application, however, only the deviations between predicted states and measurements are available. The procedure used is similar to that presented here, except that care must be taken to avoid "overfitting", i.e., the **Q** matrix must be chosen to make the observed deviations between measured and predicted values consistent with the theoretical measurement error. A more complete discussion of trial and error approaches is given by Schlee, *et al* (1967).

POTENTIAL USES OF STATE ESTIMATION IN WATER RESOURCE PROBLEMS

The use of the filter models discussed above provide estimates of two quantities not available in other modeling techniques. Firstly, an estimate of system state is provided which includes information from a measurement as well as from a system model. The classical approach in deterministic modeling is to use the data to "calibrate" the model, the measurements are assumed to represent truth. This approach inevitably leads to problems of overfitting. Secondly, state estimation techniques in addition to the estimate of state, yield an estimate of the state covariance matrix. This allows an estimate of the expected error associated with the predicted value to be made. Deterministic models cannot yield such an estimate.

The authors see several areas in which state estimation techniques might provide (and have provided) substantial improvements over existing methods. Some of these areas are briefly addressed below.

Measurement System Design

The estimate of the system error covariance matrix P is independent of the actual measurements. This allows use of the filter, exclusive of the actual state estimation equations, to set criteria for sample station location. Moore (1971, 1973) used filter methods to design a monitoring system for a reach of the Sacramento River. Perlis and Okunseinde (1974) used state estimation techniques to design a measurement system for the Passaic River subject to a criterion including measurement cost and integrated prediction error.

Substantial problems still exist, particularly in extension of the method to systems with multiple independent variables (e.g., time and several space dimensions). These problems result principally because the formulation used in navigation problems utilizes a single independent variable (usually time). The problem may be circumvented by defining a new state vector component at, for instance, each point in a spatial grid; however, this results in the manipulation of very large matrices with resultant high computation costs. Further research is required in application to systems with multiple independent variables.

Analysis of Requirements for Model Building and Assessment of Models

At present it is very difficult to assess the capabilities of water quality models, particularly in terms of the level of complexity required. State estimation techniques provide (for a given model) an estimate of the system state covariance matrix which may be used to assess potential improvements in the model. For instance, the effect of including (or ignoring) additional state variables may be assessed in terms of the reduction (or increase) in the system state covariance matrix magnitude. The authors feel that, with the proliferation of models in recent years, more effort should be spent in assessing the degree of complexity required. State estimation techniques allow one way of proceeding.

Extending the Utility of Existing Data

The amount of data available in water resource investigations is often substantially less than that desired. State estimation techniques allow interpolation and prediction (with associated uncertainty estimates) to points at which data are not available. This capability should assist planners in maximizing use of available data. Filter techniques probably have potential in data filter situations where a cause effect model could be employed to fill in missing observations in otherwise reasonably complete data time series. Current techniques usually employ linear regression methods (Texas Water Development Board 1970, 1972), and consequently ignore knowledge of system dynamics. In addition, state estimation techniques allow forecasts to be made from water resource models and yield confidence limits which accompany the forecast of the mean value. Deterministic models are frequently used in planning applications where forecasts are necessary, but confidence limits on forecasted values are rarely available. Applications of nonlinear filtering and prediction techniques in water quality modeling were demonstrated by Lee (1972), but operational utilization of state estimation in these applications has not yet occurred.

CALIBRATION OF MODELS

State estimation techniques are potentially useful in model calibration applications. Here calibration would be viewed in an essentially Bayesian sense where the actual dynamics are well established but calibration parameters need to be determined. The parameters to be estimated would be added to the state vector as were the reaeration and BOD decay constants in the extended Kalman Filter example. As each measurement is employed parameters are updated. These techniques should be applicable to a large class of water resource engineering problems where model parameters have been traditionally computed by taking measurements as deterministic quantities and obtaining a model that "best" fits these measurements.

SUMMARY

Relatively straightforward examples have been used to illustrate the mechanics of state estimation techniques. A simplified model which assumed constant BOD decay and reaeration coefficients in the Streeter-Phelps Equations illustrated an application of the linear Kalman Filter technique. The filter technique illustrated the inherent lack of validity in assuming constant parameters in this model. The extended Kalman Filter was used to examine the behavior of the Streeter-Phelps equations when the "constants" were considered to be variable quantities. Results in agreement with physical plausibility were demonstrated.

State estimation techniques have considerable potential for application in water resource systems modeling particularly in situations where combinations of measurements and model dynamics are desirable. Some useful applications include design of space-time frequency monitoring systems, data fill in, model calibration, and possibly in general, model building.

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