SYSTEM IDENTIFICATION, ESTIMATION, AND FORECASTING OF WATER QUALITY
PART I: THEORY

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PREFACE

This paper has its origins in a set of lecture notes prepared for a course entitled "Modeling and Control of River Quality" which was jointly sponsored by the Politecnico di Milano and IIASA and held in Florence during June, 1978. The initial justification for converting lecture notes into a paper lay with the observation that many people who might potentially be interested in applying techniques of system identification were discouraged from doing so by the apparent sophistication of the associated theory. There is no doubt that some of the techniques are elegant, but the purpose of this paper is certainly not one of seeking sophistication in its theoretical development. The paper originally had two objectives: to present some of the theoretical background of system identification from the starting point of basic least squares regression analysis; and then to demonstrate this theory at work by means of illustrative case studies.

However, while writing what is here Part 1 of the paper it became evident that the complete manuscript would take a long time to complete. Hence for reasons of time-constraints there is an undesirable division of the paper into a Part 1 (theory) and a Part 2 (applications). Moreover, other interests within

Resources and Environment's Task on "Models for Environmental Quality Control and Management" make it seem incomplete to discuss merely theory and its application. It ought to be possible to provide a synthesis of the major problems and future directions in identification, estimation, and forecasting of water quality; perhaps even to provide an overall framework for modeling such badly defined environmental systems. Thus when Part 2 has materialized it may well be that a Part 3, dealing with these broader issues, will have come more clearly into view.

SUMMARY

This paper presents some background theory for algorithms of system identification, estimation, and forecasting. Special attention is given to the application of these algorithms in the field of water quality modeling.

The paper starts with some qualitative definitions of the problems to be addressed, for example, problems of model structure identification, parameter estimation, state estimation, state reconstruction, and combined state-parameter estimation. The central theme of the paper, however, is the idea of an on-line, or recursive estimation algorithm. In particular a derivation of the linear Kalman filter is given; this is achieved by extending the principle of linear least squares regression analysis. Having derived the filtering algorithms, which refer to the problem of state estimation, the paper turns to the subject of recursive parameter estimation algorithms in the context of conventional time-series analysis. Finally, the algorithms of an extended Kalman filter are developed in order to treat the problem of combined state-parameter estimation.

The primary objective of the paper is to present the methods of system identification, estimation, and forecasting in a fashion which will be understandable for those more familiar with the subject of water quality modeling.

SYSTEM IDENTIFICATION, ESTIMATION, AND FORECASTING OF WATER QUALITY - PART 1: THEORY

1. INTRODUCTION

Whether one disagrees or agrees with it, mathematical modeling of water quality is a well-established field of study and research. The literature on the subject is indeed vast and the effort expended on model development and verification must be equally large. There are many ways in which to approach the problem of mathematical model construction, and probably each person involved in such an activity has his own unique collection of procedures. A major proportion of these procedures, as applied to water quality modeling, might be counted as essentially procedures of "trial and error" deterministic simulation. In other words, this is the type of informal modeling procedure whereby (see Figure 1), starting with some initial model structure and set of associated parameter (coefficient) values, the simulated performance or response of the model is compared with the actually observed behavior of the system under investigation. Then, if the model is found to be inadequate in its characterization of reality, the analyst may decide simply to adjust some of the parameter values on an ad hoc basis until the desired performance is obtained. On the other hand, the model may be so much in error that the analyst is required to alter the structure of the relationships between the variables accounted for in the model.

Reality is, of course, somewhat subject to randomness in its observed behavior, and rather strongly so in the field of environmental and water quality systems. Thus an essentially deterministic approach to modeling is incomplete in its recognition of the real system's properties. The aim of this paper is to be partly tutorial and partly review in character. In being tutorial it seeks to present a number of techniques of estimation which should permit a more formal and adequate treatment of model development by reference to noise-corrupted field data. In particular, we should like these techniques to be capable of admitting the existence of both random disturbances of process behavior and random measurement error. At the same time formal methods of estimation should be able to discriminate effectively against such ever-present noise and chance error in the field data. It is not in practice a matter of the analyst being unaware of the stochastic aspects of the modeling problems nor of the informal deterministic simulation method being wholly inadequate. For whether one models a system's behavior along the lines of Figure 1 or Figure 2, a large part of the modeling exercise is devoted precisely to the activity of filtering out the uncertainty (noise) in the observed patterns of behavior.

Yet the paper by the nature of its title deals with more than just the subject of estimation methods: it treats also the topics of system identification and forecasting. This is because the techniques of estimation that we shall introduce derive in part from the broader field of system identification, which incorporates estimation with other problems of specialized experimental design, model structure identification, model verification and model validation. Another reason is that the central theme of the paper, namely Kalman filtering, is perhaps better known within the context of on-line forecasting and control situations. All three topics, identification, estimation, and forecasting, are closely interrelated. We shall exploit these interrelationships for illustrative purposes wherever appropriate in the paper.

Most of the background technique here necessary for development of the estimation algorithms derives from control theory.

Since control theory is frequently understood, and perhaps misunderstood, to be concerned merely with black box models of input/output behavior, it is possible that matters such as system identification and estimation are by association regarded with suspicion. This suspicion may arise for two reasons. Firstly, the term "black box model" suggests a lack of desire for understanding or acknowledging the true physical mechanisms which govern process dynamic behavior. And secondly, the association with statistical features of the modeling problem is all too redolent of sterile curve-fitting exercises. The theoretical development of this paper is, therefore, especially concerned with presenting an estimation method suitable for use with what will be called internally descriptive models (see section 2.2.2). In fact both black box and internally descriptive models have important roles to play in the analysis of field data. Likewise, though an accurate model would be the ultimate goal of any modeling exercise, curve-fitting is not necessarily very meaningful in itself: the identification of mathematical models from field data is essentially a learning procedure in which models are working hypotheses about the nature of reality.

A large section of the paper is occupied by the mathematical development of the linear Kalman filter (LKF), from which is finally required a derivation of the extended Kalman filter (EKF). This particular derivation commences with a well-known and simple parameter estimation technique, linear least squares regression analysis, and then builds upwards in complexity towards the linear Kalman filter. Such an approach has previously been adopted by Young (1974). It is not necessarily an elegant or an efficient derivation; our intention is that the analysis should be as transparent as possible and that the reader will thereby obtain a picture of several other closely related recursive parameter estimation algorithms. To aim for clarity at the expense of theoretical elegance is justified by the lack of previous application of these techniques in water quality modeling (as evidenced by Beck (1978a), Jørgensen (1979), and Jørgensen and Harleman (1978)). This may have been due to the kind of suspicion we have mentioned earlier. Further, given the belief that much can be learned from

the demonstration of theory applied to practice, Part 2 of the paper has been designed to complement the theoretical development of Part 1 with a number of case study results.

The organization of the paper is as follows. Section 2 discusses the principles and qualitative features of system identification, estimation, and forecasting in the specific context of wastewater treatment and river water quality modeling. Section 3 presents the development of the linear Kalman filter from the starting point of linear least squares regression analysis; again here emphasis is placed on the qualitative features of the filtering algorithms. The evident attention to detail in Section 3 gives way to a more brief treatment in Section 4 of conventional time-series analysis and recursive parameter estimation techniques closely related to the linear Kalman filter. Likewise the development of the extended Kalman filter algorithms for combined state-parameter estimation in Section 5 is relatively brief and relies strongly on the resources of Section 3. Part 2 will then deal with illustrative examples from case studies. These examples include topics such as: designing experiments to test the behavior of a full-scale anaerobic digestion unit; estimating the parameters of a model for dissolved oxygen (DO) and biochemical oxygen demand (BOD) interaction; on-line estimation of the behavior of nitrifying organisms in an activated sludge plant; and adaptive forecasting of sewer network flows.

It is not in general the purpose of Part 1 of the paper to enter any philosophical debate regarding environmental or ecological systems modeling, as in, for example, Young (1978a) or Halfon (1978). We do assume, however, a certain pragmatism in modeling in that field data of an adequate kind and number are a priori available or necessary. And in Part 3 we shall assume the license of discussing future possible foci of attention for identification, estimation, and forecasting of water quality. With that our review of current successes and problems of this subject will be completed.

2. PROBLEMS OF SYSTEM IDENTIFICATION, ESTIMATION, AND PREDICTION

Let us start with some problem definitions. In this section we first consider a basic abstract characterization of the dynamic behavior of a system. From here onwards it is assumed that unsteady, transient, or dynamic behavior will be of primary interest. The abstract characterization is then interpreted within the context of modeling interactions in microbiological and ecological systems. Both the abstraction and the microbiological/ecological example will hence serve to illustrate the principal qualitative features of system identification, estimation, and prediction.

2.1 Definitions and Objectives

Figure 3 gives a schematic definition of the dynamic system model and variables, i.e. the component features of our portrayal of reality. To give a more immediate appreciation of this diagram let us suppose the following, that:

(i) The group of variables denoted by $\underline{u}$, measured input disturbances, might comprise the recorded day-to-day variations of total BOD, suspended solids (SS), and ammonia-N concentrations in the settled sewage influent to an activated sludge plant.

(ii) The group of variables denoted by $\underline{\xi}$ represent unmeasured (unknown) input disturbances. These might include items such as random variations in the rate of dissolved BOD and organic phosphorus addition to a river by local surface runoff. Other undetected disturbances, which in concept can be equated with input disturbances, would include random fluctuations in the mixing regime of the liquors in an activated sludge aerator unit.

(iii) The process state variables, both $\underline{x}_m$ and $\underline{x}_u$, are quantities that characterize the essential properties and behavior of a process with the passage of time. There are two types of state variable: those that can be measured (easily), $\underline{x}_m$, such as the pH level and temperature of the sludge contained in an anaerobic digester; and those that

are extremely awkward, if not impossible, to measure, $\underline{x}_u$, for example, mixed liquor nitrosomonas bacterial concentration, or the viable fraction of a biological floc.

(iv) The group of variables $\underline{y}$ are termed measured output variables. In fact, frequently these variables are merely measurements of the (measurable) state variables, $\underline{x}_m$, and the labels state and output are therefore loosely interchangeable in some cases. However, in order to emphasize the idea of an output response of the process to an input disturbance, we can visualize the time-variations of downstream DO concentration in a stretch of a river as an output response to changes in the upstream (input) BOD concentration.

(v) The last group of variables, $\underline{\eta}$, represents the respective random and systematic measurement errors which derive from process instrumentation and laboratory analysis; such errors are inherent in all measurements $\underline{y}$ thus precluding the possibility of $\underline{y}$ being an absolutely exact measure of $\underline{x}_m$.

One further group of quantitites in Figure 3 remains to be discussed -- these are the model parameters, $\underline{\alpha}$, for instance, the reaeration rate coefficient or chemical kinetic rate constants which appear in the equations of the system model. In general, the desirable property of the parameters is that they be invariant with time, i.e. truly constant. In the following, this desirable property is seen to be an extremely important feature of certain aspects of model development and analysis. The other five groups of variables, as indicated in Figure 3, are assumed to be functions of time t; they are also implicitly functions of space.

A common theme of identification, estimation, and prediction is that they are all concerned with the retrieval, manipulation, and restructuring of measured information about a system's dynamic behavior. Figure 3 indicates, therefore, that in order to compute values for $\underline{x}$ and $\underline{\alpha}$, or statistical properties of $\underline{\xi}$ and $\underline{\eta}$, the information available to the analyst is represented by the measured input and output data for $\underline{u}$ and $\underline{y}$ respectively. Given that restricted measurement facilities and considerable complexity are the dominant characteristics of microbiological/ecological systems, what is the likelihood of success in the application of the algorithms we are about to develop?

To answer this it is instructive to recast Figure 3 as the representation of Figure 4. Let us start with Block 1 of Figure 4 in which we have the fundamental microbiology and biochemistry of the system, such as phytoplankton production, or microorganism/substrate interaction. At this level a high degree of literally microscopic detail would be required to characterize (i.e. model) all the phenomena present in the process under study. Yet the structure of these relationships, and the changing patterns of dominant species in the ecological community, though microscopic in detail, cannot necessarily be ignored, for they may have gross macroscopic impacts on overall process conditions, as for example in algal blooms with the consequences of severe oxygen depletion and so forth.

For Block 2 the more macroscopic features of the process state dynamics, e.g. variations in pH and temperature, will reciprocally influence what happens at the microscopic biochemical level. In general, however, most of the microscopic detail of Block 1 falls under the category of variables which are not easily measured, $\underline{x}_u$, and hence this fine detail is "lost," as it were, to the process environment (Block 3). That is to say, direct measurement of the variables characteristic of Block 1 is extremely difficult unless specialized experimental and analytical facilities are available to the investigator. The relatively small number of variables in Block 2 which are easily measured, that is $\underline{x}_m$, amount only to the more macroscopic, sometimes

crude, measurements of quantities like chemical oxygen demand (COD), suspended solids, and dissolved oxygen concentrations.

Block 3 of Figure 4 represents in part the system environment, from which all manner of unobserved disturbances and unpredictable mechanisms of behavior ($\underline{\xi}$) will interact with the more deterministic features of the phenomena accounted for in Blocks 1 and 2. Block 3 also represents the instrumentation and analytical procedures from which arise unavoidable components of measurement error ($\underline{\eta}$). Thus Block 3 is intended to introduce elements of uncertainty into the picture of a system's behavior.

So finally the following can be stated in answer to our earlier question about the likelihood of success in the application of "sophisticated" algorithms to modeling and forecasting water quality. Clearly, if only measurements of some of the process inputs, $\underline{u}$, and of some of the process outputs, $\underline{y}$, can be obtained, then relatively very little information is available concerning the basic biochemical/ecological nature of Block 1 in Figure 4. Moreover, the relationships between $\underline{u}$, $\underline{x}$, and $\underline{y}$ are significantly obscured by the uncertainty originating from the process environment and instrumentation. In fact it will become evident that irrespective of whether the primary objective is model development or forecasting, the application of the algorithms has two major functions: (i) during analysis, to discriminate against the effects of the stochastic components $\underline{\xi}$ and $\underline{\eta}$; (ii) to assist in making inferences about the behavior of the inaccessible* "microscopic" portion of the state variables from information on the more accessible "macroscopic" sector of the process dynamics. If the algorithms can fulfill these functions, even in some small measure, then we might consider their application to have been successful. It is always important to bear in mind that the construction of large, apparently comprehensive, and detailed models does not necessarily imply that these models are either accurate or that the model-builder has a good understanding of observed process behavior.

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*intended here as not easily measurable.

2.2 System Identification

The term system identification is meant here as the complete process of deriving mathematical models from, and by reference to experimental field data. One can now perhaps call it a subject in its own right after the rapid developments of the past ten to fifteen years, see for example Eykhoff (1974) and Mehra and Lainiotis (1976); it has its roots in statistical and control theory with strong branches of application in econometrics and biometrics.

2.2.1 Experimental Design

Several separate stages can be distinguished along more or less formal lines within the procedure of system identification. The first of these stages is that of experimental design, since a prerequisite for model development is an appropriate record of the observed process dynamics. Unless otherwise stated this field data base will be required to comprise regularly and discretely sampled values of several input/output variables over a given period of time, i.e. a group of time-series.

The success of any modeling exercise which sets itself the objective of demonstrating how well, or how badly, the model simulates reality is strongly dependent upon the quality of the field data available. The ideal would be the ability to make certain specialized and deliberate experiments. Experiments of this kind are usually designed for the observation of process dynamic behavior as a response to well-defined input disturbances (forcing functions). For instance, in the case of an activated sludge unit it might be desirable to measure how the mixed liquor suspended solids concentration and the clarifier effluent BOD and SS concentrations change with time in response to a sudden step increase in the volumetric feed-rate of settled sewage to the aerator. A good experimental design involves the assessment and determination of several factors (Gustavsson (1975)), some of which -- in a circular fashion -- depend upon a reasonable knowledge of the model before the modeling exercise begins! Two factors of special importance are the rate at which sampled measurements of the system behavior should be taken, and the length

of time over which to conduct the experiment. Two very rough rules of thumb state that:

(i) The sampling interval should be at most as long as the minimum time-constant of interest; or alternatively the sampling interval should be one-sixth of the period of the fastest sinusoidal-type variation expected in the behavior of the system.

(ii) The length of the experiment would ideally cover a period with magnitude of at least ten times the magnitude of the largest time-constant of interest; to some extent this kind of determination is related to the observation that the degree of subsequent parameter estimation error is inversely proportional to the length, i.e. number of samples, of the experiment.

Both points have to do with the speeds of response of the output variables to changes in the input variables. For example, DO concentration in the mixed liquor of an activated sludge unit would be expected to respond quickly, of the order of minutes, to changes in the air blower speed; gas production in an anaerobic digester varies over a period of hours after batch feeding has been completed; and the growth of nitrifying bacteria in activated sludge flocs can be measured within the time-scale of days and weeks. So if we wished to determine a dynamic relationship between air blower speed and DO concentration, it would be necessary to take measurements of these variables at very frequent intervals, but the experiment could be completed in a few hours. On the other hand, to determine the behavior of nitrification in biological wastewater treatment, much less frequent measurements are required but the experiment would probably have to continue for several months. Thus, if the idea of a time-constant* is approximately interpreted as, say, the detention time for water in a reach of river, and assuming that the same

*Strictly speaking, for complex nonlinear systems it would be more appropriate to use the term response time.

idea roughly translates into the time-scales for biological growth of a species and rates at which nutrients are cycled in an ecological system, one has the beginnings of an experimental design.

The opportunities offered for specialized experimentation in environmental systems are, however, rare. This is because two major practical problems must be overcome:

(i) While experimenting with, for example, a unit process of wastewater treatment, satisfactory operation of the plant still has to be assured.

(ii) The manipulation of input disturbances may demand quite extraordinary facilities for implementation of the given experimental design, as for example the manipulation of variations in upstream BOD concentration of a reach of river.

These problems are not always insurmountable; but they are, nevertheless, factors contributing to the slow progress in mathematical modeling of water quality and wastewater treatment processes. On the whole, current experimental work in this area reduces simply to a matter of observing behavior under normal operating conditions, a term used by Eykhoff (1974); there are few exceptions to this rule where there has been significant intervention by the experimenter, see for example Olsson and Hansson (1976).

2.2.2 Choice of Model Type

Choosing the type of model to be used is relevant primarily in as much as the problem at hand may dictate the outcome of this choice; and once the choice is made, the nature of any parameter estimation algorithm for subsequent application to the model is also thereby broadly defined. To state the choice as one between an internally descriptive model or a black box model is merely to define the two polar extremes of a spectrum of models. An internally descriptive (or mechanistic) model exploits all the available a priori information on the physical, chemical, biological, and ecological phenomena thought to govern process dynamics. This

lends to the internally descriptive model -- thus called because it characterizes how $\underline{u}$, $\underline{x}$, and $\underline{y}$ are related to each other (Figure 3) -- the potential for universal applicability and the appearance of being grounded in theory or "the laws of nature."

The black box (or input/output) model, in contrast, while it can usually command simplicity, reflects only what changes the input disturbances $\underline{u}$ will bring about in the output responses $\underline{y}$. A black box model makes no claim to be universally applicable and the range of its validity is restricted to the sample data set from which it has been obtained. It has already been mentioned in the introduction of section 1 that black box models are regarded with a degree of suspicion for these kinds of reasons. We shall return again to this subject in greater detail in section 4. In defense of black box models, however, it must be said that they can prove to be very useful in on-line forecasting applications and as initial attempts at elucidating any basic cause/effect relationships not immediately apparent in the given field data. For instance, when the analyst comprehends but a little of the process behavior under study, the identification of which inputs affect which outputs, by how much, and how quickly, may yield important clues about the further development of internally descriptive models.

In this paper and elsewhere (Beck (1978b)) the view taken is that black box and internally descriptive models represent complementary, conceptual frameworks for system identification; more is to be gained from their joint application than from the exclusive use of either model. For much of the time system identification is confronted with the need to offer plausible hypotheses about "unexplained" relationships in a set of field data. It seems only prudent therefore to approach each such problem from a variety of different angles and to gather together all the available evidence for synthesis of the next hypothesis.

2.2.3 Model Structure Identification and Parameter Estimation

We come now to two features of system identification which are central to the subsequent technical development of the paper:

(i) Model structure identification addresses the problem of establishing how the measured system input disturbances $\underline{u}$, are related to the system's state variables $\underline{x}$, and how these latter are in turn related both to themselves and to the measured system outputs $\underline{y}$.

(ii) Parameter estimation deals with the computation of values for the parameters which appear in the model equations, once the structure of these relationships has been properly identified.

The distinction between the two concepts is important for an appreciation of the procedure of model development. In practice, as will be demonstrated later, the application of a parameter estimation algorithm is frequently implicit in the solution of the model structure identification problem, see also Beck (1978c).

It may be helpful to visualize model structure identification as analogous to the choice of whether to fit a straight line or a curve to a set of experimental data. Or again, within the above broad definition of this problem, model structure identification is also concerned with identifying the correct form of the mathematical expressions which are contained in the model equations. A simple example may serve to illustrate this point. Suppose we are investigating the uptake or removal of a nutrient/substrate in a batch chemostat reaction, and our first hypothesis is a linear model,

$$\underline{\text{Model I}}: \quad \frac{dx_1(t)}{dt} = \dot{x}_1(t) = - [\alpha_1] x_1(t) \tag{2.1}$$

in which the dot notation refers to differentiation with respect to time t; x_1, the concentration of substrate, is the state variable and α_1 is a parameter representing a first-order kinetic decay-rate constant. For our second hypothesis about the observed system behavior we might propose a Monod-type kinetic expression and the presence of a mediating micro-organism in the reaction,

$$\underline{\text{Model II}}: \quad \begin{aligned} \dot{x}_1(t) &= -[\alpha_1' x_2(t)/(\alpha_2' + x_1(t))]\, x_1(t) \\ \dot{x}_2(t) &= [\alpha_3' x_2(t)/(\alpha_2' + x_1(t))]\, x_1(t) - \alpha_4' x_2(t) \end{aligned} \tag{2.2}$$

where the additional state variable x_2 is the micro-organism concentration and we have a vector $[\alpha_1', \alpha_2', \alpha_3', \alpha_4']$ of associated model parameters. Now recall that there are presumably some noise-corrupted measurements available from this experiment, but that we do not know which, if either, of Models I and II best characterizes the nature of the observed behavior. Model structure identification is then the problem of choosing -- by reference to the in situ data -- the number of state variables to be accounted for in the model, the problem of defining how these state variables depend upon each other, and the problem of identifying the correct form of the expression to go inside the square parentheses $[\cdot]$ of equations (2.1) and (2.2). If both models are thought a priori to be good approximations of reality, we might also call this a problem of model discrimination. But if neither hypothesis is adequate and a more complex pattern of behavior is suggested by the analysis of the data, the first definition will be the most useful interpretation of model structure identification to be borne in mind for the following.

For parameter estimation, an important distinction can be made between algorithms which are <u>off-line</u> (or block data processing schemes) and algorithms which are <u>on-line</u> (or recursive). Figure 5 provides a pictorial representation of the essential differences between the two types of algorithm. An off-line procedure, Figure 5(a), holds the parameter estimates constant at their a priori values, $\underline{\hat{\alpha}}^0$, while the complete block of time-series field data -- from time $t_0 \rightarrow t_N$ of the experimental period -- is processed by the algorithm. Usually all the data are processed together at one computation. A loss function, almost certainly based on the errors between observed and model responses, is calculated at the end of each iteration; the algorithm attempts then to minimize the loss function over the parameter space and computes an updated set of parameter values, $\underline{\hat{\alpha}}^1$, for substitution into the next iteration through the data (from $t_0 \rightarrow t_N$). A

recursive algorithm, in contrast, computes updated parameter estimates, $\underline{\hat{\alpha}}^0(t_k)$, at each sampling instant t_k of the field data; the minimization of the error loss function is implicitly, rather than explicitly, included in the algorithms. At the end of the block of data the estimates $\underline{\hat{\alpha}}^0(t_N)$ are substituted for the a priori parameter values $\underline{\hat{\alpha}}^1(t_0)$ of the next iteration through the data. Because of their potential for estimating time-varying parameter values, upon which certain very useful interpretations will be placed shortly, and because of a more general interest in on-line, ergo real-time, estimation and forecasting applications, the paper will focus attention solely upon recursive algorithm development.

Equipped now with more knowledge of parameter estimation algorithms, let us return to the problem of model structure identification. Imagine that the state variables $\underline{x}$ in a model may be represented conceptually by the nodes of Figure 6(a) and that the parameter values are visualized as the "elastic" connections between the state variables. If the assumption has been made that all the parameters have values which are constant with time and yet a recursive algorithm yields an estimate of one or more of the parameters, α_4 say, which is significantly time-varying, one may question the correctness of the chosen model structure. The reason for this is as follows. The general nature of an estimation procedure is to fit the model (i.e. state variable) predictions to the field observations. Hence, when any persistent structural discrepancy is detected between the model and reality this will manifest itself as an attempt by the estimation procedure to adapt the model, i.e. the parameter values, towards reality. Such time-variations of the parameter values can, of course, occur for different reasons, for instance, the parameter may be truly time-varying in accordance with some seasonal fluctuation. But for the purposes of our example in Figure 6(a) we might suppose that the actual structure of the relationships underlying the observed system behavior is better represented by the introduction of a new state variable and two new parameters, Figure 6(b). If this were indeed the correct model structure,

recomputation of the parameter values should give recursive estimates which are essentially constant.

Our example here has two objectives. Firstly, it should emphasize the earlier statement that model structure identification and parameter estimation are closely interrelated and that the former problem can sometimes be solved by recourse to a parameter estimation routine. Secondly, it should be apparent that an exercise in accurate parameter estimation is of dubious significance if the problem of model structure identification has not been satisfactorily resolved.

2.2.4 Verification and Validation

Model verification may be defined as, among other definitions, the determination of whether the "correct" model has been obtained from a given single set of experimental data. It can thus be said that model validation, on the other hand, concerns itself with checking the accuracy with which the same model predicts the behavior observed in different independent data sets.

On reflection it must appear that our definition of verification is something of a truism. And in fact the arguments for satisfying oneself that the model is verified are also rather circular. Let us assume that the model structure has been identified, the parameters estimated, and thus a sequence of final model response errors can be computed according to Figure 7. Almost inevitably it will have been necessary at some stage in the model development and data analysis to have made assumptions about the statistical properties of the noise sequences in Figure 7, i.e. $\underline{\xi}$ and $\underline{\eta}$ in Figure 3. If these assumptions are valid, the model response errors should also conform to certain statistical properties, and in particular to those of white noise, i.e. the errors are not correlated with themselves in time and they are statistically independent of the measured system input disturbances (forcing functions). Evaluation of the error sequences in this fashion can therefore provide a check essentially on whether the final model invalidates some of the assumptions inherent in its development.

Should the error sequences not conform to their desired properties, this suggests that the model does not characterize adequately all the relatively more deterministic features of the observed dynamic behavior. A strong correlation between variations in a given input and the variations in the model response errors of a given output, for example, would indicate that the model structure should be modified to accommodate additional significant relationships between those two variables. Analysis of the model performance along these lines, therefore, directs attention once again back to the model structure identification problem. We can draw two conclusions from this. First, while not lessening the importance of model verification, it may be argued that model structure identification is the fundamental issue of overall model development, see also Beck (1978c). Second, it will be evident that model development is not rigorously constrained to the sequence of procedures outlined here.

2.3 State Estimation and Prediction

The difference between a quantity which is a state variable and a quantity which is a parameter becomes almost negligible when one considers a state variable which does not vary with time, i.e. part of the system is at steady state, or a parameter which exhibits seasonal, and therefore temporal fluctuations. To attempt to preserve a difference between state and parameter is actually not particularly useful either in the later mathematical development of estimation algorithms or for fully appreciating the scope for application of these algorithms. Perhaps an ambivalent attitude towards the distinction is desirable: sometimes the difference between state and parameter is important, and sometimes it is not!

2.3.1 A Preview of the Kalman Filter

On occasion it is helpful to have a preview of the end-point of an analysis and especially so if the analysis is lengthy; this

is the intention of the present section. In section 2.2.3 and Figure 5(b), we gave the basic ideas behind recursive parameter estimators. From Figure 5(b) it is possible to write down in skeletal form the mechanism of updating the parameter estimate, i.e. in scalar terms*,

$$\hat{\alpha}(t_k) = \hat{\alpha}(t_{k-1}) + k(t_k)\varepsilon(t_k) \qquad (2.3)$$

in which $\varepsilon(t_k)$ is the error between a model prediction of the system response at time t_k and the noise-corrupted measurement $y(t_k)$ of that output response. The gain factor $k(t_k)$ is a factor which weights the importance of the error in providing a correction of the old estimate $\hat{\alpha}(t_{k-1})$ obtained at the previous sampling instant t_{k-1}. The manner in which the gain factor is computed will eventually be seen to be of great importance, but it will not concern us at this point. It is not difficult to see that a recursive state estimator could be constructed along exactly analogous lines, namely

$$\hat{\underline{x}}(t_k^+) = \hat{\underline{x}}(t_k^-) + \underline{k}'(t_k)\varepsilon'(t_k) \qquad (2.4)$$

where again $\varepsilon'(t_k)$ and $\underline{k}'(t_k)$ are response error and gain factor respectively (the prime notation merely indicates that they may be different from the error and gain of (2.3)). $\hat{\underline{x}}(t_k^+)$ denotes the newly updated (a posteriori) state estimate immediately after the receipt of the output measurement $y(t_k)$ at time t_k, whereas $\hat{\underline{x}}(t_k^-)$ represents a "best" forward extrapolated (a priori) estimate of the state $\underline{x}$ immediately before the instant of time t_k.

A subtle but very significant distinction between (2.3) and (2.4) lies in the arguments of $\hat{\alpha}$ and $\hat{\underline{x}}$. As one would expect, the state of a system will change between the measurement sampling instants t_{k-1} and t_k; it is therefore sensible to use a dynamic

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*This is for simplicity; in general, we shall be dealing with vectors and matrices for systems with many state variables and multiple parameters.

model to make an extrapolated prediction over this interval for comparison with the measurement at time t_k. In contrast the assumed model of parameter dynamics (time-variations) is that in fact the parameter remains constant. Hence the best prediction of the value of a parameter at a later instant of time is that it has the same value as its most recent estimate.

We are now in a position to introduce a conceptual picture of the Kalman filter. This is given in Figure 8 as an extension of Figure 2. The original results of Kalman (Kalman (1960), Kalman and Bucy (1961)) refer to the problem of state estimation; they were intended for purposes of stochastic control. In other words, for a feedback controller the desired aim is to match the performance (behavior) of the measurable state variables $\underline{x}_m$ with some desired reference process performance. Such a controller usually acts upon the perceived error between the measurements $\underline{y}$ and the reference performance; but $\underline{y}$ is error-corrupted and thus the Kalman filter sets out to permit control on the basis of the error between the state estimates ($\hat{\underline{x}}_m$) and the desired performance. Figure 8 treats the case of combined state and parameter estimation for which the algorithms of an extended Kalman filter (EKF) will be required. The important difference between the EKF and linear Kalman filter (LKF) is that the EKF is an (approximate) algorithm for a system with nonlinear dynamic behavior while the LKF is an algorithm for systems with linear behavior. Suffice it to say here that the combined state and parameter estimation problem is equivalent to state estimation for a nonlinear system.

In Figure 8 we see that a model of reality is embedded in the filter. Predictions of the kind $\hat{\underline{x}}(t_k^-)$ in equation (2.4) are computed by the model and fed forward to the corrector algorithm(s) together with the current observations $\underline{y}(t_k)$ of the process output response. For the corrector algorithms, equations (2.3) and/or (2.4), it is apparent that additional computation is necessary for specification of the weighting factors $k(t_k)$ or $k'(t_k)$. This additional computation refers to a parallel set of algorithms describing the time-evolution of the estimation error magnitudes, which itself is determined by a balance of the levels of uncertainty (or error) in the model as an approximation of reality, in the

unmeasured input disturbances, and in the output response observations. But again, this is almost pre-empting the subsequent development of the paper; section 3.8 will deal with the full significance of these statements. The results of the corrector algorithm are the updated state and parameter estimates $\underline{\hat{x}}_m(t_k^+)$, $\underline{\hat{x}}_u(t_k^+)$, $\underline{\hat{a}}(t_k)$ as indicated by Figure 8. These in turn are fed back to the model for revision of the information available for subsequent predictions.

The essential character of the filtering algorithms is therefore one of information restructuring: from the input/output observations of the real system's behavior, the information is "translated" into model-related estimates of the state variables and parameters. The name "filter" suggests also the intuitive idea that here is an algorithm which attempts to filter out from the given information the unwanted influences of measurement noise and uncertain disturbances. If attention is being focused on the parameter estimates as the product of the filtering operation, information about significant unexplained parameter adaptation can clearly be used to assist solution of the model structure identification problem (see section 2.2.3). Alternatively, if the filter is tracking truly time-varying parameters, this form of parameter adaptation may be subservient to the goal of maintaining an adequate state estimation performance. In both cases, however, since modification of the model is occurring, then modification of the level of uncertainty in the model is also implied as shown in Figure 8. Lastly, and of interest also as a matter of information restructuring, notice that the filter has the potential to provide estimates of those state variables which are not measured; this is known as <u>state reconstruction</u>.

With the aid of some concise notation we can add qualification to the usage of the term estimation. Suppose the current time is t_k, then,

(i) estimation of the values $\underline{\hat{x}}(t_k|t_k)$ is also termed <u>filtering</u>, where the notation signifies an estimate at time t_k based upon all the information available up to and including the measurements $\underline{y}(t_k)$;

(ii) estimation of $\underline{\hat{x}}(t_k+\tau|t_k)$ is prediction, since the state at time $(t_k+\tau)$ in the future is being estimated from measurements up to time t_k;

(iii) estimation of $\underline{\hat{x}}(t_k-\tau|t_k)$ is known as smoothing, with the provision of state estimates for some time $(t_k-\tau)$ in the past.

Of these, smoothing will be of little interest here.

2.4 Summary

The following then can be stated to summarize the problem definitions and objectives for the remainder of the paper.

Assume that we are given:

(i) Time-series of information on the measured input disturbances $\underline{u}$ and output responses $\underline{y}$ of a dynamic process;

(ii) Some knowledge of, or a set of assumptions about the statistical properties of the unmeasured random process disturbances, $\underline{\xi}$, and random measurement errors, $\underline{\eta}$.

We wish to determine, by application of recursive estimation algorithms to the analysis of the measured information:

(i) The structure of the dynamic relationships between $\underline{u}$, the state variables $\underline{x}$, and the outputs $\underline{y}$ (model structure identification);

(ii) The values of the parameters $\underline{\alpha}$ that appear in the identified model structure (parameter estimation);

(iii) The current and future values of the state variables $\underline{x}$ (state estimation and prediction);

(iv) The values of the inaccessible state variables that are not measured $\underline{x}_u$ (state reconstruction);

(v) Simultaneously the values of $\underline{x}$ and $\underline{\alpha}$ (combined state and parameter estimation or adaptive prediction).

Natural extensions of (iii), (iv), and (v) would be the use of recursive estimation algorithms in a real-time control context. This will not be treated in any depth here. However, it is worth noting that for adaptive control, as an extension of (v), part of the function of the controller is to choose values for the control signal input, $\underline{u}$, which enhance the possibilities for system identification and parameter value updating.

3. STATE ESTIMATION: A DERIVATION OF THE LINEAR KALMAN FILTER

The problem at hand is that ultimately it will be necessary to have available an algorithm for combined state-parameter estimation, i.e. the EKF. Working backwards from this final objective, we shall previously have had to derive the linear Kalman filter (LKF); and in order to make this derivation as transparent as possible it is advisable first to introduce the basic principle of linear least squares estimation, with then subsequent special reference to a recursive least squares algorithm.

The complete sequence of development of the LKF and EKF is shown in Figure 9, a key figure to which frequent reference is made during the course of this section. Inevitably the decision concerning the degree of "transparency" of the derivation has been a difficult one. In particular, the heavy use of vector-matrix algebra might have been lightened at the expense of a longer presentation. But the reader genuinely interested in applying the methods will eventually have to invest the time and effort in acquiring familiarity with this algebra. Some compensation, nevertheless, is provided at regular intervals by reverting to scalar equivalents for explanation of various points. The original motivation for this particular route in developing the LKF derives from Young (1974), although here greater emphasis is placed on the Kalman filtering technique for its own sake. Another useful text, and a source of helpful insights, is the book on applied optimal estimation by Gelb (1974). From both of these authors the following has benefited considerably.

3.1 An Introduction to the Principle of Least Squares Estimation

Let us start with the simple and most familiar problem of parameter estimation, namely the problem of linear regression analysis. Suppose we have a substance, concentration C, which decays with first-order kinetics. We wish to estimate the rate constant, β_1 say, for the decay kinetics from (noise-corrupted)

observations of the remaining concentration of the substance at time t, i.e. C(t). Our model of the process is (for a batch, sealed-vessel reaction),

$$dC(t)/dt = -\beta_1 C(t) \tag{3.1}$$

or

$$\log_e C(t) = \log_e C(t_0) - \beta_1 t \quad , \tag{3.2}$$

where $C(t_0)$ is the initial concentration of the substance. If we define

$$\log_e C(t) \triangleq x(t) \tag{3.3a}$$

and

$$\log_e C(t_0) \triangleq \beta_0 \quad , \tag{3.3b}$$

then equation (3.2) becomes

$$x(t) = \beta_0 - \beta_1 t \quad . \tag{3.4}$$

If we have N sampled measurements of x(t), denoted $y(t_k)$, where t_k is the time of the kth sampling instant (k = 1,2,...,N) and where each observation $y(t_k)$ is corrupted by a random measurement error $\eta(t_k)$,

$$y(t_k) = x(t_k) + \eta(t_k) \quad , \tag{3.5}$$

then (3.4) becomes

$$y(t_k) = \beta_0 - \beta_1 t_k + \eta(t_k) \quad . \tag{3.6}$$

The parameter estimation problem here is defined thus:

Given: the measured information t_k and $y(t_k)$ for t_1, t_2,...,

t_N (in this exceptional case we shall visualize time as being a measurement) then,

Determine: values for the unknown parameters β_0 and β_1; that is to say, determine the intercept and slope respectively of the "best" line that can be drawn through the observations in Figure 10.

One well-known solution of this parameter estimation problem is as follows. First, define the two, two-element, vectors

$$\begin{aligned} \underline{x}^T(t_k) &= [1.0, t_k] \\ \underline{\alpha} &= [\beta_0, -\beta_1]^T \end{aligned} \tag{3.7}$$

where the superscript T denotes the transpose of a vector or matrix, so that (3.6) can be written concisely,

$$y(t_k) = \underline{x}^T(t_k)\underline{\alpha} + \eta(t_k) \quad . \tag{3.8}$$

We now wish to estimate the unknown parameter values $\underline{\alpha}$ so that the loss function defined as the sum of squared errors,

$$J \triangleq \sum_{k=1}^{N} (y(t_k) - \underline{x}^T(t_k)\hat{\underline{\alpha}})^2 \tag{3.9}$$

is minimized. The estimates $\hat{\underline{\alpha}}$ of $\underline{\alpha}$ that minimize J are called the least squares estimates. (Notice that the model response errors $\varepsilon(t_k) = y(t_k) - \underline{x}^T(t_k)\hat{\underline{\alpha}}$ are not in general identical with $\eta(t_k)$ but converge to $\eta(t_k)$ as $\hat{\underline{\alpha}}$ converges to the true values $\underline{\alpha}$.)

We can obtain the minimum value of J by differentiating J with respect to $\hat{\underline{\alpha}}$ (see Appendix 1) and then setting this vector of derivatives equal to $\underline{0}$, i.e.

$$\nabla_{\hat{\underline{\alpha}}} J \triangleq \frac{\partial J}{\partial \hat{\underline{\alpha}}} = [\sum_{k=1}^{N} \underline{x}(t_k)\underline{x}^T(t_k)]\hat{\underline{\alpha}} - \sum_{k=1}^{N} \underline{x}(t_k)y(t_k) = \underline{0} \tag{3.10}$$

Hence we have the well-known equations for the least squares parameter estimates

$$\hat{\underline{\alpha}} = \left[\sum_{k=1}^{N} \underline{x}(t_k)\underline{x}^T(t_k)\right]^{-1} \left[\sum_{k=1}^{N} \underline{x}(t_k)y(t_k)\right] \tag{3.11}$$

in which $[\,\cdot\,]^{-1}$ denotes the inverse of a matrix. According to a standard text (Draper and Smith(1966)) equation (3.11) is a "result of great importance and should be memorized" -- a point which emphasizes the fundamental role of least squares as an introduction to parameter estimation.

If we pause for a short time we may observe in passing that the estimates $\hat{\underline{\alpha}}$ will only converge to the true values $\underline{\alpha}$ of the parameters provided that the correct model structure has been identified (of which more below) and provided the following statistical properties hold for the measurement errors $\eta(t_k)$,

(i) the mean value of $\eta(t_k)$ is zero, i.e.

$$\mathcal{E}\{\eta(t_k)\} = 0 \tag{3.12}$$

($\mathcal{E}\{\cdot\}$ is the expectation operator such that the expected value of a random variable X can be computed as $\int_{-\infty}^{\infty} xf(x)dx = \mathcal{E}\{X\}$ in which f(x) is the probability density function of X).

(ii) $\eta(t_k)$ is not correlated with itself in time, i.e.

$$\mathcal{E}\{\eta(t_k)\eta(t_j)\} = r\delta_{kj} \quad ; \tag{3.13}$$

where

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

in which r is the variance of $\eta(t_k)$.

(iii) $\eta(t_k)$ is not correlated with the variables $\underline{x}(t_k)$, i.e.

$$\mathcal{E}\{\underline{x}(t_k)\eta(t_j)\} = \underline{0} \text{ for all } k, j. \tag{3.14}$$

These three conditions may be recognized from the earlier discussion of section 2.2.4 as those which define the error sequence $\eta(t_k)$ as a zero-mean white noise sequence. For the present such statistical assumptions are important only insomuch as they attribute the desirable property of unbiased convergence to the least squares algorithm, i.e. the estimates converge to the true values of the parameters. In fact when the assumption of white noise is not valid for $\eta(t_k)$, which is usually the case, the least squares parameter estimates will in general be biased -- hence the origin of many other parameter estimation routines as attempts to overcome the problem of bias. However, at this stage and for the next two steps in our development of the LKF, it is not essential to have any statistical assumptions since the intermediate algorithms of these sections are derived using deterministic arguments alone.

We may also observe that had we wished to fit a higher order polynomial to the experimental data, so that in place of equation (3.6) we have

$$y(t_k) = \beta_0 - \beta_1 t_k + \beta_2 t_k^2 + ... + \beta_n t_k^n + \eta(t_k) \quad , (3.15)$$

it would have been possible to redefine the vectors $\underline{x}$ and $\underline{\alpha}$ of (3.7) as,

$$\begin{aligned} \underline{x}^T(t_k) &= [1.0,\ t_k,\ t_k^2,\ \ldots\ ,\ t_k^n] \\ \underline{\alpha} &= [\beta_0,\ -\beta_1,\ \beta_2,\ \ldots,\ \beta_n]^T \end{aligned} \qquad (3.16)$$

and thus to arrive at an identical formulation for the least squares estimates of (3.11). This is one benefit of employing the concise vector-matrix notation for its easy accommodation of problems with different and high dimensions. Further, recalling section 2.2.3 and the discussion of model structure identification, it is possible to see how (3.15), as a model of the same data set, has a different structure from the model of (3.6). For the two structures, an estimation algorithm would almost certainly yield

different values for the parameters β_0 and β_1 depending upon the particular model to which they may belong.

3.2 Extending the Principle of Least Squares Estimation

Instead of having a single scalar observation, as in equations (3.5) or (3.6), consider the situation where we have ℓ such noise-corrupted measurements of ℓ different variables, relationships for which are to be regressed upon a number of other qualities, i.e.

$$\begin{aligned} y_1(t_k) &= \underline{x}_1^T(t_k)\underline{\alpha}_1 + \eta_1(t_k) \\ y_2(t_k) &= \underline{x}_2^T(t_k)\underline{\alpha}_2 + \eta_2(t_k) \\ &\vdots \\ y_\ell(t_k) &= \underline{x}_\ell^T(t_k)\underline{\alpha}_\ell + \eta_\ell(t_k) \end{aligned} \tag{3.17}$$

so that along the lines of (3.8) we can write concisely,

$$\underline{y}(t_k) = X(t_k)\underline{\alpha} + \underline{\eta}(t_k) \tag{3.18}$$

The vectors $\underline{y}(t_k)$ and $\underline{\eta}(t_k)$ are of dimension ℓ, $\underline{\alpha}$ is an n-element vector of parameters $\alpha_1, \alpha_2, \ldots, \alpha_n$, and $X(t_k)$ is an ℓ x n matrix containing elements of the vectors $\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_\ell$. An example will serve to illustrate the construction of equation (3.18). Suppose,

$$\begin{aligned} y_1(t_k) &= x_1(t_k)\alpha_1 + x_2(t_k)\alpha_2 + \eta_1(t_k) \\ y_2(t_k) &= x_2(t_k)\alpha_3 + x_3(t_k)\alpha_4 + \eta_2(t_k) \quad , \end{aligned} \tag{3.19}$$

then,

$$\begin{bmatrix} y_1(t_k) \\ y_2(t_k) \end{bmatrix} = \begin{bmatrix} x_1(t_k) & x_2(t_k) & 0 & 0 \\ 0 & 0 & x_2(t_k) & x_3(t_k) \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} + \begin{bmatrix} \eta_1(t_k) \\ \eta_2(t_k) \end{bmatrix} \quad (3.20)$$

$(\underline{y})$ $\quad$ (X) $\quad$ $(\underline{\alpha})$ $\quad$ $(\underline{\eta})$

Thus for (3.18) we can set up the least squares loss function (which is a scalar quantity),

$$J \triangleq \sum_{k=1}^{N} \{(\underline{y}(t_k) - X(t_k)\hat{\underline{\alpha}})^T(\underline{y}(t_k) - X(t_k)\hat{\underline{\alpha}})\} \quad (3.21)$$

and once again setting $\partial J/\partial\hat{\underline{\alpha}} = \underline{0}$, obtain (see Appendix 1) the <u>least squares estimates</u>

$$\hat{\underline{\alpha}} = [\sum_{k=1}^{N} X^T(t_k)X(t_k)]^{-1}[\sum_{k=1}^{N} X^T(t_k)\underline{y}(t_k)] \; . \quad (3.22)$$

Now let us assume that in (3.17) we know the parameters $\underline{\alpha}$, but we wish to estimate values for the quantities $\underline{x}(t_k)$, which are assumed <u>constant but unknown</u>. Taking the illustrative example of (3.19), equation (3.20) can be restated as,

$$\begin{bmatrix} y_1(t_k) \\ y_2(t_k) \end{bmatrix} = \begin{bmatrix} \alpha_1 & \alpha_2 & 0 \\ 0 & \alpha_3 & \alpha_4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} \eta_1(t_k) \\ \eta_2(t_k) \end{bmatrix} \quad (3.23)$$

$(\underline{y})$ $\quad$ (A) $\quad$ $(\underline{x})$ $\quad$ $(\underline{\eta})$

where the argument t_k has deliberately been omitted from $\underline{x}$ since by assumption $\underline{x}(t_k) = \underline{x}$, a vector of constant, time-invariant quantities. For the problem of (3.23) three quantities, x_1, x_2, x_3, are to be estimated, whereas previously in (3.20) there were four quantities, α_1, α_2, α_3, α_4, to be estimated. By analogy with the derivation of (3.22) we obtain from (3.23),

$$\underline{y}(t_k) = A\underline{x} + \underline{\eta}(t_k) \tag{3.24}$$

in which A is a matrix with the known parameters α_i as some of its elements, such that the least squares estimates of $\underline{x}$ are given by,

$$\underline{\hat{x}} = \left[\sum_{k=1}^{N} A^T A\right]^{-1} \left[\sum_{k=1}^{N} A^T \underline{y}(t_k)\right] \quad . \tag{3.25}$$

As an aside we may note that (3.25) can be simplified since A is a constant matrix and therefore independent of t_k; hence,

$$\begin{aligned} \underline{\hat{x}} &= [NA^T A]^{-1} \left[A^T \sum_{k=1}^{N} \underline{y}(t_k)\right] \\ &= (1/N)A^{-1}(A^T)^{-1}A^T \left[\sum_{k=1}^{N} \underline{y}(t_k)\right] \quad , \end{aligned} \tag{3.26}$$

so that

$$\underline{\hat{x}} = A^{-1} \left\{(1/N) \sum_{k=1}^{N} \underline{y}(t_k)\right\} \quad . \tag{3.27}$$

Notice that now the quantity $\{\cdot\}$ in (3.27) is nothing more than the sample mean value of the vector $\underline{y}(t_k)$. This means that in the simplest scalar equivalent where x is linearly proportional to y, that is $y(t_k) = \alpha x + \eta(t_k)$, the least squares estimate of x according to (3.27) is simply the mean value of y divided by α, in other words

$$\hat{x} = (1/N\alpha) \sum_{k=1}^{N} y(t_k)$$

Let us summarize then the development thus far so that in the following section the endpoint of the analysis can be restated in more detail. We refer to Figure 9. Here, having passed through the stage of multiple regression analysis, we are in a convenient position to observe in (3.22) and (3.25) an important duality between problems of parameter estimation and state estimation. The same correspondence is evident in the discussion of section 2.3. It is possible to see that (3.25) provides least squares estimates of the states of a system which is time-invariant, or at steady state, if we anticipate the future interpretation of $\underline{x}$ as a vector

of state variables. However, we are now at the transition between the limits of usefulness of the illustrative example of section 3.1 and a return to the notational and conceptual conventions of section 2.1. The remainder of section 3 focuses upon the problem of state estimation. We shall therefore depart from the problem of parameter estimation until later in sections 4 and 5.

3.3 The Desired Nature of the Kalman Filter

In order to define the desired nature of the LKF algorithms, it is first necessary to introduce briefly two versions of the internally descriptive process model discussed earlier in section 2.2.2--for more detailed presentations of these topics the reader is referred to, for example, Rinaldi et al (1979), and Szöllösi-Nagy (1976). Let us suppose, therefore, that the dynamic behavior of the state of a system can be described by the following linear vector differential equation,

$$\dot{\underline{x}}(t) = F\underline{x}(t) + G\underline{u}(t) + L\underline{\xi}(t) \qquad (3.28)$$

where from section 2.1 and Figure 3 $\underline{x}$ is an n-dimensional state vector, $\underline{u}$ is an m-dimensional vector of measured input disturbances, $\underline{\xi}$ is a p-dimensional vector of stochastic, unmeasured disturbances (system noise) and F, G, L are respectively n x n, n x m, and n x p time-invariant matrices. Equation (3.28) is often referred to as a continuous-time description of process dynamics because of the argument t of the variable quantities. If equation (3.28) is integrated over the interval $t_{k-1} \rightarrow t_k$ we may obtain the corresponding discrete-time model,

$$\underline{x}(t_k) = \Phi\underline{x}(t_{k-1}) + \Gamma\underline{u}(t_{k-1}) + \Lambda\underline{\xi}(t_{k-1}) \qquad (3.29)$$

in which

$$\Phi \triangleq \exp\left(F[t_k - t_{k-1}]\right)$$

$$= I + F[t_k - t_{k-1}] + \frac{F^2}{2!}[t_k - t_{k-1}]^2 + \ldots \qquad (3.30)$$

where I is the identity matrix, and

$$\Gamma \underline{u}(t_{k-1}) \triangleq \int_{t_{k-1}}^{t_k} \Phi(t_k, \tau)\, G(\tau)\underline{u}(\tau)d\tau \tag{3.31}$$

$$\Lambda \underline{\xi}(t_{k-1}) \triangleq \int_{t_{k-1}}^{t_k} \Phi(t_k, \tau) L(\tau)\underline{\xi}(\tau)d\tau \quad . \tag{3.32}$$

Strictly speaking, Φ in (3.29) is not time-invariant if the sampling interval $(t_k - t_{k-1})$ is not constant; unless otherwise stated, however, the sampling interval is assumed to be constant in the following.

To complete our characterization of the input and output behavior of the process we require a representation of the noise-corrupted output observations of the state variables, i.e.

$$\underline{y}(t_k) = H\underline{x}(t_k) + \underline{\eta}(t_k) \tag{3.33}$$

where $\underline{y}(t_k)$ is an ℓ-dimensional vector of output observations, $\underline{\eta}(t_k)$ is an ℓ-dimensional vector of random measurement errors (measurement noise) and H is an ℓ x n observations matrix. This discrete-time form of the output measurement process is preferred, since generally it is possible to obtain only discrete-time, digital measurements of $\underline{y}(t_k)$ and not continuous-time, analog records of system behavior.

Two points are worth noting in connection with the discrete-time representation of (3.29) and the state transition matrix Φ of (3.30), since these may be unfamiliar to the reader. First, suppose for simplicity in (3.28) that $\underline{u}(t) = \underline{\xi}(t) = \underline{0}$ and then take the scalar equivalent of an unforced system dynamic response, i.e.,

$$\dot{x}(t) = fx(t) \tag{3.34}$$

so that an analytical solution for $x(t_k)$ as a function of $x(t_{k-1})$ is given by

$$x(t_k) = \exp(f[t_k - t_{k-1}])x(t_{k-1}) = \phi x(t_{k-1}) \quad (3.35)$$

The analogy between the scalar ϕ of (3.35) and its matrix equivalent Φ of (3.30) should now be more evident. Thus we may remark that the solution (3.29) of the differential equation (3.28) is the vector-matrix equivalent of solving the general linear first-order differential equation with the aid of an integrating factor (see Dorf, 1965, Stephenson, 1966). Second, had we chosen to solve (3.34) by the following first-order finite difference approximation, for small time-intervals,

$$\dot{x}(t_k) = \frac{\Delta x}{\Delta t} = \frac{x(t_k) - x(t_{k-1})}{(t_k - t_{k-1})} = fx(t_{k-1}) \quad (3.36)$$

then we could have obtained,

$$\begin{aligned} x(t_k) &= x(t_{k-1}) + [t_k - t_{k-1}]fx(t_{k-1}) \\ &= (1 + f[t_k - t_{k-1}])x(t_{k-1}) \\ &= \phi' x(t_{k-1}) \quad . \end{aligned} \quad (3.37)$$

Hence the analogy between ϕ' as a first-order approximation of ϕ and as an equivalent of the first two terms in the Taylor series expansion of the matrix Φ should also be apparent.

But let us return to specification of the desired nature of the LKF; it is as follows. Given the two system characterizations (3.28) and (3.33), or (3.29) and (3.33), determine an "optimal," in our case least squares, estimate $\underline{\hat{x}}(t)$ for the state variables $\underline{x}(t)$ <u>together with</u> the variance-covariance matrix $P(t)$ of the estimation errors, that is

$$\underline{\hat{x}}(t) = \mathcal{E}\{\underline{x}(t)\} \quad (3.38)$$

and

$$P(t) = \mathcal{E}\{(\underline{\hat{x}}(t) - \underline{x}(t))(\underline{\hat{x}}(t) - \underline{x}(t))^T\} \quad . \quad (3.39)$$

In other words the filter is to provide a picture of the time evolution of the estimated mean, or most probable, values of the state variables; and it also attaches a measure of confidence (or uncertainty bounds) to these estimated values, as provided by the estimation error covariance matrix.

We have already noted this desired parallel development of estimates and estimation errors in Figure 8 and section 2.3. Of course, what we seek is a recursive (on-line, real-time) estimation algorithm of the type given by equation (2.4). The next step is therefore the derivation of a recursive version of the least squares algorithm of (3.25) in the preceding section. In this a crucial connecting link is that equation (3.33) above looks remarkably similar to (3.24), as indeed it is meant to.

3.4 A Recursive Version of Least Squares Estimation

All three versions of the least squares algorithms of (3.11), (3.22), and (3.25) yield estimates from <u>one</u> computation when <u>all</u> the N sampled observations are available. Clearly, in the context of Figure 5(b), a recursive algorithm should be capable of computing an updated (a posteriori) estimate at time t_k given a forward prediction (a priori estimate) based on the information available at the previous sampling instant t_{k-1}. Such a capability can be translated either into an equation of the structure of (2.4),

$$\underline{\hat{x}}(t_k^+) = \underline{\hat{x}}(t_k^-) + K(t_k)\underline{\varepsilon}(t_k) \qquad (3.40a)$$

where $\underline{\varepsilon}(t_k)$ is some form of model prediction response error, or into an equation of the type,

$$\underline{\hat{x}}(t_k^+) = M_1(t_k)\underline{\hat{x}}(t_k^-) + M_2(t_k)\underline{y}(t_k) \quad . \qquad (3.40b)$$

Both of equations (3.40) will represent the essence of the recursive estimation algorithms for our purposes. In (3.40b) the

the matrices $M_1(t_k)$ and $M_2(t_k)$ determine how the a posteriori estimate is constructed from an intelligent combination of prediction and actual observation. From Figure 8 it should be evident that $\underline{\hat{x}}(t_k^-)$ and $\underline{y}(t_k)$ are implicit in the computation of $\underline{\varepsilon}(t_k)$ in (3.40a).

Let us consider (3.33),

$$\underline{y}(t_k) = H\underline{x}(t_k) + \underline{\eta}(t_k)$$

so that if the system displayed no dynamic behavior, estimates for $\underline{x}(t_k)$ are given by direct analogy with (3.25) as,

$$\underline{\hat{x}}(t_k) = [\sum_{j=1}^{k} H^T H]^{-1} [\sum_{j=1}^{k} H^T \underline{y}(t_j)] \quad . \tag{3.41}$$

A comparison of (3.41) with (3.25) shows an important difference: in (3.41) we have inserted the argument t_k for the estimates $\underline{\hat{x}}(t_k)$. We are still assuming that the vector of quantities $\underline{x}$ does not vary with time but that the estimates $\underline{\hat{x}}(t_k)$ of those quantities will be functions of time, since as each new piece of information is serially processed by the recursive algorithm, the new value of $\underline{\hat{x}}(t_k)$ will change as it converges to the true value of $\underline{x}$. One may view this as tantamount to minimizing a loss function $J(t_k)$ which varies with time, i.e. in line with (3.21),

$$J(t_k) = \sum_{j=1}^{k} \{(\underline{y}(t_j) - H\underline{\hat{x}}(t_k))^T (y(t_j) - H\hat{x}(t_k))\} \tag{3.42}$$

The loss function varies with time because new pieces of information are continually becoming available for analysis; the estimates $\underline{\hat{x}}(t_k)$ therefore represent the new estimates which result from a recomputation and minimization of $J(t_k)$ over all the currently available observations. The significance of estimates that vary with time will become apparent, not surprisingly, when the system under consideration exhibits dynamic behavior and thus requires the estimation of time-varying quantities.

For the derivation of a recursive least squares algorithm, we first define,

$$P^*(t_k) \triangleq [\sum_{j=1}^{k} H^T H]^{-1} \tag{3.43}$$

$$\underline{b}(t_k) \triangleq [\sum_{j=1}^{k} H^T \underline{y}(t_j)]$$

so that upon substituting equations (3.43) into (3.41) we obtain,

$$\hat{\underline{x}}(t_k) = P^*(t_k)\underline{b}(t_k) \quad . \tag{3.44}$$

Now observe that the following recursive relationships can be set up, for P^* and $\underline{b}$,

$$[P^*(t_k)]^{-1} = [\sum_{j=1}^{k} H^T H] = [\sum_{j=1}^{k-1} H^T H] + H^T H$$

$$= [P^*(t_{k-1})]^{-1} + H^T H \tag{3.45a}$$

$$\underline{b}(t_k) = [\sum_{j=1}^{k} H^T \underline{y}(t_j)] = [\sum_{j=1}^{k-1} H^T \underline{y}(t_j)] + H^T \underline{y}(t_k)$$

$$= \underline{b}(t_{k-1}) + H^T \underline{y}(t_k) \tag{3.45b}$$

and thus the matrix $P^*(t_k)$ and vector $\underline{b}(t_k)$ may be computed as functions of their previous values $P^*(t_{k-1})$ and $\underline{b}(t_{k-1})$ at time t_{k-1}. The application of some matrix manipulation (see Appendix 2) yields eventually the <u>recursive least squares algorithms</u>,

$$\hat{\underline{x}}(t_k) = \hat{\underline{x}}(t_{k-1}) + P^*(t_{k-1})H^T[I+HP^*(t_{k-1})H^T]^{-1}\{\underline{y}(t_k)-H\hat{\underline{x}}(t_{k-1})\}$$

$$P^*(t_k) = P^*(t_{k-1})-P^*(t_{k-1})H^T[I+HP^*(t_{k-1})H^T]^{-1}HP^*(t_{k-1}) \quad . \tag{3.46}$$

There are a number of features to observe in the nature of the algorithms (3.46):

(i) Let us put

$$K^*(t_k) = P^*(t_{k-1})H^T[I + HP^*(t_{k-1})H^T]^{-1} \quad , \qquad (3.47)$$

then we have in the first of equations (3.46),

$$\underline{\hat{x}}(t_k) = \underline{\hat{x}}(t_{k-1}) + K^*(t_k)\{\underline{y}(t_k) - H\underline{\hat{x}}(t_{k-1})\} \qquad (3.48)$$

for comparison with (3.40a). Since by inspection of the measurement equation, (3.33), $H\underline{\hat{x}}(t_{k-1})$ in (3.48) is equivalent, as it were, to a prediction $\hat{y}(t_k)$ of the actual observations $y(t_k)$, it is possible to see explicitly how the correction applied to the old estimate $\underline{\hat{x}}(t_{k-1})$ is a function of the weighting (gain) matrix $K^*(t_k)$ and predicted observation errors.

(ii) Alternatively, by rearrangement of (3.48) we have

$$\underline{\hat{x}}(t_k) = [I - K^*(t_k)H]\underline{\hat{x}}(t_{k-1}) + [K^*(t_k)]\,\underline{y}(t_k) \qquad (3.49)$$

for comparison with (3.40b), where $\underline{\hat{x}}(t_{k-1})$ has been substituted as the best a priori estimate $\underline{\hat{x}}(t_k^-)$ of the value of $\underline{x}$ at time t_k. This accords with our current model of the system as one of steady-state behavior, see also section 2.3.

(iii) Finally, a point to which we shall return later, notice that the algorithms of (3.46) require the specification of initial conditions for the estimates $\underline{\hat{x}}(t_0)$ and the matrix $P^*(t_0)$ at the starting time $t_k = t_0$.

3.5 Incorporation of Some Statistical Information

Although occasional reference has been made to some desirable statistical properties required of the various random processes in our system characterization, we have not yet indicated how such information might be incorporated in the estimation routine. The algorithms of (3.46), for instance, have been derived by deterministic

arguments alone. This section, therefore, will modify equation (3.46) to include some statistical assumptions about the measurement errors $\underline{\eta}(t_k)$ which appear in equation (3.33) of the system model. A comparison of the algorithms (3.46) with the desired objectives of the LKF, that is equations (3.38) and (3.39), suggests that we should seek a statistical equivalent of the matrix P* for substitution into (3.46). The intention is that the interpretation of estimation error variance-covariance can be attached to such a matrix.

First, however, it is necessary to demonstrate the conditions under which the estimates of $\underline{\hat{x}}(t_k)$ from (3.46) are <u>unbiased</u>. These conditions will turn out to be equivalent to those quoted earlier in equations (3.12), (3.13), and (3.14) of section 3.1. From (3.41) we have,

$$\underline{\hat{x}}(t_k) = [\sum_{j=1}^{k} H^T H]^{-1} [\sum_{j=1}^{k} H^T \underline{y}(t_j)] \tag{3.50}$$

which, providing H is a matrix of constant valued elements which are not correlated with $\underline{y}(t_j)$, gives (compare with (3.26)),

$$\underline{\hat{x}}(t_k) = [kH^T H]^{-1} [H^T \sum_{j=1}^{k} \underline{y}(t_j)] \tag{3.51}$$

$$= (1/k) H^{-1} (H^T)^{-1} H^T \sum_{j=1}^{k} \{H\underline{x}(t_j) + \underline{\eta}(t_j)\} \tag{3.52}$$

where we have substituted $\underline{y}(t_j) = H\underline{x}(t_j) + \underline{\eta}(t_j)$ from (3.33). Rearranging (3.52),

$$\underline{\hat{x}}(t_k) = (1/k) H^{-1} H [\sum_{j=1}^{k} \underline{x}(t_j)] + (1/k) H^{-1} [\sum_{j=1}^{k} \underline{\eta}(t_j)] \tag{3.53}$$

so that taking expectations,

$$\mathcal{E}\{\underline{\hat{x}}(t_k)\} = (1/k) \sum_{j=1}^{k} \mathcal{E}\{\underline{x}(t_j)\} + (1/k) H^{-1} [\sum_{j=1}^{k} \mathcal{E}\{\underline{\eta}(t_j)\}] \ . \tag{3.54}$$

Hence, under the assumptions that since we are dealing with a system which does not exhibit dynamic behavior, i.e.

$$\underline{x}(t_1) = \underline{x}(t_2) = \ldots = \underline{x}(t_k) = \underline{x}$$

such that

$$\mathcal{E}\{\underline{x}(t_j)\} = \mathcal{E}\{\underline{x}\} = \underline{x} \quad ,$$

and that $\underline{\eta}(t_j)$ is a zero-mean vector random process, i.e.

$$\mathcal{E}\{\underline{\eta}(t_j)\} = \underline{0} \quad , \tag{3.55}$$

then (3.54) becomes,

$$\mathcal{E}\{\hat{\underline{x}}(t_k)\} = \underline{x} \quad . \tag{3.56}$$

Equation (3.56) implies that the estimates $\hat{\underline{x}}(t_k)$ are unbiased for the given conditions.

For ease of illustration perhaps we might briefly remove some sophistication from (3.54) above. If we had not applied the expectation operator to (3.53), then we should have, with the assumption concerning the time-invariance of $\underline{x}$,

$$\hat{\underline{x}}(t_k) = (1/k) \sum_{j=1}^{k} \underline{x} + H^{-1} [(1/k) \sum_{j=1}^{k} \underline{\eta}(t_j)] \quad . \tag{3.57}$$

Thus

$$\hat{\underline{x}}(t_k) = \underline{x} + H^{-1} [(1/k) \sum_{j=1}^{k} \underline{\eta}(t_j)] \quad . \tag{3.58}$$

Suppose now that we had available an infinite number of samples, $k \to \infty$, and that the population of random variables from which $\underline{\eta}(t_j)$ are drawn has a mean value of zero, equation (3.58) then states that $\hat{\underline{x}}(t_k)$ converges to $\underline{x}$ in the limit as k tends to infinity. Equation (3.54) with the assumption of (3.55) also states this but in a rather different fashion. In practice, however, one is very unlikely to have even a large number of measurements available in the kind of environmental engineering systems

under study here. The implication of this is that with a finite and small number of k samples it is improbable that the mean values of those sample realizations of $\underline{\eta}(t_j)$ are precisely zero; $\hat{\underline{x}}(t_k)$ will be accordingly inaccurate as an estimate of $\underline{x}$. The point of imposing the more rigorous statistical assumptions is therefore to acquire the comfort of knowing that the algorithm should "behave nicely" under certain limiting conditions.

Continuing the analysis, we can set up from (3.53) an expression for the variance-covariance matrix of estimation errors. We have

$$\hat{\underline{x}}(t_k) = (1/k)\sum_{j=1}^{k}\underline{x}(t_j) + (1/k)H^{-1}\sum_{j=1}^{k}\underline{\eta}(t_j) \qquad (3.59)$$

which providing $\underline{x}(t_1) = \underline{x}(t_j) = \underline{x}(t_k)$ for all j, gives

$$\hat{\underline{x}}(t_k) = \underline{x}(t_k) + (1/k)H^{-1}\sum_{j=1}^{k}\underline{\eta}(t_j) \quad . \qquad (3.60)$$

We wish now to compute the covariance matrix of the estimation errors $\tilde{\underline{x}}(t_k)$, namely the matrix P of (3.39),

$$P(t_k) = \text{cov}\{\tilde{\underline{x}}(t_k)\} = \mathcal{E}\{\tilde{\underline{x}}(t_k)\tilde{\underline{x}}^T(t_k)\}$$

$$= \mathcal{E}\{(\hat{\underline{x}}(t_k) - \underline{x}(t_k))(\hat{\underline{x}}(t_k) - \underline{x}(t_k))^T\} \qquad (3.61)$$

in which the errors are defined by,

$$\tilde{\underline{x}}(t_k) = \hat{\underline{x}}(t_k) - \underline{x}(t_k) \quad .$$

From (3.60) we can substitute for these errors giving

$$\text{cov}\{\underline{\tilde{x}}(t_k)\} = \mathcal{E}\{[(1/k)H^{-1}\sum_{j=1}^{k}\underline{\eta}(t_j)][(1/k)H^{-1}\sum_{j=1}^{k}\underline{\eta}(t_j)]^T\}$$

$$= \mathcal{E}\{(1/k^2)H^{-1}[\sum_{j=1}^{k}\underline{\eta}(t_j)][\sum_{j=1}^{k}\underline{\eta}^T(t_j)](H^{-1})^T\}$$

$$= \mathcal{E}\{(1/k^2)H^{-1}[\sum_{i=1}^{k}\sum_{j=1}^{k}\underline{\eta}(t_i)\underline{\eta}^T(t_j)](H^T)^{-1}\} \quad . \tag{3.62}$$

We now make a second assumption about the statistics of $\underline{\eta}(t_k)$ by stating that the vector sequence of $\underline{\eta}(t_k)$ is <u>not correlated with itself in time</u>, i.e.,

$$\mathcal{E}\{\underline{\eta}(t_i)\underline{\eta}^T(t_j)\} = R\,\delta_{ij} \quad . \tag{3.63}$$

Thus in (3.62), again making the assumption that $\underline{\eta}(t_j)$ is uncorrelated with the elements of H so that the expectation operator can be taken inside the summation procedure,

$$P(t_k) = (1/k^2)H^{-1}[\sum_{i=1}^{k}\sum_{j=1}^{k}\mathcal{E}\{\underline{\eta}(t_i)\underline{\eta}^T(t_j)\}](H^T)^{-1}$$

$$= (1/k^2)H^{-1}[\sum_{i=1}^{k}\sum_{j=1}^{k}R\delta_{ij}](H^T)^{-1} \quad .$$

Hence, finally

$$P(t_k) = (1/k)H^{-1}R(H^T)^{-1} \quad . \tag{3.64}$$

Equation (3.64) gives a concise expression for the estimation error variance associated with $\underline{\hat{x}}(t_k)$ as an estimate of $\underline{x}$. It is worth noting an important characteristic of this relationship by reverting once more to the scalar example. Assume we have a measurement equation from (3.33) as,

$$y(t_k) = hx(t_k) + \eta(t_k) \tag{3.65}$$

which would give for (3.64),

$$p(t_k) = (1/k)(r/h^2) \tag{3.66}$$

where r is the variance of the random variable $\eta(t_k)$, compare with equation (3.13). It is now possible to see from (3.66) that as we increase the number of measurements, i.e. k increases, the estimation error $p(t_k)$ decreases and thus our estimates $\underline{\hat{x}}(t_k)$ become progressively more accurate -- recall the discussion, therefore, of section 2.2.1.

The clue to establishing a relationship between $P(t_k)$ of (3.64) and the matrix $P^*(t_k)$ in the algorithms (3.46) is given by the definition of $P^*(t_k)$ in (3.43), i.e.

$$P^*(t_k) \triangleq [\sum_{j=1}^{k} H^T H]^{-1} = (1/k)H^{-1}(H^T)^{-1} \quad . \tag{3.67}$$

So if we post-multiply (3.64) first by H^T and then by R^{-1}, we obtain

$$P(t_k)H^T R^{-1} = (1/k)H^{-1}$$

and post-multiplying this equation by $(H^T)^{-1}$ yields

$$P(t_k)H^T R^{-1}(H^T)^{-1} = (1/k)H^{-1}(H^T)^{-1} = [kH^T H]^{-1}$$
$$= [\sum_{j=1}^{k} H^T H]^{-1} \quad .$$

Therefore,

$$P(t_k)H^T R^{-1}(H^T)^{-1} = P^*(t_k) \quad . \tag{3.68}$$

The relationship (3.68) permits us to substitute for $P^*(t_k)$ and $P^*(t_{k-1})$ in (3.46), which after some manipulation (see Appendix 3) gives the following <u>recursive least squares algorithms for the state estimate and error covariance matrix updates</u> of a system at steady state,

$$\underline{\hat{x}}(t_k) = \underline{\hat{x}}(t_{k-1}) + P(t_{k-1})H^T[HP(t_{k-1})H^T + R]^{-1}\{y(t_k) - H\underline{\hat{x}}(t_{k-1})\}$$
$$P(t_k) = P(t_{k-1}) - P(t_{k-1})H^T[HP(t_{k-1})H^T + R]^{-1}HP(t_{k-1}) \tag{3.69}$$

Reference to Figure 9 indicates that one step remains in the derivation of the LKF: that of introducing a process dynamical description and thereby relaxing the constraint of assuming time-invariance of the state of the process. Taking stock of the developments thus far we can summarize as follows.

3.5.1 Summary

For the measurements (observations) relationship of equation (3.33),

$$\underline{y}(t_k) = H\underline{x}(t_k) + \underline{n}(t_k)$$

where the state variables $\underline{x}(t_k)$ do not change with time, i.e. in terms of the discrete-time model description of (3.29),

$$\underline{x}(t_k) = \underline{x}(t_{k-1}) \tag{3.70}$$

we have that, on receipt of the measurements $\underline{y}(t_k)$ we can correct the previous (a priori) estimates $\underline{\hat{x}}(t_{k-1})$ of $\underline{x}(t_k)$ and the associated matrix $P(t_{k-1})$ of (a priori) estimation error covariances according to the algorithms of (3.69). If we draw together the earlier discussion of sections 2.3.1 and 3.4, and in particular if the notation introduced in section 2.3.1 is recalled, a useful modification of (3.69) can be suggested. Henceforth in (3.69) let us denote $\underline{\hat{x}}(t_{k-1})$ and $P(t_{k-1})$ by $\underline{\hat{x}}(t_k|t_{k-1})$ and $P(t_k|t_{k-1})$ respectively so that this signifies that $\underline{\hat{x}}(t_k|t_{k-1})$ and $P(t_k|t_{k-1})$ are the state estimates and error covariance matrix predicted at time t_k on the basis of all measured information up to and including that available at the last sampling instant t_{k-1}. Likewise $\underline{\hat{x}}(t_k)$ and $P(t_k)$ in (3.69) may be denoted by $\underline{\hat{x}}(t_k|t_k)$ and $P(t_k|t_k)$ respectively which thus represent the updated (a posteriori) estimates and covariance matrix at time t_k given $\underline{y}(t_k)$. A schematic interpretation of this procedure and the associated notation is provided by Figure 11.

The algorithms (3.69) actually characterize the LKF for the rather special system behavior of (3.70) with the measurements

of (3.33); this will become evident in the next section. The problem now, of course, is one of determining how to extrapolate, or predict, the evolution of the state estimates and covariance matrix over the interval $t_{k-1} \rightarrow t_k$ when (3.70) is no longer valid because the system displays unsteady-state behavior.

3.6 The Discrete-time Linear Kalman Filter

The "discrete-time" qualification in the title of this section derives from the fact that the algorithms are associated with a discrete-time representation of the system state variable dynamics, i.e. from (3.29),

$$\underline{x}(t_k) = \Phi\underline{x}(t_{k-1}) + \Gamma\underline{u}(t_{k-1}) + \Lambda\underline{\xi}(t_{k-1}) \qquad (3.71a)$$

and with a discrete-time observations equation

$$\underline{y}(t_k) = H\underline{x}(t_k) + \underline{\eta}(t_k) \quad . \qquad (3.71b)$$

Given this model of the system dynamics we must consider how a forward prediction, or estimate $\hat{\underline{x}}(t_k|t_{k-1})$, can be made on the basis of (3.71). Suppose we have available the most recent updated estimate, $\hat{\underline{x}}(t_{k-1}|t_{k-1})$, we have measured $\underline{u}(t_{k-1})$, and under the assumption that

$$\mathcal{E}\{\underline{\xi}(t_k)\} = \underline{0} \qquad (3.72)$$

then a "best" estimate $\hat{\underline{x}}(t_k|t_{k-1})$ is provided by

$$\hat{\underline{x}}(t_k|t_{k-1}) = \Phi\hat{\underline{x}}(t_{k-1}|t_{k-1}) + \Gamma\underline{u}(t_{k-1}) \quad . \qquad (3.73)$$

This is simply (3.71) with the state estimates substituted for $\underline{x}(t_{k-1})$ and with the stochastic sequence vector $\underline{\xi}(t_{k-1})$ set equal to zero; since we cannot know $\underline{\xi}(t_{k-1})$, then for prediction it is reasonable to assign the most probable, or mean value to this variable. We are clearly interested to know whether $\hat{\underline{x}}(t_k|t_{k-1})$ from (3.73) will be an unbiased estimate, i.e. $\mathcal{E}\{\tilde{\underline{x}}(t_k|t_{k-1})\} = \underline{0}$.

Subtracting (3.71a) from (3.73) gives, where $\underline{\tilde{x}}(t_k|t_{k-1}) = \underline{\hat{x}}(t_k|t_{k-1}) - \underline{x}(t_k)$ and $\underline{\tilde{x}}(t_k|t_k) = \underline{\hat{x}}(t_k|t_k) - \underline{x}(t_k)$,

$$\underline{\tilde{x}}(t_k|t_{k-1}) = \Phi\underline{\tilde{x}}(t_{k-1}|t_{k-1}) - \Lambda\underline{\xi}(t_{k-1}) \quad . \tag{3.74}$$

Hence,

$$\mathcal{E}\{\underline{\tilde{x}}(t_k|t_{k-1})\} = \Phi\mathcal{E}\{\underline{\tilde{x}}(t_{k-1}|t_{k-1})\} - \Lambda\mathcal{E}\{\underline{\xi}(t_{k-1})\} \tag{3.75}$$

which by assumption (3.72), that $\underline{\xi}$ is a zero-mean stochastic process, implies that $\underline{\hat{x}}(t_k|t_{k-1})$ will be unbiased provided $\underline{\hat{x}}(t_{k-1}|t_{k-1})$ is unbiased. This is almost a circular argument and will eventually require certain assumptions to be made about the initial conditions of the filter.

Given (3.74) we can also set up a relationship for $P(t_k|t_{k-1})$, the estimation error covariance matrix extrapolated across the interval $t_{k-1} \rightarrow t_k$,

$$\begin{aligned} P(t_k|t_{k-1}) = \operatorname{cov}\{\underline{\tilde{x}}(t_k|t_{k-1})\} &= \mathcal{E}\{(\Phi\underline{\tilde{x}}(t_{k-1}|t_{k-1}) - \Lambda\underline{\xi}(t_{k-1})) \\ &\qquad (\Phi\underline{\tilde{x}}(t_{k-1}|t_{k-1}) - \Lambda\underline{\xi}(t_{k-1}))^T\} \\ &= \Phi\mathcal{E}\{\underline{\tilde{x}}(t_{k-1}|t_{k-1})\underline{\tilde{x}}^T(t_{k-1}|t_{k-1})\}\Phi^T - \Lambda\mathcal{E}\{\underline{\xi}(t_{k-1})\underline{\tilde{x}}^T(t_{k-1}|t_k)\}\Phi^T \\ &\quad - \Phi\mathcal{E}\{\underline{\tilde{x}}(t_{k-1}|t_{k-1})\underline{\xi}^T(t_{k-1})\}\Lambda^T + \Lambda\mathcal{E}\{\underline{\xi}(t_{k-1})\underline{\xi}(t_{k-1})\}\Lambda^T \end{aligned} \quad . \tag{3.76}$$

Hence, under the following assumptions,

$$\mathcal{E}\{\underline{\xi}(t_{k-1})\underline{\xi}(t_{j-1})\} = Q\delta_{kj} \tag{3.77a}$$

and

$$\mathcal{E}\{\underline{\xi}(t_{k-1})\underline{\tilde{x}}^T(t_{k-1}|t_{k-1})\} = \mathcal{E}\{\underline{\tilde{x}}(t_{k-1}|t_{k-1})\underline{\xi}^T(t_{k-1})\} = \underline{0}$$

for all k, (3.77b)

which imply, inter alia, that the system noise $\underline{\xi}$ is uncorrelated with the estimation errors $\underline{\tilde{x}}$, and with

$$P(t_{k-1}|t_{k-1}) = \mathcal{E}\{\underline{\tilde{x}}(t_{k-1}|t_{k-1})\underline{\tilde{x}}^T(t_{k-1}|t_{k-1})\}$$

that

$$P(t_k|t_{k-1}) = \Phi P(t_{k-1}|t_{k-1})\Phi^T + \Lambda Q \Lambda^T \quad . \tag{3.78}$$

The reader may now be somewhat surprised to learn that equations (3.73) and (3.78) in fact complete the derivation of the LKF. We can at last summarize thus:

- o For the system characterization of (3.71) the <u>linear discrete-time Kalman filter algorithms</u> are given by,

(i) <u>Prediction</u>: between t_{k-1} and t_k from (3.73) and (3.78):

$$\underline{\hat{x}}(t_k|t_{k-1}) = \Phi \underline{\hat{x}}(t_{k-1}|t_{k-1}) + \Gamma \underline{u}(t_{k-1}) \tag{3.79a}$$

$$P(t_k|t_{k-1}) = \Phi P(t_{k-1}|t_{k-1})\Phi^T + \Lambda Q \Lambda^T \tag{3.79b}$$

(ii) <u>Correction</u>: across t_k on receipt of $\underline{y}(t_k)$, from (3.69):

$$\underline{\hat{x}}(t_k|t_k) = \underline{\hat{x}}(t_k|t_{k-1}) + K(t_k)\{\underline{y}(t_k) - H\underline{\hat{x}}(t_k|t_{k-1})\} \tag{3.79c}$$

$$P(t_k|t_k) = [I - K(t_k)H]P(t_k|t_{k-1}) \tag{3.79d}$$

where, the Kalman gain matrix $K(t_k)$ is given by

$$K(t_k) = P(t_k|t_{k-1})H^T[HP(t_k|t_{k-1})H^T + R]^{-1} \tag{3.79e}$$

In (3.79c), (3.79d) and (3.79e) observe that we have adopted the notation $\underline{\hat{x}}(t_k|t_{k-1})$ and $P(t_k|t_{k-1})$ etc., as suggested for the algorithms (3.69) of the previous section.

3.6.1 Some Initial Comments on the Filter

Later in section 3.8 some important qualitative characteristics of the filter will be discussed in detail; here we merely note a number of technical details concerning the algorithms (3.79).

(i) Gathering together the statistical assumptions of (3.55), (3.63), (3.72), and (3.77) we require,

$$\mathcal{E}\{\underline{\xi}(t_k)\} = \mathcal{E}\{\underline{\eta}(t_k)\} = \underline{0}$$

$$\mathcal{E}\{\underline{\xi}(t_k)\underline{\xi}^T(t_j)\} = Q\ \delta_{kj}$$

$$\mathcal{E}\{\underline{\eta}(t_k)\underline{\eta}^T(t_j)\} = R\ \delta_{kj}$$

$$\mathcal{E}\{\underline{\xi}(t_k)\underline{\eta}^T(t_j)\} = 0$$

(ii) If $\underline{\xi}(t_k)$ and $\underline{\eta}(t_k)$ are Gaussian normal distributions, then a least squares, a maximum likelihood, or a Bayesian minimum variance approach to the filter derivation all yield identical results. (Indeed, among several other derivations, Gelb (1974) takes the desired filter structure of (3.40b) and proceeds to obtain those forms of the matrices $M_1(t_k)$ and $M_2(t_k)$ which provide a minimum value for the variance-covariance matrix $P(t_k|t_k)$.)

(iii) Figure 12 shows an interpretation of the updating and prediction schedule of the filtering algorithms; when compared with Figure 11, Figure 12 indicates how the algorithms now permit the prediction of the time-varying state vector.

(iv) An implementation of the filter is represented by the block diagram form of Figure 13. If the discussion of section 2.1 is recalled together with Figure 4, Figure 13 re-emphasizes the crucial role of instrumentation and the measurement process in facilitating, or degrading, the performance of the filter as a means of restructuring information about the behavior of reality. Moreover, since the filter must inevitably be constructed round an imperfect model of reality its matrices Φ and H are only approximations to the true matrices Φ' and H'.

(v) The errors between the response observations and their predicted values, in (3.79c), deserve special mention, for they will subsequently become important in assessing the results of applying the filtering algorithms. They are denoted by,

$$\underline{\varepsilon}(t_k|t_{k-1}) = \underline{y}(t_k) - H\hat{\underline{x}}(t_k|t_{k-1}) \tag{3.80}$$

and are frequently referred to as the innovations process residual errors, or as the one-step ahead prediction errors.

(vi) We may also note that subtracting $\underline{x}(t_k)$ from both sides of (3.79c) yields,

$$\hat{\underline{x}}(t_k|t_k) - \underline{x}(t_k) = \hat{\underline{x}}(t_k|t_{k-1}) - \underline{x}(t_k) + K(t_k)\{\underline{y}(t_k) - H\hat{\underline{x}}(t_k|t_{k-1})\}$$

which, after substituting for $\underline{y}(t_k)$ from (3.71), gives

$$\begin{aligned}\tilde{\underline{x}}(t_k|t_k) &= \check{\underline{x}}(t_k|t_{k-1}) + K(t_k)H\underline{x}(t_k) + K(t_k)\underline{\eta}(t_k) - K(t_k)H\hat{\underline{x}}(t_k|t_{k-1}) \\ &= \check{\underline{x}}(t_k|t_{k-1}) - K(t_k)H\tilde{\underline{x}}(t_k|t_{k-1}) + K(t_k)\underline{\eta}(t_k) \\ &= [I - K(t_k)H]\tilde{\underline{x}}(t_k|t_{k-1}) + K(t_k)\,\underline{\eta}(t_k) \quad .\end{aligned} \tag{3.81}$$

Hence,

$$\mathcal{E}\{\tilde{\underline{x}}(t_k|t_k)\} = [I - K(t_k)H]\mathcal{E}\{\tilde{\underline{x}}(t_k|t_{k-1})\} + K(t_k)\mathcal{E}\{\underline{\eta}(t_k)\} \quad . \tag{3.82}$$

Equation (3.82) states, therefore, that $\hat{\underline{x}}(t_k|t_k)$ will be unbiased providing $\hat{\underline{x}}(t_k|t_{k-1})$ is unbiased, which in turn with (3.75) implies that the a priori (initial) estimates should be chosen as unbiased estimates, i.e.

$$\hat{\underline{x}}(t_0|t_0) = \underline{x}(t_0)$$

with (3.83)

$$P(t_0|t_0) = \text{cov}\{\tilde{\underline{x}}(t_0|t_0)\} \quad .$$

These represent the desired initial conditions for the filter.

(vii) Using (3.82) an alternative expression for $P(t_k|t_k)$ may be derived.

$$P(t_k|t_k) = \mathcal{E}\{\tilde{\underline{x}}(t_k|t_k)\tilde{\underline{x}}^T(t_k|t_k)\}$$

$$= \mathcal{E}\{[I - K(t_k)H]\tilde{\underline{x}}(t_k|t_{k-1})\tilde{\underline{x}}^T(t_k|t_{k-1})[I - K(t_k)H]^T$$

$$+ K(t_k)\underline{\eta}(t_k)\underline{\eta}^T(t_k)K^T(t_k) + [I - K(t_k)H]\tilde{\underline{x}}(t_k|t_{k-1})\underline{\eta}^T(t_k)K^T(t_k)$$

$$+ K(t_k)\underline{\eta}(t_k)\tilde{\underline{x}}^T(t_k|t_{k-1})[I - K(t_k)H]^T\} \qquad (3.84)$$

which with the additional assumption that*

$$\mathcal{E}\{\tilde{\underline{x}}(t_k|t_{k-1})\underline{\eta}^T(t_k)\} = \mathcal{E}\{\underline{\eta}(t_k)\tilde{\underline{x}}^T(t_k|t_{k-1})\} = \underline{0}$$

then,

$$P(t_k|t_k) = [I - K(t_k)H]P(t_k|t_{k-1})[I - K(t_k)H]^T$$

$$+ K(t_k)RK^T(t_k) \quad . \qquad (3.85)$$

(viii) Lastly, notice that if $\Phi = I$, and $\underline{u}(t_k) = \underline{\xi}(t_k) = \underline{0}$ in (3.71), i.e. the state variables are time-invariant, then (3.79a) and (3.79b) give $\hat{\underline{x}}(t_k|t_{k-1}) = \hat{\underline{x}}(t_{k-1}|t_{k-1})$ and $P(t_k|t_{k-1}) = P(t_{k-1}|t_{k-1})$ so that upon substitution of these results in (3.79c),

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* In fact, it follows from the measurement errors being uncorrelated with time that $\tilde{\underline{x}}(t_k|t_{k-1})$, being conditioned upon measurements up to and including those at time t_{k-1}, will be uncorrelated with $\eta(t_k)$.

(3.79d), (3.79e), the filter reduces to the algorithms of (3.69).

3.7 The Continuous-Discrete Linear Kalman Filter

If the discrete-time model of the system state dynamics in (3.71a) is replaced by the continuous-time, ordinary differential equation representation of (3.28) the qualification "continuous-discrete" for the LKF should become self-evident. Since we shall retain the discrete-time measurement process, in (3.33) or (3.71b), and in view of the manner in which we have derived the LKF, it should also be apparent that for the continuous-discrete version of the filter we are seeking replacements for the forward extrapolation algorithms of (3.79a) and (3.79b). In fact the objective of this section is to modify only algorithm (3.79a) and we shall not in any case proceed to the completely continuous version of the LKF. The reasons for thus restricting the argument are:

(i) that this form of the continuous-discrete filter provides the best conceptual link with the form of the extended Kalman filter to be derived in section 5;

(ii) that in practice we shall very rarely require the analysis of continuous-time observations; observations are nearly always sampled, as has been mentioned before;

(iii) that if we do require knowledge of the system behavior between t_{k-1} and t_k, then attention will almost certainly be focused upon the evolution of $\underline{\hat{x}}(t|t_{k-1})$ and not on $P(t|t_{k-1})$; it is also rather easier to derive an expression for the evolution of $\underline{\hat{x}}(t|t_{k-1})$ than it is to derive an equivalent expression for $P(t|t_{k-1})$.

Recall that from (3.28)

$$\dot{\underline{x}}(t) = F\underline{x}(t) + G\underline{u}(t) + L\underline{\xi}(t) \quad ,$$

so that for $t_{k-1} \leq t \leq t_k$, if we have available the estimate $\underline{\hat{x}}(t_{k-1}|t_{k-1})$, we have knowledge of $\underline{u}(t)$, and with $\mathcal{E}\{\underline{\xi}(t)\} = \underline{0}$, then a "best" extrapolation of $\underline{\hat{x}}(t|t_{k-1})$ is provided by the

solution of,

$$\dot{\underline{\hat{x}}}(t|t_{k-1}) = F\underline{\hat{x}}(t|t_{k-1}) + G\underline{u}(t) \qquad (3.86)$$

for $t_{k-1} \leq t \leq t_k$ and

for $\underline{\hat{x}}(t|t_{k-1}) = \hat{x}(t_{k-1}|t_{k-1})$ at $t = t_{k-1}$.

Therefore, for the continuous-discrete linear Kalman filter we have the algorithms (3.79) with (3.86) replacing (3.79a). Figure 14 shows this version of the filter in block diagram form.

3.8 Interpretations of the Filter Covariance and Gain Matrices

At the very beginning of this derivation it was observed that there is no really easy route to an appreciation of the Kalman filtering algorithms. Prior to that observation the filter was said in section 2.3.1 to behave so as to eliminate, or filter out, the random noise effects of the $\underline{\xi}$ and $\underline{\eta}$ variables. The burden of compensating for the lengthy derivation, and of fulfilling the preview of the filter, rests with this section. Not surprisingly it is to a scalar equivalent of the algorithms to which we return for purposes of illustration.

In algorithms (3.79b), (3.79d), and (3.79e) we have,

$$\text{(3.79b):}\quad p(t_k|t_{k-1}) = \phi p(t_{k-1}|t_{k-1})\phi + \lambda q \lambda = \phi^2 p(t_{k-1}|t_{k-1}) + \lambda^2 q \qquad (3.87)$$

$$\text{(3.79d):}\quad p(t_k|t_k) = [1 - k(t_k)h]p(t_k|t_{k-1}) \qquad (3.88)$$

$$\text{(3.79e):}\quad k(t_k) = p(t_k|t_{k-1})h[h^2 p(t_k|t_{k-1}) + r]^{-1} \qquad (3.89)$$

Upon substituting for $p(t_k|t_{k-1})$ from (3.87) in (3.88) and (3.89), and assuming that $h = 1$, i.e. $y(t_k) = x(t_k) + \eta(t_k)$, gives after rearrangement,

$$p(t_k|t_k) = [1 - k(t_k)]\phi^2 p(t_{k-1}|t_{k-1}) + [1 - k(t_k)]\lambda^2 q \qquad (3.90)$$

$$k(t_k) = \frac{[\phi^2 p(t_{k-1}|t_{k-1}) + \lambda^2 q]}{[\phi^2 p(t_{k-1}|t_{k-1}) + \lambda^2 q + r]} \qquad (3.91)$$

Given the relationships (3.90) and (3.91) for the estimation error variance and the gain factor, the key to an appreciation of the operating characteristics of the filter is to ascribe to the filter the properties of intelligence. In other words, how "well" or how "badly" does the filter "believe" it is replicating the behavior of reality.

Table 1 summarizes various filter operating conditions which are discussed in the following; it is important, however, to recognize that Table 1 expresses relative and qualitative statements about the expected behavior of the filtering algorithms. First, we may note that k, the filter gain, is always less than

Table 1: A Summary of Filter Operating Characteristics in Relation to the Gain and Covariance Matrices (or Scalar Equivalents).

System noise q	Measurement noise r	Gain k	Estimation error variance p	Estimate corrections kε
	large	small (→0.0)		small
	small	large (→1.0)		large
		large	large	
		small	changes slowly	
		large	changes rapidly	
large			large	

unity. Now visualize what this ration means in physical terms, since,

(i) the numerator of k is a function of

Uncertainty propagated from the initial uncertainty in the state of the system (p) + Uncertainty contributed by the system noise (q)

(ii) the denominator of k is a function of

(p) + (q) + Uncertainty in the system output response observations (r)

The implication is that if r is relatively large (in comparison with p and q), i.e. relatively inaccurate measurements, k is relatively small; and if r is small, $k \to 1.0$. The effect of p being relatively large, i.e. inaccurate estimates, is to make k large, as is the implied effect of a large q, i.e. large unknown input disturbances.*

From (3.79c) and (3.80) we may recall that the corrections applied to the forward a priori estimates $\underline{\hat{x}}(t_k|t_{k-1})$ are a product of the gain k and the innovations process residual errors $\varepsilon(t_k|t_{k-1})$, i.e. the error between actual and predicted output response. Thus if the measurement errors are known to be small (r is small), the effect is to make k large -- see Table 1 -- such that the filter "takes a lot of notice" of the errors between predictions and observations, i.e. the filter weights the errors quite heavily. Since the observations are accurate, any prediction errors must presumably result from a poor prediction which therefore requires considerable correction. Likewise, when the filter "does not know the process well," in other words inaccurate predictions and a

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* q may also be interpreted as a measure of the accuracy (uncertainty) of the process model as an approximation to reality, see Beck (1978c).

large estimation error variance (p), errors between prediction and observation are weighted strongly. On the other hand, when r is large, or p is small -- the case of good predictions and/or poor measurements -- the filter will tend to ignore the prediction errors as k becomes small. In other words, the filter will attempt to "filter out" the spurious fluctuations in ε since it assumes that the measurement noise is the source of these errors.

Table 1 also indicates that for the gain k being small, p changes slowly. This corresponds to the situation in which the filter "believes" it has adequate knowledge of process behavior, p will probably be small, and the magnitude of k will tend to settle at some constant value. When k is large and p is changing rapidly, the filter is much less certain of its ability to predict the variations in the output from the process under study. The fact that p is changing rapidly, indeed decreasing rapidly, suggests however that the filter is quickly learning the process behavior and placing more and more confidence in its own performance.

The reader should perhaps satisfy himself that the statements of Table 1 are logically consistent. Hopefully it will now be evident that the filter <u>in theory</u> responds quite intelligently to the specified uncertainty in its operating environment.

4. PARAMETER ESTIMATION AND CONVENTIONAL TIME-SERIES ANALYSIS

Let us return to Figure 9. The lengthy development of the preceding section dealt with the central topic of state estimation in which an on-line estimate of the state of a system is required for process control purposes, see also section 2. In this section attention will be transferred back to the problem of parameter estimation, principally in connection with the subject of model development and time-series analysis, but also as it relates to possible applications in adaptive prediction and adaptive control contexts. Our starting point, however, will be the introduction of a rather useful form of black box model. The reasons for so doing are that this model is regularly encountered in the literature on time-series analysis and that with suitable transformations into this form of model, many problems of parameter estimation become amenable to recursive least squares and related techniques. The remainder of the section will then pick up the development of parameter estimation algorithms beginning with a recursive form of the least squares estimator of equation (3.11) in section (3.1), see Figure 9. More detailed discussion of these techniques and conventional time-series analysis can be found in, for example, Box and Jenkins (1970), Eykhoff (1974), Young (1974), and Söderström et al (1978).

4.1 A Useful Form of Model

Some of the groundwork for introducing the model has already been covered in section 3.3. We require the discrete-time characterisation of (3.29) and (3.33), namely,

$$\underline{x}(t_k) = \Phi\underline{x}(t_{k-1}) + \Gamma\underline{u}(t_{k-1}) + \Lambda\underline{\xi}(t_{k-1}) \quad , \tag{4.1a}$$

$$\underline{y}(t_k) = H\underline{x}(t_k) + \underline{\eta}(t_k) \quad . \tag{4.1b}$$

It has already been shown how this discrete-time representation of an internally descriptive model relates to the more familiar continuous-time representation of the dynamic behaviour of a system. The intention here is to demonstrate that, by means of a

simple example, one can proceed from the continuous-time internally descriptive model via the above discrete-time formulation to a typical input/output time-series analysis model. Perhaps the origin of much of the scepticism surrounding black box models lies here with the fact that most papers dealing with such statistical models assume a priori the form of the model. Any connection back to the continuous-time internally descriptive model, and hence to "reality", is thus lost and with it also may be lost the attention and comprehension of the previously unacquainted reader.

Our development will first oblige us to make the general form of equation (4.1) more specific through a number of assumptions. For a simple, physicochemical example we shall then derive a model from a component mass balance which resembles the specific reduced form of (4.1). Hence from this meeting point of particular example and non-specific model we shall finally generalise to our proposed useful form of model.

4.1.1 From the General to the Specific

In (4.1) let us assume that the observations matrix H is equal to the identity matrix I, i.e. all the state variables can be observed linearly,

$$\underline{x}(t_k) = \Phi\underline{x}(t_{k-1}) + \Gamma\underline{u}(t_{k-1}) + \Lambda\underline{\xi}(t_{k-1}) \quad , \tag{4.2a}$$

$$\underline{y}(t_k) = \underline{x}(t_k) + \underline{\eta}(t_k) \quad . \tag{4.2b}$$

The restrictions of this assumption in practice are not great since ultimately we seek a model which merely characterises observed input/output relationships without reference to any internal state variable description of the process being modelled. With this final objective in mind let us further combine equations (4.2a) and (4.2b) such that by substituting for $\underline{x}(t_k) = \underline{y}(t_k) - \underline{\eta}(t_k)$ from (4.2b) into (4.2a) we can eliminate $\underline{x}(t_k)$, i.e.

$$\underline{y}(t_k) - \underline{\eta}(t_k) = \Phi[\underline{y}(t_{k-1}) - \underline{\eta}(t_{k-1})] + \Gamma\underline{u}(t_{k-1}) + \Lambda\underline{\xi}(t_{k-1}) \tag{4.3}$$

which after rearrangement gives,

$$\underline{y}(t_k) = \Phi \underline{y}(t_{k-1}) + \Gamma \underline{u}(t_{k-1}) + [\Lambda \underline{\xi}(t_{k-1}) + \underline{\eta}(t_k) - \Phi \underline{\eta}(t_{k-1})] \quad . \quad (4.4)$$

[lumped noise term]

If we then assume that the system has only a single output, that is the scalar $y(t_k)$, and define

$$v(t_k) = \lambda \xi(t_{k-1}) + \eta(t_k) - \phi \eta(t_{k-1}) \quad (4.5)$$

to be a corresponding scalar equivalent of the lumped noise term in (4.4), we have

$$y(t_k) = \phi y(t_{k-1}) + \underline{\gamma} \underline{u}(t_{k-1}) + v(t_k) \quad . \quad (4.6)$$

Equation (4.6) might thus be called a particular form of Multiple Input/Single Output (MISO) model representation. It is multiple input because we have retained the input $\underline{u}$ as nominally an m-dimensional vector; the restriction to single output will be discussed in due course below.

4.1.2 From the Specific to the General

For our physicochemical example we choose once again the case of a dissolved substance decaying with first-order kinetics in a continuous flow, continuously stirred tank reactor (CSTR), see Figure 15. Here $u_1(t)$, $u_2(t)$, and $x(t)$ are respectively the first influent, second influent, and effluent concentrations of the substance; V, q_1, q_2, and q_o, where $q_o = (q_1 + q_2)$, are respectively the tank liquid volume, first influent flow-rate, second influent flow-rate, and effluent flow-rate, all of which are assumed to be time-invariant. As with the example of section 3.1, β_1 is the first-order kinetic decay rate constant. A component mass balance across the tank reactor yields

$$dx(t)/dt = (q_1/V)u_1(t) + (q_2/V)u_2(t) - \beta_1 x(t) - (q_o/V)x(t) \quad , (4.7)$$

with the assumption that the substance concentration in the tank is identical to the concentration of material in the effluent. After rearrangement and upon integration over the interval $t_{k-1} \rightarrow t_k$ (4.7) becomes

$$x(t_k) = \phi x(t_{k-1}) + \gamma_1 u_1(t_{k-1}) + \gamma_2 u_2(t_{k-1}) \quad , \qquad (4.8)$$

where

$$\phi = \exp[-(\beta_1 + q_o/V)(t_k - t_{k-1})] \quad , \qquad (4.9a)$$

$$\gamma_1 = \int_{t_{k-1}}^{t_k} \{\exp[-(\beta_1 + q_o/V)(t_k - \tau)](q_1/V)\} d\tau \quad , \qquad (4.9b)$$

$$\gamma_2 = \int_{t_{k-1}}^{t_k} \{\exp[-(\beta_1 + q_o/V)(t_k - \tau)](q_2/V)\} d\tau \quad . \qquad (4.9c)$$

To be precise, note that two further assumptions are implied by (4.9):

(i) that if the sampling interval $(t_k - t_{k-1})$ is assumed constant for this discrete-time representation, then ϕ, γ_1 and γ_2 are also constants;

(ii) that $u_1(t)$ and $u_2(t)$ for the integration interval $t_{k-1} \leq t \leq t_k$ are assumed to be held constant at their instantaneously sampled values $u_1(t_{k-1})$ and $u_2(t_{k-1})$; this enables $u_1(t)$ and $u_2(t)$ to be treated outside the integrals of (4.9)--compare with the more general forms of (3.32) in section 3.3.

At present (4.8) is a purely deterministic characterisation of process dynamic behaviour; clearly, in line with previous developments, it is necessary to complete the characterisation by introducing a stochastic component into the model. From the preceding section let us therefore hypothesise a lumped term $v(t_k)$--compare with (4.5)--which accounts for all aspects of uncertainty in the observed behaviour whether they arise from unmeasured input disturbances (ξ) or from random measurement errors (η) associated with measurement of the system output response.

In other words in (4.8)

$$y(t_k) = \phi y(t_{k-1}) + \gamma_1 u_1(t_{k-1}) + \gamma_2 u_2(t_{k-1}) + v(t_k) \quad , \quad (4.9)$$

where $y(t_k) = x(t_k) + \eta(t_k)$ is the error-corrupted effluent concentration measurement. Now making the vector definitions,

$$\underline{\gamma} = [\gamma_1, \gamma_2] \quad \text{and} \quad \underline{u}(t_{k-1}) = \begin{bmatrix} u_1(t_{k-1}) \\ u_2(t_{k-1}) \end{bmatrix} \quad ,$$

we obtain

$$y(t_k) = \phi y(t_{k-1}) + \underline{\gamma}\underline{u}(t_{k-1}) + v(t_k) \quad , \quad (4.10)$$

which permits a direct comparison with (4.6). Alternatively, had we defined

$$\underline{\alpha} = [\phi, \gamma_1, \gamma_2]^T \quad \text{and} \quad \underline{z}^T(t_k) = [y(t_{k-1}), u_1(t_{k-1}), u_2(t_{k-1})] \quad ,$$

$$\text{then } y(t_k) = \underline{\alpha}^T \underline{z}(t_k) + v(t_k) = \underline{z}^T(t_k)\underline{\alpha} + v(t_k) \quad , \quad (4.11)$$

which bears a readily evident correspondence with (3.8) of section (3.1).

This is the mid-point of our development. The clue to further development depends on the interpretation of (4.9) as a kind of regression equation relationship. Notice first, therefore, that (4.9) states essentially that the current value of the output, $y(t_k)$, is a function of the previous output observation $y(t_{k-1})$--hence the term autoregressive--and past observations $u_1(t_{k-1}), u_2(t_{k-1})$ of the two inputs, together with the current unknown realisation of the noise process $v(t_k)$. Equation (4.9) is based securely, of course, on a prior knowledge of the various physical and chemical phenomena which are thought to govern process dynamic behaviour, i.e. it can be said to be an internally descriptive model. Yet what if we suppose the converse? Imag-

ine that we have time-series data $y(t_k), u_1(t_k), u_2(t_k)$, with $k = 1,2,\ldots,N$, but that we make no assumptions about the internal nature of the system and simply view it as a black box. It may then occur that analysis of the time-series suggests that the current value of the output is more probably a function of the two immediately previous output observations $y(t_{k-1}), y(t_{k-2})$ together with, say, $u_1(t_{k-1}), u_2(t_{k-1})$ and $u_2(t_{k-2})$. We could in that event try to fit a relationship which "regresses" $y(t_k)$ upon $y(t_{k-1}), y(t_{k-2}), u_1(t_{k-1}), u_2(t_{k-1}), u_2(t_{k-2})$, namely

$$y(t_k) = \phi_1 y(t_{k-1}) + \phi_2 y(t_{k-2}) + \gamma_{11} u_1(t_{k-1}) + \gamma_{21} u_2(t_{k-1}) + \gamma_{22} u_2(t_{k-2}) + v(t_k), \tag{4.12}$$

and provided we define the parameter vector $\underline{\alpha}$ and data vector $\underline{z}$ appropriately, we can still arrive at the general form of relationship given by (4.11).

There may, or may not, be some plausible explanation of why, in this particular example of the continuously stirred tank reactor, a model of the form (4.12) gives a better fit to the data than (4.9). One might hypothesise, for instance, that there is either a dead zone or imperfect mixing in the tank. However, our particular example has served its purpose in the inductive argument of deriving the proposed useful form of model. The requirement now is for a further generalisation to be made. The natural progression from (4.9) and (4.12) is to reason that for an (m) multiple input/single output system description the current value of the output can in general be a function of the n previous multiple input and output observations,

$$y(t_k) = \sum_{i=1}^{n} \phi_i y(t_{k-i}) + \sum_{j=1}^{m} \sum_{i=1}^{n} \gamma_{ji} u(t_{k-i}) + v(t_k). \tag{4.13}$$

This is one form in which the MISO time-series model is often quoted. The determination of n is a problem in itself and is known as model order determination; it is equivalent to the problem of model structure identification as we have already noted

in section 3.1. Alternatively, if we introduce the backward shift operator q^{-1}, defined by

$$q^{-1}\{y(t_k)\} = y(t_{k-1}) \tag{4.14}$$

(4.13) transforms to

$$y(t_k) = \left[\sum_{i=1}^{n} \phi_i q^{-i}\right] y(t_k) + \sum_{j=1}^{m}\left[\sum_{i=1}^{n} \gamma_{ji} q^{-i}\right] u_j(t_k) + v(t_k) \quad . \tag{4.15}$$

Hence, after rearranging, and with the following definitions of polynomials in the backward shift operator

$$\begin{aligned} A(q^{-1}) &= 1 - \phi_1 q^{-1} - \phi_2 q^{-2} - \ldots - \phi_n q^{-n} \\ B_j(q^{-1}) &= \gamma_{j1} q^{-1} + \gamma_{j2} q^{-2} + \ldots + \gamma_{jn} q^{-n} \quad ; \quad j = 1,\ldots,m \end{aligned} \tag{4.16}$$

we obtain

$$A(q^{-1})y(t_k) = \sum_{j=1}^{m} B_j(q^{-1}) u_j(t_k) + v(t_k) \quad , \tag{4.17}$$

which also represents a popular starting point for papers on time-series analysis.

There are a number of remarks to be made in conclusion of this development. For instance:

(i) The interpretations placed on equation (4.9) should emphasise the sometimes thin line of distinction between the notions of black box and internally descriptive models; the analyst could have arrived at the given model either from theory or from empirical data analysis. It is these opposite, yet complementary, approaches which would define the character of the model.

(ii) The MISO description has been chosen because it reflects current usage in the large majority of time-series analysis applications. When dealing with the more complex

multiple input/multiple output (MIMO) case, Young and Whitehead (1977), for example, employ the model formulation of (4.4). In this event it is customary to make a prior definition of the zero and non-zero elements ϕ_{ij} of the matrix Φ before applying any parameter estimation routine. This definition of non-zero ϕ_{ij} elements specifies the causal relationships between process output responses; it is in practice dictated largely by theoretical considerations of the nature of the system under study.

(iii) Any relationship which can be expressed according to (4.11),(4.13) or (4.17) becomes amenable to the parameter estimation routines which will be presented in the next section. This "useful form of model" is indeed quite flexible for it requires only that the equations be linear-in-the-parameters (Eykhoff, 1974). To appreciate this point, suppose we wish to estimate the parameters of the nonlinear relationship,

$$y(t_k) = \phi_1 y(t_{k-1}) + \gamma_1 / u(t_{k-1}) + v(t_k) \quad .$$

The problem can still be treated with ease since by defining

$$\underline{\alpha} = [\phi_1, \gamma_1]^T \quad \text{and} \quad \underline{z}^T(t_k) = [y(t_{k-1}), \{1/u(t_{k-1})\}] \quad ,$$

we have $y(t_k) = \underline{z}^T(t_k)\underline{\alpha} + v(t_k)$,

and the model remains linear in the parameters.

(iv) Lastly, we may observe that the lumped noise sequence $v(t_k)$ has carefully been left undefined. Generally $v(t_k)$ will be a non-white (or correlated, coloured) random process; the manner in which one chooses to describe it is closely tied to the particular choice of parameter estimation scheme, see, for example, Söderström et al (1978), Beck (1978c).

4.2 Recursive Parameter Estimation Algorithms

Thus armed with three forms of our useful model, (4.11), (4.13), (4.17), we shall in fact choose (4.11) as the most appropriate for the present, i.e.

$$y(t_k) = \underline{z}^T(t_k)\underline{\alpha} + v(t_k) \tag{4.18}$$

with the vector definitions

$$\left.\begin{aligned} \underline{z}^T(t_k) &= [\,y(t_{k-1}),\dots,y(t_{k-n}),u_1(t_{k-1}),\dots,u_1(t_{k-n}),\dots,u_m(t_{k-1}),\dots,u_m(t_{k-n})\,]\,, \\ \underline{\alpha} &= [\phi_1,\dots,\phi_n,\gamma_{11},\dots,\gamma_{1n},\dots,\gamma_{m1},\dots,\gamma_{mn}]^T\,, \end{aligned}\right\} \tag{4.19}$$

such that $\underline{z}^T(t_k)$ and $\underline{\alpha}$ are vectors of dimension $n(m+1)$.

4.2.1 Recursive Least Squares

A comparison of (4.18) with (3.33) shows that we can summarily quote the recursive least squares algorithm for the estimates $\hat{\underline{\alpha}}$ of the parameters $\underline{\alpha}$ by direct analogy with the arguments of section 3.4 and specifically with (3.46). Hence

$$\hat{\underline{\alpha}}(t_k) = \hat{\underline{\alpha}}(t_{k-1}) + P^*(t_{k-1})\underline{z}(t_k)[\,1+\underline{z}^T(t_k)P^*(t_{k-1})\underline{z}(t_k)\,]^{-1}\{y(t_k) - \underline{z}^T(t_k)\hat{\underline{\alpha}}(t_{k-1})\}, \tag{4.20a}$$

$$P^*(t_k) = P^*(t_{k-1}) - P^*(t_{k-1})\underline{z}(t_k)[\,1+\underline{z}^T(t_k)P^*(t_{k-1})\underline{z}(t_k)\,]^{-1}\underline{z}^T(t_k)P^*(t_{k-1})\,, \tag{4.20b}$$

in which for this case,

$$P^*(t_k) \triangleq [\,\sum_{j=1}^{k}\underline{z}(t_j)\underline{z}^T(t_j)\,]^{-1}\,. \tag{4.21}$$

An important feature of the algorithms (4.20), which is not apparent in the earlier discussion of section 3.4, is that these algorithms do not require matrix inversion since the term [...] is a scalar. If nothing else, this then is one of the benefits of working with a single output system representation. (Likewise also the LKF algorithms do not require matrix inversion for systems with a single output, see (3.79e).)

4.2.2 The Problem of Bias

The fundamental role of least squares algorithms for parameter estimation can clearly not be denied. Yet neither can it be denied that these algorithms suffer from a major restriction, namely the problem of bias in the parameter estimates. The many variants on the theme of least squares estimation have their origins in the desire to overcome this problem of bias. To see how the estimates $\underline{\hat{\alpha}}$ may be biased we can once again follow an argument developed previously in section 3.5. In line with equation (3.50) we have the non-recursive formulation of least squares estimates,

$$\underline{\hat{\alpha}}(t_k) = [\sum_{j=1}^{k} \underline{z}(t_j)\underline{z}^T(t_j)]^{-1} [\sum_{j=1}^{k} \underline{z}(t_j)y(t_j)] \quad . \tag{4.22}$$

Upon substitution of $y(t_j) = \underline{z}^T(t_j)\underline{\alpha} + v(t_j)$ and after rearrangement,

$$\underline{\hat{\alpha}}(t_k) = [\sum_{j=1}^{k} \underline{z}(t_j)\underline{z}^T(t_j)]^{-1} [\sum_{j=1}^{k} \underline{z}(t_j)\underline{z}^T(t_j)]\underline{\alpha} + [\sum_{j=1}^{k} \underline{z}(t_j)\underline{z}^T(t_j)]^{-1} [\sum_{j=1}^{k} \underline{z}(t_j)v(t_j)] \quad , \tag{4.23}$$

so that

$$\underline{\hat{\alpha}}(t_k) = \underline{\alpha} + [\sum_{j=1}^{k} \underline{z}(t_j)\underline{z}^T(t_j)]^{-1} [\sum_{j=1}^{k} \underline{z}(t_j)v(t_j)] \quad . \tag{4.24}$$

For $\underline{\hat{\alpha}}(t_k)$ to be unbiased, therefore, the following conditions must hold,

$$\mathcal{E}\{\underline{z}(t_j)v(t_j)\} = \underline{0} \quad , \quad \text{for all } k, \tag{4.25}$$

or, more specifically, recalling the definition of $\underline{z}(t_k)$ in (4.19),

$$\left.\begin{aligned}
&\mathcal{E}\{y(t_{k-1})v(t_k)\} = 0 \quad , \\
&\mathcal{E}\{y(t_{k-2})v(t_k)\} = 0 \quad , \\
&\qquad\vdots \qquad\qquad\vdots \\
&\mathcal{E}\{y(t_{k-n})v(t_k)\} = 0 \quad , \\
&\mathcal{E}\{u_1(t_{k-1})v(t_k)\} = 0 \quad , \\
&\qquad\vdots \qquad\qquad\vdots \\
&\mathcal{E}\{u_m(t_{k-n})v(t_k)\} = 0 \quad .
\end{aligned}\right\} \tag{4.26}$$

Of these the most probable conditions to be violated are those requiring no correlation between the current noise process realisations and past output observations $y(t_{k-1}),\ldots,y(t_{k-n})$. Only if $v(t_k) = e(t_k)$, where $e(t_k)$ is a white noise sequence, i.e.

$$\mathcal{E}\{v(t_k)v(t_j)\} = \mathcal{E}\{e(t_k)e(t_j)\} = 0 \ , \text{ for } k \neq j \ , \tag{4.27}$$

will the estimates be unbiased. Otherwise if $v(t_k)$ is autocorrelated, say, this implies that $v(t_k)$ is correlated with $v(t_{k-1})$ which in turn implies through (4.18) that $v(t_k)$ is correlated with $y(t_{k-1})$--since $y(t_{k-1})$ is a function of $v(t_{k-1})$--and thus

$$\mathcal{E}\{y(t_{k-1})v(t_k)\} \neq 0 \quad .$$

When the conditions of (4.25) are satisfied, and with the further assumption that the noise sequence is normally distributed with variance $\mathcal{E}\{v(t_k)v(t_k)\} = \sigma^2$, it can be easily shown by arguments similar to those of section 3.5 that

$$P(t_k) = \text{cov}\{\underline{\tilde{\alpha}}(t_k)\} = \mathcal{E}\{(\underline{\hat{\alpha}}(t_k) - \underline{\alpha})(\underline{\hat{\alpha}}(t_k) - \underline{\alpha})^T\} \quad ,$$

$$= P^*(t_k)\left[\mathcal{E}\{[\sum_{j=1}^{k} \underline{z}(t_j)v(t_j)][\sum_{j=1}^{k} v(t_j)\underline{z}^T(t_j)]\}\right]P^{*T}(t_k)$$

$$= \sigma^2 P^*(t_k) \quad . \qquad (4.28)$$

The covariance matrix of least squares parameter estimation is therefore found conveniently to be proportional (under the limiting conditions of large k) to the matrix $P^*(t_k)$ computed from the recursive algorithms (4.20)*.

4.2.3. Unbiased Recursive Estimators

The conditions under which the least squares estimates are unbiased will rarely be satisfied in practice. The outcome of such a limitation on the applicability of the method has been the generation of many other algorithms which strive to guarantee convergence of the parameter estimates to their true values. In a recent article Söderström et al (1978) report on a comparative study of four of the more commonly used variants of recursive parameter estimation algorithms. Here we shall discuss a particular form of one of these variants, as indicated in Figure 9, namely the recursive Instrumental Variable (IV) algorithm due to Young, e.g. Young (1974). Most pragmatists would probably agree that there is little difference between the performance of the various algorithms; our choice is dictated by the fact that we shall subsequently demonstrate the use of an IV algorithm in Part 2. Our choice is also influenced by current indications that the principle of the IV approach may well offer a unified and comprehensive approach to the subject of system identification itself (Young, 1976, Young and Jakeman 1978a, 1978b, Jakeman and Young, 1978, Young et al, 1978).

As we have already stated with respect to (4.26), the most likely source of biased estimates is an autocorrelated noise process giving rise to a significant correlation between the noise sequence and past values of the output y. Suppose now that from

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*In practice σ^2 would not be known but can be estimated as the variance of the residual error sequence $\varepsilon(t_k) = y(t_k) - \underline{z}^T(t_k)\underline{\hat{\alpha}}$ after the estimates $\underline{\hat{\alpha}}$ have achieved satisfactory convergence.

the model characterisation of (4.17), and given suitable estimates of the parameters in the $A(q^{-1})$ and $B_j(q^{-1})$ polynomials, denoted $\hat{A}(q^{-1})$ and $\hat{B}_j(q^{-1})$ respectively, a (deterministic) time-series $\hat{x}(t_k)$ can be computed by

$$\hat{x}(t_k) = [1 - \hat{A}(q^{-1})]\hat{x}(t_k) + \sum_{j=1}^{m} \hat{B}_j(q^{-1})u_j(t_k) \quad . \quad (4.29)$$

Viewed from the perspective of Figure 16 $\hat{x}(t_k)$ clearly corresponds to an estimate--since probably it is not generated from the true process characterisation--of the hypothetical noise-free output response of the system. And since we are in general discussing systems in which the single state variable is linearly observed, $\hat{x}(t_k)$ here bears a strong notational and physical resemblance to the notion of state estimates from the Kalman filter. Some structural similarities should therefore be evident from a comparison of Figures 16 and 8. Inspection of (4.29) and (4.17) shows further that : (i) variations in $\hat{x}(t_k)$ should be strongly correlated with variations in the noise-corrupted output observation $y(t_k)$; but (ii) these variations in $\hat{x}(t_k)$ should be uncorrelated with $v(t_k)$ providing $v(t_k)$ is not correlated with the measured input sequences $u_j(t_k)$, i.e.

$$\mathcal{E}\{u_j(t_k)v(t_\ell)\} = 0 \text{ for all } j,k,\ell \quad . \quad (4.30)$$

In fact the above two properties are precisely what is required of the instrumental variables, though it is not necessary that they be computed according to (4.29). Let us therefore call $\hat{x}(t_k)$ from (4.29) the sequence of instrumental variables and denote (4.29) by the term auxiliary model (Young,1974).

The next step in deriving the IV algorithm is one of replacing y by $\hat{x}$ in the least squares algorithms so that the conditions for unbiased estimates of (4.26) are modified to give

$$\left.\begin{aligned}
&\mathcal{E}\{\hat{x}(t_{k-1})v(t_k)\} = 0 \quad , \\
&\mathcal{E}\{\hat{x}(t_{k-2})v(t_k)\} = 0 \quad , \\
&\qquad\vdots \qquad\qquad \vdots \\
&\mathcal{E}\{\hat{x}(t_{k-n})v(t_k)\} = 0 \quad , \\
&\mathcal{E}\{u_1(t_{k-1})v(t_k)\} = 0 \quad , \\
&\qquad\vdots \qquad\qquad \vdots \\
&\mathcal{E}\{u_m(t_{k-n})v(t_k)\} = 0 \quad ,
\end{aligned}\right\} \tag{4.31}$$

which we have argued should indeed be fulfilled by the instrumental variables of (4.29). With the definition

$$\underline{\hat{z}}^T(t_k) = [\hat{x}(t_{k-1}),\ldots,\hat{x}(t_{k-n}),u_1(t_{k-1}),\ldots,u_1(t_{k-n}),\ldots,u_m(t_{k-1}),\ldots,u_m(t_{k-n})] \quad , \tag{4.32}$$

and replacing $\underline{z}(t_k)$ by $\underline{\hat{z}}(t_k)$, but <u>not</u> $\underline{z}^T(t_k)$ by $\underline{\hat{z}}^T(t_k)$, in (4.24), i.e.

$$\underline{\hat{\alpha}}(t_k) = \underline{\alpha} + [\sum_{j=1}^{k} \underline{\hat{z}}(t_j)\underline{z}^T(t_j)]^{-1}[\sum_{j=1}^{k} \underline{\hat{z}}(t_j)v(t_j)] \quad ,$$

we can work backwards with this heuristic reasoning to the desired algorithm.

In summary then, the <u>recursive instrumental variable algorithm</u> is given by

$$\underline{\hat{\alpha}}(t_k) = \underline{\hat{\alpha}}(t_{k-1}) + \hat{P}^*(t_{k-1})\underline{\hat{z}}(t_k)[1 + \underline{z}^T(t_k)\hat{P}^*(t_{k-1})\underline{\hat{z}}(t_k)]^{-1}\{y(t_k) - \underline{z}^T(t_k)\underline{\hat{\alpha}}(t_{k-1})\} \quad , \tag{4.33a}$$

$$\hat{P}^*(t_k) = \hat{P}^*(t_{k-1}) - \hat{P}^*(t_{k-1})\underline{\hat{z}}(t_k)[1 + \underline{z}^T(t_k)\hat{P}^*(t_{k-1})\underline{\hat{z}}(t_k)]^{-1}\underline{z}^T(t_k)\hat{P}^*(t_{k-1}) \quad , \tag{4.33b}$$

with

$$\hat{x}(t_k) = [\,1 - \hat{A}(q^{-1})]\hat{x}(t_k) + \sum_{j=1}^{m} \hat{B}_j(q^{-1})u_j(t_k) \quad , \qquad (4.33c)$$

where

$$\hat{P}^*(t_k) \triangleq [\sum_{j=1}^{k} \underline{\hat{z}}(t_j)\underline{z}^T(t_j)]^{-1} \qquad (4.34)$$

It should not, however, have escaped attention that we have appealed to a circular argument in order to obtain the IV algorithms: for calculation of the parameter values in (4.33a) these same values are assumed to be available for computation of $\hat{x}$ in (4.33c). Reference to Figure 16 should clarify the true intent of the argument. For any given iteration through the block of N data samples--recall Figure 5--the estimated parameters of the auxiliary model of (4.33c) are kept constant* for all t_k, k = 1, 2,...,N. At the end of each iteration they are set equal to the new estimates $\underline{\hat{\alpha}}(t_N)$ provided by (4.33a) and (4.33b); and if convergence is guaranteed then a "better" auxiliary model yields "better" estimates of $\underline{\alpha}$, and so on. Such a circular behaviour has earned the title of bootstrap estimator for this kind of IV algorithm. Of course, one question remains: what values should be assumed for the first set of parameter estimates in the auxiliary model? An intelligent and easily determined answer is to use the least squares estimates, derived from a previous iteration through the data, even though these values are probably biased.

Perhaps briefly at this point we might review some of the similarities and differences between the IV, LS, and LKF algorithms.

(i) The LS estimator of (4.20) amounts merely to a manipulation of the observed input/output time-series data. Whereas the assumed form of the model chosen to characterise the observed behaviour is implicit in the LS algorithms, through the definitions of the vectors $\underline{\alpha}$ and $\underline{z}$, it is explicit in the IV estimator (as it like-

*They may also be adaptively updated in a recursive fashion, but this form of the IV estimator will not be discussed here, see Young et al (1971).

wise in the LKF).

(ii) The similarities of structure between the LKF and IV estimator ought to be self-evident from Figures 8 and 16.

(iii) The strong suggestion of equivalence between instrumental variables and state estimates deserves special attention in connection with the earlier allusion to the duality between state and parameter estimation, see section 3.2. The IV algorithms as quoted are almost a realisation of a joint state-parameter estimator. They are, however, not quite complete in this sense because the instrumental variable computation of (4.33c) lacks a corrective element based on the perceived error between $\hat{x}$ and the actual output observation y. By joint state-parameter estimator we mean an algorithm which partitions the problem into two sub-problems: first, the use of state estimates for computation of the parameter estimates, then substitution of the new parameter estimates for the next computation of the state estimates, and so on as the recursive algorithm moves serially through the data. The same idea is actually hidden in equations (2.3) and (2.4) of section 2.3.1. One example of such a joint estimator for application to a hydrological forecasting problem is given by Todini (1978), which he calls a Mutually Interactive State Parameter (MISP) estimation algorithm. It will be seen in section 5 that the use of the term combined state-parameter estimation has a rather different interpretation.

(iv) Finally, for the purposes of completeness we can point out that the form of $v(t_k)$ is left unspecified in the case of an IV estimator. Other algorithms assume that any correlated structure of $v(t_k)$ may itself be modelled by some transformation of a white noise sequence; the additional parameters of the noise model are accordingly required to be estimated (Söderström et al, 1978).

4.3 Time-variable Parameters

There was a proposal in section 2.3 that an ambivalent attitude towards the distinction between the concepts of state and parameter should be encouraged. For the development of the linear Kalman filter algorithms considerable use was made of time-invariant state vectors; in this section we investigate the converse, that is methods for estimating time-variable parameters. There are two contexts in which the recursive estimation of time-variable parameters is of major interest:

(i) For solution of the model structure identification problem (see also section 2.2.3) whereby the analyst seeks an understanding of why certain assumed constant model parameters are not found to have time-invariant estimates.

(ii) In adaptive prediction and control (see also section 2.3.1), in which some parameters may be thought of as truly time-varying; or else the objective is to allow sufficient flexibility for the model to be adapted in accordance with the actual variations in the dynamic properties of the system under study.

An appreciation of the following time-variable parameter estimators is intimately linked with the qualitative properties of the gain matrix in the LKF which were discussed in section 3.8. We shall exploit this link wherever possible, for it not only provides us with insight, but also it strengthens the unifying themes of the paper as a whole. First, however, for the sake of illustration let us transform the LS algorithms of (4.20) by making the substitution of (4.28) such that

$$\left.\begin{aligned} \underline{\hat{\alpha}}(t_k) &= \underline{\hat{\alpha}}(t_{k-1}) + P(t_{k-1})\underline{z}(t_k)[\sigma^2 + \underline{z}^T(t_k)P(t_{k-1})\underline{z}(t_k)]^{-1}\{y(t_k) - \underline{z}^T(t_k)\underline{\hat{\alpha}}(t_{k-1})\}, \\ P(t_k) &= P(t_{k-1}) - P(t_{k-1})\underline{z}(t_k)[\sigma^2 + \underline{z}^T(t_k)P(t_{k-1})\underline{z}(t_k)]^{-1}\underline{z}^T(t_k)P(t_{k-1}) , \end{aligned}\right\} \quad (4.35)$$

and hence we have at our disposal a set of recursive equations for the parameter estimates $\underline{\hat{\alpha}}$ and their error variance-covariance matrix $P(t_k)$. For (4.35) the equivalent of the gain matrix is the gain vector defined by

$$\underline{k}(t_k) = P(t_{k-1})\underline{z}(t_k)[\sigma^2 + \underline{z}^T(t_k)P(t_{k-1})\underline{z}(t_k)]^{-1} \quad . \qquad (4.36)$$

If the simplest <u>scalar</u> example is taken, i.e. for the process model of (4.18),

$$y(t_k) = \phi_1 y(t_{k-1}) + v(t_k) \quad , \qquad (4.37)$$

(4.36) reduces to

$$k(t_k) = p(t_{k-1})y(t_{k-1})[y^2(t_{k-1})p(t_{k-1}) + \sigma^2]^{-1} \quad , \qquad (4.38)$$

which offers a clear parallel with (3.89) of section 3.8--the transposition of states and parameters should now be obvious from (3.89) and (4.38). Thus by analogy with Table 1 it can also be deduced that when the parameter estimates have achieved convergence $p(t_{k-1})$ should be relatively small and therefore $k(t_k)$ is small. But in the situation of time-varying parameters, only small corrections to the estimates would be counter-productive. Here one would argue that large errors between observed and predicted output are not so much a consequence of spurious errors in the measurements but are due primarily to changing values of the model parameters. We need, therefore, to maintain $k(t_k)$, and by implication $p(t_{k-1})$, at artificially larger values. In fact Table 1 suggests that if more information is available on how the parameters vary with time then less artificial and more natural methods of achieving our objectives are available; these are discussed later in section 4.3.2.

4.3.1 Exponential Weighting of Past Data

A continuation of the argument developed so far adopts the following attitude. If the observed process behaviour is changing with time then the <u>current</u> estimates of the parameter values should be based on the current and most recent past observations and not on the more distant past observations, when the parameters actually had quite different values. In other words, it is disadvantageous for the estimator to place equal weight on all the

data obtained since the initial time t_1; what we require is for the estimator to forget, as it were, the behaviour that was observed in the past. The method of Exponential Weighting of Past data (EWP), illustrated by the weighting function of Figure 17, is one method that staisfies the desired objectives. This method is such that the modified estimator is equivalent to minimising the loss function (compare with (3.9) and 3.42)),

$$J'(t_k) = \sum_{j=1}^{k} \mu^{k-j} \left(y(t_j) - \underline{z}^T(t_j)\hat{\underline{\alpha}}(t_k) \right)^2 \quad ; \; 0 \ll \mu \ll 1 \; , \tag{4.39}$$

where the current weighted squared error sum and the minimum value thereof yield the most recent estimate $\hat{\underline{\alpha}}(t_k)$. We notice that the current squared error at t_k is weighted by an amount 1.0, the error at t_{k-1} by μ, that at t_{k-2} by μ^2, etc. Since μ, the weighting factor, is normally chosen to be just less than unity, the most recent errors are weighted preferentially and they will thus dominate the computation of the estimates $\hat{\underline{\alpha}}(t_k)$. This is what we would wish in order to avoid attaching too much significance to distant past errors calculated using $\hat{\underline{\alpha}}(t_k)$. The choice of μ and the rate of change of the parameter values are closely tied together; a lower value of μ permits faster adaptation of the estimates in conjunction with a more rapid "forgetting" of past data.

Assuming then the loss function of (4.39) we arrive at the following recursive EWP algorithms for time-varying parameters

$$\left.\begin{aligned} \hat{\underline{\alpha}}(t_k) &= \hat{\underline{\alpha}}(t_{k-1}) + P'(t_{k-1})\underline{z}(t_k)[\mu + \underline{z}^T(t_k)P'(t_{k-1})\underline{z}(t_k)]^{-1} \\ &\quad \times \{y(t_k) - \underline{z}^T(t_k)\hat{\underline{\alpha}}(t_{k-1})\} \quad , \\ P'(t_k) &= (1/\mu)\{P'(t_{k-1}) - P'(t_{k-1})\underline{z}(t_k)[\mu + \underline{z}^T(t_k)P'(t_{k-1})\underline{z}(t_k)]^{-1} \\ &\quad \times \underline{z}^T(t_k)P'(t_{k-1})\} \quad , \end{aligned}\right\} \tag{4.40}$$

in which

$$P'(t_k) \triangleq [\sum_{j=1}^{k} \mu^{k-j} \underline{z}(t_j)\underline{z}^T(t_j)]^{-1} \quad . \tag{4.41}$$

A comparison of $P'(t_k)$ in (4.41) with $P^*(t_k)$ from the recursive LS algorithms of (4.20) and (4.21) shows that $P'(t_1) = P^*(t_1)$, i.e. these two matrices have identical initial conditions. Inspection of their respective recursive relationships

$$[P^*(t_k)]^{-1} = [\sum_{j=1}^{k-1} \underline{z}(t_j)\underline{z}^T(t_j)] + \underline{z}(t_k)\underline{z}^T(t_k)$$

$$= [P^*(t_{k-1})]^{-1} + \underline{z}(t_k)\underline{z}^T(t_k) \quad , \tag{4.42}$$

$$[P'(t_k)]^{-1} = \mu[\sum_{j=1}^{k-1} \mu^{k-j-1}\underline{z}(t_j)\underline{z}^T(t_j)] + \underline{z}(t_k)\underline{z}^T(t_k)$$

$$= \mu[P'(t_{k-1})]^{-1} + \underline{z}(t_k)\underline{z}^T(t_k) \quad , \tag{4.43}$$

reveals that the inverse of $P'(t_k)$ increases more slowly than does the inverse of $P^*(t_k)$. Hence the effect of introducing μ is to lessen the rate of decrease of P' relative to the case of $\mu = 1.0$, i.e. ordinary LS estimation. The transfer of this reasoning for evaluation of the qualitative effect of μ on the gain vector, i.e.

$$\underline{k}'(t_k) = P'(t_{k-1})\underline{z}(t_k)[\mu + \underline{z}^T(t_k)P'(t_{k-1})\underline{z}(t_k)]^{-1} \quad , \tag{4.44}$$

requires a small manipulation of $\underline{k}'(t_k)$. For example, premultiply the RHS of (4.44) by $P'(t_k)[P'(t_k)]^{-1}$ and then substituting for $[P'(t_k)]^{-1}$ from (4.43) gives

$$\underline{k}'(t_k) = P'(t_k)\{\mu[P'(t_{k-1})]^{-1} + \underline{z}(t_k)\underline{z}^T(t_k)\}P'(t_{k-1})\underline{z}(t_k)$$

$$\cdot [\mu + \underline{z}^T(t_k)P'(t_{k-1})\underline{z}(t_k)]^{-1}$$

$$= P'(t_k)\underline{z}(t_k)[\mu + \underline{z}^T(t_k)P'(t_{k-1})\underline{z}(t_k)]$$

$$\cdot [\mu + \underline{z}^T(t_k)P'(t_{k-1})\underline{z}(t_k)]^{-1}$$

or, $$\underline{k}'(t_k) = P'(t_k)\underline{z}(t_k) \quad , \tag{4.45}$$

from which the influence of μ on $\underline{k}'(t_k)$, through $P'(t_k)$, is that of maintaining the gain vector at relatively larger values.

4.3.2 Dynamic Least Squares

There are two basic limitations on the use of exponential weighting of past data as a method of allowing for recursive estimation of time-varying parameters. It does not permit any prior selection between different expected rates of change of the parameters and it is really only appropriate for the case of slowly varying parameters. It is, nevertheless, a minimally more complex algorithm than the ordinary LS algorithm.

The obvious equivalence of the state and time-variable parameter estimation problems prompts thus the question of whether a model can be postulated for a description of the way in which the parameters are expected to change. We could, for instance, assume a model by straightforward analogy with (3.71) in section 3.6, i.e.

$$\underline{\alpha}(t_k) = \Theta\underline{\alpha}(t_{k-1}) + \Psi\underline{\zeta}(t_{k-1}) \quad , \tag{4.46}$$

where $\underline{\zeta}(t_{k-1})$ is a white-noise disturbance, and hence proceed to a set of predictor and corrector equations in line with the LKF of (3.79). This presupposes, however, a far greater knowledge of parameter variations than would probably be available in practice. A much simpler model is that in which the paramters are defined as random walk variables, i.e.

$$\underline{\alpha}(t_k) = \underline{\alpha}(t_{k-1}) + \underline{\zeta}(t_{k-1}) \quad , \tag{4.47}$$

which captures the tendency of the parameters to exhibit behaviour that is partly autocorrelated and partly random, without demanding any excessive prior knowledge of these variations. The individual rates of parameter variations are governed by the choice of the matrix D where

$$D = \mathcal{E}\{\underline{\zeta}(t_k)\underline{\zeta}^T(t_k)\} \quad , \tag{4.48}$$

and with D being diagonal in the absence of any more precise information to the contrary. For parameter estimation we thus have, first,

Prediction:

$$\left.\begin{aligned} \underline{\hat{\alpha}}(t_k|t_{k-1}) &= \underline{\hat{\alpha}}(t_{k-1}|t_{k-1}) \quad , \\ P(t_k|t_{k-1}) &= P(t_{k-1}|t_{k-1}) + D \quad , \end{aligned}\right\} \tag{4.49}$$

and then by suitable substitution in the LS algorithms of (4.35),

Correction:

$$\left.\begin{aligned} \underline{\hat{\alpha}}(t_k|t_k) &= \underline{\hat{\alpha}}(t_k|t_{k-1}) + P(t_k|t_{k-1})\underline{z}(t_k)[\sigma^2 + \underline{z}^T(t_k)P(t_k|t_{k-1})\underline{z}(t_k)]^{-1} \\ &\qquad \times \{y(t_k) - \underline{z}^T(t_k)\underline{\hat{\alpha}}(t_k|t_{k-1})\} \\ P(t_k|t_k) &= P(t_k|t_{k-1}) - P(t_k|t_{k-1})\underline{z}(t_k)[\sigma^2 + \underline{z}^T(t_k)P(t_k|t_{k-1})\underline{z}(t_k)]^{-1} \\ &\qquad \times \underline{z}^T(t_k)P(t_k|t_{k-1}) \quad . \end{aligned}\right\} \tag{4.50}$$

Equations (4.49) and (4.50) readily combine to give the dynamic least squares algorithms

$$\begin{aligned} \underline{\hat{\alpha}}(t_k) &= \underline{\hat{\alpha}}(t_{k-1}) + \{P(t_{k-1}) + D\}\underline{z}(t_k)[\sigma^2 + \underline{z}^T(t_k)\{P(t_{k-1}) + D\}\underline{z}(t_k)]^{-1} \\ &\qquad \times \{y(t_k) - \underline{z}^T(t_k)\underline{\hat{\alpha}}(t_{k-1})\} \quad , \end{aligned}$$

$$\begin{aligned} P(t_k) &= \{P(t_{k-1}) + D\} - \{P(t_{k-1}) + D\}\underline{z}(t_k) \\ &\qquad \times [\sigma^2 + \underline{z}^T(t_k)\{P(t_{k-1}) + D\}\underline{z}(t_k)]^{-1} \underline{z}^T(t_k)\{P(t_{k-1}) + D\} \quad , \end{aligned} \tag{4.51}$$

in which the simpler notation is retained. As with μ in the EWP algorithm, the net effect of inserting D is to reduce the rates of decrease in the $P(t_k)$ matrix and in the gain vector. Of course, though more sophisticated, the specification of D remains a problem for practical implementation of this algorithm.

5. COMBINED STATE AND PARAMETER ESTIMATION: THE EXTENDED KALMAN FILTER

In section 3 we derived a set of algorithms for on-line, recursive state estimation; in section 4 we have now derived a set of on-line, recursive parameter estimation algorithms. And we have further shown that a duality exists between state estimation and parameter estimation--the reader has not been spared the repeated references to this point in sections 2.3,3.2,4.2, and 4.3. The purpose of the present section is to demonstrate how the combined state-parameter estimation problem leads to a nonlinear filtering problem. Since the filtering algorithms of section 3 can deal only with linear system descriptions it will be necessary to develop a different filter, the extended Kalman filter (EKF), which is capable of application to a nonlinear system representation. In practice the EKF is actually a first-order linear approximation to the ideal of a nonlinear filter.

5.1 Problem Formulation

From the foregoing discussion one might anticipate that the derivation will attempt to make some appropriate combination of the algorithms already stated in sections 3 and 4. But this would miss the most useful aspect of erasing the distinction between states and parameters. Let us therefore return briefly to the very first preview of the Kalman filter. For the multivariable situation we have the following equivalent of equation (2.4) in section 2.3.1,

$$\underline{\hat{x}}(t_k|t_k) = \underline{\hat{x}}(t_k|t_{k-1}) + K_s(t_k)\underline{\varepsilon}(t_k|t_{k-1}) \quad , \tag{5.1}$$

and an equivalent of (2.3),

$$\underline{\hat{\alpha}}(t_k|t_k) = \underline{\hat{\alpha}}(t_k|t_{k-1}) + K_p(t_k)\underline{\varepsilon}(t_k|t_{k-1}) \quad . \tag{5.2}$$

Here we are suggesting that both equations come from some filtering algorithm formulation and thus the notational conventions are consistent with those used elsewhere. From previous arguments K_s, the state estimation gain matrix, is in principle a function

of the system parameters and the state estimation error covariances--compare with (3.89)--while K_p, the parameter estimation gain matrix, is in principle a function of the system observations (inputs and outputs) and the parameter estimation errors--compare with (4.38).

What is really required conceptually for combined state-parameter estimation is to begin not by trying to combine equations (5.1) and (5.2), but to list all those quantities that one wishes to estimate, say a vector $\underline{x}^*$, and then to write down the equations for the dynamic behaviour of these quantities $\underline{x}^*$. We can still expect the kernel of the filtering algorithms to take the form of

$$\hat{\underline{x}}^*(t_k|t_k) = \hat{\underline{x}}^*(t_k|t_{k-1}) + K^*(t_k)\underline{\varepsilon}(t_k|t_{k-1}) \quad , \qquad (5.3)$$

in which $\underline{\varepsilon}(t_k|t_{k-1})$ is preserved as nominally similar to $\underline{\varepsilon}(t_k|t_{k-1})$ in (5.1) and (5.2) because a rearrangement of the internal description of the system does not alter the "external" observations against which some appropriate prediction is to be evaluated.

After our brief excursion, however, it is now necessary to set up the nonlinear system description upon which the problem of combined state parameter estimation will be constructed. The complete development of the extended Kalman filtering algorithms is shown in Figure 18 as an extension of Figure 9. Let us start by restating the continuous-discrete representation of system behaviour of equations (3.28) and (3.33) in section 3.3,that is, the state vector dynamics

$$\dot{\underline{x}}(t) = F\underline{x}(t) + G\underline{u}(t) + L\underline{\xi}(t) \quad , \qquad (5.4a)$$

and the sampled output observations,

$$\underline{y}(t_k) = H\underline{x}(t_k) + \underline{\eta}(t_k) \quad . \qquad (5.4b)$$

From here onwards we shall assume, with no loss of generality, that L = I, the identity matrix, in (5.4a).

Suppose now that some of the unknown, or imprecisely known, elements of the matrices F,G, and H, that is a vector of parameters $\underline{\alpha}$, say, are required to be estimated simultaneously with the estimation of the state vector $\underline{x}$. We can infer from the preceding development of equation (5.3) that one approach to realizing a simultaneous, combined state-parameter estimator is to augment the state vector $\underline{x}$ with the parameter vector $\underline{\alpha}$ and accordingly to postulate a set of additional differential equations representing the parameter dynamics. As a consequence, if the augmented state vector $\underline{x}^*$ is defined by

$$\underline{x}^* \triangleq \begin{bmatrix} \underline{x} \\ \hline \underline{\alpha} \end{bmatrix} , \tag{5.5}$$

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

$$\underline{x}^*(t) = \underline{f}\{\underline{x}^*(t), \underline{u}(t)\} + \underline{\xi}^*(t) , \tag{5.6a}$$

$$\underline{y}(t_k) = \underline{h}\{\underline{x}^*(t_k)\} + \underline{\eta}(t_k) . \tag{5.6b}$$

The functions $\underline{f}\{\cdot\}$ and $\underline{h}\{\cdot\}$ are vector functions; they are nonlinear principally because of the product terms involving elements of $\underline{\alpha}$ with elements of $\underline{x}$ and $\underline{u}$. In (5.6a) $\underline{\xi}^*$ indicates that this vector of stochastic disturbances is now of a different order to that defined for $\underline{\xi}$ in (5.4a). Note also that had we begun with a set of nonlinear state variable dynamics, the estimation problem to be solved would still be posed according to equations (5.6).

Let us consider the matter of specifying the dynamics of the parameters $\underline{\alpha}$. Of particular importance are two such specifications: (i) we might naturally assume that the parameters are constant, i.e. time-invariant

$$\dot{\underline{\alpha}}(t) = 0 , \tag{5.7}$$

or (ii) it might be proposed that they vary in an unknown random

walk fashion, as has been suggested earlier in section 4.3.2,

$$\dot{\alpha}(t) = \zeta(t) \quad , \tag{5.8}$$

in which $\zeta(t)$ is a white noise process. The vector $\underline{\xi}^*$ in (5.6a) is thus nominally composed of disturbances $\underline{\xi}$ of the state variables, and disturbances $\underline{\zeta}$ of some of the parameters. Were there to be more a priori information on the parameter variations, then it would be appropriate, for instance, to define the dynamics of the parameters as oscillatory in accordance with some diurnal or seasonal fluctuation.

5.2 Major Steps in the Derivation of the Extended Kalman Filter

The customary procedure for dealing with nonlinear system descriptions is to approximate their behaviour by a set of linear equations. As we have said before, the EKF is a linear approximation of the nonlinear filter which would ideally be required to provide estimates of $\underline{x}^*$ in the system of (5.6). The virtue of this linearisation is that the problem, whatever it may be, becomes amenable to the many powerful techniques of analysis available from linear systems theory. The linear Kalman filter is just one such technique. Bearing this in mind we can take the first step in deriving the EKF.

5.2.1 Linearisation of the Nonlinear Augmented state Equations

For small perturbations $\delta\underline{x}^*(t)$ of the state-parameter vector $\underline{x}^*(t)$ about some nominal deterministic reference trajectory $\bar{\underline{x}}^*(t)$, a set of linear dynamic equations in $\delta\underline{x}^*(t)$ may be obtained by taking a first-order Taylor series expansion of the nonlinear function $\underline{f}$ in (5.6a). In other words, if the perturbations $\delta\underline{x}^*(t)$ and $\delta\underline{u}(t)$ are defined by

$$\left.\begin{aligned} \delta\underline{x}^*(t) &\triangleq \underline{x}^*(t) - \bar{\underline{x}}^*(t) \quad , \\ \delta\underline{u}(t) &\triangleq \underline{u}(t) - \bar{\underline{u}}(t) \quad , \end{aligned}\right\} \tag{5.9}$$

the assumption is that dynamic variations of $\delta\underline{x}^*(t)$ are linear

in the vicinity of the solution $\underline{\bar{x}}^*(t)$ of the deterministic reference dynamic system

$$d\underline{x}^*(t)/dt = \underline{f}\{\underline{\bar{x}}^*(t),\underline{\bar{u}}(t)\} \quad ; \quad \underline{\bar{x}}^*(t) = \underline{\bar{x}}^*(t_o) \text{ for } t = t_o \ . \tag{5.10}$$

In (5.10) $\underline{\bar{u}}(t)$ is a known function of time describing the variations in the measured system inputs; $\underline{\bar{x}}^*(t)$ is therefore determined for all t by the specification of $\underline{\bar{u}}(t)$ and by the choice of the initial conditions $\underline{\bar{x}}^*(t_o)$.

A first-order Taylor series expansion of $\underline{f}\{\underline{x}^*(t),\underline{u}(t)\}$ in (5.6a) about the reference trajectory is given by

$$\underline{f}\{\underline{x}^*(t),\underline{u}(t)\} = \underline{f}\{\underline{\bar{x}}^*(t),\underline{\bar{u}}(t)\} + F^*\{\underline{\bar{x}}^*(t_o),\underline{\bar{u}}(t)\}[\underline{x}^*(t) - \underline{\bar{x}}^*(t)] + G^*\{\underline{\bar{x}}^*(t_o),\underline{\bar{u}}(t)\}[\underline{u}(t) - \underline{\bar{u}}(t)] + \ldots \ , \tag{5.11}$$

where the matrices $F^*\{\cdot\}$ and $G^*\{\cdot\}$ are defined as

$$F^*\{\underline{\bar{x}}^*(t_o),\underline{\bar{u}}(t)\} \triangleq \left[\frac{\partial f_i\{\underline{x}^*(t),\underline{u}(t)\}}{\partial x_j}\right]_{\substack{\underline{x}^*(t)=\underline{\bar{x}}^*(t) \\ \underline{u}(t)=\underline{\bar{u}}(t)}} \ , \tag{5.12}$$

$$G^*\{\underline{\bar{x}}^*(t_o),\underline{\bar{u}}(t)\} \triangleq \left[\frac{\partial f_i\{\underline{x}^*(t),\underline{u}(t)\}}{\partial x_j}\right]_{\substack{\underline{x}^*(t)=\underline{\bar{x}}^*(t) \\ \underline{u}(t)=\underline{\bar{u}}(t)}} \ . \tag{5.13}$$

The argument $\underline{\bar{x}}^*(t_o)$ of $F^*\{\cdot\}$ and $G^*\{\cdot\}$ signifies that these matrices are dependent on the choice of initial conditions for the deterministic reference state vector.

Now substituting for $\underline{x}^*(t)$ from (5.9) in (5.6a) we have

$$\frac{d}{dt}(\underline{\bar{x}}^*(t) + \delta\underline{x}^*(t)) = d\underline{\bar{x}}^*(t)/dt + d(\delta\underline{x}^*(t))/dt = \underline{f}\{\underline{x}^*(t),\underline{u}(t)\} + \underline{\xi}^*(t) \ , \tag{5.14}$$

so that substitution of $d\underline{\bar{x}}^*(t)/dt$ from (5.10) gives

$$d(\delta\underline{x}^*(t))/dt = \underline{f}\{\underline{x}^*(t),\underline{u}(t)\} - \underline{f}\{\underline{\bar{x}}^*(t)\underline{\bar{u}}(t)\} + \underline{\xi}^*(t) \ . \tag{5.15}$$

Hence using (5.11) with the definitions (5.9), we obtain from (5.15)

$$d(\delta\underline{x}^*(t))/dt = F^*\{\bar{\underline{x}}^*(t),\bar{\underline{u}}(t)\}\delta\underline{x}^*(t) + G^*\{\bar{\underline{x}}^*(t),\bar{\underline{u}}(t)\}\delta\underline{u}(t) + \underline{\xi}^*(t) \quad , \tag{5.16}$$

which is the desired linear dynamic relationship for the small perturbations $\delta\underline{x}^*(t)$.

5.2.2 Linearisation of the Nonlinear Observations Equation

Similarly for the nonlinear observations equation (5.6b), i.e.

$$\underline{y}(t_k) = \underline{h}\{\underline{x}^*(t_k)\} + \underline{n}(t_k) \quad ,$$

a first-order Taylor series expansion of $\underline{h}\{\cdot\}$ may be taken about the reference trajectory, giving

$$\underline{h}\{\underline{x}^*(t_k)\} = \underline{h}\{\bar{\underline{x}}^*(t_k)\} + H^*\{\bar{\underline{x}}^*(t_0)\}\delta\underline{x}^*(t_k) + \ldots \quad , \tag{5.17}$$

with the definition

$$H^*\{\bar{\underline{x}}^*(t_0)\} \triangleq \left[\frac{\partial h_i\{\underline{x}^*(t_k)\}}{\partial x^*_j}\right]_{\underline{x}^*(t_k)=\bar{\underline{x}}^*(t_k)} \quad , \tag{5.18}$$

where again, like $F^*\{\cdot\}$ and $G^*\{\cdot\}$, the matrix $H^*\{\cdot\}$ is ultimately dependent upon $\bar{\underline{x}}^*(t_0)$. If we define also a nominal measurement sequence $\bar{\underline{y}}(t_k)$,

$$\bar{\underline{y}}(t_k) \triangleq \underline{h}\{\bar{\underline{x}}^*(t_k)\} \quad , \tag{5.19}$$

and an associated small perturbation

$$\delta\underline{y}(t_k) \triangleq \underline{y}(t_k) - \bar{\underline{y}}(t_k) \quad , \tag{5.20}$$

the required linear observations equation for the small perturbations $\delta\underline{x}^*(t)$ is obtained

$$\delta\underline{y}(t_k) = H^*\{\bar{\underline{x}}^*(t_0)\}\delta\underline{x}^*(t_k) + \underline{n}(t_k) \quad . \tag{5.21}$$

5.2.3 Application of the Linear Kalman Filter to the Small Perturbations Equations

Gathering together equations (5.16),(5.21) and (5.10),(5.19) our system characterisation comprises

(i) The Linear Small Perturbations Equations:

$$\delta\dot{\underline{x}}^*(t) = F^*\delta\underline{x}^*(t) + G^*\delta\underline{u}(t) + \underline{\xi}^*(t) \quad , \tag{5.22a}$$

$$\delta\underline{y}(t_k) = H^*\delta\underline{x}^*(t_k) + \underline{\eta}(t_k) \quad ; \tag{5.22b}$$

(ii) The Deterministic Reference Trajectory and Reference Observations:

$$\dot{\bar{\underline{x}}}^*(t) = \underline{f}\{\bar{\underline{x}}^*(t),\bar{\underline{u}}(t)\} \quad ; \; \bar{\underline{x}}^*(t) = \bar{\underline{x}}^*(t_o) \text{ for } t = t_o \tag{5.23a}$$

$$\bar{\underline{y}}(t_k) = \underline{h}\{\bar{\underline{x}}^*(t_k)\} \quad , \tag{5.23b}$$

in which the arguments of F*, G*, and H* have been omitted for brevity and for ease of comparison of equations (5.22) with equations (5.4) in section 5.1.

We may observe that equations (5.22) are in principal amenable to the application of a linear Kalman filtering algorithm. However, one further step is required before we can complete this interim stage in the development of the EKF. As with the original analysis of section 3.3 we need an equivalent discrete-time representation of (5.22a), i.e.

$$\begin{aligned}\delta\underline{x}^*(t_k) = {} & \Phi^*\{t_k,t_{k-1};\bar{\underline{x}}^*(t_{k-1}),\bar{\underline{u}}(t_{k-1})\}\delta\underline{x}^*(t_{k-1}) \\ & + \Gamma^*\{t_k,t_{k-1};\bar{\underline{x}}^*(t_{k-1}),\bar{\underline{u}}(t_{k-1})\}\delta\underline{u}(t_{k-1}) + \underline{\xi}^*(t_{k-1}) \quad ,\end{aligned} \tag{5.24}$$

where

$$\Phi^*\{t_k,t_{k-1};\bar{\underline{x}}^*(t_{k-1}),\bar{\underline{u}}(t_{k-1})\} \triangleq \exp(F^*\{\bar{\underline{x}}^*(t_{k-1}),\bar{\underline{u}}(t_{k-1})\}[t_k - t_{k-1}]) \quad , \tag{5.25}$$

$$\Gamma^*\{t_k,t_{k-1};\bar{\underline{x}}^*(t_{k-1}),\bar{\underline{u}}(t_{k-1})\} \triangleq \int_{t_{k-1}}^{t_k} \Phi^*\{t_k,\tau;\bar{\underline{x}}^*(t_{k-1})\bar{\underline{u}}(t_{k-1})\} \times G^*\{\bar{\underline{x}}^*(t_{k-1})\bar{\underline{u}}(t_{k-1})\}d\tau \quad , \tag{5.26}$$

$$\underline{\xi}^*(t_{k-1}) \triangleq \int_{t_{k-1}}^{t_k} \Phi^*\{t_k,\tau;\bar{\underline{x}}^*(t_{k-1})\bar{\underline{u}}(t_{k-1})\}\underline{\xi}^*(\tau)d\tau \quad . \tag{5.27}$$

A word of explanation is required for the cumbersome, yet precise notation of the above definitions. In practice, the evaluation of $\Phi^*\{\cdot\}$ and $\Gamma^*\{\cdot\}$ will be carried out by evaluation of the matrices $F^*\{\cdot\}$ and $G^*\{\cdot\}$ given a knowledge of the reference variables $\bar{\underline{x}}^*(t_{k-1})$ and $\bar{\underline{u}}(t_{k-1})$ at the previous sampling instant t_{k-1}. It is also assumed in the definition of $\Gamma^*\{\cdot\}$ that $\bar{\underline{u}}(t)$ is constant over the interval $t_{k-1} \rightarrow t_k$ and equal to $\bar{\underline{u}}(t_{k-1})$. For conciseness in the following we shall retain only part of the arguments for $\Phi^*\{\cdot\}$ and $\Gamma^*\{\cdot\}$ so that (5.24) may be written more clearly as

$$\delta\underline{x}^*(t_k) = \Phi^*\{t_k,t_{k-1}\}\delta\underline{x}^*(t_{k-1}) + \Gamma^*\{t_k,t_{k-1}\}\delta\underline{u}(t_{k-1}) + \underline{\xi}^*(t_{k-1}) \quad , \tag{5.28}$$

and can thus be compared with equation (3.71a) in section 3.6.

What now are the possibilities for obtaining recursive estimates of the augmented state-parameter vector $\underline{x}^*$? We know $\bar{\underline{u}}(t)$ and $\bar{\underline{x}}^*(t_0)$ such that $\bar{\underline{x}}^*(t)$ and $\bar{\underline{y}}(t_k)$ can be generated from (5.23), and then from (5.9) and (5.20) the measurement deviations $\delta\underline{u}(t_k)$ and $\delta\underline{y}(t_k)$ may be computed from the actual observations $\underline{u}(t_k)$ and $\underline{y}(t_k)$. Given $\delta\underline{u}(t_k)$ and $\delta\underline{y}(t_k)$, and given either of the system characterisations of equations (5.22) or equations (5.28) and (5.22b), we could apply an LKF algorithm to obtain estimates $\hat{\delta\underline{x}}^*(t_k|t_k)$ of the small perturbations $\delta\underline{x}^*(t_k)$. Finally, working backwards through the definition of (5.9) our knowledge of $\bar{\underline{x}}^*(t_k)$, the reference trajectory, can be combined with $\hat{\delta\underline{x}}^*(t_k|t_k)$ to yield the estimates $\hat{\underline{x}}^*(t_k|t_k)$ by

$$\hat{\underline{x}}^*(t_k|t_k) = \bar{\underline{x}}^*(t_k) + \hat{\delta\underline{x}}^*(t_k|t_k) \quad . \tag{5.29}$$

A schematic picture of the procedure we have just described is given in Figure 19. This procedure might be called an indirect method of nonlinear state estimation since it requires the coupled computation of a set of reference system deterministic dynamics and a set of estimates for small perturbations in the vicinity of the reference state trajectory. It is not yet the procedure of the extended Kalman filter.

We might also remark that the derivation of (5.28) serves a second purpose other than demonstrating simply the discrete-time dynamics of the small perturbations. Recall, therefore, that both the discrete and continuous-discrete LKF algorithms of sections 3.6 and 3.7 use the state transition matrix, here $\Phi^*\{\cdot\}$, for computing the evolution of the state estimation error covariance matrix. Indeed, it is important, since we have not already mentioned it, to check that the error covariance matrix for the small perturbations is identical to the error covariance matrix of the actual state-parameter vector estimates. Thus

$$\begin{aligned}\tilde{\underline{x}}^*(t_k|t_k) = \underline{x}^*(t_k) - \hat{\underline{x}}^*(t_k|t_k) &= \bar{\underline{x}}^*(t_k) + \delta\underline{x}^*(t_k) - \bar{\underline{x}}^*(t_k) - \hat{\delta\underline{x}}^*(t_k|t_k) \\ &= \delta\underline{x}^*(t_k) - \hat{\delta\underline{x}}^*(t_k|t_k) \\ &= \delta\tilde{\underline{x}}^*(t_k|t_k) \quad ,\end{aligned}$$

in other words

$$\mathrm{cov}\{\tilde{\underline{x}}^*(t_k|t_k)\} = \mathrm{cov}\{\delta\tilde{\underline{x}}^*(t_k|t_k)\} \triangleq P(t_k|t_k) \quad . \qquad (5.30)$$

5.2.4 The Choice of Nominal Reference Trajectory

Two factors in the arguments leading to the interim solution of our problem in the preceding section are of crucial significance. These are:

(i) the specification for $\underline{u}(t)$ as a known function of time;

(ii) the choice of $\bar{\underline{x}}(t_0)$,

both of which strongly influence the ability to obtain accurate estimates of the augmented state-parameter vector $\underline{x}^*$. Consider then the implications of Figure 19. A basic flaw in this coupled

indirect estimation method is that it operates in an "open loop" situation; in other words there is no feedback of information, such as the state estimates, with which to correct for the possibility of the reference model performance being inaccurate. Consequently if the choice of $\underline{\bar{u}}(t)$ does not closely resemble the measured variations $\underline{u}(t)$, and further if the unknown disturbances $\underline{\xi}(t)$ are amplified as they pass through to the process output response--which may well happen in a complex nonlinear system--then $\underline{\bar{x}}^*(t)$ may diverge considerably from $\underline{x}^*(t)$. The primary result of such divergence, other than the persistent mismatch between actual output, y, and reference output $\underline{\bar{y}}$, is that the perturbation $\delta\underline{x}^*(t)$ can no longer be assumed to be small. Hence the linearised system of equations, upon which the filtering algorithms are constructed, are not a valid approximation to the behaviour of small perturbations in the vicinity of the reference trajectory.

Two eminently sensible modifications can therefore be made. One of these modifications, a matter of repeatedly adapting the reference trajectory, is the principal defining characteristic of the EKF and leads to the formulation of the algorithms directly in terms of the vector $\underline{x}^*$ (as opposed to the perturbations $\delta\underline{x}^*$). First, however, since by definition the nature of the input disturbances $\underline{u}$ is that they can be measured and therefore known, it makes little sense to specify $\underline{\bar{u}}(t)$ differently from $\underline{u}(t)$. So let us propose the modification,

(i) that $\underline{\bar{u}}(t) = \underline{u}(t)$ and by definition, i.e. equation (5.9), $\delta\underline{u}(t) = \underline{0}$ in equations (5.22a) and (5.28).

Secondly, instead of making one initial choice $\underline{\bar{x}}^*(t) = \underline{\bar{x}}^*(t_0)$ at time t_0 for the reference state vector, let us choose $\underline{\bar{x}}^*(t_0) = \underline{\hat{x}}^*(t_0|t_0)$ and subsequently at each instant t_k put $\underline{\bar{x}}^*(t_k) = \underline{\hat{x}}^*(t_k|t_k)$ as soon as $\underline{\hat{x}}^*(t_k|t_k)$ becomes available. Thus we make the modification

(ii) that the solution of the reference trajectory is given by

$$d\underline{\bar{x}}^*(t)/dt = d\underline{\hat{x}}^*(t|t_{k-1})/dt = \underline{f}\{\underline{\hat{x}}^*(t|t_{k-1}), \underline{u}(t)\} \quad \text{for } t_{k-1} \leq t \leq t_k \,. \tag{5.31}$$

By this second modification, a procedure known as relinearisation, it is possible to obtain a set of linearised small perturbations equations, as (5.22) and (5.28), which are (hopefully) valid for small perturbations in the neighbourhood of the most recently derived state estimates. The definitions of the matrices F^*, G^*, H^*, Φ^*, and Γ^* will be accordingly altered as a consequence of the above two modifications. Figure 19 indicates by dashed lines the qualitative features of the modification.

Some inductive reasoning is used to complete the development of the EKF. If we initially linearise about $\hat{\underline{x}}^*(t_0|t_0)$, i.e. $\bar{\underline{x}}^*(t_0) = \hat{\underline{x}}^*(t_0|t_0)$ for the reference trajectory, then a best estimate of the small perturbations about the reference trajectory is that in fact there is initially no such small deviation from $\bar{\underline{x}}^*(t_0)$, or

$$\delta\hat{\underline{x}}^*(t_0|t_0) = \underline{0} \quad .$$

A best forward prediction, namely $\delta\hat{\underline{x}}^*(t_1|t_0)$ on the basis of (5.28), with $\delta\underline{u}(t_0) = \underline{0}$ by definition and with $\underline{\xi}^*(t_0) = \underline{0}$ by assumption (i.e. $\underline{\xi}^*(t_k)$ is a zero-mean, Gaussian, white-noise sequence), would therefore be

$$\delta\hat{\underline{x}}^*(t_1|t_0) = \Phi^*\{t_1,t_0\}\delta\hat{\underline{x}}^*(t_0|t_0) = \underline{0} \quad .$$

And since we would relinearise about $\hat{\underline{x}}^*(t_1|t_1)$, or in general about $\hat{\underline{x}}^*(t_k|t_k)$, we may state that

$$\delta\hat{\underline{x}}^*(t|t_{k-1}) = \underline{0} \quad \text{for } t_{k-1} \leq t \leq t_k \quad . \tag{5.32}$$

Thus by our choice of reference trajectory the small perturbation estimate equations over the interval $t_{k-1} \rightarrow t_k$ are equivalent to an unforced system initially at rest.

Given (5.32), and recalling how previously, for example in (5.29), the state estimate was intuitively obtained as the sum of the reference state and the best estimate of the small perturbations, then

$$\dot{\hat{\underline{x}}}^*(t|t_{k-1}) = \underline{f}\{\hat{\underline{x}}^*(t|t_{k-1}), \underline{u}(t)\} \; ; \quad \hat{\underline{x}}(t|t_{k-1}) = \hat{\underline{x}}(t_{k-1}|t_{k-1}) \quad ,$$
$$\text{for } t = t_{k-1} \text{ and } t_{k-1} \leq t \leq t_k \quad , \qquad (5.33)$$

yields the best forward extrapolated state-parameter estimates $\hat{\underline{x}}^*(t_k|t_{k-1})$ between the sampling instants t_{k-1} and t_k. Here, of course, we are assuming as before that the nonlinear differential equation (5.33) can be solved by some appropriate numerical routine. From (5.6a), (5.23a), and (5.33) one would hope that the relative variations of the true state, the uncorrected reference state, and the state estimates with updating of the reference state, respectively, might be as shown in Figure 20.

To summarise, we have now a procedure for extrapolation of the augmented state-parameter estimates between sampling instants, i.e. equation (5.33), but we are still required to examine the nature of the estimate updating mechanism. Thus, from a linear filter applied to the small perturbations equations we should obtain

$$\delta\hat{\underline{x}}^*(t_k|t_k) = \delta\hat{\underline{x}}^*(t_k|t_{k-1}) + K(t_k)[\,\delta\underline{y}(t_k) - H^*(t_k)\,\delta\hat{\underline{x}}^*(t_k|t_{k-1})] \quad . \qquad (5.34)$$

Let us consider what is really meant by $\delta\hat{\underline{x}}^*(t_k|t_k)$ in (5.34) in view of the chosen relinearisation procedure. Since $\delta\hat{\underline{x}}^*(t_k|t_{k-1}) = \underline{0}$ and after substituting for $\delta\underline{y}(t_k)$ from (5.19) and (5.20)

$$\delta\hat{\underline{x}}^*(t_k|t_k) = K(t_k)[\,\underline{y}(t_k) - \underline{h}\{\bar{\underline{x}}^*(t_k)\}] \quad . \qquad (5.35)$$

At time t_k, therefore, before correction of the estimates, but given $\underline{y}(t_k)$, the best estimate of $\bar{\underline{x}}^*(t_k)$ is $\hat{\underline{x}}^*(t_k|t_{k-1})$ so that in (5.35)

$$\delta\hat{\underline{x}}^*(t_k|t_k) = K(t_k)[\,\underline{y}(t_k) - \underline{h}\{\hat{\underline{x}}^*(t_k|t_{k-1})\}] \quad . \qquad (5.36)$$

So providing $K(t_k)$ can be suitably computed, and noticing that (5.36) is precisely the correction that would be applied to the a priori estimate in order to obtain the a posteriori estimate,

i.e.

$$\hat{\delta \underline{x}}^*(t_k|t_k) = \hat{\underline{x}}^*(t_k|t_k) - \hat{\underline{x}}^*(t_k|t_{k-1}) \quad , \tag{5.37}$$

then we have the desired estimate updating procedure: combining (5.36) and (5.37)

$$\hat{\underline{x}}^*(t_k|t_k) = \hat{\underline{x}}^*(t_k|t_{k-1}) + K(t_k)[\underline{y}(t_k) - \underline{h}\{\hat{\underline{x}}^*(t_k|t_{k-1})\}] \quad . \tag{5.38}$$

Figure 21 attempts to give further explanation of this procedure.

At this point both the prediction and correction algorithms for the state estimates can be written directly in terms of $\hat{\underline{x}}^*$ instead of in terms of $\hat{\delta \underline{x}}^*$. These algorithms were derived under the assumptions that:

(i) we are still employing a linear filter applied to the perturbation system representation;

(ii) we have made a prudent substitution for the deterministic reference trajectory.

It remains only for us to show that the estimation error covariances for the perturbation system are equivalent to those for the actual system. We already have that such an equivalence holds for $P(t_k|t_k)$, by equation (5.30), and now writing

$$\tilde{\underline{x}}^*(t_k|t_{k-1}) = \underline{x}^*(t_k) - \hat{\underline{x}}^*(t_k|t_{k-1}) = \bar{\underline{x}}^*(t_k) + \delta \underline{x}^*(t_k) - \hat{\underline{x}}^*(t_k|t_{k-1}) \ . \tag{5.39}$$

Noting that we have chosen $\bar{\underline{x}}^*(t_k^-) = \hat{\underline{x}}^*(t_k|t_{k-1})$ and that $\hat{\delta \underline{x}}^*(t_k|t_{k-1}) = \underline{0}$, then

$$\tilde{\underline{x}}^*(t_k|t_{k-1}) = \delta \underline{x}^*(t_k) - \hat{\delta \underline{x}}^*(t_k|t_{k-1}) = \delta \tilde{\underline{x}}^*(t_k|t_{k-1}) \ . \tag{5.40}$$

Thus

$$\mathrm{cov}\{\tilde{\underline{x}}^*(t_k|t_{k-1})\} = \mathrm{cov}\{\delta \tilde{\underline{x}}^*(t_k|t_{k-1})\} = P(t_k|t_{k-1}) \quad . \tag{5.41}$$

5.3 The Algorithms

The arguments leading to the EKF algorithms have been as follows. First, a linear Kalman filter can be applied to a set of linearised equations which result from the formulation of the combined state-parameter estimation problem. Second, however, if we choose always to relinearise about the most recent augmented state estimates $\hat{\underline{x}}^*(t_k|t_k)$, the algorithms for the direct prediction and correction of the state-parameter estimates are obtained which employ the original nonlinear functions of the system characterisation in (5.6), i.e. equations (5.33) and (5.38). Third, the linearised system dynamics representation will still have to be used for computation of the evolution of the estimation error covariance matrix.

In line with the statement of the LKF algorithms of equations (3.79), the extended Kalman filter algorithms are given by

(i) Prediction: between t_{k-1} and t_k

$$\hat{\underline{x}}^*(t_k|t_{k-1}) = \hat{\underline{x}}^*(t_{k-1}|t_{k-1}) + \int_{t_{k-1}}^{t_k} \underline{f}\{\hat{\underline{x}}^*(t|t_k),\underline{u}(t)\}dt \quad , \tag{5.42a}$$

$$P(t_k|t_{k-1}) = \Phi^*\{t_k,t_{k-1}\}P(t_{k-1}|t_{k-1})\Phi^{*T}\{t_k,t_{k-1}\} + Q^* \quad , \tag{5.42b}$$

(ii) Correction: at time t_k on receipt of $y(t_k)$

$$\hat{\underline{x}}^*(t_k|t_k) = \hat{\underline{x}}^*(t_k|t_{k-1}) + K(t_k)[\underline{y}(t_k) - \underline{h}\{\hat{\underline{x}}^*(t_k|t_{k-1})\}] \quad , \tag{5.42c}$$

$$P(t_k|t_k) = [I - K(t_k)H^*(t_k)]P(t_k|t_{k-1})[I - K(t_k)H^*(t_k)]^T + K(t_k)RK^T(t_k) \quad , \tag{5.42d}$$

with $K(t_k)$ given by

$$K(t_k) = P(t_k|t_{k-1})H^{*T}(t_k)[H^*(t_k)P(t_k|t_{k-1})H^{*T}(t_k) + R]^{-1} \quad . \tag{5.42e}$$

The notational abbreviations

$$\Phi^*\{t_k,t_{k-1}\} = \Phi^*\{t_k,t_{k-1};\hat{\underline{x}}^*(t_{k-1}|t_{k-1}),\underline{u}(t_{k-1})\} \quad , \tag{5.43a}$$

$$H^*(t_k) = H^*\{\hat{\underline{x}}^*(t_k|t_{k-1})\} \quad , \tag{5.43b}$$

have been used for purposes of clarity; the more precise arguments for these matrices of the linearised small perturbation equations indicate the manner in which the state estimates are substituted for the nominal reference trajectory--compare with the definitions of (5.18) and (5.25). The measurement noise covariance matrix is as previously defined for the LKF, since although we are estimating both parameters and states we have not altered the external (i.e. input/output) description of the system. The system noise covariance matrix Q*, however, is defined by

$$Q^* = \mathcal{E}\{\underline{\xi}^*(t_k)\underline{\xi}^{*T}(t_k)\} \quad ,$$

where $\underline{\xi}^*(t_k)$ is a zero-mean, white, Gaussian sequence. As before for the LKF, the variances of $\underline{\xi}^*(t_k)$ and $\underline{\eta}(t_k)$ are assumed to be constant with time, i.e. stationary. If this assumption is not valid, the algorithms are not made more complex; one is simply required to have knowledge of $Q^*(t_k)$ and $R(t_k)$ as functions of t_k.

5.3.1 Some Comments

Much of what has been said of the linear filter, for example in section 3.8, applies equally well to the EKF. But certain features should be clarified. Indeed, throughout sections 3 and 5 we have neatly avoided two awkward questions: one is a matter of theory and the other is a matter of practice. The notion of a continuous-time white noise process, say $\underline{\xi}(t)$, is a mathematical fiction since a physical realisation thereof does not exist. For this reason we have preferred merely to define covariance matrices for the discrete-time equivalents, say $\underline{\xi}(t_k)$ or $\underline{\xi}^*(t_k)$, of such a fictional process. Next, if in practice it is not possible to observe the system's outputs in the absence of errors, how can we assume, as we have done, that the measured system inputs, $\underline{u}$, are free of noise? Here again, the assumption is a device useful for the theoretical development of the filtering algorithms. Any uncertainty in $\underline{u}$ could have been made explicit in the covariance propagation equations, though it is much more convenient here to state that this category of uncertainty can be absorbed into the definition of the system noise covariance matrix

Q, or Q*. The system noise covariance matrix will also, incidentally, accommodate the analyst's specification of the uncertainty (or error) in his model as an approximation to reality.

Figure 22 provides a schematic diagram of the EKF algorithms. We have chosen this time to represent the filter differently from the schemes of Figures 13 and 14 for the linear Kalman filter by including a block diagram of the covariance prediction and correction computations. The intention is first to show the parallel nature of the state-parameter estimate propagation and the estimation error covariance propagation and second to emphasise the interaction that takes place between these two parallel functions. Notice, therefore, how the predicted and corrected state-parameter estimates are fed into the computation of the $H^*(t_k)$ and $\Phi^*\{t_k, t_{k-1}\}$ matrices respectively, compare with eqns (5.43). In the reverse direction it can be seen that the filter gain matrix $K(t_k)$ is fed back from the covariance algorithms to the state-parameter estimate algorithms. Now let us consider what would be the equivalent situation for the LKF. In this case the elements of the matrices Φ and H, see eqns (3.79), are completely known, i.e. the model parameter values are known precisely. Thus the evaluation of Φ and H is decoupled from the prediction and correction algorithms for the state-parameter estimates and hence the covariance algorithms operate autonomously, although they are subject, of course, to the analyst's specification of the Q and R matrices.

The two-way interaction of the EKF is in principle attractive since it holds out the tempting possibility of <u>adaptive</u> estimation. That is to say, like the bootstrap estimation characteristics discussed in section 4.2.3, the adaptation of the parameter values will improve the state estimation capabilities which in turn will enhance the likelihood of more accurate parameter estimation and so on. Unfortunately, there is a great difference between what is possible in principle and what is attainable in practice. For the EKF to perform at its most useful it is almost certainly necessary to have available reasonable estimates of the paramters a priori,as we shall see in later parts of the paper.

6. CONCLUSIONS

In this, Part 1 of a two-part paper, the basic components of recursive estimation have been presented. We have shown that a fundamental feature of the recursive estimator is the way in which the estimates are corrected by a weighted model response error function. In other words, the algorithm continually adapts its estimates on the basis of feedback information about the discrepancy between model prediction and actually observed behaviour. The principal theoretical development of the paper has been concerned with the linear Kalman filter. For this particular algorithm the weighting factors of the correcting mechanism for the estimates are computed in part from the estimation error covariance matrix.

Six forms of recursive (state or parameter) estimation algorithms have been discussed. These are: the recursive least squares algorithm, equations (4.20) or (4.35); a recursive instrumental variable estimator, equation (4.33); a recursive algorithm with exponential weighting of past data, equation (4.40); a dynamic least squares algorithm, equation (4.51); the linear Kalman filter, equations (3.79); and the extended Kalman filter, equation (5.42). In Part 2, which deals with the application of these algorithms, the specific character of some of the case studies will require additional, but only minor, modification of these six basic algorithms.

Appendix 1: Minimising the Squared-error Loss Function

Analytical derivations are given for minimising a squared-error loss function. We consider first the case of scalar observations and then the case of vector observations.

(i) Scalar Observations

From equation (3.9) we have the loss function

$$J = \sum_{k=1}^{N} (y(t_k) - \underline{x}^T(t_k)\hat{\underline{\alpha}})^2 \quad , \tag{A1.1}$$

so that differentiating J with respect to the parameter vector $\hat{\underline{\alpha}}$ gives

$$\nabla_{\hat{\underline{\alpha}}} J = \sum_{k=1}^{N} \nabla_{\hat{\underline{\alpha}}} \{ y^2(t_k) - 2y(t_k)\underline{x}^T(t_k)\hat{\underline{\alpha}} + \underline{x}^T(t_k)\hat{\underline{\alpha}}\,\underline{x}^T(t_k)\hat{\underline{\alpha}} \}$$

$$= \sum_{k=1}^{N} \nabla_{\hat{\underline{\alpha}}} \{ y^2(t_k) - 2_y(t_k)\underline{x}^T(t_k)\hat{\underline{\alpha}} + \hat{\underline{\alpha}}^T\underline{x}(t_k)\underline{x}^T(t_k)\hat{\underline{\alpha}} \} \quad . \tag{A1.2}$$

Carrying out the differentiation in (A1.2) on each term yields:

$$\nabla_{\hat{\underline{\alpha}}} \{ y^2(t_k) \} = \underline{0} \quad , \tag{A1.3}$$

$$\nabla_{\hat{\underline{\alpha}}} \{ -2y(t_k)\underline{x}^T(t_k)\hat{\underline{\alpha}} \} = -2y(t_k)\underline{x}(t_k) \quad , \tag{A1.4}$$

$$\nabla_{\underline{\hat{\alpha}}}\{\underline{\hat{\alpha}}^T[\underline{x}(t_k)\underline{x}^T(t_k)]\underline{\hat{\alpha}}\} = [\underline{x}(t_k)\underline{x}^T(t_k)]\underline{\hat{\alpha}} + [\underline{x}(t_k)\underline{x}^T(t_k)]^T\underline{\hat{\alpha}}$$

$$= 2[\underline{x}(t_k)\underline{x}^T(t_k)]\underline{\hat{\alpha}} \quad , \qquad \text{(A1.5)}$$

where in the last step the matrix $[\underline{x}(t_k)\underline{x}^T(t_k)]$ is symmetric and thus the transpose of this matrix equals the matrix itself. Gathering together the derivatives of (A1.3), (A1.4), and (A1.5) and putting the result to zero gives the conditions for the minimum value of J, i.e.

$$\nabla_{\underline{\hat{\alpha}}}J = 2[\sum_{k=1}^{N}\underline{x}(t_k)\underline{x}^T(t_k)]\underline{\hat{\alpha}} - 2[\sum_{k=1}^{N}\underline{x}(t_k)y(t_k)] = \underline{0} \quad , \qquad \text{(A1.6)}$$

which is the result of euqation (3.10) in section 3.1.

(ii) Vector Observations

From equation 3.21 we have the loss function

$$J = \sum_{k=1}^{N}\{(\underline{y}(t_k) - X(t_k)\underline{\hat{\alpha}})^T(\underline{y}(t_k) - X(t_k)\underline{\hat{\alpha}})\} \quad . \qquad \text{(A1.7)}$$

Differentiating J with respect to $\underline{\hat{\alpha}}$ gives,

$$\nabla_{\underline{\hat{\alpha}}}J = \sum_{k=1}^{N}\nabla_{\underline{\hat{\alpha}}}\{(\underline{y}^T(t_k) - \underline{\hat{\alpha}}^TX^T(t_k))(\underline{y}(t_k) - X(t_k)\underline{\hat{\alpha}})\}$$

$$= \sum_{k=1}^{N}\nabla_{\underline{\hat{\alpha}}}\{\underline{y}^T(t_k)\underline{y}(t_k) - \underline{\hat{\alpha}}^TX^T(t_k)\underline{y}(t_k) - \underline{y}^T(t_k)X(t_k)\underline{\hat{\alpha}} + \underline{\hat{\alpha}}^TX^T(t_k)X(t_k)\underline{\hat{\alpha}}\}$$

$$= \sum_{k=1}^{N}\{\underline{0} - X^T(t_k)\underline{y}(t_k) - X^T(t_k)\underline{y}(t_k) + X^T(t_k)X(t_k)\underline{\hat{\alpha}} + X^T(t_k)X(t_k)\underline{\hat{\alpha}}\}$$

$$= \sum_{k=1}^{N}\{2X^T(t_k)X(t_k)\underline{\hat{\alpha}} - 2X^T(t_k)\underline{y}(t_k)\} \quad . \qquad \text{(A1.8)}$$

Hence when the derivative of (A1.8) is set equal to

zero, we have

$$\nabla_{\underline{\hat{\alpha}}} J = 2\left[\sum_{k=1}^{N} X^T(t_k)X(t_k)\right]\underline{\hat{\alpha}} - 2\left[\sum_{k=1}^{N} X^T(t_k)\underline{y}(t_k)\right] \quad , \qquad \text{(A1.9)}$$

which leads to the result quoted in equation (3.22) of section 3.2.

Appendix 2: The Recursive Least Squares Algorithm

From section 3.4 the following recursive relationships, equations (3.45), are given as the starting point for the derivation of the recursive least squares algorithm,

$$[P^*(t_k)]^{-1} = [P^*(t_{k-1})]^{-1} + H^T H \quad , \tag{A2.1}$$

$$\underline{b}(t_k) = \underline{b}(t_{k-1}) + H^T \underline{y}(t_k) \quad . \tag{A2.2}$$

If (A2.1) is premultiplied by $P^*(t_k)$ and then post-multiplied by $P^*(t_{k-1})$, then

$$P^*(t_{k-1}) = P^*(t_k) + P^*(t_k)H^T H P^*(t_{k-1}) \quad . \tag{A2.3}$$

Postmultiplying (A2.3) by H^T gives,

$$P^*(t_{k-1})H^T = P^*(t_k)H^T[I + HP^*(t_{k-1})H^T] \quad , \tag{A2.4}$$

so that further post-multiplication by $[I + HP^*(t_{k-1})H^T]^{-1}HP^*(t_{k-1})$ yields

$$P^*(t_{k-1})H^T[I + HP^*(t_{k-1})H^T]^{-1}HP^*(t_{k-1}) = P^*(t_k)H^T H P^*(t_{k-1}) \quad . \tag{A2.5}$$

Substituting for $P^*(t_k)H^THP^*(t_{k-1})$ from (A2.3) gives finally:

$$P^*(t_k) = P^*(t_{k-1}) - P^*(t_{k-1})H^T[I + HP^*(t_{k-1})H^T]^{-1}HP^*(t_{k-1}) \quad . \tag{A2.6}$$

This is the second of equations (3.46). The recursive algorithm for $\hat{\underline{x}}(t_k)$ can now be developed by substituting for $\underline{b}(t_k)$ from (A2.2) and for $P^*(t_k)$ from (A2.6) into the equation,

$$\hat{\underline{x}}(t_k) = P^*(t_k)\underline{b}(t_k) \quad , \tag{A2.7}$$

i.e.

$$\hat{\underline{x}}(t_k) = [P^*(t_{k-1}) - P^*(t_{k-1})H^T[I + HP^*(t_{k-1})H^T]^{-1}HP^*(t_{k-1})]\{\underline{b}(t_{k-1}) + H^T\underline{y}(t_k)\} \quad , \tag{A2.8}$$

and since $\hat{\underline{x}}(t_{k-1}) = P^*(t_{k-1})\underline{b}(t_{k-1})$ this expression can be expanded to give

$$\begin{aligned}
\hat{\underline{x}}(t_k) &= \hat{\underline{x}}(t_{k-1}) - P^*(t_{k-1})H^T[I + HP^*(t_{k-1})H^T]^{-1}H\hat{\underline{x}}(t_{k-1}) \\
&\quad + P^*(t_{k-1})H^T\underline{y}(t_k) - P^*(t_{k-1})H^T[I + HP^*(t_{k-1})H^T]^{-1}HP^*(t_{k-1})H^T\underline{y}(t_k) \\
&= \hat{\underline{x}}(t_{k-1}) - P^*(t_{k-1})H^T[I + HP^*(t_{k-1})H^T]^{-1}H\hat{\underline{x}}(t_{k-1}) \\
&\quad + P^*(t_{k-1})H^T[I + HP^*(t_{k-1})H^T]^{-1}\{(I + HP^*(t_{k-1})H^T) \\
&\quad - HP^*(t_{k-1})H^T\}\underline{y}(t_k) \quad .
\end{aligned} \tag{A2.9}$$

Hence from (A2.9), we have:

$$\hat{\underline{x}}(t_k) = \hat{\underline{x}}(t_{k-1}) + P^*(t_{k-1})H^T[I + HP^*(t_{k-1})H^T]^{-1}\{\underline{y}(t_k) - H\hat{\underline{x}}(t_{k-1})\} \quad . \tag{A2.10}$$

This is the first of equations (3.46).

Appendix 3: Recursive Least Squares Algorithms for State and Covariance Correction in a System at Steady State

In equation (3.68) of section 3.5 a relationship is given for the matrix $P^*(t_k)$ in terms of the estimation error covariance matrix $P(t_k)$, i.e.

$$P^*(t_k) = P(t_k)H^T R^{-1}(H^T)^{-1} \quad . \tag{A3.1}$$

We wish to substitute this expression for $P^*(t_k)$ in the recursive least squares algorithms of (3.46). Thus, in the first of algorithms (3.46),

$$\underline{\hat{x}}(t_k) = \underline{\hat{x}}(t_{k-1}) + P(t_{k-1})H^T R^{-1}(H^T)^{-1}H^T[I + HP(t_{k-1})H^T R^{-1}(H^T)^{-1}H^T]^{-1}\{\underline{y}(t_k) - H\underline{\hat{x}}(t_{k-1})\} \ , \tag{A3.2}$$

$$= \underline{\hat{x}}(t_{k-1}) + P(t_{k-1})H^T R^{-1}[I + HP(t_{k-1})H^T R^{-1}]^{-1}\{\underline{y}(t_k) - H\underline{\hat{x}}(t_{k-1})\}$$

$$= \underline{\hat{x}}(t_{k-1}) + P(t_{k-1})H^T[R + HP(t_{k-1})H^T R^{-1}R]^{-1}\{\underline{y}(t_k) - H\underline{\hat{x}}(t_{k-1})\} \ , \tag{A3.3}$$

That is,

$$\underline{\hat{x}}(t_k) = \hat{x}(t_{k-1}) + K(t_k)\{\underline{y}(t_k) - H\underline{\hat{x}}(t_{k-1})\} \quad , \tag{A3.4}$$

where

$$K(t_k) = P(t_{k-1})H^T[HP(t_{k-1})H^T + R]^{-1} \quad . \tag{A3.5}$$

Now compare (A3.5) with the previous expression for $K^*(t_k)$ given by (3.47), i.e.

$$K^*(t_k) = P^*(t_{k-1})H^T[HP^*(t_{k-1})H^T + I]^{-1} \quad . \tag{A3.6}$$

Noting thus that the manipulations (A3.2) → (A3.5) allow, in effect, the substitution of $K(t_k)$ for $K^*(t_k)$, we have after substituting for $P^*(t_k)$ in the second of algorithms (3.46)

$$P(t_k)H^TR^{-1}(H^T)^{-1} = P(t_{k-1})H^TR^{-1}(H^T)^{-1} - K(t_k)HP(t_{k-1})H^TR^{-1}(H^T)^{-1} \quad . \tag{A3.7}$$

All terms in (A3.7) have a common factor of $H^TR^{-1}(H^T)^{-1}$; hence,

$$P(t_k) = P(t_{k-1}) - K(t_k)HP(t_{k-1}) \quad . \tag{A3.8}$$

Or

$$P(t_k) = [I - K(t_k)H]P(t_{k-1}) \quad . \tag{A3.9}$$

In fact, from (A3.9) and (A3.4) we see that we have transformed (3.46) into:

$$\left.\begin{aligned} \underline{\hat{x}}(t_k) &= \underline{\hat{x}}(t_{k-1}) + P(t_{k-1})H^T[HP(t_{k-1})H^T + R]^{-1}\{\underline{y}(t_k) - H\underline{\hat{x}}(t_{k-1})\} \quad , \\ P(t_k) &= P(t_{k-1}) - P(t_{k-1})H^T[HP(t_{k-1})H^T + R]^{-1}HP(t_{k-1}) \quad , \end{aligned}\right\} \tag{A3.10}$$

which are the algorithms of equation (3.69) in section 3.5.

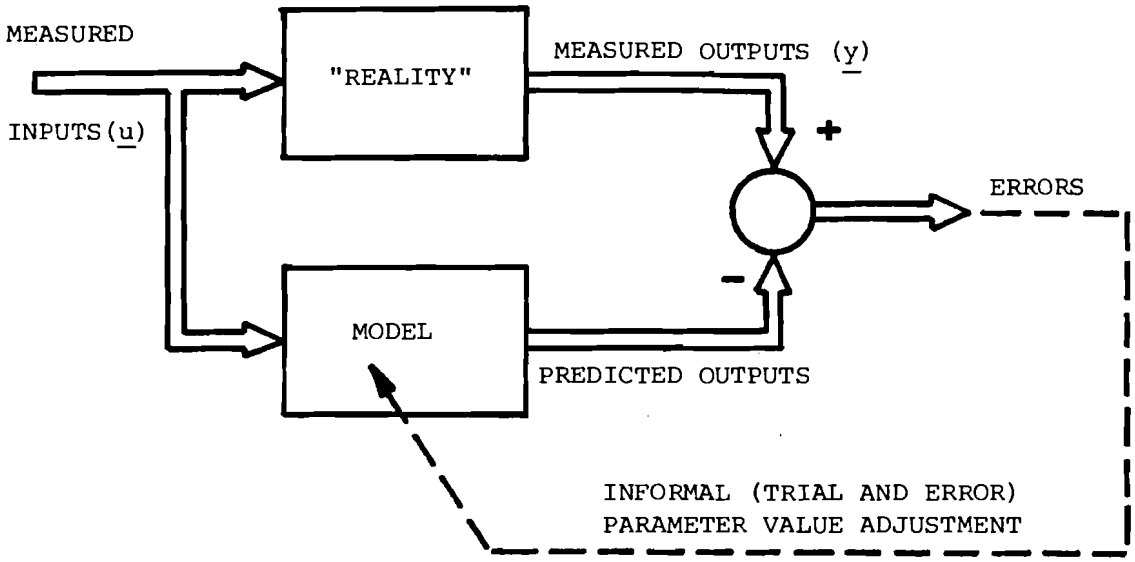

Figure 1. A rudimentary method of model calibration.

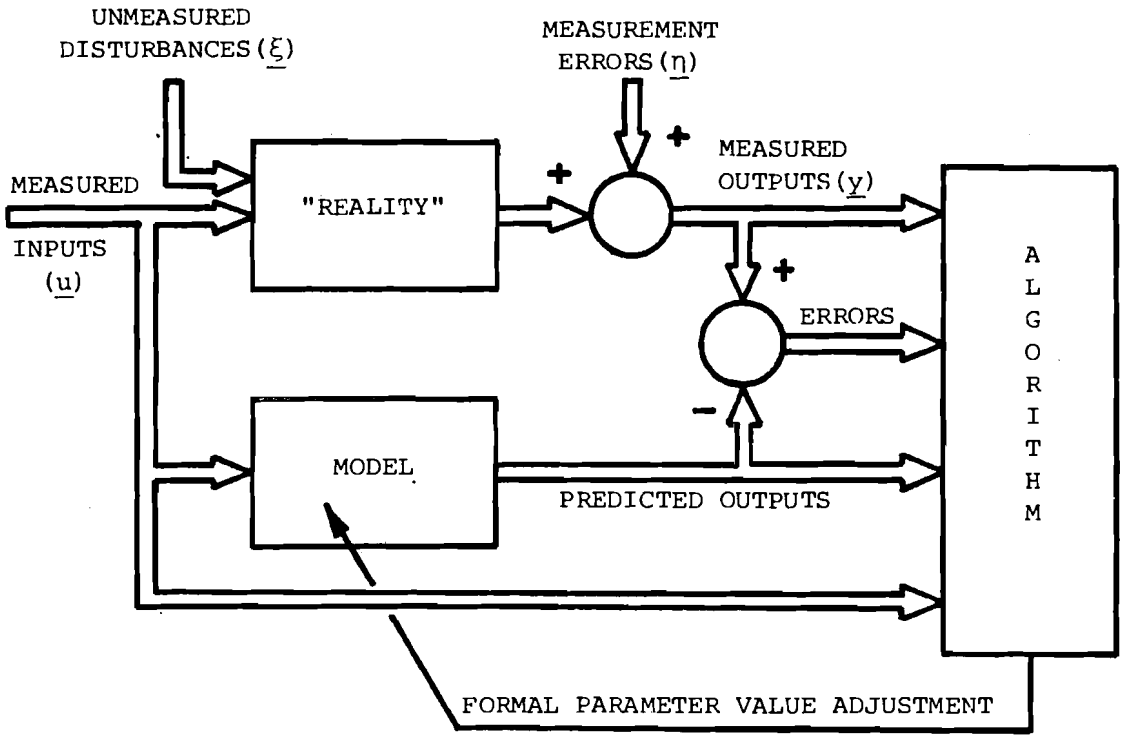

Figure 2. A more formal method of model calibration.

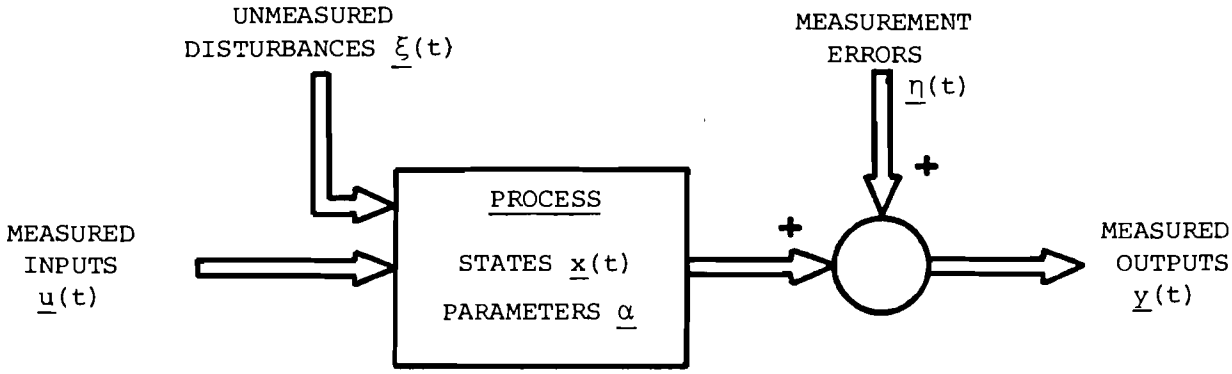

Figure 3. Definition of the system and variables.

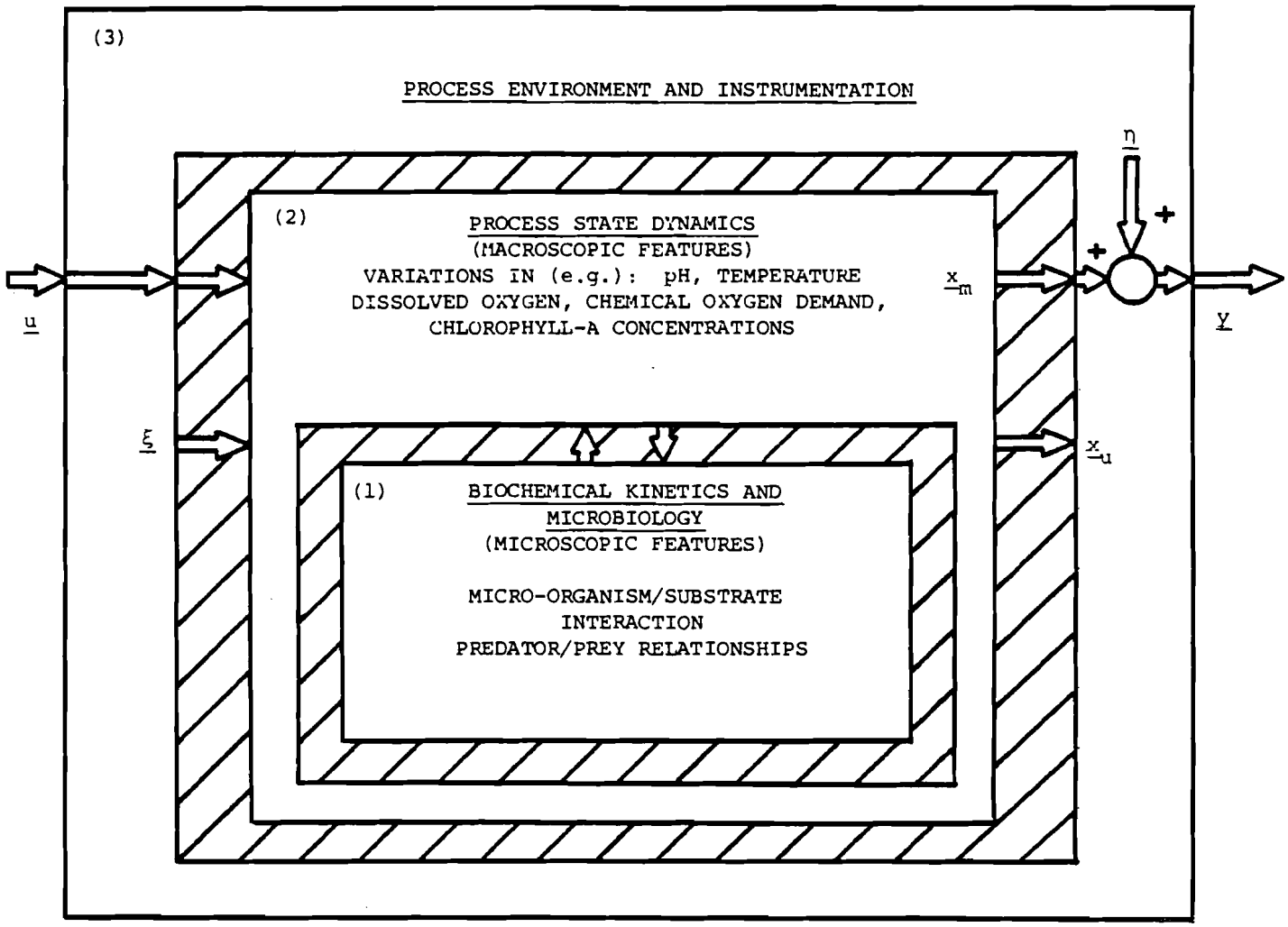

Figure 4. A schematic representation of how the input/output observations are related to the biochemical and microbiological aspects of the process dynamics.

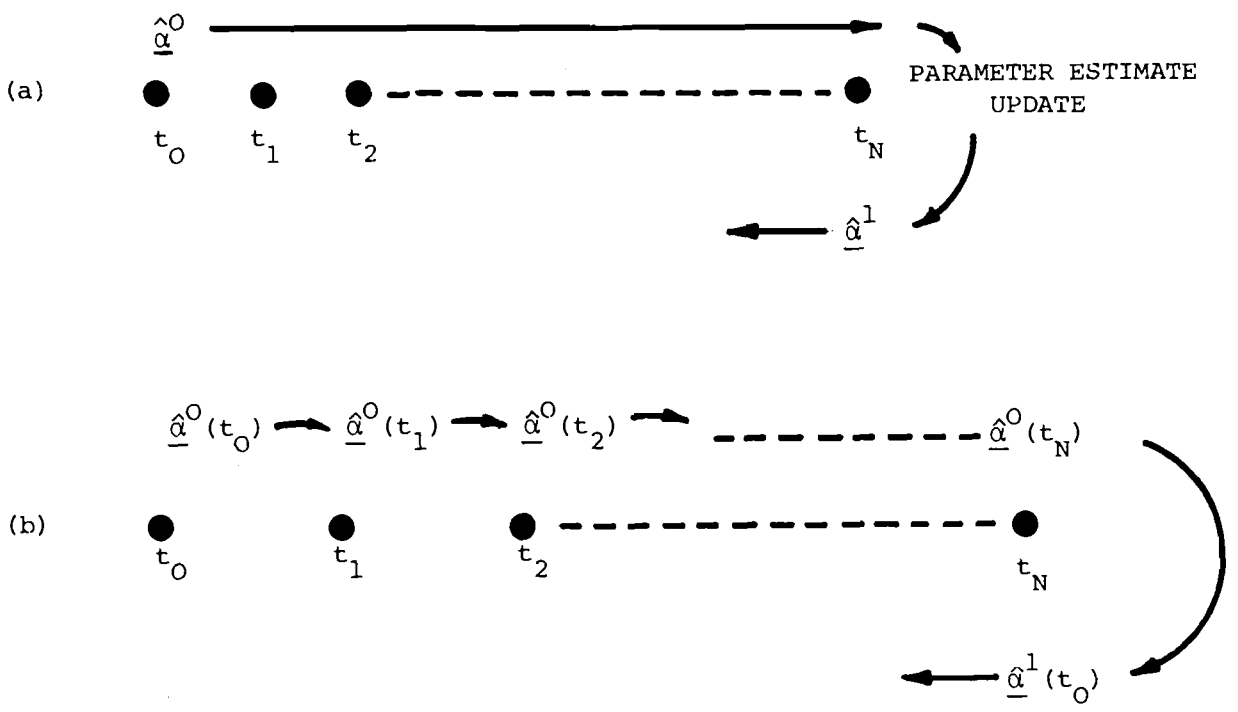

Figure 5. Methods of parameter estimation: (a) off-line; (b) recursive. The notation t_k in this example denotes the kth discrete sampling instant in a time-series with N samples; the superscript i in $\hat{\underline{\alpha}}^i$ denotes the estimate at the beginning of the (i + 1)th iteration through the data.

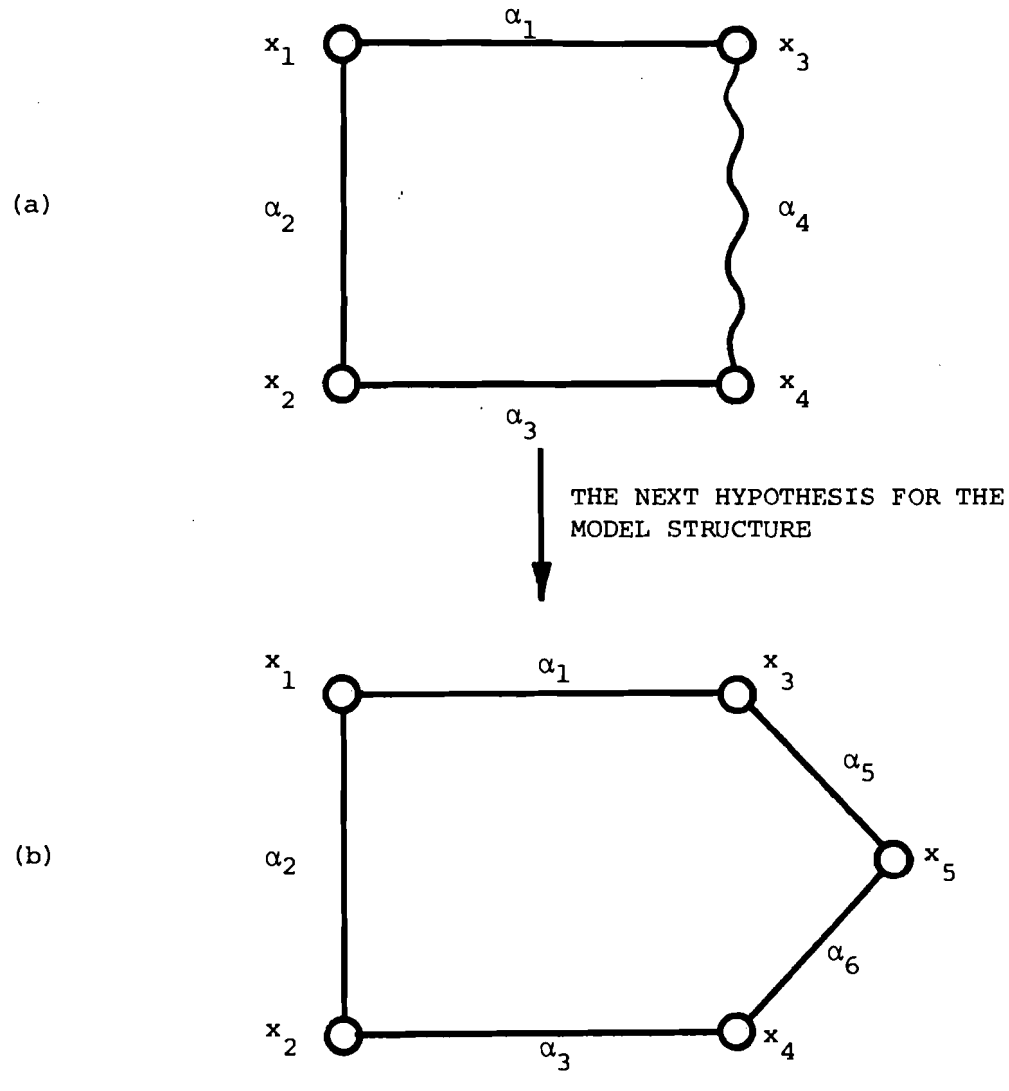

Figure 6. A conceptual picture of the problem of model structure identification.

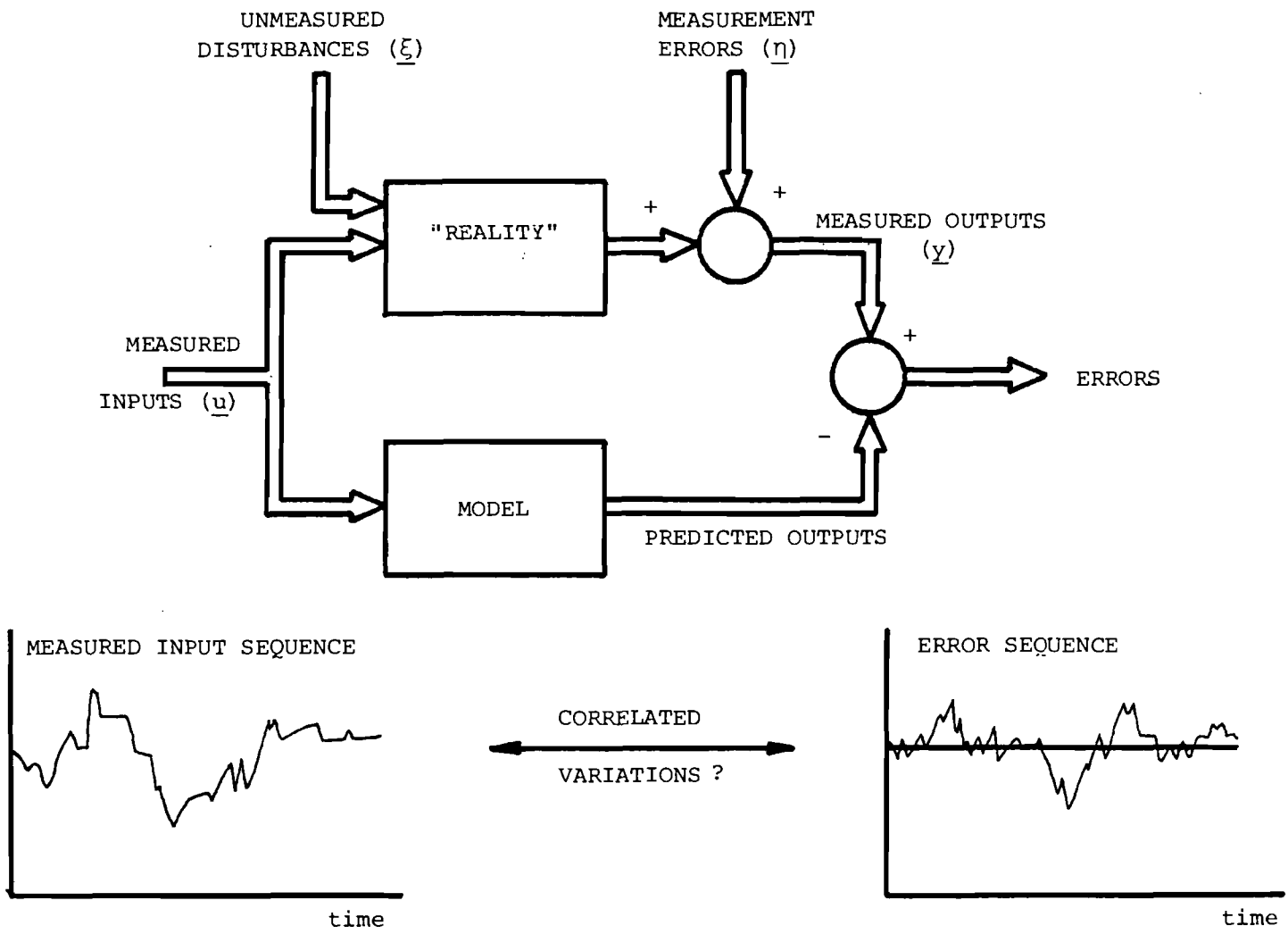

Figure 7. Model verification: computing the residual error sequences and checking their statistical properties.

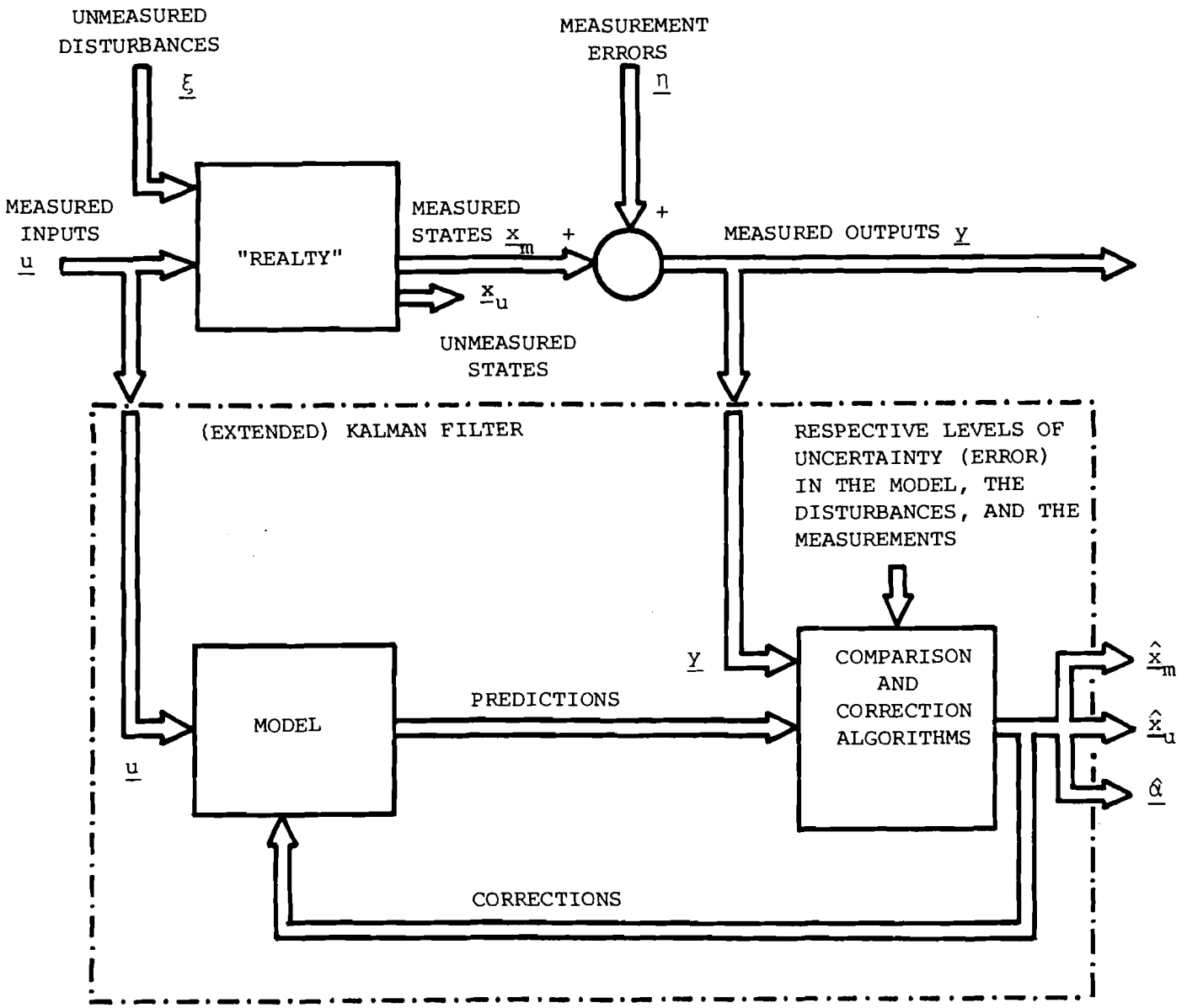

Figure 8. Basic conceptual features of the Kalman filter.

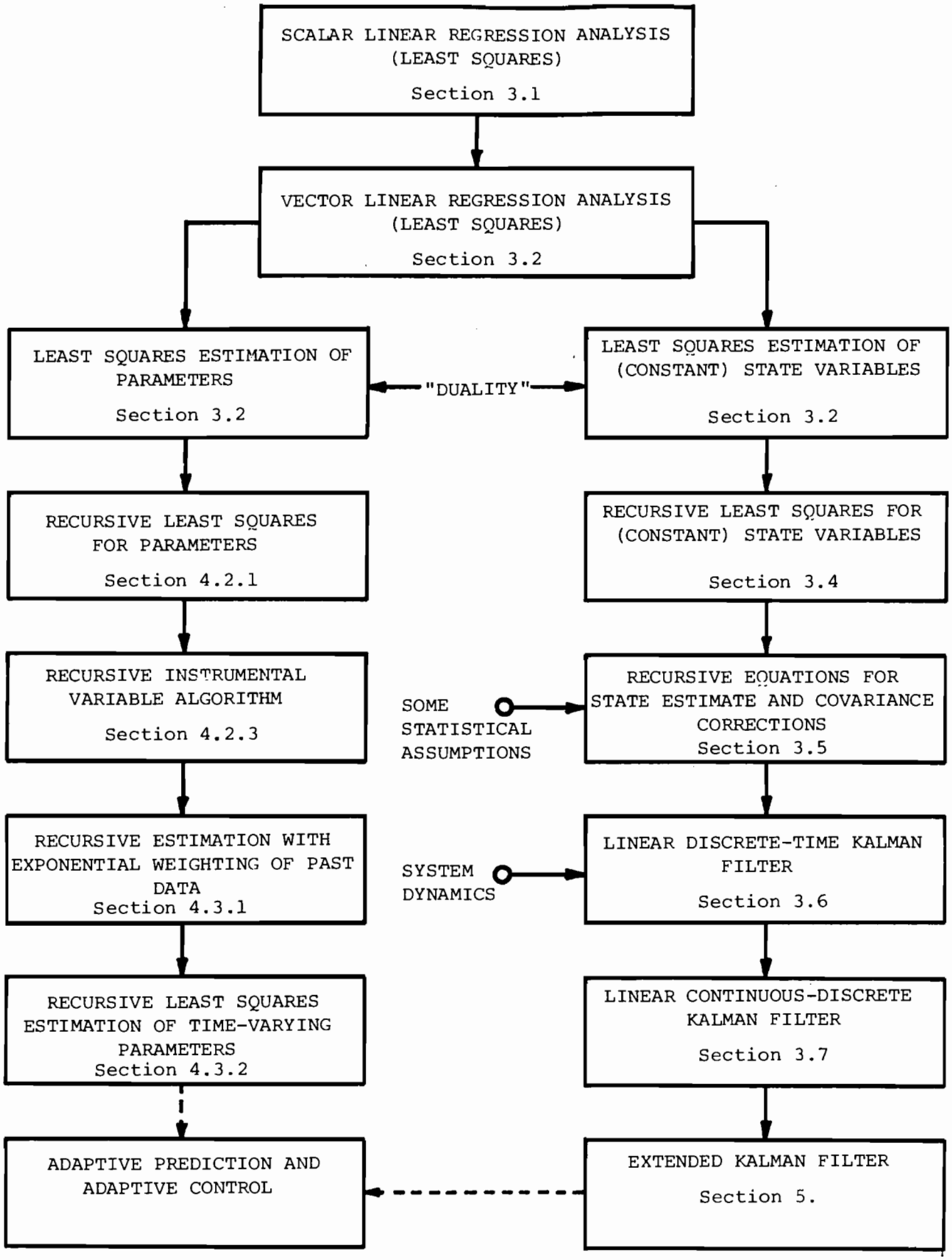

Figure 9. Recursive estimation algorithms: an outline of the derivation of the linear Kalman filter.

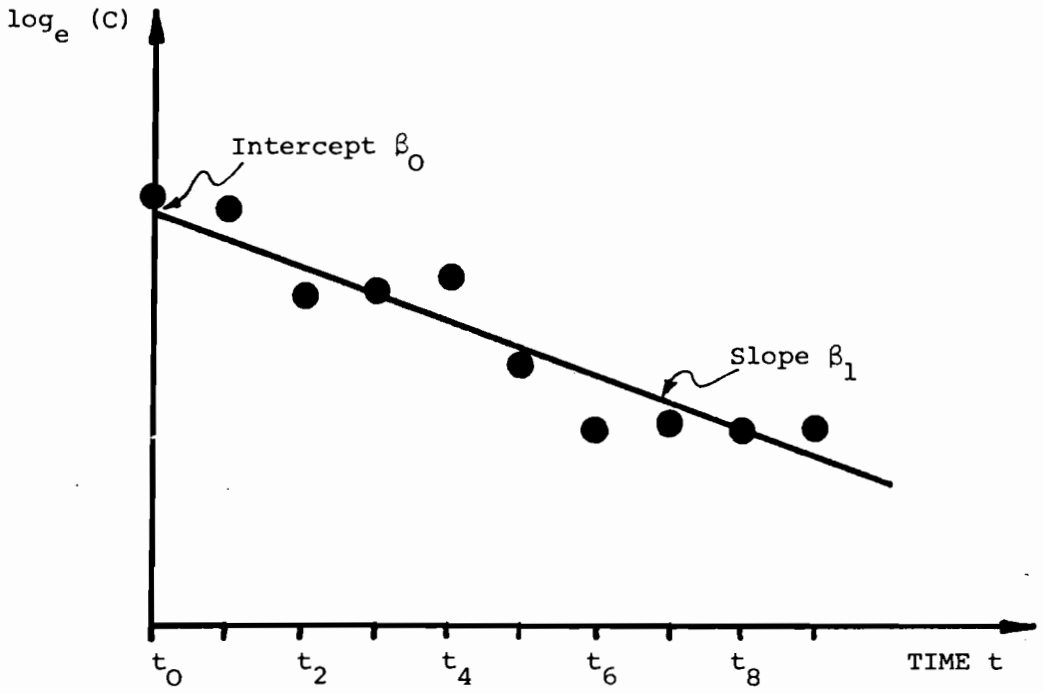

Figure 10. Linear regression analysis of observations on the decay of a substance, concentration C, with time t.

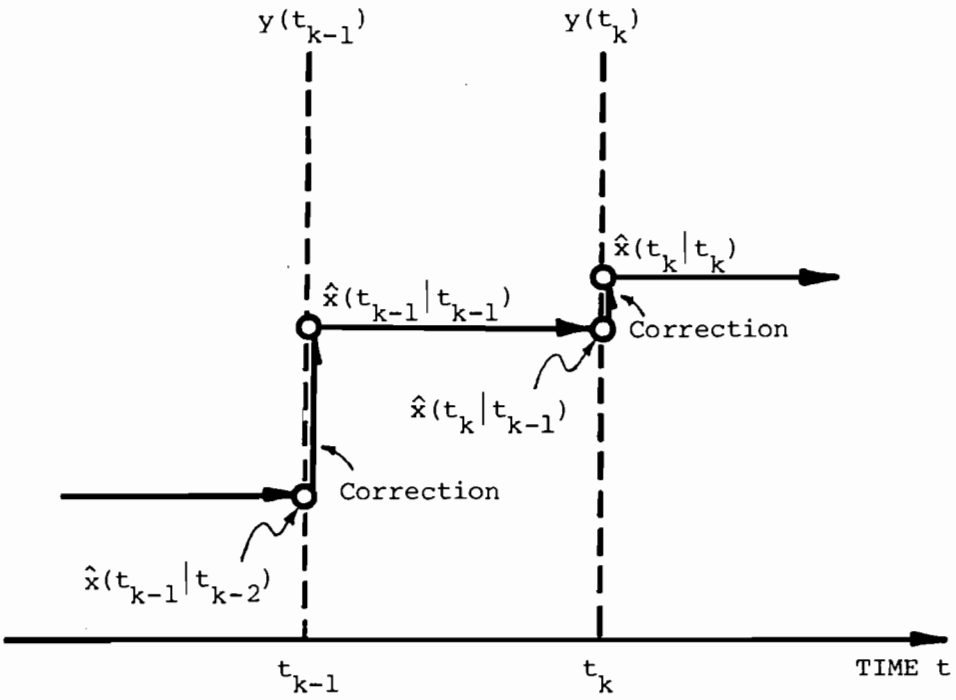

Figure 11. A priori state estimates, a posteriori estimates and estimate corrections for a system not exhibiting dynamic behavior.

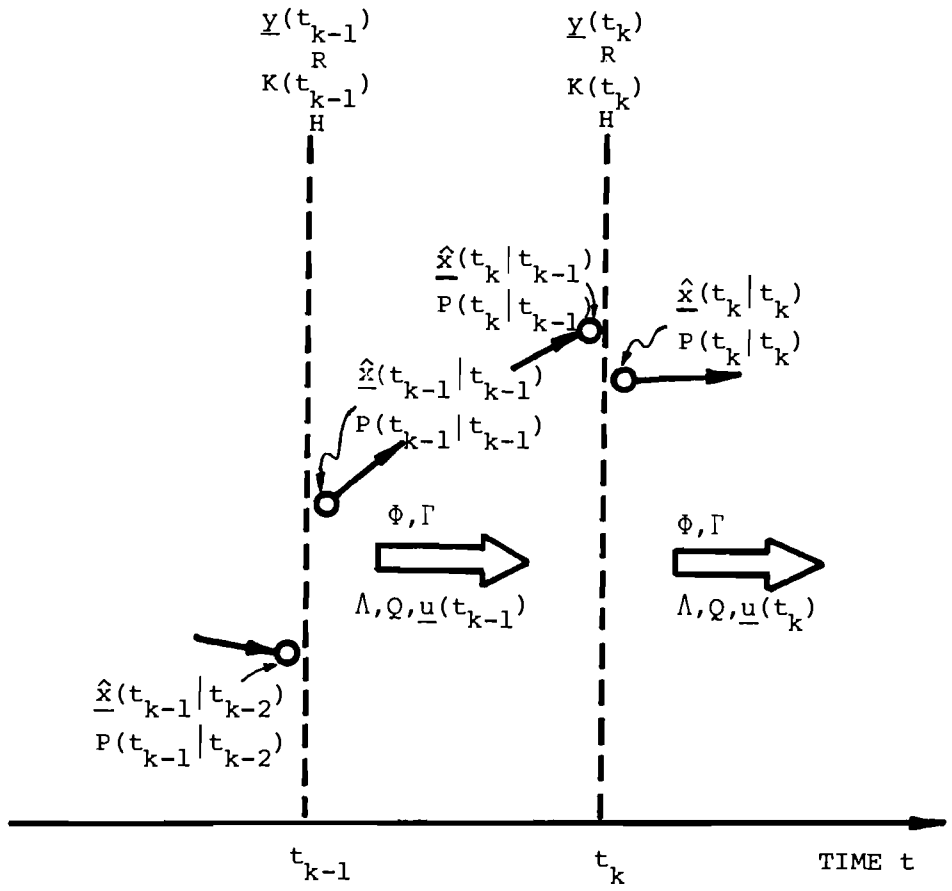

Figure 12. Updating and prediction schedule for the linear discrete-time Kalman filter.

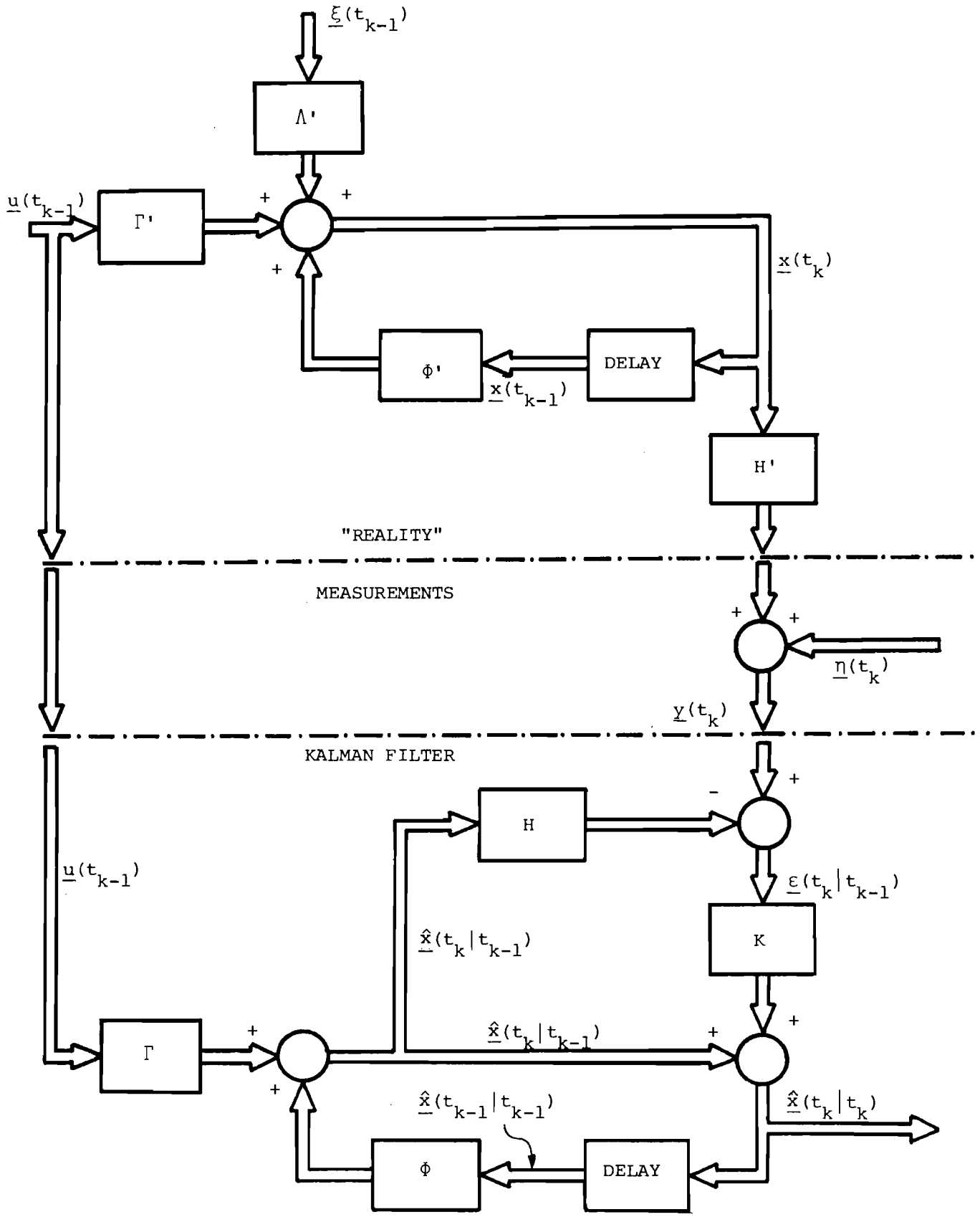

Figure 13. Block diagram of the linear discrete-time Kalman filter. The prime notation indicates that the matrices assumed for the filter are not necessarily identical with those of reality.

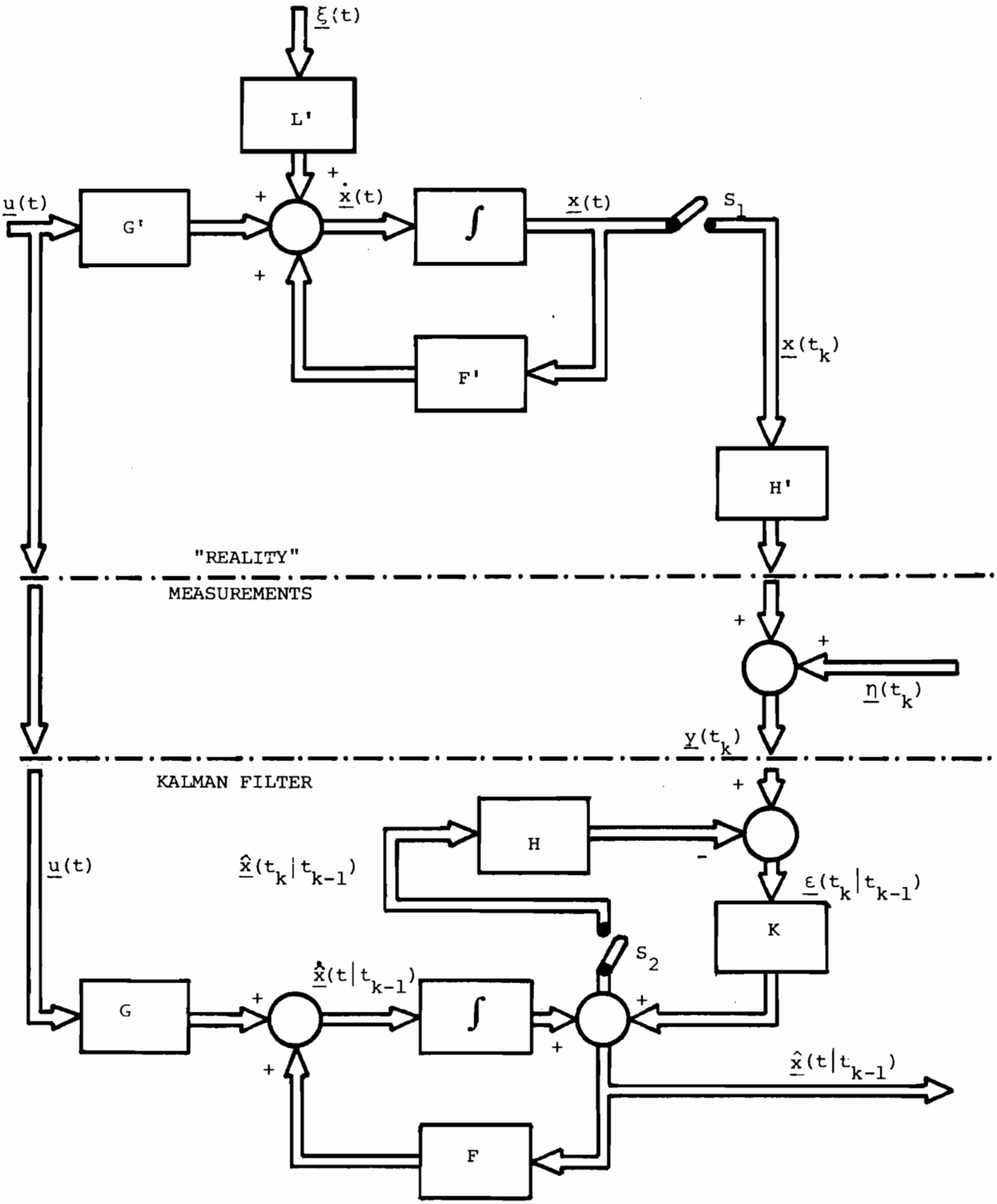

Figure 14. Block diagram of the linear continuous-discrete Kalman filter. The sampling switches S_1 and S_2 close instantaneously at time t_k.

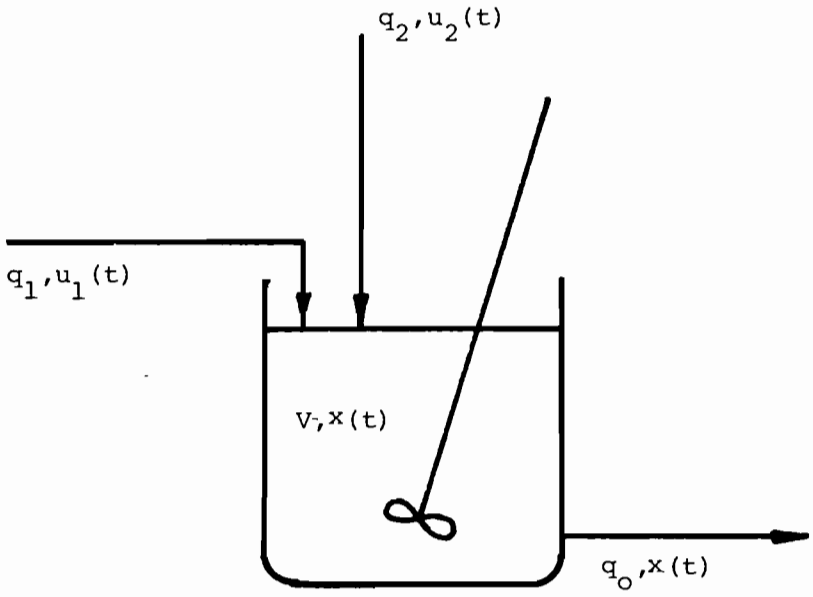

Figure 15. Continuously stirred tank reactor in which a substance, concentration x(t), decays with first-order rate kinetics.

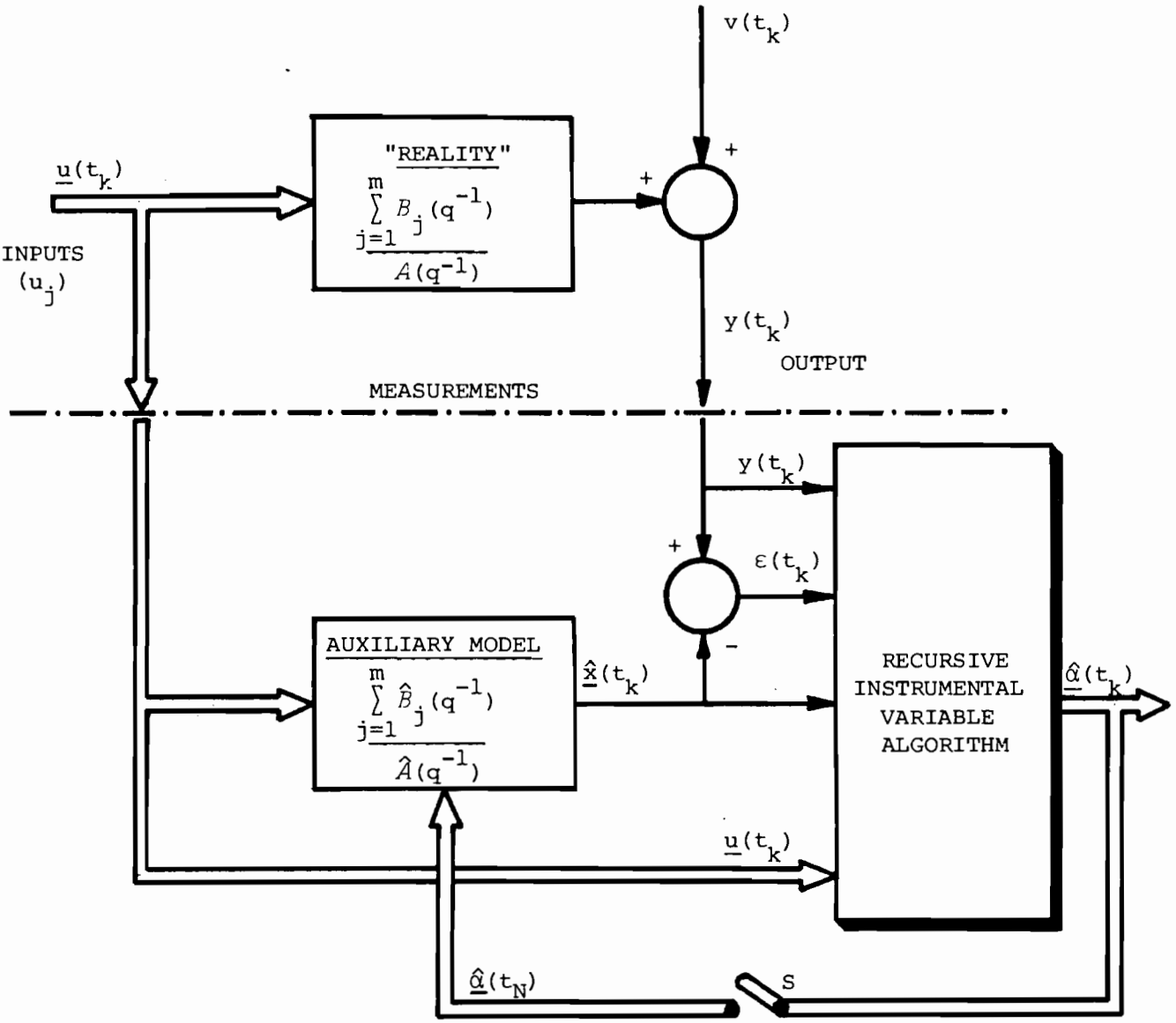

Figure 16. Block diagram of the recursive Instrumental Variable algorithm (compare with Figures 2 and 8). The switch S closes at the end, t_N, of each pass through the block of N data samples.

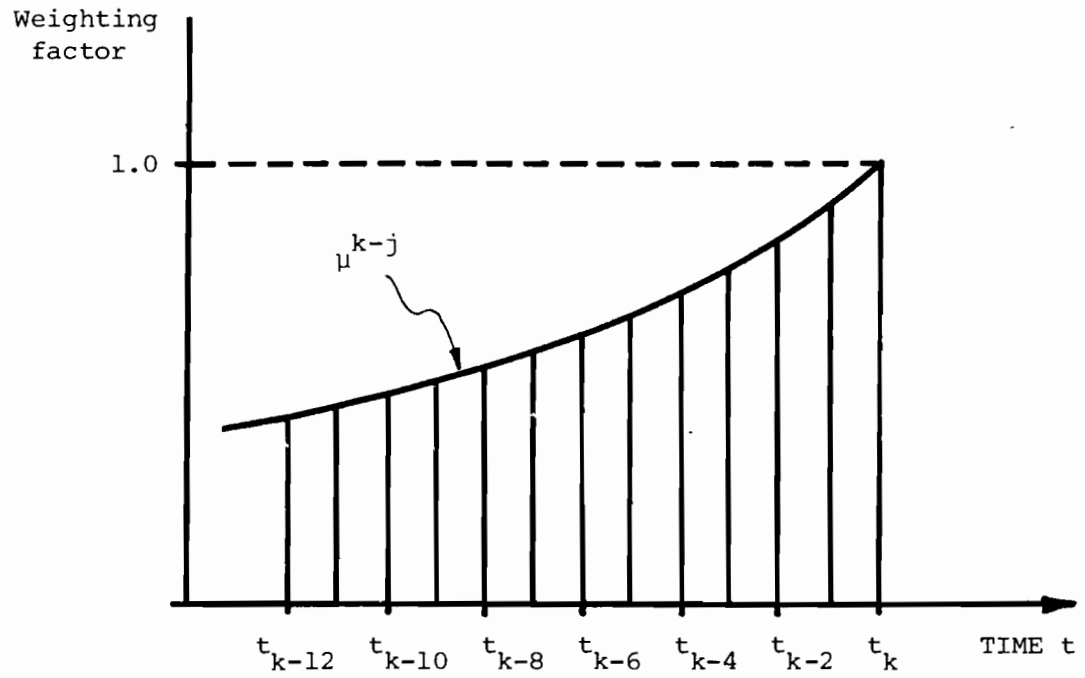

Figure 17. Weighting factors for exponential weighting of past data.

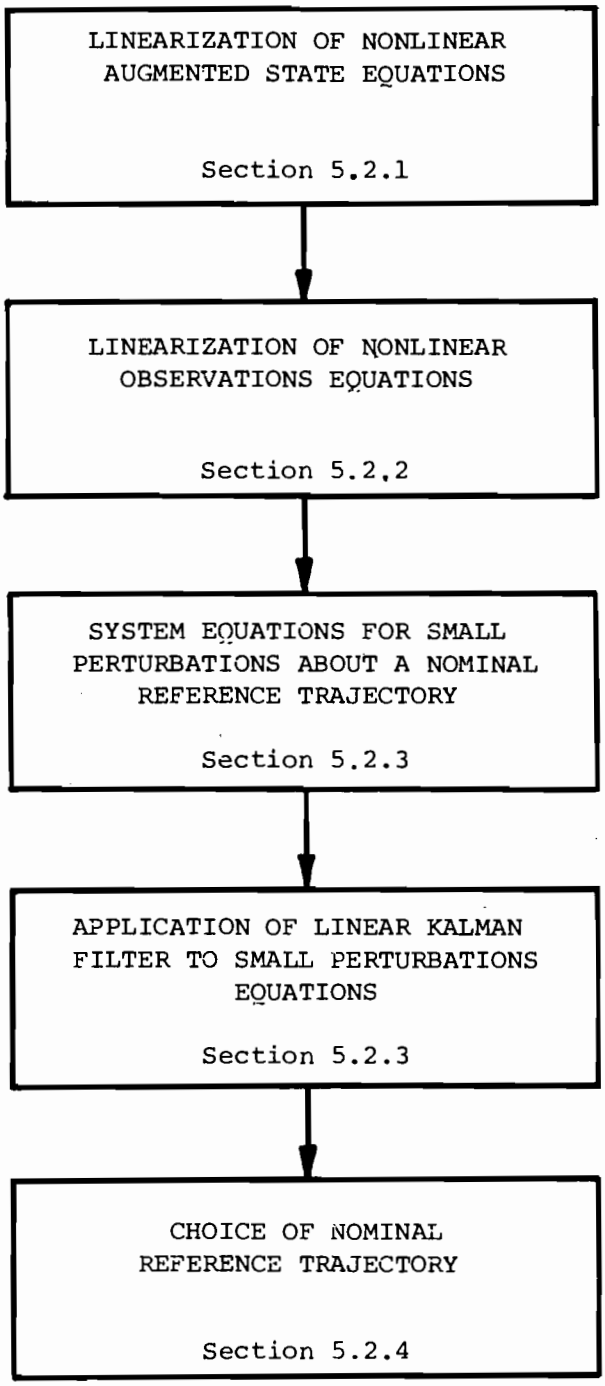

Figure 18. Steps in the derivation of the extended Kalman filtering algorithms.

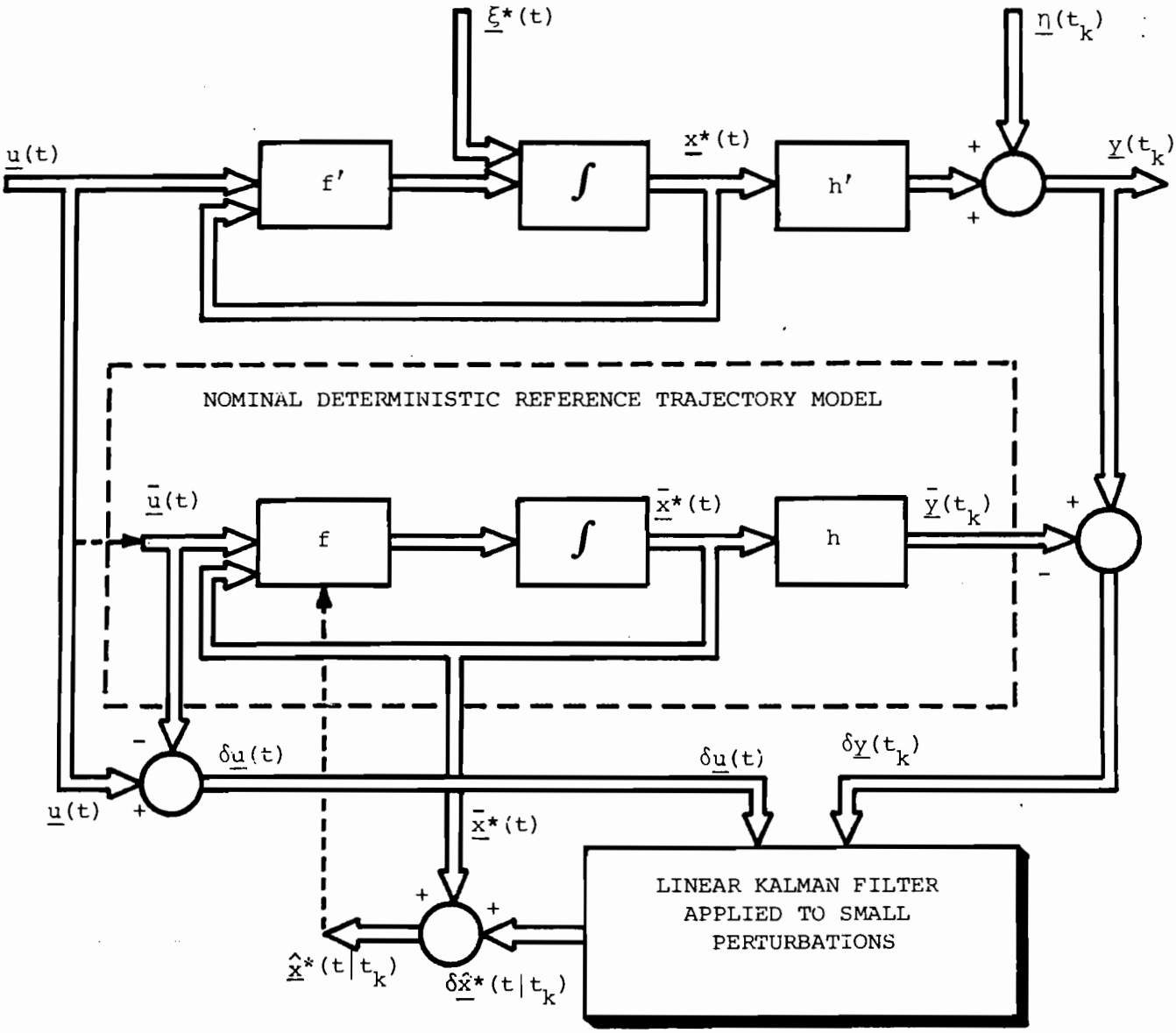

Figure 19. A linear Kalman filter applied to the small perturbation equations for estimation of state and parameters in a non-linear system with known reference trajectory (the dashed lines indicate modifications required for the extended Kalman filter).

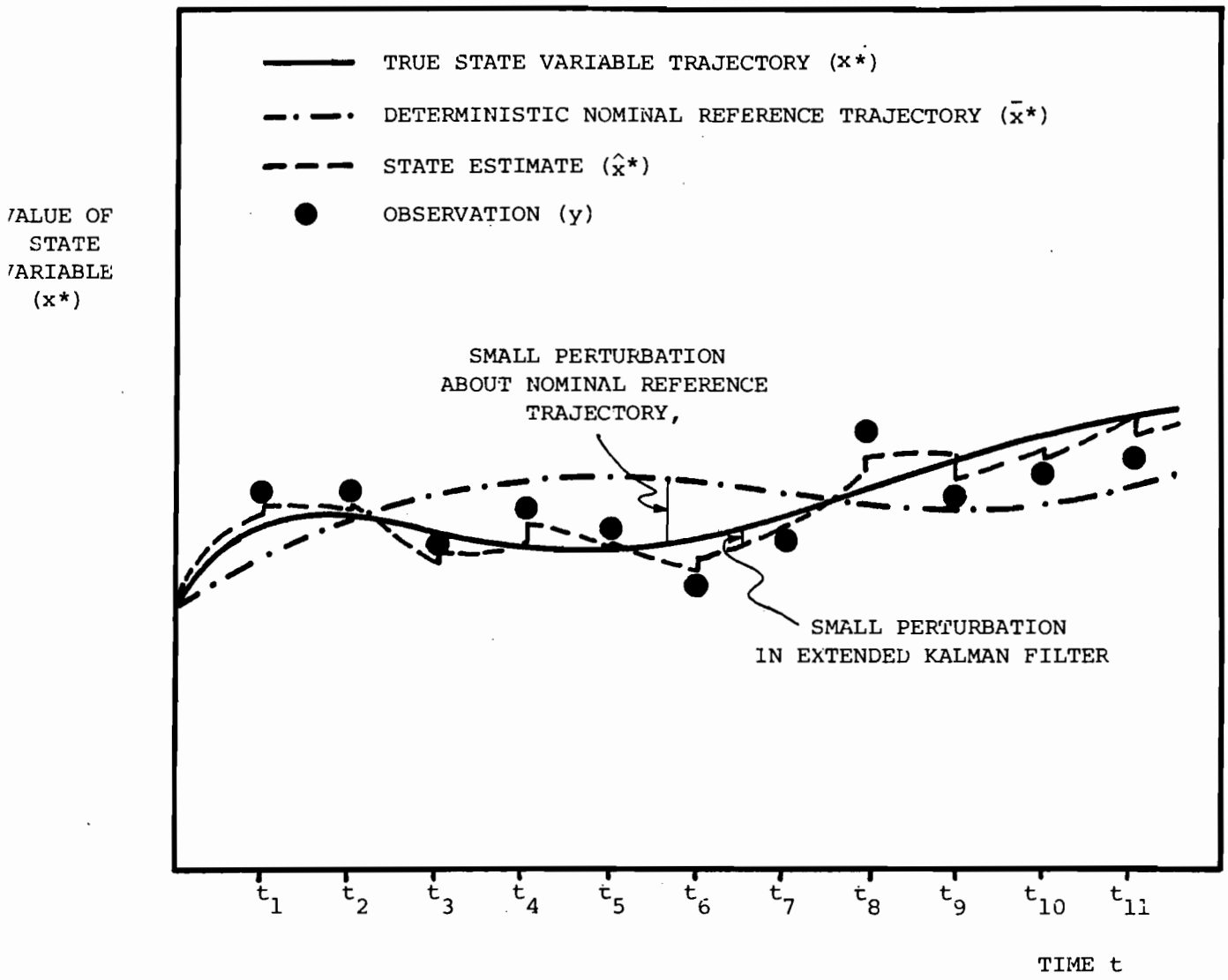

Figure 20. An example showing how the relinearization procedure of the extended Kalman filter is capable of preserving only small perturbations about the reference trajectory (in the EKF the current state estimates are substituted for the reference trajectory).

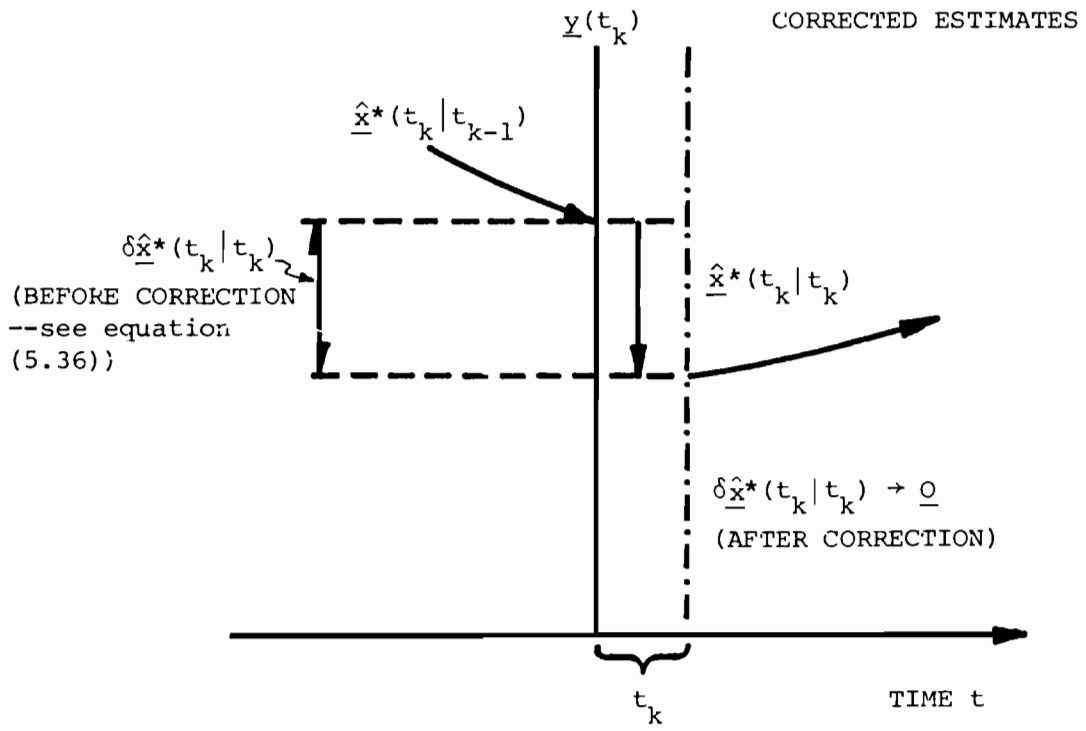

Figure 21. The estimate updating procedure at time t_k in the extended Kalman filter.

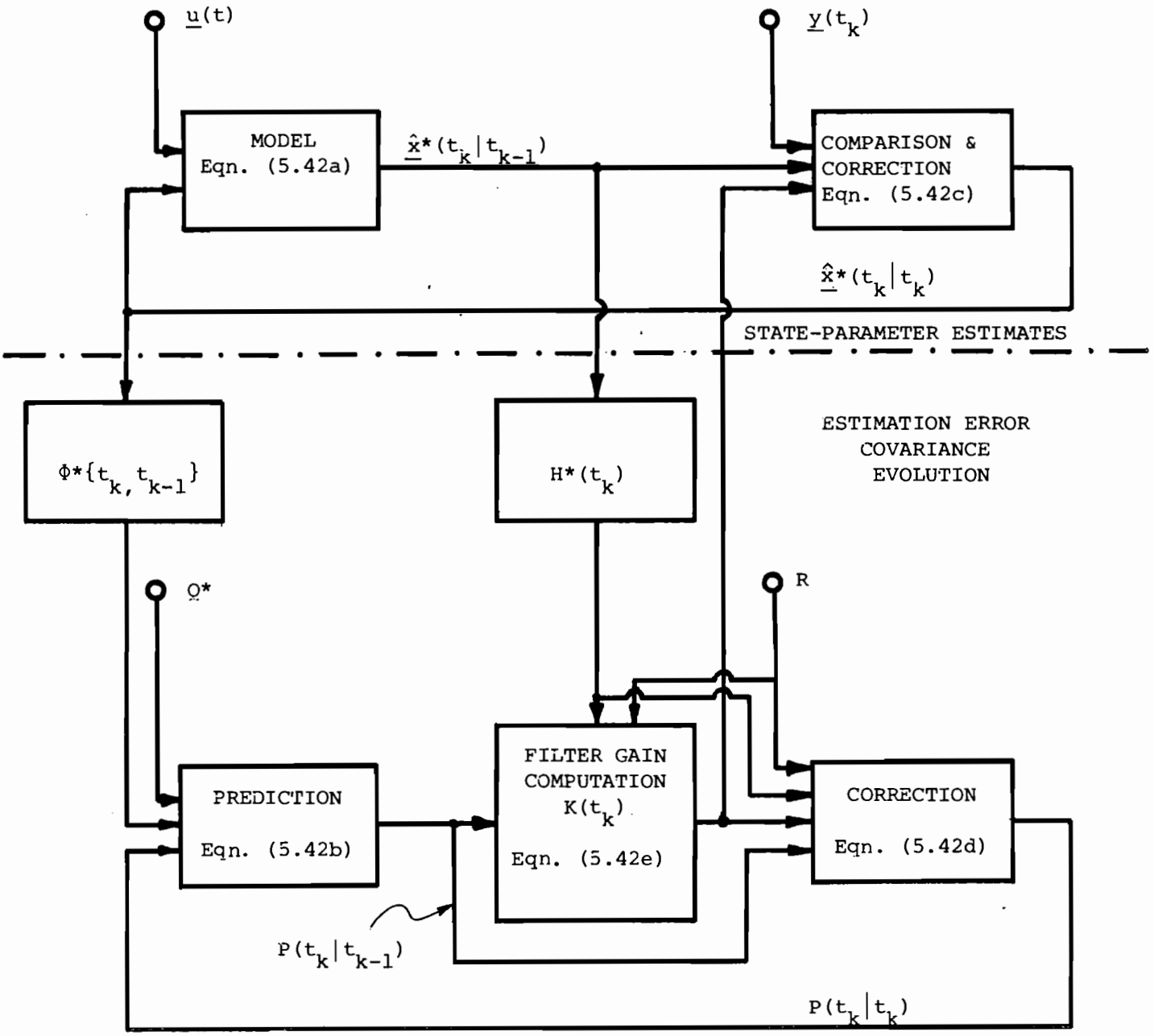

Figure 22. Block diagram of the extended Kalman filter algorithms showing both the computation of the state-parameter estimates and the computation of the covariance matrix.

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