MODEL STRUCTURE IDENTIFICATION FROM EXPERIMENTAL DATA

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PREFACE

In recent years there has been considerable interest in the development of models for river and lake ecological systems. Much of this interest has been directed toward the development of progressively larger and more complex simulation models. In contrast, relatively little attention has been devoted to the problems of uncertainty and errors in the field data, of inadequate numbers of field data, of uncertainty in the relationships between the important system variables, and of uncertainty in the model parameter estimates. The International Institute for Applied Systems Analysis Resources and Environment Area's Task on Models for Environmental Quality Control and Management addresses problems such as these.

The subject of this paper is model calibration. But rather than solving the customary problem of model parameter estimation, given an established structure for the model, the paper attempts to answer the prior question of identifying the dominant relationships between the system inputs, state variables, and output responses. That, then, is the problem that needs to be solved *before* one can consider how to estimate the model parameter values accurately. And it *is* a problem because, despite very many laboratory-scale experiments and a number of major field studies, our knowledge of the relationships between the mineral, organic, and microbiological components of an aquatic ecosystem is still quite uncertain.

SUMMARY

This paper is reprinted from the book *Theoretical Systems Ecology: Advances and Case Studies*, edited by E. Halfon of the Canada Centre for Inland Waters and published by Academic Press, New York. Acknowledging that systems ecology has had a large impact on all aspects of environmental research, the book aims to bridge the gap in communication between theoreticians, modelers, and field ecologists. Three classes of problems are treated in the book. They separate approximately into (a) how the model should be developed and analyzed prior to the collection and use of field data, (b) how the model should be developed or modified when it is evaluated against field data, and (c) the desired properties of the models for control and management purposes. The objective of this paper is to emphasize the fact that the second of these three problem categories is not simply a matter of straightforward model parameter estimation.

The basic problem of model calibration – or system identification – is that information about the "externally" observed behavior of a system is required to be translated into information about the model-based description of the system's "internal" mechanisms of behavior. The measured input and output variables represent the system's external description, whereas state variables and parameter values refer to the system's internal description. In other words, during model calibration, and especially in the process of identifying the model's structure, we seek improved understanding of those physical, chemical, and biological phenomena that are thought to govern the system's observed behavior. Model structure identification is important in many water quality modeling exercises because the analyst is frequently confronted with the need to offer plausible hypotheses about "unexplained" relationships in a set of field data.

In order to discuss model structure identification, this paper first provides a brief review of the essential steps of system identification – experimental design; choice of model type; model structure identification; parameter estimation; and verification and validation. Two case studies are then presented that illustrate approaches to the solution of the model structure identification

problem. A key feature of these approaches is the use of recursive parameter estimation schemes, which, through their ability to estimate time-varying model parameter values, can yield useful insight into where and how the structure of the model relationships is inadequate. For example, an estimated parameter value that varies significantly with time is an indication of the invalidity of the common hypothesis that the model coefficients are constant with time. Such diagnostic information, however, while it reveals what is wrong with the model, does not prescribe a formal means of finding a better formulation for the model structure. The methods of the paper are therefore clearly limited in their ability to solve completely the problem of model structure identification.

ABSTRACT

Methods for identifying the structure of dynamic mathematical models for water quality by reference to experimental field data are discussed. The context of the problem of model structure identification is described by briefly reviewing the steps involved in the overall process of system identification. These steps include experimental design; choice of model type; model structure identification; parameter estimation; and verification/validation. Two examples of approaches to solving the problem of model structure identification are presented. The first example is concerned with identifying the structure of a black box (input/output) model for the variations of gas production in the anaerobic digestion process of wastewater treatment. Correlation analysis is used as the principal method of solution, although it is found to have significant limitations for certain kinds of data. The second example addresses the more difficult problem of identifying the structure of an internally descriptive ("mechanistic") model form. The application of an extended Kalman-filtering algorithm to this problem is discussed in detail. The approach is illustrated with a model for phytoplankton–biochemical-oxygen-demand (BOD) interaction in a freshwater river system.

Chapter 11

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1. INTRODUCTION

Dynamic model structure definition (identification) is arguably one of the major unresolved technical problems in the field of system identification and parameter estimation. It is certainly true in practice that model structure identification from experimental field data gives rise to all manner of difficulties. This chapter has the objective of presenting some theoretical techniques which can be applied to the solution of the identification problem.

Throughout the chapter we shall assume a pragmatic approach to modeling: Namely, the act of modeling implies the collection of experimental field data. In order to avoid confusion we may state that the term *system identification* is interpreted herein as the complete process of deriving mathematical models from, and by reference to experimental data; the term *identification* means the specific process of model structure identification. If the system under investigation can be represented by the (dynamic) model of Fig. 1, all variables thus being functions of time t, a broad definition of model structure identification can be given as the establishment of how the measured system inputs $\mathbf{u}$ are related to the system's state variables $\mathbf{x}$ and how these latter are in turn related both to themselves and to the measured system outputs $\mathbf{y}$. The *dynamic* modeling context arises for the following reason: An experimenter studying a system under laboratory conditions wishes to keep that system as close to steady state as possible while he tests the relationship between, say, two particular variables. Such steady-state conditions, and especially so for ecological systems, rarely prevail in the field. Hence in order to establish any significant theory of the system's behavior it is necessary to set up the problem within a framework which recognizes the dynamic and stochastic (random) nature of experimental data. We are, however, concerned exclusively here with identifying a structure for the deterministic component

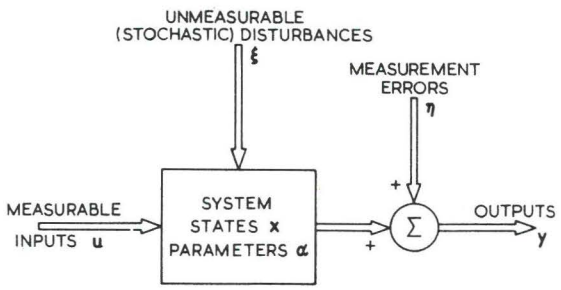

Figure 1. System and variables definition.

of the model. The techniques employed in the modeling analysis should therefore operate so as to discriminate effectively against the ever-present random noise component of measured signals. The motivation for solving the model structure identification problem stems from the experience of studying river water quality modeling and control (Beck, 1977); the following illustrative examples are drawn from this subject area.

2. SYSTEM IDENTIFICATION: A BRIEF REVIEW

The field of system identification has developed rapidly over the past decade, and like any other discipline which has emerged and matured so quickly, its accompanying literature is vast but not well coordinated. For the reader previously unacquainted with system identification a carefully guided introduction to the literature is appropriate.

The book by Eykhoff (1974) is to be recommended as giving the broadest and most comprehensive treatment of system identification; for a more brief survey of the subject and its earlier literature there is the review by Åström and Eykhoff (1971). Box and Jenkins' (1970) detailed account of discrete-time, input/output, black box modeling must also receive due

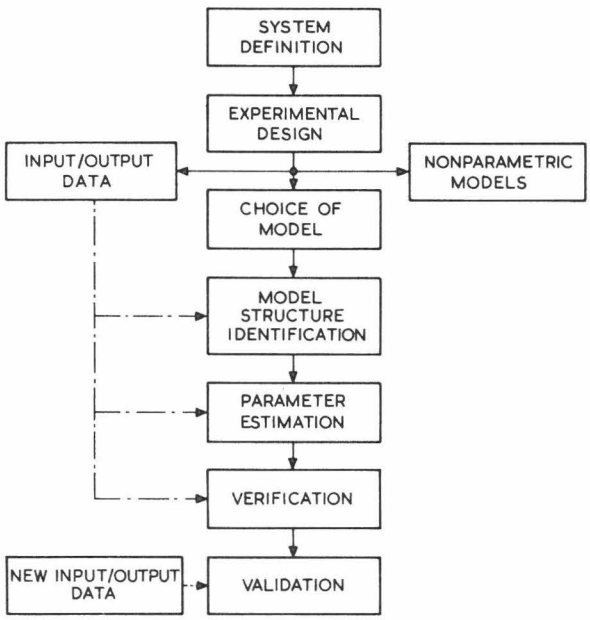

Figure 2. Individual steps in the procedure of system identification.

reference: This text, probably more so than others, has had a very significant impact on the application of time-series analysis in many diverse technical fields. Among the multitude of publications on methods of parameter estimation the easily readable article by Young (1974) provides an excellent introduction to recursive estimation techniques, or alternatively, these same techniques are given a rigorous treatment in Söderström *et al.* (1974).

Each of the above publications offers a suitable point of departure into the subject of system identification. The purpose of this section is to outline a scheme of individual steps in the procedure of system identification, thereby describing the context of the model structure identification problem (see Fig. 2).

2.1. Experimental Design

Besides the definition of the system and its variables, which we have assumed to be according to Fig. 1, a prerequisite of system identification is an appropriate record of the observed process dynamics. Any *a priori* knowledge of the system's dynamic behavior is an advantage, since this knowledge can be used in assessing the following important aspects of experimental design (Gustavsson, 1975): (a) major process time constants; (b) sampling (measurement) frequency; (c) duration of the experiment; (d) choice of input test signals **u**; (e) noise levels; (f) process nonlinearities. When confronted with a modeling problem it is thus not particularly encouraging to reflect upon the fact that a good experimental design, and hence the likelihood of useful results, is strongly dependent upon a good *a priori* knowledge (model) of the system! A particularly thorny problem with respect to ecological systems is the inability to probe the process dynamics with artificially manipulated signals such as step, impulse, or pseudorandom binary sequence (PRBS) inputs **u**. In other words, our experiments reduce simply to the observation of behavior without any intervention on behalf of the experimenter, that is, "normal operating conditions" (Eykhoff, 1974). Later sections of the chapter will illustrate how difficult it can be to undertake modeling exercises under the very limiting constraints of data derived from normal operating conditions.

2.2. Choice of Model

A distinction should be drawn between parametric and nonparametric classes of models since Fig. 2 assumes implicitly that only the former are to be dealt with here. Nonparametric models, such as Volterra series, impulse, and step response representations, are *intrinsically of infinite order*; they are

characterized, in principle, by an *infinite number of parameters*. For instance, if a system with simple first-order dynamics (an exponential lag) were to be represented by its discrete-time impulse response, an infinite number of response coefficients (parameters) would be required to characterize those dynamics completely. Parametric models, in contrast, are characterized by a *finite* (and usually small) *number of parameters*. Indeed, we may remark that the translation of a nonparametric model into a parametric model representation constitutes the basis of the black box model identification problem (see Section 2.3).

Broadly speaking, a choice can be made between two parametric model forms: (a) a black box (or input/output) model and (b) an internally descriptive (or mechanistic) model. These two model representations reflect two opposite, yet complementary, approaches to modeling. Either one takes existing theory (that is, physical, chemical, biological, ecological theory) and develops this model so that it may be tested against experimental data—a deductive reasoning approach associated with a model of type b, or, assuming no *a priori* knowledge (theory) of process behavior, one attempts to develop the specific information acquired from the data into a more general model—an inductive reasoning approach closely related to black box model representations.

2.2.1. Black Box Model

For simplicity and brevity a *linear* form of the black box model is given by the discrete-time, difference equation

$$A(q^{-1})y(t_k) = \sum_{i=1}^{v} q^{-\delta_i} B_i(q^{-1})u_i(t_k) + E(q^{-1})e(t_k) \tag{1}$$

in which $u_i(t_k)$, $i = 1, 2, \ldots, v$, and $y(t_k)$ are, respectively, observations of the multiple (v) system inputs and the system output at the kth sampling instant; $e(k)$ is a sequence of independent, Gaussian, random variables and q^{-1} is the backward shift operator

$$q^{-1}\{y(t_k)\} = y(t_{k-1}), \qquad \text{etc.}$$

$A(q^{-1})$ and $B_i(q^{-1})$ are polynomials in q^{-1}, of orders n and m_i, respectively, with parameters a_j and b_{ij} to be estimated

$$\begin{aligned} A(q^{-1}) &= 1 + a_1 q^{-1} + \cdots + a_n q^{-n}, \\ B_i(q^{-1}) &= b_{i0} + b_{i1} q^{-1} + \cdots + b_{im_i} q^{-m_i}; \qquad i = 1, 2, \ldots, v, \end{aligned} \tag{2}$$

and δ_i, $i = 1, 2, \ldots, v$, represents a pure time delay in the response between output and input u_i. The form of $E(q^{-1})$ is left unspecified, except to state that it is in general a rational function. The precise description of the *lumped*

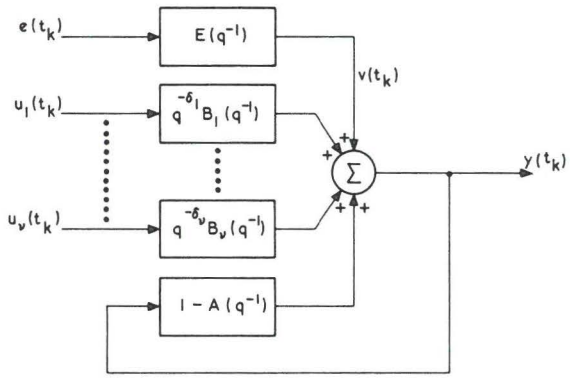

Figure 3. Schematic representation of the black box model [Eq. (1)].

stochastic process $v(t_k)$ in Fig. 3, which accounts for the combined effects of system noise ξ and measurement error η (in Fig. 1) as white noise $e(t_k)$ passed through this "shaping filter" $E(q^{-1})$, depends partly on the type of parameter estimation method to be applied (see Section 2.4). Details of this stochastic process description will not concern us greatly here since we are trying to establish the nature of deterministic relationships between **u** and y.

Equation (1) states essentially that the current value of the output $y(t_k)$ is a (scalar) function, f, of current and past measurements of the inputs u_i, of past measurements of the output, and of current and past realizations of the stochastic process v, as in Fig. 3,

$$y(t_k) = f\{y(t_{k-1}), \ldots, y(t_{k-n}), u_1(t_{k-\delta_1}), \ldots, u_1(t_{k-\delta_1-m_1}), \ldots, u_\nu(t_{k-\delta_\nu}), \ldots, u_\nu(t_{k-\delta_\nu-m_\nu}), v(t_k), \ldots, v(t_{k-\tau})\}. \quad (3)$$

Here τ denotes that $y(t_k)$ depends upon a finite number of realizations of v. Such a black box model, being specific to the sample data set from which it is derived, is unlikely to be a universal description of a system's dynamics. Nor is this model necessarily amenable to interpretations on the perceived physical nature of process behavior. The *black box* is literally a fair reflection of our insight into the internal mechanisms of the system. As a model it is a first attempt at elucidating any observed basic cause/effect relationships, such as which inputs affect which output, by how much, and how quickly. Yet these are just the advantages that a black box modeling approach can offer: It is simple, and there are many situations where an internally descriptive model, although available, has a form which is too unwieldy or complex to be properly verified against field data.

We have, however, imposed a restriction on the model of Eq. (1) in

that it refers to a *single*-output process. It is worth noting that the majority of applications of black box models have been similarly so restricted, although this is not a justification for imposing the constraint. Multivariate forms of the model are discussed in greater detail in Rowe (1970) and Young and Whitehead (1977).

2.2.2. *Internally Descriptive Model*

An internally descriptive model exploits much more, if not all, of the available *a priori* information on the physical, chemical, biological, and ecological phenomena governing process dynamics. As with Eq. (1) we confine the discussion to linear forms of the model for ease of illustration. The internally descriptive model may then be represented by the following *linear*, continuous-time, state vector differential equation (see also Fig. 4)

$$\dot{\mathbf{x}}(t) = \mathbf{F}\mathbf{x}(t) + \mathbf{G}\mathbf{u}(t) + \boldsymbol{\xi}(t) \tag{4a}$$

with sampled, noise-corrupted observations

$$\mathbf{y}(t_k) = \mathbf{H}\mathbf{x}(t_k) + \boldsymbol{\eta}(t_k) \tag{4b}$$

in which the dot notation refers to differentiation with respect to time t. The variables are defined as: $\mathbf{x}$, the l-dimensional state vector; $\mathbf{u}$, the v-dimensional input vector; $\mathbf{y}$, the p-dimensional vector of outputs; $\boldsymbol{\xi}$, l-dimensional vector of zero-mean, white, Gaussian disturbances; $\boldsymbol{\eta}$, p-dimensional vector of zero-mean, white, Gaussian measurement errors; $\mathbf{F}, \mathbf{G}, \mathbf{H}$, are accordingly $l \times l$, $l \times v$, and $p \times l$ matrices whose elements are the parameters that characterize the system.

The attractions of working with this type of model are its potentially universal applicability and its apparent grounding in theory or *the laws of nature*. But in a sense this latter feature is the source of many model structure identification problems because theory, at least in the ecological

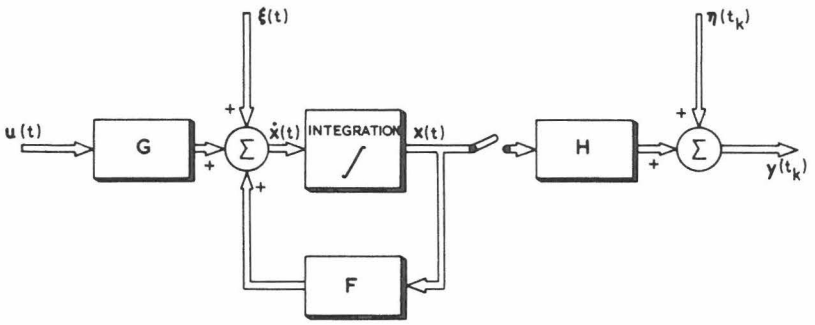

Figure 4. Schematic representation of the (linear) internally descriptive model [Eq. (4)].

microcosms of wastewater treatment processes (Curds, 1973; Olsson, 1975) and rivers (Thomann *et al.*, 1974), may diverge considerably from what is observed to happen in practice.

2.3. Model Structure Identification: Problem Definition

2.3.1. Black Box Model

Recalling the introductory definition of model structure identification we note that the problem for a black box model is considerably simplified since only input → output relationships are being sought. There are two specific identification problems to be solved with respect to Eqs. (1) and (2). The first sounds deceptively easy: For the multiple-input case it concerns the determination of which of these several input variables are in any way significantly related to the output y. Let us call this problem the identification of *cause/effect* relationships, that is, examination of the existence of a deterministic connection between inputs and output. The second identification problem is associated with defining the *time dependence* of the relationships between inputs and outputs. Of interest is the determination of factors such as the speed and nature of the output response to changes in a given input variable.

In formal terms we require a definition of the values of n, m_i, and δ_i in Eqs. (1) and (2); or, rather more precisely, we need to know further which of the b_{ij} parameters of the $B_i(q^{-1})$ polynomials are significantly nonzero. And last, although Eq. (1) is restricted to a linear form, it is also necessary to investigate possible nonlinearities in the terms of the model. Postulation of the correct structure for the nonlinearity, as an identification problem, is not at all trivial. However, providing the model remains "linear-in-the-parameters"—a term defined by Eykhoff (1974) and illustrated below—such nonlinearities present no additional difficulties in the subsequent parameter estimation phase of modeling.

The black box model structure identification problem may be loosely summarized as a problem of transferring from a nonparametric to a parametric representation with minimal loss of accuracy.

2.3.2. Internally Descriptive Model

If the principles of mass, momentum, and energy conservation are applied for the description of our system's behavior, we should be in a position to test the identifiability of the resulting internally descriptive model, as Eq. (4), with a view to *subsequent* planned experimentation. This kind of *a priori* identifiability analysis is presented rigorously elsewhere in this volume by Cobelli *et al.* (Chapter 10); it is not the model structure identification problem to be tackled here.

Our *a posteriori* identification problem is defined as follows: Given a set of measurements of **u** and **y**, determine an appropriate state vector **x**, the number of elements l in that vector, and which of the elements of the matrices $\mathbf{F}, \mathbf{G}, \mathbf{H}$ are significantly nonzero. The essence of the internally descriptive model structure identification problem is the testing of hypotheses and the evolution of a theory. So identification can be viewed as a procedure of repeated *hypothesis testing* and *decision making*—an intuitive interpretation which has been illustrated earlier in Beck (1978). There are two points about this view which are of some considerable importance: First, it reinforces the notion that modeling is subjective—it depends on the analyst's choice of criteria and his decision to accept or reject a hypothesis (model) on the basis of those criteria; second, it emphasizes the fact that the ultimate problem of modeling is the generation of a subsequent hypothesis given that the current hypothesis is inadequate.

The earlier assumption that an internally descriptive model derived from the application of basic theoretical principles has a linear structure is not a restriction on the following discussion. In fact, a nonlinear model structure arises frequently in the analysis of ecological (Di Cola *et al.*, 1976) and microbiological systems (Beck, 1977), although no explicit examples thereof are presented here. The assumption that the model form is lumped, thus enabling us to use ordinary differential equation representations in preference to partial differential equations, is much more restrictive. However, it is our intention to uphold this latter simplifying assumption in order to avoid consideration of the problem of identifying a correct lumping of the parameters from a distributed-parameter system. The problem already posed is quite sufficiently difficult, and not the least of these difficulties is that, unlike the black box model which may take a rather arbitrary structural form, the abstractions $\mathbf{x}, \mathbf{F}, \mathbf{G}, \mathbf{H}$ of the internally descriptive model must bear some resemblance to the real world.

2.4. Parameter Estimation

The estimation of parameters is required in two different contexts: It is often implicit in the solution of the identification problem, as will be seen later; and parameter estimation is, of course, the means whereby the coefficients appearing in the finally identified differential/difference equations are accurately evaluated.

A basic principle of parameter estimation is that the estimates $\hat{\boldsymbol{\beta}}$, say, of the model parameters $\boldsymbol{\beta}$ are obtained by minimizing some function of the error

$$\varepsilon(t_k) = y(t_k) - \hat{y}\{\hat{\boldsymbol{\beta}}, t_k\} \tag{5}$$

between the output observation y and a (model) prediction $\hat{y}$ of that output variable. One of the simplest and most well known of parameter estimation schemes is that of *least-squares estimation* where the loss (error) function

$$J(t_N) = \sum_{j=1}^{N} \varepsilon^2(t_j) \tag{6}$$

is minimized; N is the number of data samples. A more complete discussion of least-squares estimation and its fundamental role in time-series analysis is given in Young (1974).

2.4.1. Black Box Models

In most cases of practical interest least-squares estimation gives parameter estimates $\hat{\boldsymbol{\beta}}$ that are biased, that is,

$$\mathscr{E}\{\hat{\boldsymbol{\beta}}\} \neq \boldsymbol{\beta}$$

in which $\mathscr{E}\{\cdot\}$ is the expectation operator, because the statistical properties of $v(t_k)$ (see Fig. 3) do not satisfy the conditions,

$$v(t_k) = e(t_k). \tag{7}$$

But this is not to deny the importance of least-squares estimation; it is a ubiquitous technique and can be employed to good advantage as evidenced elsewhere in this book (see Chapter 13 by Ivakhnenko *et al.*). Indeed, the variety of parameter estimation methods stems from the many diverse attempts to overcome the problem of bias. Noting that Eq. (7) implies $E(q^{-1}) = 1$ in Eq. (1), the principal alternative methods of estimation are each associated with different noise process characterizations:

Generalized least-squares (Clarke, 1967; Hastings-James and Sage, 1969)

$$E(q^{-1}) = 1/C(q^{-1}).$$

Maximum likelihood (Åström and Bohlin, 1966)

$$E(q^{-1}) = D(q^{-1}).$$

Instrumental variable–approximate maximum likelihood as in Young (1976)

$$E(q^{-1}) = A(q^{-1})D(q^{-1})/C(q^{-1})$$

with the additional polynomials $C(q^{-1}), D(q^{-1})$ being defined in a fashion similar to $A(q^{-1})$ in Eq. (2).

2.4.2. *Internally Descriptive Models*

The number of techniques available for estimating parameters in Eq. (4) is remarkable for its smallness. To the best of our knowledge only a maximum likelihood (Källström *et al.*, 1976) method and variants on the extended Kalman filtering (EKF) (Jazwinski, 1970) theme have been applied to the analysis of field data. This latter method, however, we shall consider in detail as a method for solving the model structure identification problem.

2.5. Verification and Validation

In deriving the models of Eqs. (1) and (4) some important assumptions (see Section 2.2) have been made about the statistics of e, $\boldsymbol{\xi}$, and $\boldsymbol{\eta}$. Model *verification*, in our terminology, sets out accordingly to check that the sample statistics of, say, the one-step-ahead prediction errors (residual errors, innovations process errors),

$$\varepsilon(t_k|t_{k-1}) = y(t_k) - \hat{y}(t_k|t_{k-1}) \tag{8}$$

approximate the conditions

$$\mathscr{E}\{\varepsilon(t_k|t_{k-1})\} = 0, \tag{9a}$$

$$\mathscr{E}\{\varepsilon(t_k|t_{k-1})\varepsilon(t_j|t_{j-1})\} = \sigma^2\delta_{kj}, \tag{9b}$$

$$\mathscr{E}\{\varepsilon(t_k|t_{k-1})u_i(t_j)\} = 0; \qquad \text{for all } k,j; \quad i = 1,2,\ldots,v, \tag{9c}$$

where δ_{kj} is the Kronecker delta function such that

$$\delta_{kj} = \begin{cases} 0 & \text{for } k \neq j \\ 1 & \text{for } k = j \end{cases}$$

and $\hat{y}(t_k|t_{k-1})$ is the one-step-ahead prediction of $y(t_k)$ given all past sampled observations of the input and output time-series. Conditions (9a) and (9b) specify that the residuals are a zero-mean, white noise sequence, that is, not correlated with themselves in time, with variance σ^2; condition (9c) requires the residuals to be independent of the inputs u_i. If these conditions hold then our statistical assumptions are valid and it is reasonable to conclude that the model is an adequate characterization of the process behavior observed in the sampled data set from which the model is derived.

There is, however, no guarantee that the model's validity extends beyond this specific set of data. *Validation* is, then, the testing of the model's adequacy against a new set of field data and this will almost certainly entail the design and implementation of new experiments. So finally it can be seen how model building is properly accommodated within the easily recognizable scientific tradition of repeated experiment/analysis/and synthesis.

3. MODEL STRUCTURE IDENTIFICATION: BLACK BOX MODELS

Solutions to the problem of identifying a black box model structure are dealt with first since a black box modeling approach may sometimes be employed as a prelude to working with internally descriptive models.

The identification problems outlined in Section 2.3 (cause–effect; time-dependence) can both be partially solved by computing sample cross-correlation functions from the data

$$\rho_{uy}(\theta) = \frac{1}{N\sigma_u\sigma_y}\sum_{j=1}^{N-\theta}(u(t_j)-\mu_u)(y(t_{j+\theta})-\mu_y); \qquad \theta = 0,1,\ldots,\theta_{\max};$$
$$\rho_{uy}(-\theta) = \rho_{yu}(\theta); \qquad \theta = 1,2,\ldots,\theta_{\max}. \tag{10}$$

Here μ_u, μ_y, and σ_u^2, σ_y^2, are, respectively, the sample means and variances of the chosen input and output observation sequences. If $\rho_{uy}(\theta)$ is not significantly nonzero for $\theta = -\theta_{\max},\ldots,0,\ldots,\theta_{\max}$, then it can be concluded that no dynamic relationship exists between u and y (cause/effect identification).

In an ideal situation it is desirable to have $u(t_k)$ approximating a white noise sequence, for it can then be shown (for example, Box and Jenkins, 1970) that $\rho_{uy}(\theta)$ approximates the *impulse response* $h(\theta)$ between input and output. Hence it is possible to see how the solution of the time-dependence identification problem is to be constructed as a matter of transferring from a nonparametric to a parametric model representation, as has already been mentioned in Section 2.3. The statistical properties of $u(t_k)$ do not generally, however, approximate those of white noise, although it may be justified to assume that $u(t_k)$ can be characterized by

$$u(t_k) = W(q^{-1})u^*(t_k) \tag{11}$$

in which $W(q^{-1})$, a rational function, is termed a "shaping filter," and $u^*(t_k)$ is a white noise sequence. If Eq. (11) is a valid assumption, and provided we can find $W(q^{-1})$, then (Box and Jenkins, 1970),

$$\rho_{u^*y^*}(\theta) \simeq h(\theta), \tag{12}$$

where $\rho_{u^*y^*}(\theta)$ is the cross-correlation function between the prefiltered (or prewhitened) time series

$$u^*(t_k) = W^{-1}(q^{-1})u(t_k); \qquad y^*(t_k) = W^{-1}(q^{-1})y(t_k).$$

In theory it is then possible to determine *by inspection* of the computed impulse response the pure time delay δ_i and appropriate orders n and m_i for the $A(q^{-1})$ and $B_i(q^{-1})$ polynomials of Eqs. (1) and (2). For the interested reader an exhaustive treatment of solving the identification problem in this manner is given in Box and Jenkins (1970). Note that the impulse response

determined through Eqs. (12) and (10) is a truncated approximation of the true impulse response function since it has only a finite number of coefficients for $\theta = 0, 1, \ldots, \theta_{\max}$ (compare with Section 2.2).

The values so derived for n, m_i, and δ_i should at best be regarded as initial intelligent guesses. The cross-correlation function, while it is an indispensable component of any data analysis, has its limitations (see below). Moreover, it is important to note also that the use of input prewhitening involves a second subproblem of identification, namely, the specification of the orders of the numerator and denominator polynomials of $W(q^{-1})$. And even with δ_i, n, m_i specified we have yet to examine whether each b_{ij} parameter is significantly nonzero.

Not all methods of black box model structure identification require the use of input/output cross-correlation functions as described above. A distinguishing feature of this first approach to the identification problem is that it attempts to solve model order determination (that is, obtain values for δ_i, n, m_i) without recourse to any subsequent estimation of parameters. A transposed version of this approach, as it were, takes trial values (hypotheses) of n, δ_i, and m_i and analyzes the variance and statistical properties of the error sequences $\varepsilon(t_k)$ from the resulting fully estimated model (see, for instance, Åström and Eykhoff, 1971; Chan *et al.*, 1974). Other methods which rely on the estimation of parameters as an index of a properly identified model structure include the novel *auxiliary system* method of Wellstead (1976) and the notion of "time-invariance of recursive parameter estimates" illustrated by Whitehead and Young (1975) and Whitehead (1976) (see also Section 4.4). Rather more unorthodox approaches to model structure identification include Ivakhnenko's (1968) group method of data handling (GMDH) algorithm (see also Chapter 13 by Ivakhnenko *et al.* in this volume) and the application of methods of pattern recognition (Kittler and Whitehead, 1976). For other reviews of specific details of this problem the reader is referred to the papers by Van den Boom and Van den Enden (1974) and Unbehauen and Göhring (1974).

3.1. An Example: Anaerobic Digestion of Waste Organic/Biological Sludges

The results presented in this example are taken from an analysis of gas production dynamics in the anaerobic digestion of waste municipal/domestic sludges (Beck, 1976). The principal biochemical feature of the process is the multistage breakdown of complex (insoluble) organic substrates to simple end products, primarily methane and carbon dioxide. The last stage of the overall reaction, in which methanogenic bacteria metabolize the volatile acid intermediates with the release of methane, is generally believed

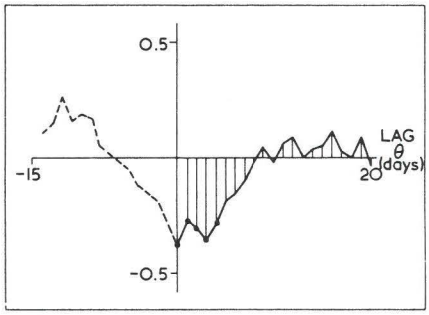

Figure 5. Cross-correlation function ρ_{uy} between volatile acids concentration (u) and gas production rate (y); correlation coefficients marked with ● denote (assumed) significant correlation between input and output.

to be rate limiting (Graef and Andrews, 1974) and thus crucial to an investigation of digester dynamics. Volatile acid concentration and gas production rate are frequently used to monitor process stability.

In the original study a multiple-input/single-output model representation is identified; for the purposes of illustration, however, merely the identification of a single-input/single-output model for volatile acid concentration, input u, and volumetric gas flow rate, output y, is selected. Figure 5 shows, thus, the cross-correlation function ρ_{uy}; the experimental data represent normal operating conditions at the Norwich Sewage Works in England. Initial conclusions from Fig. 5 are that, according to Eqs. (1) and (2), $\delta = 0$ and $m = 4$, approximately. So together with the assumption of $n = 1$ (by inspection of the autocorrelation function of the output time series) we can broadly state that there exists the following deterministic time-dependence relationship between volatile acids and gas production [compare with Eq. (3)]

$$y(t_k) = f\{y(t_{k-1}), u(t_k), u(t_{k-1}), u(t_{k-2}), u(t_{k-3}), u(t_{k-4})\}. \tag{13}$$

The inclusion of the term $u(t_k)$ in Eq. (13) probably occurs as a consequence of the relatively slow sampling frequency of the data which obscures some of the faster dynamic aspects of the relationship between volatile acids and gas production. This observation, apart from the several other attendant difficulties, is a cautionary message on the use of data from badly designed experiments, that is, normal operating conditions.

The interpretation of values for δ and m from Fig. 5 is clearly somewhat speculative. But any attempt at circumventing such imprecision by designing a prewhitening filter results in a cross-correlation function $\rho_{u^*y^*}$ which is equally inconclusive (Fig. 6). It is necessary, ultimately, to incorporate repeated parameter estimation of trial model structures, within

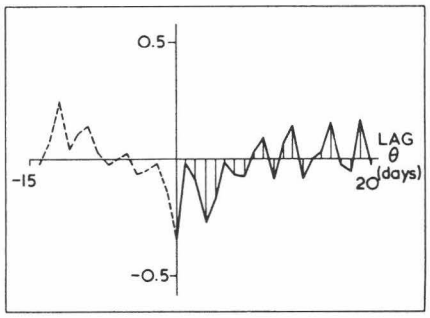

Figure 6. Cross-correlation function $\rho_{u^*y^*}$ for the prewhitened volatile acid concentration series (u^*) and prewhitened gas production rate series (y^*).

the range of combinations allowed by Eq. (13), as a method of identification. At this stage we can exploit an intuitively useful criterion which states simply that if

$$(\hat{\sigma}_{\hat{\beta}}/\hat{\beta}) \geqslant 1 \tag{14}$$

for any model parameter estimate $\hat{\beta}$, where

$$\hat{\sigma}_{\hat{\beta}}^2 \simeq \mathscr{E}\{(\beta-\hat{\beta})^2\}$$

is an estimate of the parameter estimation error, then the parameter β is not significantly nonzero and its associated term can be dropped from the model structure.

A final structure of the model obtained in such a fashion is given by

$$y(t_k) = a_1 y(t_{k-1}) + b_0 u'(t_k) + b_2 u'(t_{k-2})$$

with $u'(t_k) = (\mu_u/u(t_k))$ where μ_u is a sample mean value for $u(t_k)$. The interesting point here is the fact that the model remains linear-in-the-parameters (Section 2.3) but is quite nonlinear in terms of $u(t_k)$.

What can be concluded from the example presented? Primarily it is observed that solving the identification problem is subjective, clearly so in the inspection of cross-correlation functions and rather less obviously so in the use of Eq. (14). Second, it should be evident that there are good reasons for avoiding the analysis of normal operating data where at all possible.

4. MODEL STRUCTURE IDENTIFICATION: INTERNALLY DESCRIPTIVE MODELS

The technique to be applied exclusively to internally descriptive model structure identification is the extended Kalman filter (EKF). In order to see

how the need for the EKF develops from the linear Kalman filter (Kalman, 1960; Kalman and Bucy, 1961) it is first necessary to pose the problem of combined state parameter estimation. Hence model structure identification in this case can be constructed as a problem of assessing diagnostic information on recursive parameter estimates and residual error sequences—a notion already introduced in Section 3.

A formal derivation of the EKF is given in the source reference of Jazwinski (1970). Alternatively, Young (1974) provides an outline of how the EKF algorithms can be obtained from an extension of linear regression analysis.

4.1. Formulation of the Combined State Parameter Estimation Problem

For the linear system of Eq. (4) the linear Kalman filter would provide recursive estimates $\hat{\mathbf{x}}(t_k|t_k)$ of the state vector $\mathbf{x}(t_k)$ conditioned upon all sampled process measurements up to and including those at time t_k.

Suppose now that some of the unknown, or imprecisely known elements of the matrices $\mathbf{F}, \mathbf{G}, \mathbf{H}$, that is, a vector of parameters $\boldsymbol{\alpha}$, say, are required to be estimated simultaneously with the estimation of the state vector. One approach to realizing a simultaneous state parameter estimator is to augment the state vector $\mathbf{x}$ with the parameter vector $\boldsymbol{\alpha}$ and accordingly to postulate a set of additional differential equations representing the parameter dynamics. If the augmented state vector $\mathbf{x}^*$ is defined by

$$\mathbf{x}^* \triangleq \begin{bmatrix} \mathbf{x} \\ \cdots \\ \boldsymbol{\alpha} \end{bmatrix}$$

the state parameter dynamics and observation equation are given in the following general nonlinear form

$$\dot{\mathbf{x}}^*(t) = \mathbf{f}\{\mathbf{x}^*(t), \mathbf{u}(t)\} + \boldsymbol{\xi}^*(t), \tag{15a}$$

$$\mathbf{y}(t_k) = \mathbf{g}\{\mathbf{x}^*(t_k)\} + \boldsymbol{\eta}(t_k). \tag{15b}$$

The functions $\mathbf{f}\{\cdot\}$ and $\mathbf{g}\{\cdot\}$ are vector functions; they are nonlinear because of the product terms involving elements of $\boldsymbol{\alpha}$ with elements of $\mathbf{x}$ and $\mathbf{u}$. $\boldsymbol{\xi}^*(t)$ denotes that the vector of stochastic disturbances in Eq. (15a) is now of a different order to that defined for $\boldsymbol{\xi}(t)$ in Eq. (4a).

Let us consider the problem of specifying the dynamics of the parameters $\boldsymbol{\alpha}$. Of particular importance to the subsequent discussion are two such specifications: (a) we might assume that the parameters are constant, that is, time invariant

$$\dot{\boldsymbol{\alpha}}(t) = \mathbf{0}, \tag{16}$$

or (b) it might be proposed that they vary in an unknown "random walk" fashion,

$$\dot{\boldsymbol{\alpha}}(t) = \boldsymbol{\xi}(t). \tag{17}$$

Were there to be more *a priori* information on the parameter variations, then it would be appropriate, for instance, to define the dynamics as oscillatory in accordance with some diurnal or seasonal fluctuation.

4.2. The Extended Kalman Filtering Algorithms

The EKF is a linear approximation of the nonlinear filter which would ideally be needed to provide estimates of $\mathbf{x}^*$ in Eq. (15). The principal steps in its derivation are listed as follows.

(a) *Linearization of the nonlinear augmented state equations.* For *small* perturbations $\boldsymbol{\delta}\mathbf{x}^*(t)$ of the state $\mathbf{x}^*(t)$ about some nominal reference trajectory $\bar{\mathbf{x}}^*(t)$, a set of linear dynamic equations in $\boldsymbol{\delta}\mathbf{x}^*(t)$ are obtained by taking a first-order Taylor series expansion of $\mathbf{f}$ in Eq. (15). Here $\boldsymbol{\delta}\mathbf{x}^*(t)$ is defined by

$$\boldsymbol{\delta}\mathbf{x}^*(t) = \mathbf{x}^*(t) - \bar{\mathbf{x}}^*(t) \tag{18}$$

and

$$\mathrm{d}\bar{\mathbf{x}}^*(t)/\mathrm{d}t = \mathbf{f}\{\bar{\mathbf{x}}^*(t), \mathbf{u}(t)\}. \tag{19}$$

(b) *Linearization of the nonlinear observation equation.* By defining a nominal measurement trajectory in terms of $\bar{\mathbf{x}}^*(t)$ we can similarly derive the linear small perturbation observation equation for $\boldsymbol{\delta}\mathbf{y}(t_k)$.

(c) *Application of a linear Kalman filter to the perturbational equations.* From step a we have

$$\mathrm{d}\{\boldsymbol{\delta}\mathbf{x}^*(t)\}/\mathrm{d}t = \mathbf{F}^*\{\bar{\mathbf{x}}^*(t_0), \mathbf{u}(t)\}\boldsymbol{\delta}\mathbf{x}^*(t) + \boldsymbol{\xi}^*(t), \tag{20}$$

where

$$\mathbf{F}^*\{\bar{\mathbf{x}}^*(t_0), \mathbf{u}(t)\} \triangleq \left[\frac{\partial f_i\{\bar{\mathbf{x}}^*(t), \mathbf{u}(t)\}}{\partial x_j^*}\right]. \tag{21}$$

Integration of Eq. (20) over the interval $t_k \to t_{k+1}$ gives

$$\boldsymbol{\delta}\mathbf{x}^*(t_{k+1}) = \boldsymbol{\Phi}\{t_{k+1}, t_k; \bar{\mathbf{x}}^*(t_k), \mathbf{u}(t_k)\}\boldsymbol{\delta}\mathbf{x}^*(t_k) + \boldsymbol{\omega}(t_{k+1}), \tag{22a}$$

and from step b we have

$$\boldsymbol{\delta}\mathbf{y}(t_k) = \mathbf{H}^*\{\bar{\mathbf{x}}^*(t_k)\}\boldsymbol{\delta}\mathbf{x}^*(t_k) + \boldsymbol{\eta}(t_k) \tag{22b}$$

with the definitions

$$\boldsymbol{\Phi}\{t_{k+1}, t_k; \bar{\mathbf{x}}^*(t_k), \mathbf{u}(t_k)\} \triangleq \exp(\mathbf{F}^*\{\bar{\mathbf{x}}^*(t_k), \mathbf{u}(t_k)\}(t_{k+1} - t_k)) \tag{23}$$

and

$$\mathbf{H}^*\{\bar{\mathbf{x}}^*(t_k)\} \triangleq \left[\frac{\partial g_i\{\bar{\mathbf{x}}^*(t_k)\}}{\partial x_j^*}\right]. \tag{24}$$

Note that Eqs. (20) and (21) imply that $\mathbf{F}^*\{\cdot\}$ and hence $\boldsymbol{\Phi}\{\cdot\}$ are determined for all t by the choice of the initial conditions $\bar{\mathbf{x}}^*(t_0)$ of the reference trajectory; note also that $\omega(t_{k+1})$ is the discrete-time equivalent of $\boldsymbol{\xi}^*(t)$.

By applying a linear (discrete-time) Kalman filter to the linear system of Eq. (22) estimates $\hat{\boldsymbol{\delta}}\hat{\mathbf{x}}^*$ of the small perturbations can be derived and hence through Eq. (18) we see a means of "reconstructing" estimates of the state $\mathbf{x}^*$, that is,

$$\hat{\mathbf{x}}^*(t_k|t_k) = \bar{\mathbf{x}}^*(t_k) + \hat{\boldsymbol{\delta}}\hat{\mathbf{x}}^*(t_k|t_k). \tag{25}$$

(d) *A suitable choice of reference trajectory.* Clearly the choice of reference trajectory is crucial to the operation of the filter. If the choice of $\bar{\mathbf{x}}^*(t_0)$ were inaccurate then there is no guarantee that the perturbations about the reference trajectory are small, and thus the linearization is no longer a valid approximation. For the EKF the particular substitution of *the current state estimate as the reference trajectory* is made; in step e below we shall discuss how the term "current" is interpreted.

(e) *The algorithms.* The EKF algorithms provide for prediction of the estimates and estimation error covariances between sampling instants,

Prediction:

$$\hat{\mathbf{x}}^*(t_{k+1}|t_k) = \hat{\mathbf{x}}^*(t_k|t_k) + \int_{t_k}^{t_{k+1}} \mathbf{f}\{\hat{\mathbf{x}}^*(t|t_k), \mathbf{u}(t)\}\, \mathrm{d}t, \tag{26a}$$

$$\mathbf{P}(t_{k+1}|t_k) = \boldsymbol{\Phi}\{t_{k+1}, t_k; \hat{\mathbf{x}}^*(t_k|t_k), \mathbf{u}(t_k)\}\mathbf{P}(t_k|t_k) \times \boldsymbol{\Phi}^{\mathrm{T}}\{t_{k+1}, t_k; \hat{\mathbf{x}}^*(t_k|t_k), \mathbf{u}(t_k)\} + \mathbf{Q}(t_{k+1}), \tag{26b}$$

and for corrections to be applied to those predictions at the sampling instant,

Correction:

$$\hat{\mathbf{x}}^*(t_{k+1}|t_{k+1}) = \hat{\mathbf{x}}^*(t_{k+1}|t_k) + \mathbf{K}(t_{k+1})[\mathbf{y}(t_{k+1}) - \mathbf{g}\{\hat{\mathbf{x}}^*(t_{k+1}|t_k)\}], \tag{26c}$$

$$\mathbf{P}(t_{k+1}|t_{k+1}) = [\mathbf{I} - \mathbf{K}(t_{k+1})\mathbf{H}^*(t_{k+1})]\mathbf{P}(t_{k+1}|t_k)[\mathbf{I} - \mathbf{K}(t_{k+1})\mathbf{H}^*(t_{k+1})]^{\mathrm{T}} + \mathbf{K}(t_{k+1})\mathbf{R}(t_{k+1})\mathbf{K}^{\mathrm{T}}(t_{k+1}), \tag{26d}$$

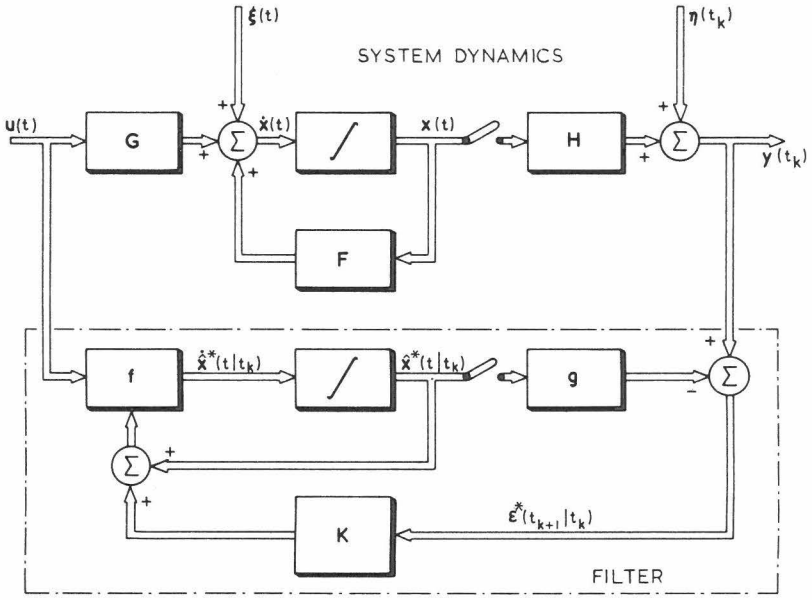

Figure 7. Block diagram of the extended Kalman filter and the (linear) system dynamics.

where $\mathbf{K}$, the Kalman gain matrix, is given by

$$\mathbf{K}(t_{k+1}) = \mathbf{P}(t_{k+1}|t_k)\mathbf{H}^{*\mathrm{T}}(t_{k+1})[\mathbf{H}^*(t_{k+1})\mathbf{P}(t_{k+1}|t_k) \times \mathbf{H}^{*\mathrm{T}}(t_{k+1}) + \mathbf{R}(t_{k+1})]^{-1}. \quad (26e)$$

$\mathbf{I}$ denotes the identity matrix and superscript T denotes the transpose of a vector or matrix.

In Eq. (26), $\mathbf{P}(t|t_k)$ is the estimation error covariance matrix defined as

$$\mathbf{P}(t|t_k) \triangleq \mathscr{E}\{(\mathbf{x}^*(t) - \hat{\mathbf{x}}^*(t|t_k))\,(\mathbf{x}^*(t) - \hat{\mathbf{x}}^*(t|t_k))^{\mathrm{T}}\}$$

and $\mathbf{Q}(t_k)$ and $\mathbf{R}(t_k)$ are, respectively, the system noise covariance and measurement noise covariance matrices

$$\mathscr{E}\{\boldsymbol{\omega}(t_k)\boldsymbol{\omega}^{\mathrm{T}}(t_j)\} = \mathbf{Q}(t_k)\delta_{kj} \qquad \text{and} \qquad \mathscr{E}\{\boldsymbol{\eta}(t_k)\boldsymbol{\eta}^{\mathrm{T}}(t_j)\} = \mathbf{R}(t_k)\delta_{kj}$$

with $\mathscr{E}\{\boldsymbol{\omega}(t_k)\} = \mathscr{E}\{\boldsymbol{\eta}(t_k)\} = \mathbf{0}$.

To conclude the arguments leading to the EKF algorithms of Eq. (26) we note that the matrices $\boldsymbol{\Phi}\{\cdot\}$ and $\mathbf{H}^*\{\cdot\}$ of the perturbational system (Eq. 22) are required only in the computation of the covariances, Eqs. (26b) and (26d), and for the gain matrix, Eq. (26e). This is so since the substitution

$$\bar{\mathbf{x}}^*(t_{k+1}) = \hat{\mathbf{x}}^*(t_{k+1}|t_k)$$

for the evaluation of $\mathbf{H}^*$ and the substitution

$$\bar{\mathbf{x}}^*(t_k) = \hat{\mathbf{x}}^*(t_k|t_k)$$

for the evaluation of $\boldsymbol{\Phi}$ enable us to employ the original nonlinear system functions $\mathbf{f}\{\cdot\}$ and $\mathbf{g}\{\cdot\}$ in Eqs. (26a) and (26c). Hence also by these substitutions the nonlinear equations are effectively relinearized at each sampling instant t_k. Because of the prudent choice of reference trajectory the filtering algorithms can be formulated directly in terms of the augmented state vector $\mathbf{x}^*$ instead of, as suggested at step c, a linear filter applied to the perturbation vector $\delta\mathbf{x}^*$ together with the solution of Eq. (19) for $\bar{\mathbf{x}}^*$. A block diagram of the EKF is given in Fig. 7.

4.3. Operation of the EKF Algorithms

In order to implement the algorithms of Eq. (26) there are three matrices and one vector which must be quantified. These comprise the *initial conditions* of the filter, in other words, the *a priori* state parameter estimates $\hat{\mathbf{x}}^*(t_0|t_0)$; the *a priori* estimation error covariances $\mathbf{P}(t_0|t_0)$; and the *noise covariances*, system noise covariances $\mathbf{Q}(t_k)$; and measurement noise covariances $\mathbf{R}(t_k)$. Any identification (and parameter estimation) results obtained with the EKF are open to debate because the specification of these "unknowns," and especially that of $\mathbf{Q}(t_k)$, may depend strongly on the subjective judgement of the analyst. There are also analytical problems in that global convergence of the estimates is not guaranteed and thus the choice of $\hat{\boldsymbol{\alpha}}(t_0|t_0)$ in $\hat{\mathbf{x}}^*(t_0|t_0)$ should reflect a vector of *a priori* parameter estimates which are within the locality of the true parameter values.

Only a few guidelines can be offered on the mechanics of implementing the filter for any given system. First, it is probably common sense to evaluate $\hat{\mathbf{x}}^*(t_0|t_0)$, in particular $\hat{\boldsymbol{\alpha}}(t_0|t_0)$, by prior trial and error deterministic simulation comparisons with the experimental field data. Second, if

$$\mathbf{y}(t_k) = \mathbf{x}(t_k) + \boldsymbol{\eta}(t_k) \tag{27}$$

as is often the case, then $\mathbf{R}(t_k)$ and that submatrix of $\mathbf{P}(t_0|t_0)$ which refers to estimates of the state vector $\mathbf{x}$ can be quantified on the basis of standard instrumentation and laboratory analysis measurement errors. Third, it is customary to assume that $\mathbf{Q}$ and $\mathbf{R}$ are time invariant and further that $\mathbf{P}(t_0|t_0)$, $\mathbf{Q}$ and $\mathbf{R}$ are diagonal, unless there is evidence supporting an alternative choice.

For the quantification of $\mathbf{Q}$ there is indeed little that can be stated categorically. Loosely speaking, one might suggest that the $\mathbf{Q}$ matrix diagonal elements for $\mathbf{x}$ be evaluated from the *relative* accuracy (un-

certainty) of the model dynamics (Eq. 4) with respect to the accuracy (uncertainty) of the measurements, that is, the corresponding elements of the **R** matrix. Quantification of those portions of $\mathbf{P}(t_0|t_0)$ and **Q** which refer to the parameter vector $\boldsymbol{\alpha}$ are discussed later in Section 4.5. Otherwise the reader is referred to Bowles and Grenney (1978) for further discussion of covariance matrices specification for the EKF.

4.4. Intuitive Criteria for Model Structure Identification with the EKF

With some understanding of the EKF and its limitations we are now in a position to consider how the filter can be used to solve the model structure identification problem. In the following our heuristic approach hinges primarily upon interpretation of the recursive parameter estimates $\hat{\boldsymbol{\alpha}}(t_k|t_k)$ as indices of an adequate/inadequate model structure.

An internally descriptive model will in general have an inadequate model structure if it does not contain explicit representations of all the significant physical, chemical, biological, or ecological processes associated with the system. Significance in this context implies that the effects of such relationships between inputs and states can be measured in the output observations **y**. The filter has a tendency to provide estimates $\hat{\mathbf{x}}$ of the state vector that track the observations **y** unless the system model is very accurate. If the model is inaccurate, which is more probable, then the filter attempts to adapt this model to the dynamic characteristics observed between **u** and **y**. Clearly the filter cannot adapt the model structure and thus *significant parameter adaptation* results.

On the basis of this argument it is possible to define a first intuitive criterion for model structure identification:

Criterion 1. A model structure is adequate if the recursive estimates $\hat{\boldsymbol{\alpha}}(t_k|t_k)$ of all parameters defined to be time invariant according to Eq. (16) display trajectories which are sensibly stationary once any initial transients have decayed away.

Now suppose we have estimated $\boldsymbol{\alpha}$ such that the matrices $\mathbf{F}, \mathbf{G}, \mathbf{H}$ in the original *linear* system dynamics of Eq. (4) are completely specified. In this event it would be possible to pass through the experimental data with the linear Kalman filter applied to Eq. (4) (note that for the functions **f** and **g** being linear the EKF algorithms of Eq. (26) reduce to those of the linear filter). The sequence of *innovations process residual errors*

$$\boldsymbol{\varepsilon}(t_k|t_{k-1}) = \mathbf{y}(t_k) - \mathbf{H}\hat{\mathbf{x}}(t_k|t_{k-1}) \tag{28}$$

thereby generated should have certain statistical properties—providing our

initial assumptions about ξ and η are valid—and a second intuitive criterion can be introduced:

Criterion 2. A model structure is adequate if the residual errors $\varepsilon(t_k|t_{k-1})$ of the linear Kalman filter for the original linear system model, Eq. (4), approximate zero–mean, white, Gaussian sequences.

Clearly the use of criterion 2 is somewhat restricted since the original system dynamics are required to be linear. Notice, however, that Eq. (28) is equivalent to

$$\varepsilon(t_k|t_{k-1}) = \mathbf{y}(t_k) - \hat{\mathbf{y}}(t_k|t_{k-1})$$

which has obvious similarities with Eq. (8)—compare also with the analogous situation for the EKF in Fig. 7.

It should be apparent that Criterion 1 is the more readily applicable criterion of model structure identification: Its use naturally precedes the application of Criterion 2. The reader should also note that, in principle, nonlinear system dynamics present no additional analytical problems for the implementation of the EKF. Nevertheless, having defined two criteria for model structure identification, it must be admitted that there will be few modeling exercises in which these criteria can be applied in any systematic manner!

4.5. Parameter Dynamics and Model Structure Identification

A familiar means of formulating a dynamic model from the available biological and ecological theory is the application of component mass balances across the system boundaries. For our specific purposes these components are usually the concentrations of dissolved substances, for example nutrients, or the magnitudes of microorganism populations. Thus Eq. (4a) might be rearranged to give

$$\dot{\mathbf{x}}(t) = \mathscr{S}\{\mathbf{x}(t), \mathbf{u}(t)\} + \mathscr{T}\{\mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\alpha}_1\} + \mathscr{U}\{\boldsymbol{\alpha}_2(t)\} + \boldsymbol{\xi}(t), \tag{29}$$

where $\mathscr{S}\{\cdot\}$ represents the bulk transport (flux) of components into and out of the system, and $\mathscr{T}\{\cdot\}$ includes *a priori well-known* theoretical relationships for population growth, death, nutrient uptake, respiration, and so on. $\mathscr{U}\{\cdot\}$ accounts for all physical, chemical, biological, and ecological phenomena whose presence in the observed data is a matter of speculation and for which no well-established formal mathematical relationships are available *a priori*. The distinction drawn between $\mathscr{T}$ and $\mathscr{U}$ is, of course, rather arbitrary. There tends to be a complete spectrum of shades of

confidence in the theories incorporated in the model; the distinction serves primarily to illustrate both how to characterize the respective parameter dynamics and how to quantify the associated submatrices of $\mathbf{P}(t_0|t_0)$ and $\mathbf{Q}$.

Let us denote by $\mathbf{P}_1(t_0|t_0)$, $\mathbf{P}_2(t_0|t_0)$, and $\mathbf{Q}_1, \mathbf{Q}_2$ the submatrices of $\mathbf{P}(t_0|t_0)$ and $\mathbf{Q}$ corresponding to $\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_2$. In principle the parameter vector $\boldsymbol{\alpha}_1$ in Eq. (29) is defined as time invariant according to Eq. (16), whereas the dynamics of $\boldsymbol{\alpha}_2$ may be said to conform to Eq. (17), that is, random walk idealizations. The *a priori* estimates $\hat{\boldsymbol{\alpha}}_1(t_0|t_0)$ ought to be quantifiable from previous empirical evidence or prior simulation results. Suitable initial guesses for $\boldsymbol{\alpha}_2$ might be that

$$\hat{\boldsymbol{\alpha}}_2(t_0|t_0) = \mathbf{0}. \tag{30}$$

If $\mathbf{P}_1(t_0|t_0)$ is evaluated in terms of the (albeit subjective) confidence bounds on $\hat{\boldsymbol{\alpha}}_1(t_0|t_0)$, then $\mathbf{P}_2(t_0|t_0)$ should express the intuitively reasonable assumption that *relatively* less initial confidence is placed in the estimates $\hat{\boldsymbol{\alpha}}_2(t_0|t_0)$ than in $\hat{\boldsymbol{\alpha}}_1(t_0|t_0)$. Our objectives in so specifying $\mathbf{P}_2(t_0|t_0)$ are to permit the rapid adaptation of subsequent recursive estimates, $\hat{\boldsymbol{\alpha}}_2(t_k|t_k)$, to values more "realistic" than those of Eq. (30). It is important to note, however, that for the EKF the matrix $\mathbf{P}(t_k|t_k)$ cannot be interpreted as an *a posteriori* measure of the true estimation error covariances. Finally, by virtue of Eq. (16) it is easy to see that

$$\mathbf{Q}_1 = \mathbf{0},$$

and on a very approximate ad hoc basis $\mathbf{Q}_2$ could be chosen such that

$$\mathbf{Q}_2 \leqslant 0.1\mathbf{P}_2(t_0|t_0).$$

The procedure for model structure testing according to Eq. (29) is formulated with the hope that various hypotheses about the form and combination of $\mathscr{T}$ and $\mathscr{U}$ can be assessed. The ideal objective would be to eliminate $\mathscr{U}$ from Eq. (29) by modification and/or expansion of the structure of $\mathscr{T}$. In this last respect it is particularly useful either to seek relationships, that is, correlated variations, between $\hat{\boldsymbol{\alpha}}_2(t_k|t_k)$ and $\mathbf{x}(t_k), \mathbf{u}(t_k)$; or, with $\mathscr{U}\{\cdot\} = \mathbf{0}$, to check any dependence of the innovations errors $\boldsymbol{\varepsilon}(t_k|t_{k-1})$ of Eq. (28) on variations in $\mathbf{u}(t_k)$.

4.6. Problems of Stability and Partially Observed State Vectors

The majority of the discussion so far has been centered implicitly upon the assumption that Eq. (27) is valid, namely,

$$\mathbf{y}(t_k) = \mathbf{x}(t_k) + \boldsymbol{\eta}(t_k).$$

If this assumption is not valid, for instance,

$$\mathbf{y}(t_k) = [\mathbf{I} \,\vdots\, \mathbf{0}]\mathbf{x}(t_k) + \boldsymbol{\eta}(t_k),$$

then Criterion 1 cannot be applied with any confidence since there is the likelihood that filter estimates of those states not measured directly are adapted in preference to $\hat{\boldsymbol{\alpha}}(t_k|t_k)$. Model structure identification under these constraints becomes an almost impossible task of checking the statistical properties of the residual errors (Criterion 2) for each set of trial (known) values for the vector $\boldsymbol{\alpha}$. It is unfortunate, therefore, that such models arise naturally and readily in water quality and wastewater treatment systems where substrate and metabolic end product concentrations are measurable but the magnitudes of mediating enzyme and microorganism populations cannot be measured (see, for example, Beck, 1977).

We note, furthermore, as did Di Cola *et al.* (1976), that for certain microbiological and ecological constituents the state vector dynamics of Eq. (4) reduce to the (deterministic) form

$$\dot{x}(t) = \alpha(t)x(t). \tag{31}$$

For any $x(t_1) > x(t_2)$, $t_2 > t_1$, that is, population growth, it is implied that Eq. (31) exhibits temporary, marginal instability. Thus a small inaccuracy in the filter estimate $\hat{\alpha}(t_k|t_k)$ can lead to severe computational problems—in physical terms, estimates $\hat{x}(t_k|t_k)$ of organism populations, for example, assume erroneously large proportions. Yet even here such adversity can be turned to our advantage, for if the filter estimates remain reasonably bounded this is evidence of a kind that the chosen model structure is adequate.

4.7. Further Considerations of the Measurement Process

The primary objective of identification is to determine the structure of the state vector dynamics (Eq. 4a), rather than the nature of the measurement process (Eq. 4b). Nevertheless, a correct characterization of Eq. (4b) is clearly of fundamental importance to identification of the correct model structure. Two commonly occurring variations on the theme of Eq. (4b) which can be easily accommodated within the analytical framework of the EKF are: (a) the situation of systematic measurement error bias

$$y(t_k) = x(t_k) + \alpha(t_k) + \eta(t_k), \tag{32}$$

and (b) the case of a single observation of multiple state variables

$$y(t_k) = x_1(t_k) + x_2(t_k) + x_3(t_k) + \eta(t_k). \tag{33}$$

In Eq. (32) the bias is estimated as an additional parameter α, which may or may not be time varying. A typical example of Eq. (33) is the measurement of suspended solids in an aquatic environment which may embrace a number of bacterial populations at different states in their life cycle (see, for instance, Busby and Andrews, 1975).

A rather more improbable version of the measurement process concerns the analytical determination of biochemical oxygen demand (BOD), a macromeasure best defined as the amount of oxygen consumed in supporting the breakdown of organic matter by aerobic bacteria. (In fact, BOD is frequently interpreted even more loosely as a measure of the polluting strength of typical municipal/domestic effluents.) A BOD measurement is carried out over a period of 5 days under laboratory conditions in a sealed vessel, at constant temperature, and in the absence of light. The BOD of the sample, for instance river water, is defined as the change in dissolved oxygen (DO) concentration of that sample between the beginning and end of the 5-day period. This measurement, therefore, is itself a dynamic process since it resembles a batch reaction in a closed system. In the example of the following section we shall deal with a modeling exercise which leads ultimately to a description of DO–BOD–algae interaction in a reach of river. The correct characterization of the BOD measurement process turns out to be crucial in interpreting the results of model structure identification. Suppose the BOD measurement is represented as

$$y(t_k) = x_1(t_k) + \int_0^5 g_1\{x_2'(\zeta), x_3'(\zeta)\}\, \mathrm{d}\zeta + \eta(t_k), \tag{34}$$

where

$$x_2'(\zeta) = x_2(t_k) \qquad \text{for} \qquad \zeta = 0$$

and where y is the measured value of BOD, x_1 is the *in situ* river BOD concentration, and g_1 is some function of x_2', the concentration of live algae in the bottle, and of x_3', the bottled sample DO concentration. x_2 is the concentration of live algae in the river, and ζ is a dummy variable of time (in days). It is thus not at all clear which of the following two mechanisms is responsible for an apparent increase in river BOD concentration, x_1: death and decay of algal matter in the river—a phenomenon which would be described by an appropriate term in $\mathscr{T}$ (Eq. 29); or respiration (in the absence of light), and subsequent death, of a live algal population caught in the river water sample of the BOD measurement, as described by Eq. (34).

Although we shall not discuss these latter stages of the identification analysis below, it may be noted that it is impossible to resolve the above issue for this particular example.

4.8. An Example: The Interaction between BOD and an Algal Population in a Freshwater River

This example, as has been mentioned already, forms a part of a larger model for river water quality, that is, DO–BOD–algae interaction (Beck, 1975); the experimental data are taken from a field study of the River Cam in eastern England (Beck and Young, 1975). The DO balance in a river is generally believed, among other factors, to be determined by: (i) the withdrawal of oxygen by BOD decay; and (ii) the photosynthetic/respiratory activity of plants and algae. Our treatment here is necessarily brief and sets out to examine how a dead and decaying algal population places an additional BOD load on the river's oxygen resources. We assume, therefore, that this is the dominant of the two alternative mechanisms suggested in Section 4.7. A comprehensive report on the use of the EKF in this specific model structure identification context is given in Beck and Young (1976). The primary aim in presenting the example is to illustrate some of the basic principles of internally descriptive model structure identification summarized in Sections 4.4 and 4.5.

An *a priori* model for the BOD dynamics can be derived from the classical studies of Streeter and Phelps (1925)

$$\dot{x}(t) = \mathscr{S}(t) - \alpha_1 x(t) + \xi(t) \tag{35}$$

in which, according to the scheme of Eq. (29),

$$\mathscr{T}\{x(t), u(t), \alpha_1\} = -\alpha_1 x(t); \qquad \mathscr{U}\{\alpha_2(t)\} = 0.$$

x is the concentration of BOD in the river, and α_1 is a parameter representing the BOD decay rate constant under the assumption of simple,

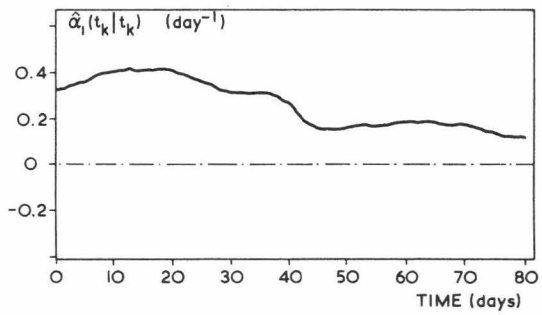

Figure 8. Recursive EKF estimates of the BOD decay rate constant, α_1, in the model of Eq. (35).

Table I *A Priori* Estimates and Covariance Specifications for the Example of Section 4.8

State parameter	$\hat{x}_i^*(t_0\|t_0)$	$p_{ii}(t_0\|t_0)$	q_{ii}	r_{ii}
x (gm^{-3})	1.4	1.0	0.4	0.4
α_1 (day^{-1})	0.32	0.005	0	—
α_2 ($gm^{-3}\,day^{-1}$)	0	2.0	0.05	—

first-order kinetics. The augmented state vector of the EKF is

$$\mathbf{x}^*(t) = [x(t), \alpha_1]^T$$

with the observation equation $y(t_k) = x(t_k) + \eta(t_k)$ and the *a priori* estimates and covariance specifications are given in Table I. The recursive estimation trajectory for $\hat{\alpha}_1(t_k|t_k)$ shown in Fig. 8 is clearly nonstationary and considerable adaptation of the parameter occurs, in particular, at about day t_{40}. It is known that over this period of the experiment the weather was warm and sunny with very low flows in the river, in other words, conditions likely to stimulate algal growth. We may conclude that the *a priori* model does not satisfy Criterion 1 of Section 4.4.

By means of a modification of the Streeter–Phelps theory due to Dobbins (1964) a term

$$\mathscr{U}\{\alpha_2(t)\} = \alpha_2(t)$$

can be incorporated into Eq. (35) such that

$$\dot{x}(t) = \mathscr{S}(t) - \alpha_1 x(t) + \alpha_2(t) + \xi(t), \tag{36}$$

where $\alpha_2(t)$ is, in effect, a time-variable parameter which accounts for the rate of addition (removal) of BOD in the river by unknown physical, chemical, or biological mechanisms. The estimates $\hat{\alpha}_1(t_k|t_k)$ in Fig. 9 are thereby much improved, that is, they are more stationary. The variations in $\hat{\alpha}_2(t_k|t_k)$, on the other hand, can be shown to be strongly correlated with the day-to-day variations in the hours of sunlight, $u(t_k)$, incident on the river system during each 24-hr period. However, for the purpose of illustrating the use of Criterion 2 from Section 4.5 this same result can be presented in an alternative fashion. Assuming $\alpha_1 = 0.32$ a linear Kalman filter applied to Eq. (35) generates the residual errors $\varepsilon(t_k|t_{k-1})$ from Eq. (28) shown in Fig. 10. The cross-correlation function between these $\varepsilon(t_k|t_{k-1})$ and $u(t_k)$ is given in Fig. 11.

Beyond this point the analysis becomes less straightforward. It is sufficient to say that we now have to establish how and why u is related through α_2 to x. In fact a final version of the DO–BOD–algae interaction model assumes that algal population growth obeys Monod (1942) kinetics

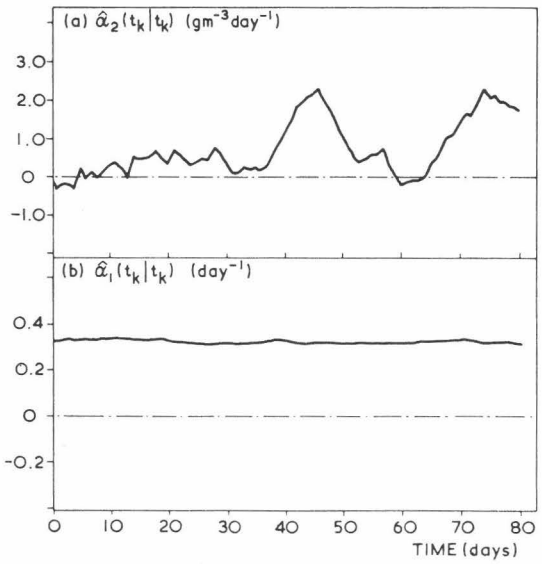

Figure 9. Recursive EKF estimates of (a) α_2 and (b) α_1 in the model of Eq. (36).

with sunlight, u, being growth-rate limiting; after death some of the particulate, algal cell material redissolves, thus creating an apparent additional BOD load in the river (Beck, 1975). During the course of the complete analysis (Beck, 1978) the order of the overall model state vector l (see Section 2.2) is expanded from two states [DO, BOD] to four states [DO, BOD, live algae, dead algae].

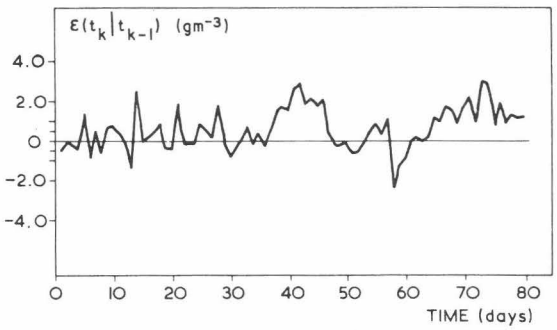

Figure 10. Residual errors $\varepsilon(t_k|t_{k-1})$ for the linear Kalman filter applied to Eq. (35); $\alpha_1 = 0.32\,day^{-1}$.

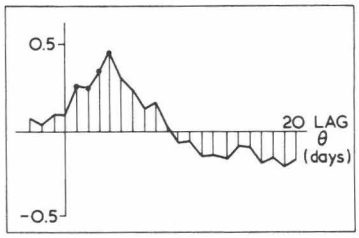

Figure 11. Cross-correlation function between $u(t_k)$, the hours of sunlight incident on the river during each day, and $\varepsilon(t_k|t_{k-1})$; correlation coefficients marked with● denote (assumed) significant correlation between $u(t_k)$ and $\varepsilon(t_k|t_{k-1})$.

5. CONCLUSIONS

There are three points to be stressed about the model structure identification problem. The first, and most fundamental, is that its solution is in many ways unavoidably subjective. There is no "best" model of a system and, indeed, different types of models are required to fulfill different roles and objectives. Our specific objectives in this instance have been to increase the degree of understanding of a system's dynamic behavior. The second point concerns the distinction made between black box and internally descriptive models. Such a distinction is necessary only in terms of presenting the various theoretical techniques for model structure identification. In an actual problem-solving context solutions evolve from the interplay between both approaches to modeling (see, for example, Beck, 1978). Third, emphasis has been placed upon the extended Kalman filter as a method of identification. It is not an easy technique with which to work and perhaps this is one reason why it appears to have received less-than-fair treatment in the system identification literature. Another reason may be that the EKF lacks certain theoretical guarantees (convergence, efficiency of estimation) on its performance. But then, in a more general sense, the analysis of field data rarely yields elegant solutions, especially when these data are derived from the predominant "normal operating conditions" of microbiological and ecological systems.

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