

OPTIMAL FILTERING FOR SYSTEMS GOVERNED BY COUPLED
ORDINARY AND PARTIAL DIFFERENTIAL EQUATIONS

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Thomas King Lin Yu

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This thesis is dedicated
to my wife, May Ling,
to her parents and
to my parents.

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ABSTRACT

The recursive estimation of states or parameters of stochastic dynamical systems with partial and imperfect measurements is generally referred to as filtering. The estimator itself is called the filter. In this dissertation optimal filters are derived for three important classes of nonlinear stochastic dynamical systems.

The first class of systems, considered in Chapter II, is that governed by stochastic nonlinear hyperbolic and parabolic partial differential equations in which the dynamical disturbances in the system and in the boundary conditions can be both additive and nonadditive. This class of systems is important for it encompasses a large group of systems of practical interest, such as chemical reactors and heat exchangers. The optimal filter obtained can estimate, not only the state, but also constant parameters appearing at the boundary and in the volume of the system. The computational application of this filter is illustrated in an example of the feedback control of a styrene polymerization reactor.

Many physical systems contain time delays in one form or another. Often, this kind of delay system is accompanied by some other processes such as dissipation of mass and energy, fluid mixing, and chemical reaction. In Chapter III within a single framework new optimal filters are obtained for the following classes of stochastic systems:

1. Nonlinear lumped parameter systems containing multiple constant and time-varying delays;

2. Mixed nonlinear lumped and hyperbolic distributed parameter systems; and
3. Nonlinear lumped parameter systems with functional time delays.

The performance of the filter is illustrated through estimates of the temperatures in a system consisting of a well-stirred chemical reactor and an external heat exchanger.

In Chapter IV filtering equations are derived for a completely general class of stochastic systems governed by coupled nonlinear ordinary and partial differential equations of either first order hyperbolic or parabolic type with both volume and boundary random disturbances. Thus, the results of Chapter III can be shown to be a special case of those obtained in Chapter IV.

A related important concept to filtering is observability. For deterministic linear lumped parameter systems, observability refers to the ability to recover some prior state of a dynamical system based on partial observations of the state over some period of time. Under certain conditions, observability of the corresponding deterministic system is a sufficient condition for convergence of the optimal linear filter for a linear system with white noise disturbances. In Chapter V the concept of observability and filter convergence is developed for a class of stochastic linear distributed parameter systems whose solutions can be expressed as eigenfunction expansions. Two important questions examined are: (1) the effect of measurement locations on observability, and (2) the optimal location of measurements for state estimation.

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Chapter I

INTRODUCTION

A dynamical system is characterized by a set of differential equations*. In particular, a dynamical system characterized by a set of ordinary differential equations is commonly called a lumped parameter system, whereas a dynamical system characterized by a set of partial differential equations is referred to as a distributed parameter system. The state of a dynamical system is a set of numbers and/or functions, the knowledge of which and the input will, with the equations describing the dynamics, provide the future state and output of the system.

A majority of the physical systems fall into the class of lumped parameter systems and distributed parameter systems. There exist, however, important physical systems whose characterizations require the use of differential-difference equations and functional differential equations. Notably, these are systems which contain time delays. For example, a system with β constant time delays $\alpha_1 < \dots < \alpha_\beta$ may be represented by

$$\dot{x}(t) = f(x(t), x(t-\alpha_1), \dots, x(t-\alpha_\beta), t)$$

$$x(t) = \phi(t) \quad , \quad -\alpha_\beta \leq t \leq 0 \quad (1)$$

*The term differential equations used here shall be sufficiently general that it includes ordinary differential equations, partial differential equations, integro-differential equations (or functional differential equations), differential-difference equations, and any mixture of these various types of equations.

A system with functional time delay may be described by the following functional differential equation

$$\dot{x}(t) = \int_0^{\alpha_\beta} K(x(t-\alpha), \alpha, t) d\alpha$$
$$x(t) = \psi(t) \quad -\alpha_\beta \leq t \leq 0 \quad (2)$$

In both (1) and (2), $x(t)$ is an n -dimensional vector. The state at time t is the vector function $\{x(\alpha): t - \alpha_\beta \leq \alpha \leq t\}$.

If a set of differential equations is an accurate characterization of a physical system, then any analysis on the dynamical behavior of the system can be done using the set of equations. Unfortunately, all descriptions of physical systems contain some degree of inherent uncertainty due to the idealization of real processes. When the uncertainties are significant, the representation of a physical system by a deterministic set of differential equations is inappropriate. In addition, it is often not possible to measure all components of the system state (partial or incomplete measurement) and the measurement errors are not negligible. Under this situation, it is evident that the modeling of the physical system must be done in a more satisfactory manner. A common approach is to add a random dynamical disturbance term to each of the original differential equations. These disturbances account for the system uncertainties, as a result of random interactions between the system and its environment and possible modeling errors. On the other hand, there are also situations where uncertainties are caused by the ignorance of the exact value of some constant parameters in the physical system. Measurement errors are often lumped as an

additive random process. In this way the physical system is being modeled as a stochastic dynamical system. For instance, a stochastic lumped parameter system may be of the form

$$\begin{aligned}\dot{x}(t) &= f(x(t), k, t) + \xi(t) \\ y(t) &= h(x(t), t) + \eta(t)\end{aligned}\tag{3}$$

$x(t)$ is the state vector, $y(t)$ is the observation vector and k is an unknown constant parameter vector. $\xi(t)$ and $\eta(t)$ are zero-mean vector random processes with unknown statistical properties.

A problem of fundamental interest to engineers is the recursive estimation, generally referred to as filtering, of states and parameters of stochastic dynamical systems based on imperfect and partial observations of the state of the system. Basically, the estimation problem consists in determining sequentially an approximation to the time history of the system's state or of some physical parameters of the system from erroneous and incomplete measurements. A performance measure is introduced to assess the quality of the approximation or estimate, and the estimate is to be chosen so that this measure is minimized. Implicit here is the development of an algorithm for processing the measurements. Such algorithm is commonly referred to as the filter. Since a performance measure is minimized, the term optimal filter is often used.

The first significant contributions in the area of filtering are those of Kalman and Bucy [12,13], in which the optimal minimum variance estimate of the state of a linear lumped parameter system

with white noise disturbances was determined as the solution of an initial value problem of ordinary differential equations, the so-called Kalman-Bucy filter. The problem of filtering for stochastic nonlinear lumped parameter systems has been studied exhaustively since about 1962. However, all the filters derived have one thing in common, i.e., they all have the form (using (3), and assuming k is known and hence deleting it for convenience)

$$\dot{\hat{x}}(t) = f(\hat{x}(t), t) + g(P(t), y(t), \hat{x}(t)) \quad (4)$$

where \hat{x} denotes the estimate of x . That is, the filter equation can be lumped into two terms; one accounts for the dynamics of the system while the other accounts for the continuous updating of new information from the measurements. In (4), $P(t)$ is a weighting matrix function whose time evolution is governed by another ordinary differential equation. In the linear case (with white noise disturbances), $P(t)$ is the covariance matrix of the estimate errors and is governed by the so-called Riccati equation.

Recently there has been interest in filtering for systems described by partial differential equations and for lumped parameter systems containing time delays. Filtering in linear distributed parameter systems has been considered by Balakrishnan and Lions [2], Falb [6], Kushner [18], Meditch [21], Pell and Aris [23], Sakawa [25], Thau [27], and Tzafestas and Nightingale [28-30,32,33]. Tzafestas and Nightingale [31] derived a maximum-likelihood filter for nonlinear distributed systems with white Gaussian noise disturbances in the

volume and observations. Seinfeld et al. [26] and Hwang et al. [10] have derived optimal least-square filters for nonlinear distributed systems with unknown volume, boundary and observation noise. The former derivation was based on conversion of the distributed system to a differential-difference system by spatial discretization, application of a lumped parameter filter and performing a limiting process on the spatial increment; the latter employed invariant imbedding after conversion of the filtering problem to an optimal control problem. Filtering in linear lumped parameter systems with multiple constant time delays and in linear lumped parameter systems with functional time delays have been studied by Kwakernaak [19], Lindquist [20], and Koivo [16].

In this dissertation optimal filters are derived for three important classes of nonlinear stochastic dynamical systems using an approach termed filter decomposition. This approach has several desirable features:

1. No a priori assumptions regarding the form of the filter are required;
2. The exact interpretation of the so-called covariance matrices results readily; and
3. An indication of the form of the exact filter results.

The first class of systems, considered in Chapter II, is governed by stochastic nonlinear hyperbolic and parabolic partial differential equations in which the dynamical disturbances in the volume and at the boundary can be both additive and nonadditive. This class of systems is important for it encompasses many distributed systems of practical

interest and, in particular, chemical reactors and heat conduction systems. The optimal filter obtained can estimate, not only the state, but also constant parameters appearing at the boundary and in the volume of the systems. Hwang et al. [10] previously derived an identical filter for the same class of systems using the invariant imbedding approach.

Many physical systems contain time delays in one form or another. For example, systems like rocket or aircraft engines with piping to fuel tanks will have valve delays as well as transport delays due to the piping. Time delays are important in the modeling of drug distribution, as in the case of cancer chemotherapy. Often, delay systems are accompanied by some other processes, such as dissipation of mass and energy, fluid mixing, and chemical reactions. In Chapter III within a single framework new optimal filters are obtained for the following classes of stochastic systems:

1. Nonlinear lumped parameter systems containing multiple constant and time-varying delays;
2. Mixed nonlinear lumped and hyperbolic distributed parameter systems; and
3. Nonlinear lumped parameter systems with functional time delays.

The performance of the filter is illustrated through estimates of the temperatures in a system consisting of a well-stirred chemical reactor with external heat exchange.

In Chapter IV an optimal filter is derived for a completely general class of stochastic systems governed by coupled nonlinear ordinary and partial differential equations of either first order hyperbolic or parabolic type with both volume and boundary random disturbances. The results of Chapter III can be shown to be a special case of those obtained in Chapter IV.

A related important concept to filtering is observability. Originally defined by Kalman [12,13] for linear lumped parameter systems, observability refers to the ability to recover completely some prior state of a dynamical system based on partial observations of the state over some period of time. Thus, observability is a fundamental consideration in the planning of how measurements are to be taken on a system. Kalman showed, in fact, that under certain circumstances observability of the corresponding deterministic system is a sufficient condition for convergence of the optimal linear filter (the Kalman-Bucy filter) for a linear system with white noise disturbances. Therefore, in order for estimates of the states to converge to the best possible estimates, it is sufficient to make measurements such that the system is observable.

Observability of linear distributed parameter systems has received only limited attention. Wang [35], the first to define distributed system observability, based his definition on the existence of the inverse of a certain self-adjoint observation operator. Goodson and Klein [7] defined distributed observability as the ability to establish the uniqueness of a solution of the system. Prado [24] has presented an elegant analysis of distributed observability from the

point of view of semi-group theory. His ultimate results are similar to those of Goodson and Klein. What is lacking, however, is a practical, general method of establishing observability of a wide class of systems governed by linear partial differential equations.

As an example, consider the problem of estimating the temperature distributions in a heat exchanger based on the observed temperature response of one fluid to a perturbation in the inlet temperature of the other fluid. The first question we must ask is, can we estimate theoretically the temperature distribution even if our measurements contain no errors whatsoever? In other words, have we made enough measurements of the right type to be able to calculate the temperature profile from our data if the data were error-free?

In Chapter V, the concept of observability and filter convergence is developed for a class of stochastic linear distributed parameter systems whose solutions can be expressed as eigenfunction expansions. Since observations of a distributed system can, in principle, be placed anywhere in the spatial domain of the system, an important related question is the effect of the measurement locations on observability. Also, it is appropriate to ask what are the measurement locations that lead to the best estimates of the state of the system. These two questions are both addressed in this study. Finally, necessary and sufficient conditions for observability are derived for a separate class of linear hyperbolic distributed parameter systems.

Chapter II

OPTIMAL FILTERING FOR NONLINEAR DISTRIBUTED PARAMETER SYSTEMS

1. Introduction

In this chapter we derive an optimal filter for a wide class of nonlinear hyperbolic and parabolic distributed parameter systems with additive volume, boundary and observation disturbances. In addition, to account for nonadditive disturbances or constant parameters which must also be estimated, volume and boundary dynamical inputs governed by stochastic ordinary differential equations are included.

2. Statement of the Problem

We consider the class of well-posed systems governed by the vector nonlinear partial differential equation

$$x_t(r,t) = f[r,t,x,x_r,x_{rr},a(t)] + \xi_1(r,t) \quad (1)$$

defined for $t \geq 0$ on the normalized domain $(0,1)$. $x(r,t)$ is the n -vector state, and x_t , x_r , x_{rr} denote $\partial x/\partial t$, $\partial x/\partial r$, $\partial^2 x/\partial r^2$, respectively. The ℓ_1 -vector input $a(t)$ is governed by

$$\dot{a}(t) = A[t,a(t)] + \xi_2(t) \quad (2)$$

and the boundary conditions of the system are given by the ℓ -vector ($\ell \leq n$) functions

$$g_0(t,x,x_r) + \xi_3(t) = 0 \quad r = 0 \quad (3)$$

$$g_1(t, x, x_r, b(t)) + \xi_4(t) = 0 \quad r = 1 \quad (4)$$

with the ℓ_2 -vector input $b(t)$ governed by

$$\dot{b}(t) = B[t, b(t)] + \xi_5(t) \quad (5)$$

Observations of the system consist of the m -vector $y(r, t)$ related to the state by

$$y(r, t) = h[r, t, x(r, t)] + \eta(r, t) \quad (6)$$

We assume that $\xi_1(r, t)$, $\xi_k(t)$, $k=2, \dots, 5$ and $\eta(r, t)$ are zero-mean random processes with unknown statistical properties. The initial conditions for (1), (2) and (5) are not known in general.

We have included the auxiliary states $a(t)$ and $b(t)$ for two reasons. First, they may account for dynamical disturbances in the volume and boundary which do not enter (1) in an additive fashion. Second, it is often necessary to estimate not only the state of the system but also constant parameters. Constant parameters occurring on the right hand side of (1) or in the boundary conditions (3) and (4) (we have chosen equation (4) for illustration) can be considered for estimation purposes as auxiliary state variables satisfying equations of the form $\dot{a} = \dot{b} = 0$. Thus, in order to estimate states and parameters simultaneously it is necessary to include equations of the type (2) and (5).

The derivation of the optimal filter consists of two major steps. First, we formulate the problem of fixed final time smoothing for system (1)-(6) and derive the necessary conditions for optimality using variational calculus. Second, we convert the smoothing problem

into the filtering problem by the filter decomposition technique [22].

We first formulate the problem of smoothing: given any $T > 0$ and observations $y(r,t)$, $0 \leq t \leq T$, $r \in [0,1]$, it is desired to estimate $x(r,t)$, $a(t)$ and $b(t)$ for $0 \leq t \leq T$, $r \in [0,1]$ such that the least square error functional

$$\begin{aligned} \Psi = & \int_0^T \left[\int_0^1 \int_0^1 \langle y(r,t) - h(r,t,x), Q(r,s,t)(y(s,t) - h(s,t,x)) \rangle dr ds \right. \\ & + \int_0^1 \int_0^1 \langle x_t(r,t) - f(r,t,x,x_r,x_{rr},a(t)), R(r,s,t)(x_t(s,t) \\ & \quad \left. - f(s,t,x,x_s,x_{ss},a(t))) \rangle dr ds \right. \\ & + \langle g_0(t,x,x_r), R_3(t)(g_0(t,x,x_r)) \rangle \\ & + \langle g_1(t,x,x_r,b), R_4(t)(g_1(t,x,x_r,b)) \rangle \\ & + \langle \dot{a}(t) - A(t,a), R_2(t)(\dot{a}(t) - A(t,a)) \rangle \\ & \left. + \langle \dot{b}(t) - B(t,b), R_5(t)(\dot{b}(t) - B(t,b)) \rangle \right] dt \end{aligned} \quad (7)$$

is minimized. The weighting matrices $Q(r,s,t)$ and $R_k(t)$, ($k=2, \dots, 5$) are positive-definite and symmetric: $R_k(t) = R_k^T(t)$, $Q(r,s,t) = Q^T(s,r,t)$. $R(r,s,t)$ is defined by [21,33]

$$\int_0^1 R^+(r,\rho,t) R(\rho,s,t) d\rho = I \delta(r-s) \quad (8)$$

where $R^+(r,s,t)$ is a positive-definite, symmetric matrix: $R^+(r,s,t) = (R^+(s,r,t))^T$. $\delta(\cdot)$ is the Dirac delta function and I is the identity matrix.

3. Necessary Conditions for Optimality

The problem of smoothing can be reformulated as a constrained minimization problem, i.e., the minimization of

$$\begin{aligned}
 L_1 = & \int_0^T \left\{ \int_0^1 \int_0^1 \langle y(r,t) - h(r,x,t), Q(r,s,t)[y(s,t) - h(s,x,t)] \rangle dr ds \right\} dt \\
 & + \int_0^T \left\{ \int_0^1 \int_0^1 \langle u_1(r,t), R(r,s,t) u_1(s,t) \rangle dr ds \right. \\
 & \left. + \sum_{k=2}^5 \langle u_k(t), R_k(t) u_k(t) \rangle \right\} dt \quad (9)
 \end{aligned}$$

subject to the constraints

$$x_t(r,t) = f[r,t,x,x_r,x_{rr},a(t)] + u_1(r,t)$$

$$\dot{a}(t) = A[t,a(t)] + u_2(t)$$

$$g_0(t,x,x_r) + u_3(t) = 0 \quad r = 0$$

$$g_1(t,x,x_r,b(t)) + u_4(t) = 0 \quad r = 1$$

$$\dot{b}(t) = B[t,b(t)] + u_5(t)$$

where the u_i are considered as the control vectors.

With the aid of the vector Lagrange multipliers $\lambda(r,t)$, $\tau(t)$, $\sigma(t)$, $\mu_0(t)$ and $\mu_1(t)$ we convert the constrained minimization problem into an unconstrained minimization problem [14]. The performance index (known as the Lagrangian) now takes the form

$$L = L_1 + L_2 \quad (10)$$

where

$$\begin{aligned}
 L_1 = & \int_0^T \left\{ \int_0^1 \int_0^1 \langle y(r,t) - h(r,x,t), Q(r,s,t)[y(s,t) - h(s,x,t)] \rangle dr ds \right. \\
 & + \int_0^T \left\{ \int_0^1 \int_0^1 \langle u_1(r,t), R(r,s,t) u_1(s,t) \rangle dr ds \right. \\
 & \left. \left. + \sum_{k=2}^5 \langle u_k(t), R_k(t) u_k(t) \rangle \right\} dt \quad (11)
 \end{aligned}$$

$$\begin{aligned}
 L_2 = & \int_0^T \left\{ \int_0^1 \langle -\lambda(r,t), x_t(r,t) - f(r,t,x,x_r,x_{rr},a(t)) - u_1(r,t) \rangle dr \right. \\
 & + \langle -\tau(t), \dot{a}(t) - A(t,a) - u_2(t) \rangle \\
 & + \langle -\sigma(t), \dot{b}(t) - B(t,b) - u_5(t) \rangle \\
 & + \langle \mu_0(t), g_0(t,x,x_r) + u_3(t) \rangle \\
 & \left. + \langle \mu_1(t), g_1(t,x,x_r,b) + u_4(t) \rangle \right\} dt \quad (12)
 \end{aligned}$$

We assume that the inverses of $g_{0x_r}^T$ and $g_{1x_r}^T$ (denoted by $g_{0x_r}^{-1}$ and $g_{1x_r}^{-1}$) exist when they are square matrices. If not square $g_{0x_r}^{-1}$ and $g_{1x_r}^{-1}$ are to be interpreted as the left pseudo inverses

$$\begin{aligned}
 g_{0x_r}^{-1} &= (g_{0x_r} g_{0x_r}^T)^{-1} g_{0x_r} \\
 g_{1x_r}^{-1} &= (g_{1x_r} g_{1x_r}^T)^{-1} g_{1x_r} \quad (13)
 \end{aligned}$$

We now give the necessary conditions for optimality obtained from the vanishing of the first variation of L (see Appendix II-B). We will use the symbol $\hat{}$ to denote the optimal values. In addition, since the

optimal solution depends on the observation time T , we will indicate this for the variables by $\hat{x}(r,t/T)$, $\hat{a}(t/T)$, $\hat{b}(t/T)$, etc.

The necessary conditions assume the form of a two-point boundary value problem and are

$$\hat{x}_t(r,t/T) = f(r,t,\hat{x},\hat{x}_r,\hat{x}_{rr},\hat{a}) - \frac{1}{2} \int_0^1 R^+(r,s,t) \hat{\lambda}(s,t/T) ds \quad (14)$$

$$g_0(t,\hat{x},\hat{x}_r) - \frac{1}{2} R_3^{-1}(t) \hat{\mu}_0(t/T) = 0 \quad r = 0 \quad (15)$$

$$g_1(t,\hat{x},\hat{x}_r,\hat{b}) - \frac{1}{2} R_4^{-1}(t) \hat{\mu}_1(t/T) = 0 \quad r = 1 \quad (16)$$

$$\hat{a}_t(t/T) = A(t,\hat{a}) - \frac{1}{2} R_2^{-1}(t) \hat{\tau}(t/T) \quad (17)$$

$$\hat{b}_t(t/T) = B(t,\hat{b}) - \frac{1}{2} R_5^{-1}(t) \hat{\sigma}(t/T) \quad (18)$$

$$\begin{aligned} \hat{\lambda}_t(r,t/T) = 2 \int_0^1 h_x^T(r,t,\hat{x}) Q(r,s,t) [y(s,t) - h(s,t,\hat{x})] ds \\ - \hat{f}_x^T \hat{\lambda} + (\hat{f}_{x_r}^T \hat{\lambda})_r - (\hat{f}_{x_{rr}}^T \hat{\lambda})_{rr} \end{aligned} \quad (19)$$

$$\hat{\tau}_t(t/T) = - \int_0^1 \hat{f}_a^T \hat{\lambda}(s,t/T) ds - \hat{A}_a^T \hat{\tau} \quad (20)$$

$$\hat{\sigma}_t(t/T) = - \hat{B}_b^T \hat{\sigma} - \hat{g}_{1_b}^T \hat{\mu}_1 \quad r = 1 \quad (21)$$

$$\hat{\lambda}(r,T/T) = \hat{\sigma}(T/T) = \hat{\tau}(T/T) = 0 \quad (22)$$

$$\hat{\lambda}(r,0/T) = \hat{\tau}(0/T) = \hat{\sigma}(0/T) = 0 \quad (23)$$

$$\hat{\mu}_0(t/T) = \hat{g}_{0_{x_r}}^{-1} \hat{f}_{x_{rr}}^T \hat{\lambda} \quad r = 0 \quad (24)$$

$$\hat{\mu}_1(t/T) = -\hat{g}_{1_{x_r}}^{-1} \hat{f}_{x_{rr}}^T \hat{\lambda} \quad r = 1 \quad (25)$$

$$\hat{g}_{0x}^T \hat{g}_{0x_r}^{-1} \hat{f}_{x_{rr}}^T \hat{\lambda} - \hat{f}_{x_r}^T \hat{\lambda} + (\hat{f}_{x_{rr}}^T \hat{\lambda})_r = 0 \quad r = 0 \quad (26)$$

$$\hat{g}_{1x}^T \hat{g}_{1x_r}^{-1} \hat{f}_{x_{rr}}^T \hat{\lambda} - \hat{f}_{x_r}^T \hat{\lambda} + (\hat{f}_{x_{rr}}^T \hat{\lambda})_r = 0 \quad r = 1 \quad (27)$$

4. Differential Sensitivities

Since (14)-(27) constitute a two-point boundary value problem (we assume it to be well-posed), the end conditions (22)-(23) uniquely determine the solution $\hat{x}(r,t/T)$, $\hat{a}(t/T)$, $\hat{b}(t/T)$, $\hat{\lambda}(r,t/T)$, $\hat{\tau}(t/T)$ and $\hat{\sigma}(t/T)$ for all $0 \leq t \leq T$, $0 \leq r \leq 1$. On the other hand, with $\hat{\lambda}(s,0/T) = \hat{\tau}(0/T) = \hat{\sigma}(0/T) = 0$ ($0 \leq s \leq 1$), $\hat{x}(r,t/T)$, $\hat{a}(t/T)$ and $\hat{b}(t/T)$ will be uniquely determined from $\hat{\lambda}(s,t/T)$ ($0 \leq s \leq 1$), $\hat{\tau}(t/T)$ and $\hat{\sigma}(t/T)$ for any $0 < t \leq T$ and $0 \leq r \leq 1$. Hence, we can express $\hat{x}(r,t/T)$, $\hat{a}(t/T)$ and $\hat{b}(t/T)$ in terms of the Lagrange multipliers by

$$\hat{x}(r,t/T) = x[r, \hat{\lambda}(s,t/T), \hat{\tau}(t/T), \hat{\sigma}(t/T)]$$

$$\hat{a}(t/T) = a[\hat{\lambda}(s,t/T), \hat{\tau}(t/T), \hat{\sigma}(t/T)] \quad s \in [0,1] \quad (28)$$

$$\hat{b}(t/T) = b[\hat{\lambda}(s,t/T), \hat{\tau}(t/T), \hat{\sigma}(t/T)]$$

Let $\delta/\delta\hat{\lambda}$ denote the functional derivative [34] and define the first order differential sensitivity matrices $P^{vv}(r,s,t/T), \dots, P^{bb}(t/T)$ by

$$P^{vv}(r,s,t/T) = -2 \frac{\delta \hat{x}(r,t/T)}{\delta \hat{\lambda}(s,t/T)}$$

$$P^{av}(s,t/T) = -2 \frac{\delta \hat{a}(t/T)}{\delta \hat{\lambda}(s,t/T)}$$

$$\begin{aligned}
 p^{bv}(s, t/T) &= -2 \frac{\hat{\delta b}(t/T)}{\delta \lambda(s, t/T)} \\
 p^{va}(r, t/T) &= -2 \frac{\hat{\partial x}(r, t/T)}{\partial \tau(t/T)} \\
 p^{aa}(t/T) &= -2 \frac{\hat{\partial a}(t/T)}{\partial \tau(t/T)} \\
 p^{ba}(t/T) &= -2 \frac{\hat{\partial b}(t/T)}{\partial \tau(t/T)} \\
 p^{vb}(r, t/T) &= -2 \frac{\hat{\partial x}(r, t/T)}{\partial \sigma(t/T)} \\
 p^{ab}(t/T) &= -2 \frac{\hat{\partial a}(t/T)}{\partial \sigma(t/T)} \\
 p^{bb}(t/T) &= -2 \frac{\hat{\partial b}(t/T)}{\partial \sigma(t/T)} \tag{29}
 \end{aligned}$$

Again, the differential sensitivities clearly depend on the length T of the observation interval.

We shall assume that the order of differentiation is interchangeable, for example,

$$\begin{aligned}
 \frac{\delta}{\delta \hat{\lambda}(s, t/T)} [\hat{x}_r(r, t/T)] &= \frac{\partial}{\partial r} \left[\frac{\hat{\delta x}(r, t/T)}{\delta \hat{\lambda}(s, t/T)} \right] \\
 \frac{\hat{\partial x}_{rr}(r, t/T)}{\partial \sigma(t/T)} &= \frac{\partial^2}{\partial r^2} \frac{\hat{\partial x}(r, t/T)}{\partial \sigma(t/T)} \tag{30}
 \end{aligned}$$

We want to compute the partial derivatives with respect to T of \hat{x} , \hat{x}_r , \hat{x}_{rr} , \hat{a} and \hat{b} , since these will be needed shortly. Using the chain rule of calculus for these partial derivatives, and employing

(29) and (30), we obtain

$$\hat{x}_T(r, t/T) = -\frac{1}{2} \left\{ \int_0^1 P^{vv}(r, s, t/T) \hat{\lambda}_T(s, t/T) ds + P^{va}(r, t/T) \hat{\tau}_T(t/T) + P^{vb}(r, t/T) \hat{\sigma}_T(t/T) \right\} \quad (31)$$

$$\hat{x}_{r_T}(r, t/T) = -\frac{1}{2} \left\{ \int_0^1 P_r^{vv}(r, s, t/T) \hat{\lambda}_T(s, t/T) ds + P_r^{va}(r, t/T) \hat{\tau}_T(t/T) + P_r^{vb}(r, t/T) \hat{\sigma}_T(t/T) \right\} \quad (32)$$

$$\hat{x}_{rr_T}(r, t/T) = -\frac{1}{2} \left\{ \int_0^1 P_{rr}^{vv}(r, s, t/T) \hat{\lambda}_T(s, t/T) ds + P_{rr}^{va}(r, t/T) \hat{\tau}_T(t/T) + P_{rr}^{vb}(r, t/T) \hat{\sigma}_T(t/T) \right\} \quad (33)$$

$$\hat{a}_T(t/T) = -\frac{1}{2} \left\{ \int_0^1 P^{av}(s, t/T) \hat{\lambda}_T(s, t/T) ds + P^{aa}(t/T) \hat{\tau}_T(t/T) + P^{ab}(t/T) \hat{\sigma}_T(t/T) \right\} \quad (34)$$

$$\hat{b}_T(t/T) = -\frac{1}{2} \left\{ \int_0^1 P^{bv}(s, t/T) \hat{\lambda}_T(s, t/T) ds + P^{ba}(t/T) \hat{\tau}_T(t/T) + P^{bb}(t/T) \hat{\sigma}_T(t/T) \right\} \quad (35)$$

These equations describe the time evolution of the optimal solutions \hat{x} , \hat{a} and \hat{b} as T , the length of the observation interval, varies.

5. Decomposition of the Filtering Process

Let $q(t/T)$ be whatever we desire to estimate in the system, based on observations $y(s, \tau)$, $s \in [0, 1]$, $\tau \in [0, T]$, and denote the

optimal estimate of $q(t/T)$ by $\hat{q}(t/T)$. Since we are interested in the optimal filter estimate, we seek $\hat{q}(T/T)$ and, in particular, the total derivative $d\hat{q}(T/T)/dT$. We note that

$$\frac{d\hat{q}(T/T)}{dT} = \hat{q}_t(t/T)\Big|_{t=T} + \hat{q}_T(t/T)\Big|_{t=T} \quad (36)$$

which we write for convenience as

$$\frac{d\hat{q}(T/T)}{dT} = \hat{q}_t(T/T) + \hat{q}_T(T/T) \quad (37)$$

Thus, the total derivative of the quantity $\hat{q}(T/T)$ is a sum of two terms, one representing the dynamics of the system $\hat{q}_t(t/T)\Big|_{t=T}$, and the second the updating of the estimate in the face of new observations $\hat{q}_T(t/T)\Big|_{t=T}$. This result was demonstrated for lumped parameter systems by Padmanabhan [22].

When \hat{q} is also a function of one or more spatial variables $\hat{q}(r,s,t/T)$, then (36) becomes

$$\frac{\partial \hat{q}(r,s,T/T)}{\partial T} = \hat{q}_t(r,s,t/T)\Big|_{t=T} + \hat{q}_T(r,s,t/T)\Big|_{t=T} \quad (38)$$

which we write for convenience as

$$\frac{\partial \hat{q}(r,s,T/T)}{\partial T} = \hat{q}_t(r,s,T/T) + \hat{q}_T(r,s,T/T) \quad (39)$$

We emphasize that each term in (38), and hence (39), represents a different partial derivative. In particular, the L.H.S. of (38) and (39) is the analog to the total derivative in (36), whereas the R.H.S. of (38) and (39) consists of partial derivatives with respect to each of the arguments t and T in $(\cdot, t/T)$, respectively.

6. State Filter Equations

We now want to derive the dynamical equations which govern $\hat{x}(r, T/T)/\partial T$, $\hat{a}(T)/dT$ and $\hat{b}(T)/dT$. First, (22) implies that

$$\frac{\partial \hat{\lambda}(s, T/T)}{\partial T} = 0 \quad \frac{d\hat{\tau}(T/T)}{dT} = 0 \quad \frac{d\hat{\sigma}(T/T)}{dT} = 0 \quad (40)$$

Using (37) and (39), (40) can be written as

$$\begin{aligned} \hat{\lambda}_T(s, T/T) + \hat{\lambda}_t(s, T/T) &= 0 \\ \hat{\tau}_T(T/T) + \hat{\tau}_t(T/T) &= 0 \\ \hat{\sigma}_T(T/T) + \hat{\sigma}_t(T/T) &= 0 \end{aligned} \quad (41)$$

Then (19)-(22), (25) and (41) give

$$\begin{aligned} \hat{\lambda}_T(s, T/T) &= -2 \int_0^1 h_X^T(s, T, \hat{x}) Q(s, \rho, T) [y(\rho, T) - h(\rho, T, \hat{x})] d\rho \\ \hat{\tau}_T(T/T) &= 0 \\ \hat{\sigma}_T(T/T) &= 0 \end{aligned} \quad (42)$$

Substituting (42) into (31), (34) and (35), we obtain, respectively

$$\begin{aligned} \hat{x}_T(r, T/T) &= \int_0^1 \int_0^1 P^{vv}(r, \zeta, T/T) h_X^T(\zeta, T, \hat{x}) Q(\zeta, v, T) [y(v, T) - h(v, T, \hat{x})] d\zeta dv \\ \hat{a}_T(T/T) &= \int_0^1 \int_0^1 P^{av}(\zeta, T/T) h_X^T(\zeta, T, \hat{x}) Q(\zeta, v, T) [y(v, T) - h(v, T, \hat{x})] d\zeta dv \\ \hat{b}_T(T/T) &= \int_0^1 \int_0^1 P^{bv}(\zeta, T/T) h_X^T(\zeta, T, \hat{x}) Q(\zeta, v, T) [y(v, T) - h(v, T, \hat{x})] d\zeta dv \end{aligned} \quad (43)$$

On the other hand, (14), (17), (18) and (22) give

$$\begin{aligned}\hat{x}_t(r, T/T) &= f(r, T, \hat{x}, \hat{x}_r, \hat{x}_{rr}, \hat{a}) \\ \hat{a}_t(T/T) &= A(T, \hat{a}) \\ \hat{b}_t(T/T) &= B(T, \hat{b})\end{aligned}\tag{44}$$

Finally, the application of (37) and (39) yields the state filter equations

$$\begin{aligned}\frac{\partial \hat{x}(r, T/T)}{\partial T} &= \hat{x}_t(r, T/T) + \hat{x}_T(r, T/T) \\ \frac{d\hat{a}(T/T)}{dT} &= \hat{a}_t(T/T) + \hat{a}_T(T/T) \\ \frac{d\hat{b}(T/T)}{dT} &= \hat{b}_t(T/T) + \hat{b}_T(T/T)\end{aligned}\tag{45}$$

The boundary conditions for the filter equations (45) are obtained by setting $t = T$ in (15), (16), (24), (25) and using (22). These are simply

$$\begin{aligned}g_0(T, \hat{x}, \hat{x}_r) &= 0 & r = 0 \\ g_1(T, \hat{x}, \hat{x}_r, \hat{b}) &= 0 & r = 1\end{aligned}\tag{46}$$

7. Dynamical Equations for the Differential Sensitivities

We now need to derive the dynamical equations for the differential sensitivities $p^{vv}(r, s, T/T), \dots, p^{bb}(T/T)$ to complete the specification of the filter. First, however, we determine the $r = 0$ and $r = 1$ boundary conditions for the differential sensitivities. For

$r = 0$, combine equations (15) and (24) to give

$$g_0(t, \hat{x}, \hat{x}_r) - \frac{1}{2} R_3^{-1}(t) \hat{g}_{0_{x_r}}^{-1} \hat{f}_{x_{rr}}^T \hat{\lambda}(r, t/T) = 0 \quad r = 0 \quad (47)$$

Since (47) holds for all T , we can differentiate it with respect to T , yielding

$$\begin{aligned} & \hat{g}_{0_x} \int_0^1 \frac{\partial \hat{x}(r, t/T)}{\partial \hat{\lambda}(s, t/T)} \hat{\lambda}_T(s, t/T) ds + \hat{g}_{0_{x_r}} \int_0^1 \frac{\partial \hat{x}_r(r, t/T)}{\partial \hat{\lambda}(s, t/T)} \hat{\lambda}_T(s, t/T) ds \\ & - \frac{1}{2} R_3^{-1}(t) \hat{g}_{0_{x_r}}^{-1} \hat{f}_{x_{rr}}^T \hat{\lambda}_T(r, t/T) - \frac{1}{2} [R_3^{-1}(t) \hat{g}_{0_{x_r}}^{-1} \hat{f}_{x_{rr}}^T]_T \hat{\lambda}(r, t/T) \\ & + \hat{g}_{0_x} \frac{\partial \hat{x}(r, t/T)}{\partial \tau(t/T)} \hat{\tau}_T(t/T) + \hat{g}_{0_{x_r}} \frac{\partial \hat{x}_r(r, t/T)}{\partial \tau(t/T)} \hat{\tau}_T(t/T) \\ & + \hat{g}_{0_x} \frac{\partial \hat{x}(r, t/T)}{\partial \sigma(t/T)} \hat{\sigma}_T(t/T) + \hat{g}_{0_{x_r}} \frac{\partial \hat{x}_r(r, t/T)}{\partial \sigma(t/T)} \hat{\sigma}_T(t/T) = 0 \end{aligned} \quad (48)$$

Note that we can write

$$\begin{aligned} R_3^{-1}(t) \hat{g}_{0_{x_r}}^{-1} \hat{f}_{x_{rr}}^T \hat{\lambda}_T(r, t/T) \Big|_{r=0} &= \int_0^1 R_3^{-1}(t) [\hat{g}_{0_{x_r}}^{-1} \hat{f}_{x_{rr}}^T]_{r=0} \\ &\times \delta(s) \hat{\lambda}_T(s, t/T) ds \end{aligned} \quad (49)$$

If we apply (A.13) of Appendix II-A and substitute (49) into (48), and bear in mind that since $\hat{\lambda}$, $\hat{\tau}$ and $\hat{\sigma}$ are considered as independent vector Lagrange multipliers in our formulation of (28), each coefficient of $\hat{\lambda}_T(s, t/T)$, $\hat{\tau}_T(t/T)$ and $\hat{\sigma}_T(t/T)$ must identically be zero in order that (48) holds, we obtain for $t = T$ and $r = 0$

$$\begin{aligned} \hat{g}_{0x} P^{VV}(r,s,T/T) + \hat{g}_{0x_r} P_r^{VV}(r,s,T/T) + R_3^{-1}(T) \hat{g}_{0x_r}^{-1} \hat{f}_{x_{rr}}^T \delta(s) &= 0 \\ \hat{g}_{0x} P^{Va}(r,T/T) + \hat{g}_{0x_r} P_r^{Va}(r,T/T) &= 0 \\ \hat{g}_{0x} P^{Vb}(r,T/T) + \hat{g}_{0x_r} P_r^{Vb}(r,T/T) &= 0 \end{aligned} \quad (50)$$

Similarly, the boundary conditions at $r = 1$ are

$$\begin{aligned} \hat{g}_{1x} P^{VV}(r,s,T/T) + \hat{g}_{1x_r} P_r^{VV}(r,s,T/T) + \hat{g}_{1b} P^{bV}(s,T/T) \\ - R_4^{-1}(T) \hat{g}_{1x_r}^{-1} \hat{f}_{x_{rr}}^T \delta(s-1) &= 0 \\ \hat{g}_{1x} P^{Va}(r,T/T) + \hat{g}_{1x_r} P_r^{Va}(r,T/T) + \hat{g}_{1b} P^{ba}(T/T) &= 0 \\ \hat{g}_{1x} P^{Vb}(r,T/T) + \hat{g}_{1x_r} P_r^{Vb}(r,T/T) + \hat{g}_{1b} P^{bb}(T/T) &= 0 \end{aligned} \quad (51)$$

Now we proceed to the derivation of the partial differential equations governing $P^{VV}(r,s,T/T), \dots, P^{bb}(T/T)$. These equations are often referred to as the "covariance equations" by analogy to the Kalman filter. In order to derive these equations, we need the total derivatives with respect to T of $P^{VV}(r,s,T/T), \dots, P^{bb}(T/T)$, as in (45) for the state filter equations. As we know, each $\partial P(\cdot, T/T)/\partial T$ will be a sum of two terms, $P_t(\cdot, T/T)$ and $P_T(\cdot, T/T)$. For the general nonlinear case which we are considering, it can be shown (Section 8) that $P_T(\cdot, T/T)$ involves the second order differential sensitivities and, likewise, the second order differential sensitivities involve the third order differential sensitivities, etc. Thus, in general, it is

not possible to close the system of equations. For this reason, we will approximate $\partial P^{VV}(r,s,T/T)/\partial T, \dots, dP^{bb}(T/T)/dT$ by $P_t^{VV}(r,s,T/T), \dots, P_t^{bb}(T/T)$, respectively. This enables us to obtain a closed set of equations.

The basic approach is that we shall derive two expressions for each of the quantities,

$$\frac{\partial}{\partial t} [\hat{x}_T(r,t/T)] \quad \frac{\partial}{\partial t} [\hat{a}_T(t/T)] \quad \frac{\partial}{\partial t} [\hat{b}_T(t/T)] \quad (52)$$

and equate the two expressions for each of the quantities, and set $t = T$. Since each of the quantities above is a continuous function of t and T , we can write

$$\frac{\partial}{\partial t} [\hat{x}_T(r,t/T)] = \frac{\partial}{\partial T} [\hat{x}_t(r,t/T)] \quad (53)$$

$$\frac{\partial}{\partial t} [\hat{a}_T(t/T)] = \frac{\partial}{\partial T} [\hat{a}_t(t/T)] \quad (54)$$

$$\frac{\partial}{\partial t} [\hat{b}_T(t/T)] = \frac{\partial}{\partial T} [\hat{b}_t(t/T)] \quad (55)$$

Let $\hat{f}(r)$, \hat{A} and \hat{B} denote $f(r,t,\hat{x},\hat{x}_r,\hat{x}_{rr},\hat{a})$, $A(t,\hat{a})$ and $B(t,\hat{b})$, respectively. Using (14) in (53) gives

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{x}_T(r,t/T)] &= \hat{f}_x(r) \hat{x}_T(r,t/T) + \hat{f}_{x_r}(r) \hat{x}_{rT}(r,t/T) \\ &\quad + \hat{f}_{x_{rr}}(r) \hat{x}_{rrT}(r,t/T) \\ &\quad + \hat{f}_a(r) \hat{a}_T(t/T) - \frac{1}{2} \int_0^1 R^+(r,s,t) \hat{\lambda}_T(s,t/T) ds \end{aligned} \quad (56)$$

Substituting (17) and (18) in (54) and (55), respectively, we obtain

$$\frac{\partial}{\partial t} [\hat{a}_T(t/T)] = \hat{A}_a \hat{a}_T(t/T) - \frac{1}{2} R_2^{-1}(t) \hat{\tau}_T(t/T) \quad (57)$$

$$\frac{\partial}{\partial t} [\hat{b}_T(t/T)] = \hat{B}_b \hat{b}_T(t/T) - \frac{1}{2} R_5^{-1}(t) \hat{\sigma}_T(t/T) \quad (58)$$

With the help of (31)-(35), we can rewrite (56)-(58) as

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{x}_T(r, t/T)] = & - \frac{1}{2} \left[\int_0^1 [\hat{f}_x(r) P^{vv}(r, s, t/T) + \hat{f}_{x_r}(r) P_r^{vv}(r, s, t/T) \right. \\ & + \hat{f}_{x_{rr}}(r) P_{rr}^{vv}(r, s, t/T) + \hat{f}_a(r) P^{av}(s, t/T) \\ & \left. + R^+(r, s, t)] \hat{\lambda}_T(s, t/T) ds \right] \\ & - \frac{1}{2} \left[[\hat{f}_x(r) P^{va}(r, t/T) + \hat{f}_{x_r}(r) P_r^{va}(r, t/T) \right. \\ & + \hat{f}_{x_{rr}}(r) P_{rr}^{va}(r, t/T) + \hat{f}_a(r) P^{aa}(t/T)] \hat{\tau}_T(t/T) \left. \right] \\ & - \frac{1}{2} \left[[\hat{f}_x(r) P^{vb}(r, t/T) + \hat{f}_{x_r}(r) P_r^{vb}(r, t/T) \right. \\ & \left. + \hat{f}_{x_{rr}}(r) P_{rr}^{vb}(r, t/T) + \hat{f}_a(r) P^{ab}(t/T)] \hat{\sigma}_T(t/T) \right] \quad (59) \end{aligned}$$

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{a}_T(t/T)] = & - \frac{1}{2} \int_0^1 \hat{A}_a P^{av}(s, t/T) \hat{\lambda}_T(s, t/T) ds \\ & - \frac{1}{2} [\hat{A}_a P^{aa}(t/T) + R_2^{-1}(t)] \hat{\tau}_T(t/T) \\ & - \frac{1}{2} \hat{A}_a P^{ab}(t/T) \hat{\sigma}_T(t/T) \quad (60) \end{aligned}$$

$$\begin{aligned}
 \frac{\partial}{\partial t} [\hat{b}_T(t/T)] = & -\frac{1}{2} \int_0^1 \hat{B}_b p^{bv}(s, t/T) \hat{\lambda}_T(s, t/T) ds \\
 & - \frac{1}{2} \hat{B}_b p^{ba}(t/T) \hat{\tau}_T(t/T) \\
 & - \frac{1}{2} [\hat{B}_b p^{bb}(t/T) + R_5^{-1}(t)] \hat{\sigma}_T(t/T)
 \end{aligned} \tag{61}$$

On the other hand, inserting (31), (34) and (35) into the three quantities of (52) respectively, and carrying out the differentiation with respect to t , we obtain

$$\begin{aligned}
 \frac{\partial}{\partial t} [\hat{x}_T(r, t/T)] = & -\frac{1}{2} \left[\int_0^1 p_t^{vv}(r, s, t/T) \hat{\lambda}_T(s, t/T) ds \right. \\
 & \left. + p_t^{va}(r, t/T) \hat{\tau}_T(t/T) + p_t^{vb}(r, t/T) \hat{\sigma}_T(t/T) \right] \\
 & - \frac{1}{2} \left[\int_0^1 p^{vv}(r, s, t/T) \frac{\partial}{\partial t} [\hat{\lambda}_T(s, t/T)] ds \right. \\
 & \left. + p^{va}(r, t/T) \frac{\partial}{\partial t} [\hat{\tau}_T(t/T)] \right. \\
 & \left. + p^{vb}(r, t/T) \frac{\partial}{\partial t} [\hat{\sigma}_T(t/T)] \right]
 \end{aligned} \tag{62}$$

$$\begin{aligned}
 \frac{\partial}{\partial t} [\hat{a}_T(t/T)] = & -\frac{1}{2} \left[\int_0^1 p_t^{av}(s, t/T) \hat{\lambda}_T(s, t/T) ds \right. \\
 & \left. + p_t^{aa}(t/T) \hat{\tau}_T(t/T) + p_t^{ab}(t/T) \hat{\sigma}_T(t/T) \right] \\
 & - \frac{1}{2} \left[\int_0^1 p^{av}(s, t/T) \frac{\partial}{\partial t} [\hat{\lambda}_T(s, t/T)] ds \right. \\
 & \left. + p^{aa}(t/T) \frac{\partial}{\partial t} [\hat{\tau}_T(t/T)] + p^{ab}(t/T) \frac{\partial}{\partial t} [\hat{\sigma}_T(t/T)] \right]
 \end{aligned} \tag{63}$$

$$\begin{aligned}
 \frac{\partial}{\partial t} [\hat{b}_T(t/T)] = & -\frac{1}{2} \left[\int_0^1 p_t^{bv}(s, t/T) \hat{\lambda}_T(s, t/T) ds \right. \\
 & + p_t^{ba}(t/T) \hat{\tau}_T(t/T) + p_t^{bb}(t/T) \hat{\sigma}_T(t/T) \left. \right] \\
 & -\frac{1}{2} \left[\int_0^1 p^{bv}(s, t/T) \frac{\partial}{\partial t} [\hat{\lambda}_T(s, t/T)] ds \right. \\
 & + p^{ba}(t/T) \frac{\partial}{\partial t} [\hat{\tau}_T(t/T)] \\
 & \left. + p^{bb}(t/T) \frac{\partial}{\partial t} [\hat{\sigma}_T(t/T)] \right] \quad (64)
 \end{aligned}$$

Finally, we successively equate (59) and (62), (60) and (63), and (61) and (64), and set $t = T$. In each case for the equality to hold, we must have the coefficients of $\hat{\lambda}_T(s, t/T)$, $\hat{\tau}_T(t/T)$, $\hat{\sigma}_T(t/T)$, $\hat{\lambda}_T(0, t/T)$ and $\hat{\lambda}_T(1, t/T)$ be identically zero at $t = T$. Using the results in the Appendix II-A it is straightforward to show that

$$\begin{aligned}
 P_t^{vv}(r, s, T/T) = & \hat{f}_x(r) P^{vv}(r, s, T/T) + P^{vv}(r, s, T/T) \hat{f}_x^T(s) \\
 & + \hat{f}_{x_r}(r) P_r^{vv}(r, s, T/T) + P_s^{vv}(r, s, T/T) \hat{f}_{x_s}^T(s) \\
 & + \hat{f}_{x_{rr}}(r) P_{rr}^{vv}(r, s, T/T) + P_{ss}^{vv}(r, s, T/T) \hat{f}_{x_{ss}}^T(s) \\
 & + \hat{f}_a(r) P^{av}(s, T/T) + P^{va}(r, T/T) \hat{f}_a^T(s) \\
 & + N_1^{vv}(r, s, T/T) + U_1^{vv}(r, s, T/T) \\
 & + R^+(r, s, T) \quad (65)
 \end{aligned}$$

$$\begin{aligned}
 P_t^{va}(r, T/T) &= \hat{f}_x(r) P^{va}(r, T/T) + \hat{f}_{x_r}(r) P_r^{va}(r, T/T) \\
 &+ \hat{f}_{x_{rr}}(r) P_{rr}^{va}(r, T/T) + \hat{f}_a(r) P^{aa}(T/T) \\
 &+ P^{va}(r, T/T) \hat{A}_a^T \\
 &+ N_1^{va}(r, T/T) + U_1^{va}(r, T/T)
 \end{aligned} \tag{66}$$

$$\begin{aligned}
 P_t^{vb}(r, T/T) &= \hat{f}_x(r) P^{vb}(r, T/T) + \hat{f}_{x_r}(r) P_r^{vb}(r, T/T) \\
 &+ \hat{f}_{x_{rr}}(r) P_{rr}^{vb}(r, T/T) + \hat{f}_a(r) P^{ab}(T/T) \\
 &+ P^{vb}(r, T/T) \hat{B}_b^T \\
 &+ N_1^{vb}(r, T/T) + U_1^{vb}(r, T/T)
 \end{aligned} \tag{67}$$

$$\begin{aligned}
 P_t^{aa}(T/T) &= \hat{A}_a P^{aa}(T/T) + P^{aa}(T/T) \hat{A}_a^T \\
 &+ N_2^{va}(T/T) + U_2^{va}(T/T) \\
 &+ R_2^{-1}(T)
 \end{aligned} \tag{68}$$

$$\begin{aligned}
 P_t^{ab}(T/T) &= \hat{A}_a P^{ab}(T/T) + P^{ab}(T/T) \hat{B}_b^T \\
 &+ N_2^{vb}(T/T) + U_2^{vb}(T/T)
 \end{aligned} \tag{69}$$

$$\begin{aligned}
 P_t^{bb}(T/T) &= \hat{B}_b P^{bb}(T/T) + P^{bb}(T/T) \hat{B}_b^T \\
 &+ N_3^{vb}(T/T) + U_3^{vb}(T/T) \\
 &+ R_5^{-1}(T)
 \end{aligned} \tag{70}$$

with the symmetry properties

$$\begin{aligned}
 P^{vv}(r,s,T/T) &= (P^{vv}(s,r,T/T))^T, \quad P^{aa}(T/T) = (P^{aa}(T/T))^T \\
 P^{va}(r,T/T) &= (P^{av}(r,T/T))^T, \quad P^{ab}(T/T) = (P^{ba}(T/T))^T \\
 P^{vb}(r,T/T) &= (P^{bv}(r,T/T))^T, \quad P^{bb}(T/T) = (P^{bb}(T/T))^T
 \end{aligned} \tag{71}$$

Thus, there is no need to present the equations for $P_t^{av}(s,T/T)$, $P_t^{bv}(s,T/T)$ and $P_t^{ba}(T/T)$, and the boundary conditions for $P^{vv}(r,s,T/T)$, $P^{av}(s,T/T)$ and $P^{bv}(s,T/T)$ at $s = 0$ and $s = 1$ because they follow directly from (71). The terms $N_1^{vv}(r,s,T/T), \dots, U_3^{vb}(T/T)$ are defined in Appendix II-A.

The entire filter is summarized in Table 1. In the column of initial conditions, $\hat{x}(r,0/0)$, $\hat{a}(0/0)$ and $\hat{b}(0/0)$ represent our best guesses of the initial states $x(r,0)$, $a(0)$ and $b(0)$. The initial conditions $P^{vv}(r,s,0/0), \dots, P^{bb}(0/0)$ are basically arbitrary. In the linear, white noise case it can be shown that

$$P^{vv}(r,s,T/T) = E \{ (x(r,T) - \hat{x}(r,T/T))(x(s,T) - \hat{x}(s,T/T))^T \}$$

$$P^{va}(r,T/T) = E \{ (x(r,T) - \hat{x}(r,T/T))(a(T) - \hat{a}(T/T))^T \}$$

$$\begin{aligned}
 p^{vb}(r, T/T) &= E\{(x(r, T) - \hat{x}(r, T/T))(b(T) - \hat{b}(T/T))^T\} \\
 p^{aa}(T/T) &= E\{(a(T) - \hat{a}(T/T))(a(T) - \hat{a}(T/T))^T\} \\
 p^{ab}(T/T) &= E\{(a(T) - \hat{a}(T/T))(b(T) - \hat{b}(T/T))^T\} \\
 p^{bb}(T/T) &= E\{(b(T) - \hat{b}(T/T))(b(T) - \hat{b}(T/T))^T\} \quad (72)
 \end{aligned}$$

These relations may be used as a guide in choosing $p^{vv}(r, s, 0/0), \dots, p^{bb}(0/0)$.

Table 1. Optimal Filter for System (1)-(6)

	Equations	Initial Conditions	Boundary Conditions
<u>Estimates</u>			
$\hat{x}(r, T/T)$	(43)-(45)	$\hat{x}(r, 0/0)$	(46)
$\hat{a}(T/T)$	(43)-(45)	$\hat{a}(0/0)$	NONE
$\hat{b}(T/T)$	(43)-(45)	$\hat{b}(0/0)$	NONE
<u>First Order Differential Sensitivities</u>			
$p^{vv}(r, s, T/T)$	(65)	$p^{vv}(r, s, 0/0)$	(50)-(51)
$p^{va}(r, T/T)$	(66)	$p^{va}(r, 0/0)$	(50)-(51)
$p^{vb}(r, T/T)$	(67)	$p^{vb}(r, 0/0)$	(50)-(51)
$p^{aa}(T/T)$	(68)	$p^{aa}(0/0)$	NONE
$p^{ab}(T/T)$	(69)	$p^{ab}(0/0)$	NONE
$p^{bb}(T/T)$	(70)	$p^{bb}(0/0)$	NONE

8. Discussion of the Results

The theoretically required relations for the covariance equations are

$$\begin{aligned} \frac{\partial P^{VV}(r,s,T/T)}{\partial T} &= P_t^{VV}(r,s,T/T) + P_T^{VV}(r,s,T/T) \\ &\vdots \\ \frac{dP^{bb}(T/T)}{dT} &= P_t^{bb}(T/T) + P_T^{bb}(T/T) \end{aligned} \quad (73)$$

We noted earlier that we would neglect the second terms on the right hand sides of (73). Let us now give some indication as to how these neglected terms might be calculated. Employing the chain rule, we have

for P_T^{VV}

$$\begin{aligned} P_T^{VV}(r,s,t/T) &= \int_0^1 \frac{\delta P^{VV}(r,s,t/T)}{\delta \hat{\lambda}(v,t/T)} \hat{\lambda}_T(v,t/T) dv \\ &+ \frac{\partial P^{VV}(r,s,t/T)}{\partial \hat{\tau}(t/T)} \hat{\tau}_T(t/T) + \frac{\partial P^{VV}(r,s,t/T)}{\partial \hat{\sigma}(t/T)} \hat{\sigma}_T(t/T) \end{aligned} \quad (74)$$

The terms,

$$\frac{\delta P^{VV}(r,s,t/T)}{\delta \hat{\lambda}(v,t/T)} \quad \frac{\partial P^{VV}(r,s,t/T)}{\partial \hat{\tau}(t/T)} \quad \frac{\partial P^{VV}(r,s,t/T)}{\partial \hat{\sigma}(t/T)}$$

are $n \times n \times n$, $n \times n \times \ell_1$, and $n \times n \times \ell_2$ matrices, respectively, which are the second order differential sensitivities. Thus, the neglected terms in (73) involve the second order differential sensitivities.

However, in order to calculate the second order sensitivities, we will need the third order sensitivities, etc. Thus, the exact form of the optimal filter for system (1)-(6) is in general composed of an

infinite set of equations which cannot be closed. In the linear, white noise case, the second and higher order differential sensitivities are identically zero.

For discrete spatial measurements at J locations, $Q(\zeta, \nu, T)$ should be replaced by $Q_d(\zeta, \nu, T)$ where

$$Q_d(\zeta, \nu, T) = \sum_{k=1}^J \sum_{\ell=1}^J Q_{k\ell}(T) \delta(\zeta - r_k) \delta(\nu - r_\ell) \quad (75)$$

The $mJ \times mJ$ weighting matrix $[Q_{k\ell}]$ is symmetric and positive definite. When (75) is used in the filter equations, the integrations become summations.

If $g_{0_{x_r}} = 0$, (24) and (26) should be replaced by

$$\hat{\mu}_0(t/T) = -\hat{g}_{0_x}^{-1} (\hat{f}_{x_{rr}}^T \hat{\lambda})_r \quad r = 0 \quad (76)$$

$$\hat{\lambda}(r, t/T) = 0 \quad r = 0 \quad (77)$$

The last term of the first equation of (50) must then be replaced by $R_3^{-1}(T) \hat{g}_{0_x}^{-1} \hat{f}_{x_{rr}}^T \delta'(s)$, where $\delta'(s)$ denotes $d\delta(s)/ds$ [3, p.320].

Similarly, if $g_{1_{x_r}} = 0$, (25) and (27) should be replaced by

$$\hat{\mu}_1(t/T) = \hat{g}_{1_x}^{-1} (\hat{f}_{x_{rr}}^T \hat{\lambda})_r \quad r = 1 \quad (78)$$

$$\hat{\lambda}(r, t/T) = 0 \quad r = 1 \quad (79)$$

The last term of the first equation of (51) must also be replaced by

$$-R_4^{-1}(T) \hat{g}_{1_x}^{-1} \hat{f}_{x_{rr}}^T \delta'(s-1) .$$

In Appendix II-C the computational application of the filter is illustrated in an example of the feedback control of a styrene polymerization reactor.

Appendix II-A

This appendix evaluates the last three terms of (62), (63) and (64). We consider first the term

$$\int_0^1 M_i(\cdot, s, t/T) \frac{\partial}{\partial t} [\hat{\lambda}_T(s, t/T)] ds \quad (A.1)$$

where the matrix $M_i(\cdot, s, t/T)$ represents $P^{VV}(r, s, t/T)$, $P^{AV}(s, t/T)$, or $P^{BV}(s, t/T)$ according to $i=1, 2$, or 3 . Hence, the unspecified argument of $M_i(\cdot, s, t/T)$ is r if $i=1$ and does not exist otherwise. With the help of (19), (A.1) can be rewritten as

$$\begin{aligned} & 2 \int_0^1 M_i(\cdot, s, t/T) \left\{ \int_0^1 V(s, \rho, t/T) d\rho \right\}_T ds \\ & + \int_0^1 M_i(\cdot, s, t/T) \left\{ -\hat{f}_X^T \hat{\lambda} + (\hat{f}_{X_S}^T \hat{\lambda})_s - (\hat{f}_{X_{SS}}^T \hat{\lambda})_{ss} \right\}_T ds \end{aligned} \quad (A.2)$$

where the vector

$$V(s, \rho, t/T) = h_X^T(s, t, \hat{x}) Q(s, \rho, t) [y(\rho, t) - h(\rho, t, \hat{x})] \quad (A.3)$$

Since we can write [34, p. 28]

$$\begin{aligned} \left\{ \int_0^1 V(s, \rho, t/T) d\rho \right\}_T &= \int_0^1 S_\rho(s, \rho, t/T) \hat{x}_T(\rho, t/T) d\rho \\ &+ \int_0^1 S_s(s, \rho, t/T) \hat{x}_T(s, t/T) d\rho \end{aligned} \quad (A.4)$$

where the matrices

$$S_{\rho}(s, \rho, t/T) = \frac{\partial V(s, \rho, t/T)}{\partial \hat{x}(\rho, t/T)}$$

$$S_s(s, \rho, t/T) = \frac{\partial V(s, \rho, t/T)}{\partial \hat{x}(s, t/T)} \quad (\text{A.5})$$

and if we use (31) in (A.4), it is straightforward to show that

$$\int_0^1 M_i(\cdot, s, t/T) \left[\int_0^1 V(s, \rho, t/T) d\rho \right]_T ds$$

$$= -\frac{1}{2} \int_0^1 [N_i^{vv}(\cdot, s, t/T) + U_i^{vv}(\cdot, s, t/T)] \hat{\lambda}_T(s, t/T) ds$$

$$- \frac{1}{2} [N_i^{va}(\cdot, t/T) + U_i^{va}(\cdot, t/T)] \hat{\tau}(t/T)$$

$$- \frac{1}{2} [N_i^{vb}(\cdot, t/T) + U_i^{vb}(\cdot, t/T)] \hat{\sigma}_T(t/T) \quad (\text{A.6})$$

where

$$N_i^{vv}(\cdot, s, t/T) = \int_0^1 \int_0^1 M_i(\cdot, \zeta, t/T) S_v(\zeta, \nu, t/T) P^{vv}(\nu, s, t/T) d\zeta d\nu$$

$$U_i^{vv}(\cdot, s, t/T) = \int_0^1 \int_0^1 M_i(\cdot, \zeta, t/T) S_{\zeta}(\zeta, \nu, t/T) P^{vv}(\zeta, s, t/T) d\zeta d\nu$$

$$N_i^{va}(\cdot, t/T) = \int_0^1 \int_0^1 M_i(\cdot, \zeta, t/T) S_v(\zeta, \nu, t/T) P^{va}(\nu, t/T) d\zeta d\nu$$

$$U_i^{va}(\cdot, t/T) = \int_0^1 \int_0^1 M_i(\cdot, \zeta, t/T) S_{\zeta}(\zeta, \nu, t/T) P^{va}(\zeta, t/T) d\zeta d\nu$$

$$N_i^{vb}(\cdot, t/T) = \int_0^1 \int_0^1 M_i(\cdot, \zeta, t/T) S_v(\zeta, \nu, t/T) P^{vb}(\nu, t/T) d\zeta d\nu$$

$$U_i^{vb}(\cdot, t/T) = \int_0^1 \int_0^1 M_i(\cdot, \zeta, t/T) S_{\zeta}(\zeta, \nu, t/T) P^{vb}(\zeta, t/T) d\zeta d\nu \quad (\text{A.7})$$

The unspecified argument of each term of (A.6) and (A.7) is r if $i = 1$ and does not exist otherwise. Further, (A.5) possesses the symmetry properties

$$\begin{aligned} S_s(s, \rho, t/T) &= S_s^T(s, \rho, t/T) \\ S_\rho(s, \rho, t/T) &= S_s^T(\rho, s, t/T) \end{aligned} \quad (\text{A.8})$$

Now let us consider the second term in (A.2), the integration of which by parts yields

$$\begin{aligned} & \int_0^1 M_i(\cdot, s, t/T) \left\{ -\hat{f}_x^T \hat{\lambda} + (\hat{f}_{x_s}^T \hat{\lambda})_s - (\hat{f}_{x_{ss}}^T \hat{\lambda})_{ss} \right\}_T ds \\ &= - \int_0^1 (M \hat{f}_x^T + M_s \hat{f}_{x_s}^T + M_{ss} \hat{f}_{x_{ss}}^T) \hat{\lambda}_T(s, t/T) ds \\ &+ \left\{ M(\hat{f}_{x_s}^T \hat{\lambda})_T - M[(\hat{f}_{x_{ss}}^T \hat{\lambda})_s]_T + M_s(\hat{f}_{x_{ss}}^T \hat{\lambda})_T \right\}_{s=0}^{s=1} \\ &- \int_0^1 \left\{ M(\hat{f}_x^T)_T + M_s(\hat{f}_{x_s}^T)_T + M_{ss}(\hat{f}_{x_{ss}}^T)_T \right\} \hat{\lambda}(s, t/T) ds \end{aligned} \quad (\text{A.9})$$

where M denotes $M_i(\cdot, s, t/T)$. (A.7)-(A.9) are used to evaluate the third to last term in (62)-(64).

The second to last term of (62)-(64) can be written with the help of (20) as

$$\begin{aligned} P \frac{\partial}{\partial t} [\hat{\tau}_T(t/T)] &= - \int_0^1 P \hat{f}_a^T(s) \hat{\lambda}_T(s, t/T) ds - P \hat{A}_a^T \hat{\tau}_T(t/T) \\ &- \int_0^1 P(\hat{f}_a^T(s))_T \hat{\lambda}(s, t/T) ds - P(\hat{A}_a^T)_T \hat{\tau}(t/T) \end{aligned} \quad (\text{A.10})$$

where the matrix P denotes $P^{va}(r,t/T)$, $P^{aa}(t/T)$, or $P^{ba}(t/T)$.

The last term of (62)-(64) can be written as

$$K \frac{\partial}{\partial t} [\hat{\sigma}_T(t/T)] = -K \hat{B}_b^T \hat{\sigma}_T(t/T) + K \hat{g}_{1_b}^T \hat{g}_{1_{x_s}}^{-1} \hat{f}_{x_{ss}}^T \hat{\lambda}_T(s,t/T) - K(\hat{B}_b^T)_T \hat{\sigma}(t/T) + K(\hat{g}_{1_b}^T \hat{g}_{1_{x_s}}^{-1} \hat{f}_{x_{ss}}^T)_T \hat{\lambda}(s,t/T) \quad s = 1 \quad (A.11)$$

where the matrix K represents $P^{vb}(r,t/T)$, $P^{ab}(t/T)$, or $P^{bb}(t/T)$, and we have used (21) and (25) to obtain (A.11).

In (A.9) the term corresponding to $s = 0$ and $s = 1$ can be evaluated with the help of (26) and (27).

Finally, in (A.9)-(A.11), there are terms which have $\hat{\lambda}(s,t/T)$, $\hat{\lambda}(0,t/T)$, $\hat{\lambda}(1,t/T)$, $\hat{\tau}(t/T)$, or $\hat{\sigma}(t/T)$ as coefficients, e.g., the last term of (A.11). These terms do not contribute to the filter because they vanish at $t = T$. To show this, we consider a matrix \hat{H} which can be expressed as

$$\hat{H} = H[r,t,\hat{x}(r,t/T), \hat{x}_r(r,t/T), \hat{x}_{rr}(r,t/T), \hat{a}(t/T), \hat{b}(t/T)] \quad (A.12)$$

Let $\hat{x}(r,t/T)$, $\hat{a}(t/T)$ and $\hat{b}(t/T)$ be functionals of the Lagrange multipliers as in (28). Let the vector \hat{e} denote either $\hat{\lambda}(r,t/T)$, $\hat{\tau}(t/T)$, or $\hat{\sigma}(t/T)$. Hence, $\hat{e} = 0$ at $t = T$. Further, let the operation $\hat{H}\hat{e}$ be defined. Then, it is easily shown that there exist matrices \hat{H}_i , $i=1,2,3$, such that

$$\hat{H}_T \hat{e} = \int_0^1 \hat{H}_1 \hat{\lambda}_T(v,t/T) dv + \hat{H}_2 \hat{\tau}_T(t/T) + \hat{H}_3 \hat{\sigma}_T(t/T) \quad (A.13)$$

and $\hat{H}_i = 0$ at $t = T$ for all i . Further,

$$\int_0^1 \hat{H}_T \hat{e} \, dr = \int_0^1 \left\{ \int_0^1 \hat{H}_1 \, dv \right\} \hat{\lambda}_T(r, t/T) \, dr + \left\{ \int_0^1 \hat{H}_2 \, dv \right\} \hat{\tau}_T(t/T) + \left\{ \int_0^1 \hat{H}_3 \, dv \right\} \hat{\sigma}_T(t/T) \quad (\text{A.14})$$

where we have interchanged the dummy variables r and v on the right hand side of (A.14).

Appendix II-B

In this appendix we obtain the necessary conditions for optimality corresponding to the minimization of (10). This is achieved by setting the first variation of L (denoted by δL) to zero [14]. We emphasize that δL is the total first variation. Suppose L depends functionally on parameters p_i , $i=1,2,\dots,J$, then we can write $\delta L = \sum_{i=1}^J \delta L(p_i)$ where $\delta L(p_i)$ is the first variation of L with respect to a variation of p_i (denoted by δp_i) over the appropriate domain. In this way, we can write

$$\begin{aligned} \delta L = & \delta L(\mu_0(t)) + \delta L(\mu_1(t)) + \delta L(\tau(t)) \\ & + \delta L(\sigma(t)) + \delta L(\lambda(r,t)) \\ & + \delta L(u_1(r,t)) + \delta L(u_1(s,t)) + \sum_{i=2}^5 \delta L(u_i(t)) \\ & + \delta L(x(r,t)) + \delta L(x(s,t)) \\ & + \delta L(x_t(r,t)) + \delta L(x_r(r,t)) + \delta L(x_{rr}(r,t)) \\ & + \delta L(x(0,t)) + \delta L(x(1,t)) + \delta L(x_r(0,t)) + \delta L(x_r(1,t)) \\ & + \delta L(a(t)) + \delta L(\dot{a}(t)) \\ & + \delta L(b(t)) + \delta L(\dot{b}(t)) \end{aligned}$$

We proceed to evaluate various variations. For convenience, we denote $f(r,t,x,x_r,x_{rr},a(t))$, $A(t,a)$, $B(t,b)$, $g_0(t,x,x_r)$, $g_1(t,x,x_r,b)$ by f , A , B , g_0 , g_1 , respectively.

$$\delta L(\mu_0(t)) = \int_0^T \langle \delta\mu_0(t), g_0 + u_3(t) \rangle dt$$

$$\delta L(\mu_1(t)) = \int_0^T \langle \delta\mu_1(t), g_1 + u_4(t) \rangle dt$$

$$\delta L(\tau(t)) = \int_0^T \langle -\delta\tau(t), \dot{a}(t) - A - u_2(t) \rangle dt$$

$$\delta L(\sigma(t)) = \int_0^T \langle -\delta\sigma(t), \dot{b}(t) - B - u_5(t) \rangle dt$$

$$\delta L(\lambda(r,t)) = \int_0^T \int_0^1 \langle -\delta\lambda(r,t), x_t(r,t) - f - u_1(r,t) \rangle dr dt$$

$$\delta L(u_1(r,t)) = \int_0^T \left[\int_0^1 \int_0^1 \langle \delta u_1(r,t), R(r,s,t) u_1(s,t) \rangle dr ds + \int_0^1 \langle \delta u_1(r,t), \lambda(r,t) \rangle dr \right] dt$$

$$\delta L(u_1(s,t)) = \int_0^T \int_0^1 \int_0^1 \langle \delta u_1(r,t), R(r,s,t) u_1(s,t) \rangle dr ds dt$$

$$\delta L(u_2(t)) = \int_0^T \langle \delta u_2(t), 2R_2(t) u_2(t) + \tau(t) \rangle dt$$

$$\delta L(u_3(t)) = \int_0^T \langle \delta u_3(t), 2R_3(t) u_3(t) + \mu_0(t) \rangle dt$$

$$\delta L(u_4(t)) = \int_0^T \langle \delta u_4(t), 2R_4(t) u_4(t) + \mu_1(t) \rangle dt$$

$$\delta L(u_5(t)) = \int_0^T \langle \delta u_5(t), 2R_5(t) u_5(t) + \sigma(t) \rangle dt$$

$$\delta L(x(r,t)) = \int_0^T \left[\int_0^1 \int_0^1 \langle -\delta x(r,t), h_x^T(r,t,x) Q(r,s,t) \right. \\ \left. \times (y(s,t) - h(s,t,x)) \rangle dr ds \right. \\ \left. + \int_0^1 \langle \delta x(r,t), f_x^T \lambda \rangle dr \right] dt$$

$$\delta L(x(s,t)) = \int_0^T \left[\int_0^1 \int_0^1 \langle -\delta x(r,t), h_x^T(r,t,x) Q(r,s,t) \right. \\ \left. \times (y(s,t) - h(s,t,x)) \rangle dr ds \right] dt$$

$$\delta L(x_t(r,t)) = \int_0^1 \int_0^T \langle -\delta x_t(r,t), \lambda \rangle dt dr \\ = \int_0^1 \langle -\delta x(r,T), \lambda(r,T) \rangle dr + \int_0^1 \langle \delta x(r,0), \lambda(r,0) \rangle dr \\ + \int_0^T \int_0^1 \langle \delta x(r,t), \lambda_t \rangle dr dt$$

$$\delta L(x_r(r,t)) = \int_0^T \int_0^1 \langle \delta x_r(r,t), f_{x_r}^T \lambda \rangle dr dt \\ = \int_0^T \langle \delta x(r,t), f_{x_r}^T \lambda \rangle \Big|_{r=0}^{r=1} dt \\ - \int_0^T \int_0^1 \langle \delta x(r,t), (f_{x_r}^T \lambda)_r \rangle dr dt$$

$$\begin{aligned}
 \delta L(x_{rr}(r,t)) &= \int_0^T \int_0^1 \langle \delta x_{rr}(r,t), f_{x_{rr}}^T \lambda \rangle dr dt \\
 &= \int_0^T \langle \delta x_r(r,t), f_{x_{rr}}^T \lambda \rangle \Big|_{r=0}^{r=1} dt \\
 &\quad - \int_0^T \langle \delta x(r,t), (f_{x_{rr}}^T \lambda)_r \rangle \Big|_{r=0}^{r=1} dt \\
 &\quad + \int_0^T \int_0^1 \langle \delta x(r,t), (f_{x_{rr}}^T \lambda)_{rr} \rangle dr dt
 \end{aligned}$$

$$\delta L(x(0,t)) = \int_0^T \langle \delta x(0,t), g_{0x}^T \mu_0 \rangle dt$$

$$\delta L(x(1,t)) = \int_0^T \langle \delta x(1,t), g_{1x}^T \mu_1 \rangle dt$$

$$\delta L(x_r(0,t)) = \int_0^T \langle \delta x_r(0,t), g_{0x_r}^T \mu_0 \rangle dt$$

$$\delta L(x_r(1,t)) = \int_0^T \langle \delta x_r(1,t), g_{1x_r}^T \mu_1 \rangle dt$$

$$\delta L(a(t)) = \int_0^T \langle \delta a(t), A_a^T \tau \rangle dt + \int_0^T \int_0^1 \langle \delta a(t), f_a^T \lambda \rangle dr dt$$

$$\begin{aligned}
 \delta L(\dot{a}(t)) &= \int_0^T \langle -\delta \dot{a}(t), \tau \rangle dt \\
 &= \langle -\delta a(t), \tau \rangle \Big|_{t=0}^{t=T} + \int_0^T \langle \delta a(t), \tau_t \rangle dt
 \end{aligned}$$

$$\delta L(b(t)) = \int_0^T \langle \delta b(t), B_b^T \sigma + g_{1b}^T \mu_1 \rangle dt$$

$$\begin{aligned} \delta L(\dot{b}(t)) &= \int_0^T \langle -\delta \dot{b}(t), \sigma \rangle dt \\ &= \langle -\delta b(t), \sigma \rangle \Big|_{t=0}^{t=T} + \int_0^T \langle \delta b(t), \sigma_t \rangle dt \end{aligned}$$

In order that $\delta L = 0$ for arbitrary δp_i , the coefficient of each of the following δp_i must identically be zero. Let $\phi(\delta p_i)$ denote the coefficient of δp_i , then

$$\phi(\delta \mu_0(t)) = 0 \quad \text{implies}$$

$$g_0 + u_3(t) = 0 \quad r = 0$$

$$\phi(\delta \mu_1(t)) = 0 \quad \text{implies}$$

$$g_1 + u_4(t) = 0 \quad r = 1$$

$$\phi(\delta \tau(t)) = 0 \quad \text{implies}$$

$$\dot{a}(t) = A + u_2(t)$$

$$\phi(\delta \sigma(t)) = 0 \quad \text{implies}$$

$$\dot{b}(t) = B + u_5(t)$$

$$\phi(\delta \lambda(r,t)) = 0 \quad \text{implies}$$

$$x_t(r,t) = f + u_1(r,t) \quad r \in (0,1)$$

$$\phi(\delta u_1(r,t)) = 0 \quad \text{implies}$$

$$u_1(r,t) = -\frac{1}{2} \int_0^1 R^+(r,s,t) \lambda(s,t) ds$$

$$\phi(\delta u_i(t)) = 0, \quad i=2,3,4,5, \quad \text{imply}$$

$$u_2(t) = -\frac{1}{2} R_2^{-1}(t) \tau(t)$$

$$u_3(t) = -\frac{1}{2} R_3^{-1}(t) \mu_0(t)$$

$$u_4(t) = -\frac{1}{2} R_4^{-1}(t) \mu_1(t)$$

$$u_5(t) = -\frac{1}{2} R_5^{-1}(t) \sigma(t)$$

$$\phi(\delta x(r,t)) = 0 \quad \text{implies}$$

$$\lambda_t(r,t) = 2 \int_0^1 h_x^T(r,t,x) Q(r,s,t) (y(s,t) - h(s,t,x)) ds \\ - f_x^T \lambda + (f_{x_r}^T \lambda)_r - (f_{x_{rr}}^T \lambda)_{rr}$$

$$\phi(\delta a(t)) = 0 \quad \text{implies}$$

$$\tau_t = - \int_0^1 f_a^T \lambda(s,t) ds - A_a^T \tau$$

$$\phi(\delta b(t)) = 0 \quad \text{implies}$$

$$\sigma_t = - B_b^T \sigma - g_{1_b}^T \mu_1 \quad r = 1$$

$$\phi(\delta x(r,T)) = \phi(\delta a(T)) = \phi(\delta b(T)) = 0 \quad \text{implies}$$

$$\lambda(r,T) = \tau(T) = \sigma(T) = 0$$

$$\phi(\delta x(r,0)) = \phi(\delta a(0)) = \phi(\delta b(0)) = 0 \quad \text{implies}$$

$$\lambda(r,0) = \tau(0) = \sigma(0) = 0$$

$\phi(\delta x(0,t)) = 0$ implies

$$g_{0x}^T \mu_0 - f_{x_r}^T \lambda + (f_{x_{rr}}^T \lambda)_r = 0 \quad r = 0$$

$\phi(\delta x(1,t)) = 0$ implies

$$g_{1x}^T \mu_1 + f_{x_r}^T \lambda - (f_{x_{rr}}^T \lambda)_r = 0 \quad r = 1$$

$\phi(\delta x_r(0,t)) = 0$ implies

$$g_{0x_r}^T \mu_0 - f_{x_{rr}}^T \lambda = 0 \quad r = 0$$

$\phi(\delta x_r(1,t)) = 0$ implies

$$g_{1x_r}^T \mu_1 + f_{x_{rr}}^T \lambda = 0 \quad r = 1$$

Control of Stochastic Distributed-Parameter Systems¹

T. K. YU² AND J. H. SEINFELD³

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Abstract. A scheme is proposed for the feedback control of distributed-parameter systems with unknown boundary and volume disturbances and observation errors. The scheme consists of employing a nonlinear filter in the control loop such that the controller uses the optimal estimates of the state of the system. A theoretical comparison of feedback proportional control of a styrene polymerization reactor with and without filtering is presented. It is indicated how an approximate filter can be constructed, greatly reducing the amount of computing required.

Notation

$a(t)$	l -vector noisy dynamic input to system
$A(t, a)$	l -vector function
A'	frequency factor for first-order rate law ($5.68 \times 10^6 \text{ sec}^{-1}$)
b	distance to the centerline between two coil banks in the reactor (4.7 cm)
B	k -vector function defining the control action
$c(x, \tau)$	concentration of styrene monomer, mole l^{-1}
C_p	heat capacity ($0.43 \text{ cal} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$)
C_{ij}	constants in approximate filter, Eqs. (49)–(52)
E	activation energy ($20330 \text{ cal} \cdot \text{mole}^{-1}$)
\mathcal{E}	expectation operator
$f(t, \dots)$	n -vector function
$g_0, g_1(t, \dots)$	n -vector functions
$h(t, u)$	m -vector function relating observations to states

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² Graduate Research Assistant, Department of Chemical Engineering, California Institute of Technology, Pasadena, California.

³ Associate Professor, Department of Chemical Engineering, California Institute of Technology, Pasadena, California.

$H(t)$	function defined in Eq. (36)
k	dimensionality of control vector $v(x, t)$
k_i	constants in approximate filter, Eqs. (49)–(52)
K	dimensionless proportional gain
l	dimensionality of dynamic input $a(t)$
m	dimensionality of observation vector $y(t)$
n	dimensionality of state vector $u(x, t)$
$P^{(vv)}(x, s, t)$	$n \times n$ matrix governed by Eq. (9)
$P^{(va)}(x, t)$	$n \times l$ matrix governed by Eq. (10)
$P^{(aa)}(t)$	$l \times l$ matrix governed by Eq. (11)
$q_i(t)$	diagonal elements of $m \times m$ matrix $Q(x, s, t)$
$Q(x, s, t)$	$m \times m$ weighting matrix
R	universal gas constant ($1.987 \text{ cal} \cdot \text{mole}^{-1} \cdot \text{K}^{-1}$)
$R(x, s, t)$	$n \times n$ weighting matrix
$R_i(t)$	$n \times n$ weighting matrix
s	dimensionless spatial variable
$S(x, s, t)$	matrix defined in Eq. (11)
t	dimensionless time variable
$T(x, \tau)$	temperature, K
$u(x, t)$	n -dimensional state vector
$u_c(t)$	wall temperature
u_d	desired value of $u_1(1, t)$
u_c^*	reference control value of u_c
u_c^{\max}	maximum value of u_c
u_c^{\min}	minimum value of u_c
$v(x, t)$	k -dimensional control vector
$W(t)$	$l \times l$ weighting matrix
x	dimensionless spatial variable
$y(t)$	m -dimensional observation vector
α_i	constants in approximate filter, Eqs. (49)–(52)
β	dimensionless parameter defined in Eq. (29)
ΔH	heat of reaction ($17500 \text{ cal} \cdot \text{mole}^{-1}$)
ϵ	dimensionless activation energy, defined in Eq. (29)
$\delta(x)$	Dirac delta function
$\eta(x, t)$	m -dimensional observation noise
κ	thermal conductivity ($0.43 \times 10^{-3} \text{ cal} \cdot \text{cm}^{-1} \cdot \text{sec}^{-1} \cdot \text{K}^{-1}$)
ρ	density ($1 \text{ g} \cdot \text{cm}^{-3}$)
τ	time, sec
ϕ	dimensionless parameter defined in Eq. (29)
χ	spatial variable, cm
*	reference value
^	estimated value

1. Introduction

In most real processes that must be controlled, there exists some degree of uncertainty. The uncertainty may be a result of observations of the output which are corrupted with noise or of the use of a mathematical model which is only an approximation to the true behavior of the system. The control of stochastic systems has received much attention in recent years. (Refs. 1-4). The control of linear stochastic distributed-parameter systems subject to white noise disturbances has been considered by Tzafestas and Nightingale (Ref. 5), Kushner (Ref. 6), Thau (Ref. 7), Pell and Aris (Ref. 8), and Sholar and Wiberg (Ref. 9). Here we consider the feedback control of nonlinear distributed-parameter systems subject to noisy inputs and measurement errors. No assumptions concerning the statistical nature of the noisy inputs and measurement errors, other than that they are zero mean random processes, will be made.

The scheme which we propose is inherently quite simple. In particular, the measurements of the system are to be processed by an on-line computer in a nonlinear filtering or recursive estimation algorithm to produce optimal least-square estimates of the true state of the system. These estimates, which include all of the states of the system, not only the measured ones, are then used as inputs to the controller in the feedback loop. The scheme has been demonstrated for lumped-parameter systems in Ref. 10. Here, we develop the theory for the same control strategy for distributed-parameter systems. We will first present the general scheme and then illustrate the application of the scheme for the control of a styrene polymerization reactor.

2. General Control Scheme

We assume that the system can be described by a set of partial differential equations of known form but perhaps containing unknown parameters. The stochastic nature of the problem is assumed to arise from noisy inputs and measurement errors. We consider the class of systems governed by

$$u_i(x, t) = f(x, t, u, u_x, u_{xx}, v(x, t), a(t)) + \xi_1(x, t), \quad (1)$$

defined for $t \geq 0$ on the normalized domain $(0, 1)$, where $u(x, t)$ is the n -vector state, $v(x, t)$ is a k -vector of controls, and $\xi_1(x, t)$ is an unknown

n -vector disturbance. The symbols u_t, u_x, u_{xx} denote $\partial u/\partial t, \partial u/\partial x,$ and $\partial^2 u/\partial x^2,$ respectively. The l -vector input $a(t)$ is governed by

$$da/dt = A(t, a(t)) + \xi_2(t), \tag{2}$$

where $a(t)$ represents a noisy dynamic input to the system. We note that both additive and nonadditive noisy inputs are included by $\xi_1(t)$ and $a(t),$ respectively.

The boundary conditions are given by

$$g_0(t, u, u_x, v) + \xi_3(t) = 0, \quad x = 0, \tag{3}$$

$$g_1(t, u, u_x, v) + \xi_4(t) = 0, \quad x = 1, \tag{4}$$

where ξ_2, ξ_3, ξ_4 are independent zero-mean random processes with unknown statistical characteristics. Observations of the system consist of the m -vector $y(x, t),$ related to the state by

$$y(x, t) = h(x, t, u(x, t)) + \eta(x, t), \tag{5}$$

where $\eta(x, t)$ is an m -vector of unknown measurement noise.

We want to consider the feedback control of the system (1)–(5). Thus, the control variable $v(x, t)$ will be determined on the basis of the measurements $y(x, t), v(x, t) = B(y(x, t)).$ This represents the usual situation of feedback control. However, if the noise is significant or the control is critical to the proper functioning of the system, then control based directly on the measurements may be quite poor. What we would like to have is the control action determined on the basis of the actual state of the system rather than the noisy measurements. Therefore, the problem is to generate continuously optimal estimates of the system state based on the observations. This is exactly the filtering or recursive estimation problem for a dynamical system. The use of a filter in the control loop will offer two important advantages: (i) optimal estimates of *all* the components of the state vector $u(x, t)$ will be provided in real time, not just those components which appear in (5); and (ii) since estimates of all the components of $u(x, t)$ are available, we can formulate a controller based on unmeasured as well as measured states. Thus, we will let the control function be represented by

$$v(x, t) = B(\hat{u}(x, t)), \tag{6}$$

where $\hat{u}(x, t)$ is the estimated value of $u(x, t).$

3. Filtering in Distributed-Parameter Systems

The subject of filtering in systems described by partial differential equations has received only limited attention. Filtering in linear distributed systems with white noise disturbances has been treated in Refs. 11-17, wherein results analogous to the Kalman filter were obtained. Filtering in nonlinear distributed systems has been considered in Refs. 18-20. The most general filter has been derived in Ref. 20, based on an optimal control approach and invariant embedding. A nonlinear least-square filter based on Eqs. (1)-(5) is given by [one assumes that Eq. (6) has been substituted into Eq. (1)]

$$\begin{aligned} \hat{u}_t &= f(x, t, \hat{u}, \hat{u}_x, \hat{u}_{xx}, \hat{a}) \\ &+ \int_0^1 \int_0^1 P^{(vv)}(x, \xi, t) h_u^T(\xi, t, \hat{u}) Q(\xi, \nu, t) [y(\nu, t) - h(\nu, t, \hat{u})] d\xi d\nu \\ &+ P^{(vv)}(x, 0, t) h_u^T(0, t, \hat{u}) Q(0, 0, t) [y(0, t) - h(0, t, \hat{u})], \end{aligned} \quad (7)$$

$$\begin{aligned} \hat{a}_t &= A(t, \hat{a}) \\ &+ \int_0^1 \int_0^1 P^{(av)}(\xi, t) h_u^T(\xi, t, \hat{u}) Q(\xi, \nu, t) [y(\nu, t) - h(\nu, t, \hat{u})] d\xi d\nu \\ &+ P^{(av)}(0, t) h_u^T(0, t, \hat{u}) Q(0, 0, t) [y(0, t) - h(0, t, \hat{u})], \end{aligned} \quad (8)$$

$$\begin{aligned} P_t^{(vv)}(x, s, t) &= f_u(x) P^{(vv)} + P^{(vv)} f_u^T(s) + f_{u_x}(x) P_x^{(vv)} + P_s^{(vv)} f_{u_s}^T(s) \\ &+ f_{u_{xx}}(x) P_{xx}^{(vv)} + P_{ss}^{(vv)} f_{u_{ss}}^T(s) + f_a(x) P^{(va)T}(s, t) + P^{(va)}(x, t) f_a^T(s) \\ &+ \int_0^1 \int_0^1 P^{(vv)}(x, \xi, t) S(\xi, \nu, t) P^{(vv)}(\nu, s, t) d\xi d\nu \\ &+ P^{(vv)}(x, 0, t) S(0, 0, t) P^{(vv)}(0, s, t) + R^{-1}(x, s, t), \end{aligned} \quad (9)$$

$$\begin{aligned} P_t^{(va)}(x, t) &= f_u(x) P^{(va)} + f_{u_x}(x) P_x^{(va)} + f_{u_{xx}}(x) P_{xx}^{(va)} + f_a(x) P^{(aa)} \\ &+ P^{(va)} \hat{A}_a^T + \int_0^1 \int_0^1 P^{(vv)}(x, \xi, t) S(\xi, \nu, t) P^{(va)}(\nu, t) d\xi d\nu \\ &+ P^{(vv)}(x, 0, t) S(0, 0, t) P^{(va)}(0, t), \end{aligned} \quad (10)$$

$$\begin{aligned} P_t^{(aa)}(t) &= \hat{A}_a P^{(aa)} + P^{(aa)} \hat{A}_a^T + \int_0^1 \int_0^1 P^{(va)T}(\xi, t) S(\xi, \nu, t) P^{(va)}(\nu, t) d\xi d\nu \\ &+ P^{(va)T}(0, t) S(0, 0, t) P^{(va)}(0, t) + W^{-1}(t), \end{aligned} \quad (11-1)$$

$$S(x, s, t) = [h_u^T(x, t, \hat{u}) Q(x, s, t) [y(s, t) - h(s, t, \hat{u})]]_{u(s, t)}, \quad (11-2)$$

where $Q(x, s, t)$, $R(x, s, t)$, and $W(t)$ are arbitrary positive-definite weighting matrices.

The initial and boundary conditions are

$$\hat{u}(x, 0) = \hat{u}_0(x), \tag{12}$$

$$\hat{a}(0) = \hat{a}_0, \tag{13}$$

$$g_0(t, \hat{u}, \hat{u}_x) = 0, \tag{14}$$

$$g_1(t, \hat{u}, \hat{u}_x) = 0, \tag{15}$$

$$P^{(vv)}(x, s, 0) = P_0^{(vv)}(x, s), \tag{16}$$

$$P^{(va)}(x, 0) = P_0^{(va)}(x), \tag{17}$$

$$P^{(aa)}(0) = P_0^{(aa)}, \tag{18}$$

$$\hat{g}_{0u} P^{(vv)} + \hat{g}_{0u_x} P_x^{(vv)} + R_1^{-1}(t) \hat{g}_{0u_x}^{-1} f_{u_{xx}}^T \delta(s) = 0, \quad x = 0, \tag{19}$$

$$\hat{g}_{1u} P^{(vv)} + \hat{g}_{1u_x} P_x^{(vv)} - R_2^{-1}(t) \hat{g}_{1u_x}^{-1} f_{u_{xx}}^T \delta(s - 1) = 0, \quad x = 1, \tag{20}$$

$$\hat{g}_{0u} P^{(va)} + \hat{g}_{0u_x} P_x^{(va)} = 0, \quad x = 0, \tag{21}$$

$$\hat{g}_{1u} P^{(va)} + \hat{g}_{1u_x} P_x^{(va)} = 0, \quad x = 1, \tag{22}$$

where $R_1^{-1}(t)$ and $R_2^{-1}(t)$ are arbitrary positive-definite weighting matrices.

The initial conditions $\hat{u}_0(x)$ and \hat{a}_0 represent our best guesses of the initial state and the noisy input $a(t)$. The initial conditions on the auxiliary equations, which we will refer to as the covariance equations, $P_0^{(vv)}(x, s)$, $P_0^{(va)}(x)$, and $P_0^{(aa)}$, are somewhat arbitrary. For measurements at M discrete spatial locations, we replace $Q(x, s, t)$ by

$$Q_d(x, s, t) = (1/M^2) \sum_{k=1}^M \sum_{l=1}^M Q(x_k, s_l, t) \delta(x - x_k) \delta(s - s_l), \tag{23}$$

so that the integrations in Eqs. (7)–(11) become summations.

If, in addition to the system states, it is necessary to estimate constant parameters appearing in Eq. (1), then these parameters can be considered as components of $a(t)$ for which $A_i(t, a) = 0$. Although to conserve space we have not presented the most general form of the filter here, the estimation of dynamical inputs of the form of Eq. (2) in the boundary conditions (3) and (4) can also be included. In the example to follow, we will consider only measurement errors, that is,

$$\xi_1 = \xi_3 = \xi_4 = 0.$$

Thus, $R(x, s, t)$, $R_1^{-1}(t)$, and $R_2^{-1}(t)$ will not be required. Also, there will be no noisy dynamical inputs of the form of Eq. (2), so that the matrices $P^{(av)}(x, t)$ and $P^{(aa)}(t)$ will not appear.

In summary, the system dynamics are described by Eqs. (1)–(6). The filter is governed by Eqs. (7)–(11), subject to Eqs. (12)–(22). Thus, the dynamics of the closed loop in the absence of filtering are described by Eqs. (1)–(5) and $v(x, t) = B[y(x, t)]$. With the filter, the dynamics are described by Eqs. (1)–(22). We now wish to compare the closed loop dynamics of a complex distributed system with and without a filter in the control loop. We will pay particular attention to the practical aspects of the scheme.

4. Control of a Styrene Polymerization Reactor

A common process for styrene polymerization, particularly high-impact polystyrene, is mass or batch operation, wherein styrene monomer is fed to the reactor, a predetermined temperature and agitation program is followed, and the product is removed after a set time of operation. Problems encountered in reactor design and control stem from the highly exothermic nature of styrene polymerization and the high viscosity of polystyrene melts, making adequate heat transfer a key design consideration. Since agitation rates are limited by the viscosity of the reactor contents, heat transfer is accomplished by banks of internal coils containing circulating oil, the temperature of which can be controlled externally. In order to prevent the formation of local hot spots which can lead to an unstable reactor, heat transfer surfaces are generally separated by a few inches at most.

The typical high-impact polystyrene polymerization process can be divided into two phases: an agitated phase and a nonagitated phase. Initially, the reactor contains mostly low-viscosity monomer, and heat transfer is accomplished by agitation. However, as the polymerization proceeds, the viscosity increases sharply and agitation can no longer be used. During this second phase, heat transfer occurs by conduction only. Close control of the temperature of the coils is important so that the polymerization will proceed at a significant rate but with temperatures kept below the point at which hot spots can develop with the reactor becoming unstable.

Let us assume that the reactor contains several parallel coil banks, separated by a distance $2b$. We consider the reaction to be confined to the space $\chi = 0$ to $\chi = 2b$. The polymerization of pure styrene has been thoroughly studied (Ref. 21). The mass thermal polymerization of

styrene can be considered a first-order kinetic process with respect to styrene monomer concentration (Ref. 22). Denote the temperature and monomer concentration by $T(\chi, \tau)$ and $c(\chi, \tau)$. In the absence of agitation, they are governed by

$$T_{\tau}(\chi, \tau) = (\kappa/\rho C_p) T_{xx} + (\Delta HA'c/\rho C_p) \exp(-E/RT), \quad (24)$$

$$c_{\tau}(\chi, \tau) = -A'c \exp(-E/RT), \quad (25)$$

$$T(\chi, 0) = T_0, \quad c(\chi, 0) = c_0, \quad (26)$$

$$T(0, \tau) = T_c(\tau), \quad (27)$$

$$T_x = 0, \quad \chi = b. \quad (28)$$

Molecular diffusion of monomer in the highly viscous melt has been neglected. T_0 and c_0 are the temperature and concentration at $\tau = 0$, and condition (28) implies symmetry at the centerline between the heat transfer surfaces at $\chi = 0$ and $\chi = 2b$.

We define the dimensionless variables

$$\begin{aligned} x &= \chi/b, & \phi &= \Delta HA'c^*b^2/\kappa T^*, \\ t &= \kappa\tau/\rho C_p b^2, & \beta &= A'b^2\rho C_p/\kappa, \\ u_1 &= T/T^*, & \epsilon &= E/RT^*, \\ u_2 &= c/c^*, & u_{1_0} &= T_0/T^*, \\ u_c &= T_c/T^*, & u_{2_0} &= c_0/c^*, \end{aligned} \quad (29)$$

where T^* and c^* are a reference temperature and concentration. In dimensionless terms, the system becomes

$$u_{1_t} = u_{1_{xx}} + \phi u_2 \exp(-\epsilon/u_1), \quad (30)$$

$$u_{2_t} = -\beta u_2 \exp(-\epsilon/u_1), \quad (31)$$

$$u_1(x, 0) = u_{1_0}, \quad u_2(x, 0) = u_{2_0}, \quad (32)$$

$$u_1(0, t) = u_c(t), \quad (33)$$

$$u_{1_x} = 0, \quad x = 1. \quad (34)$$

Temperature control is exercised through $u_c(t)$. We consider the case in which u_c is determined by a feedback proportional law based on the

deviation of the centerline temperature $u_1(1, t)$ from a desired operating temperature u_d , that is,

$$u_c(t) = \begin{cases} u_c^{\max}, & H(t) > u_c^{\max}, \\ H(t), & u_c^{\min} < H(t) < u_c^{\max}, \\ u_c^{\min}, & H(t) < u_c^{\min}, \end{cases} \quad (35)$$

$$H(t) = u_c^* - K[y_1(t) - u_d], \quad (36)$$

where u_c^* is a reference control level, u_c^{\max} and u_c^{\min} are maximum and minimum control temperatures, K is the proportional gain, and $y_1(t)$ is the measured value of $u_1(1, t)$.

We want to study the effectiveness of the stochastic control scheme when the measurements of $u_1(1, t)$ are corrupted with noise. The parameter values used in the study are those for styrene polymerization (see the nomenclature for the values of individual parameters), specifically,

$$\begin{aligned} \phi &= 1.39 \times 10^{11}, & u_{1_0} &= 1.25, \\ \beta &= 1.25 \times 10^{11}, & u_{2_0} &= 1.0, \\ \epsilon &= 34.1, & u_d &= 1.27, \\ u_c^* &= 1.16667, & u_c^{\max} &= 1.22, \\ K &= 5.0, & u_c^{\min} &= 1.1. \end{aligned}$$

Figure 1 shows the dynamics of the system of Eqs. (30)–(36) when the temperature measurements at $x = 1$, $u_1(1, t)$, are noise-free, and corrupted with additive Gaussian noise with standard deviation 10% and 20% of the value of $u_1(1, t)$. We note that with 20% noise, the system becomes unstable because of the erratic action of the controller. It is the behavior shown in Figure 1 that we wish to avoid by means of the proposed control scheme. Let us first consider the performance of the filter in estimating temperature and concentration profiles in the reactor.

4.1. Estimation of Temperature and Concentration in the Reactor. We assume that it is possible to make a maximum of three measurements, consisting of the temperature at $x = 1$ and the concentration at $x = 0$ and $x = 1$, that is,

$$y_1(t) = u_1(1, t) + \eta_1(t), \quad (37)$$

$$y_2(t) = u_2(1, t) + \eta_2(t), \quad (38)$$

$$y_3(t) = u_2(0, t) + \eta_3(t). \quad (39)$$

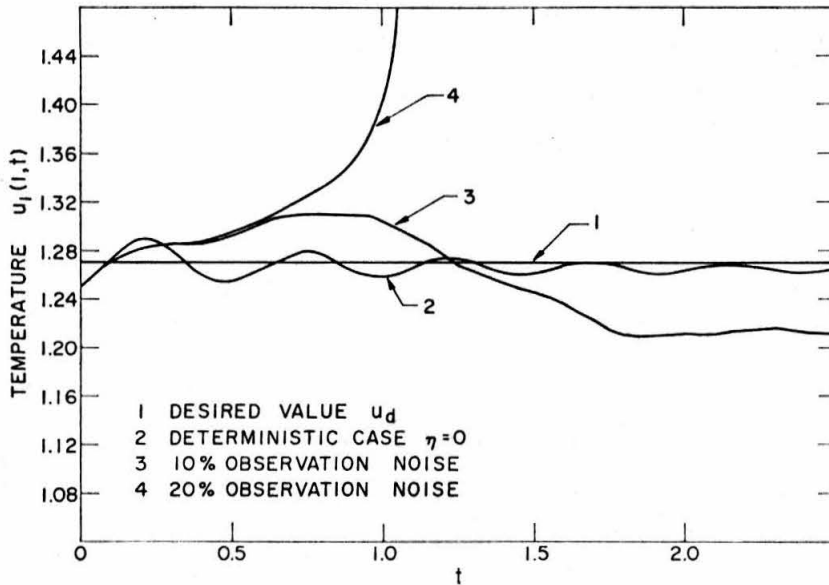


Fig. 1. Comparison of true centerline temperature under feedback proportional control with no filter at observation noise of 0% (curve 2), 10% (curve 3), and 20% (curve 4).

The estimation equations for u_1 and u_2 corresponding to these three measurements are obtained from Eq. (7), that is,

$$\begin{aligned} \hat{u}_{1,t} = & \hat{u}_{1,m} + \phi \hat{u}_2 \exp(-\epsilon/\hat{u}_1) + q_1(t) P_{11}^{(vv)}(x, 1, t)[y_1(t) - \hat{u}_1(1, t)] \\ & + q_2(t) P_{12}^{(vv)}(x, 1, t)[y_2(t) - \hat{u}_2(1, t)] \\ & + q_3(t) P_{12}^{(vv)}(x, 0, t)[y_3(t) - \hat{u}_2(0, t)], \end{aligned} \tag{40}$$

$$\begin{aligned} \hat{u}_{2,t} = & -\beta \hat{u}_2 \exp(-\epsilon/\hat{u}_1) + q_1(t) P_{21}^{(vv)}(x, 1, t)[y_1(t) - \hat{u}_1(1, t)] \\ & + q_2(t) P_{22}^{(vv)}(x, 1, t)[y_2(t) - \hat{u}_2(1, t)] \\ & + q_3(t) P_{22}^{(vv)}(x, 0, t)[y_3(t) - \hat{u}_2(0, t)], \end{aligned} \tag{41}$$

the boundary conditions of which follow directly from Eqs. (33) and (34).

The equations for $P_{11}^{(vv)}$, $P_{12}^{(vv)}$, $P_{21}^{(vv)}$, $P_{22}^{(vv)}$ can readily be obtained from Eq. (9) and will not be presented. The boundary conditions are

obtained from Eqs. (14), (15), (19), (20). The initial conditions (16) were selected as follows (these particular forms will be justified later):

$$P_{11}^{(vv)}(x, s, 0) = C_{11}xs[\exp - |x - s|], \quad (42)$$

$$P_{12}^{(vv)}(x, s, 0) = C_{12}[1 - (x - 1)^2], \quad (43)$$

$$P_{21}^{(vv)}(x, s, 0) = C_{21}[1 - (s - 1)^2], \quad (44)$$

$$P_{22}^{(vv)}(x, s, 0) = C_{22}. \quad (45)$$

Figures 2 and 3 show estimated and true temperature and concentration, respectively, for 10% measurement errors in each of the three observations [Eqs. (37)–(39)]. In the cases shown in Figs. 2 and 3, $u_c(t)$ was held constant at u_c^* . The errors were generated by

$$y_1(t) = u_1(1, t)[1 + \nu G(0, 1)],$$

where ν is the fraction of error and $G(0, 1)$ is a normally distributed random variable with mean zero and standard deviation one. The following parameter values were used: $C_{11} = 100$, $C_{12} = -50$, $C_{21} = -50$, $C_{22} = 100$, $\hat{u}_{1_0} = 1.325$, $\hat{u}_{2_0} = 0.9$, $q_1 = 1$, $q_2 = 1$, $q_3 = 0.25$ for $t \leq 0.015$ and $q_3 = 1$ for $t > 0.015$. This case represents a rather severe test of the filter, since measurement errors in u_1 of 10% correspond to a standard deviation in the temperature measurements of 37°C, a value far exceeding that to be expected in actual practice. The estimates of $u_1(1, t)$ and $u_1(0.5, t)$ converge at about the same rate, whereas the estimates of $u_2(0, t)$ and $u_2(1, t)$ converge somewhat faster than those of $u_2(0.5, t)$.

Cases similar to those shown in Figs. 2 and 3 were run with the two observations y_1 and y_2 . The filter performance in this case was very similar to that shown in Figs. 2 and 3 for three observations, and we do not present these results here. Estimation using only one observation y_1 was also attempted. In this case, u_1 was estimated quite accurately for all x , but u_2 was estimated rather poorly. However, if our only objective of filtering is to obtain a good estimate of $u_1(1, t)$, then we need only make the one measurement y_1 . This is of some practical interest, because it may be quite difficult to measure continuously the degree of polymerization u_2 . Presumably, this measurement, if necessary, could be made by a viscosity-measuring device.

Numerical integration of the state and filter partial differential equations was carried out using an IBM 360/75. The integration was carried out until $t = 2.75$ (approximately 17 h of reaction time) with a time step $\Delta t = 0.005$. Computing time required to solve the filtering equations was 6 min and 40 sec.

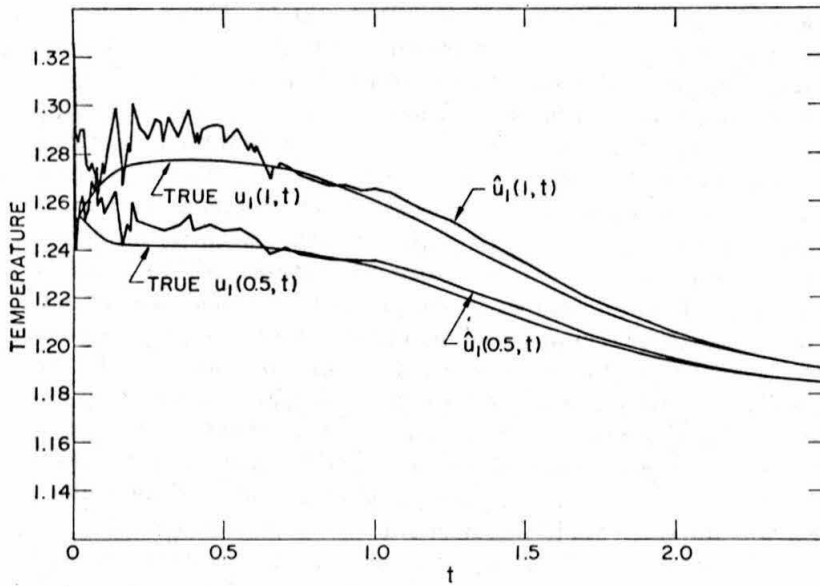


Fig. 2. True and filtered values of temperature at locations $x = 1$ and $x = 0.5$ at 10% observation noise with three observations and $u_e(t) = 1.16667$.

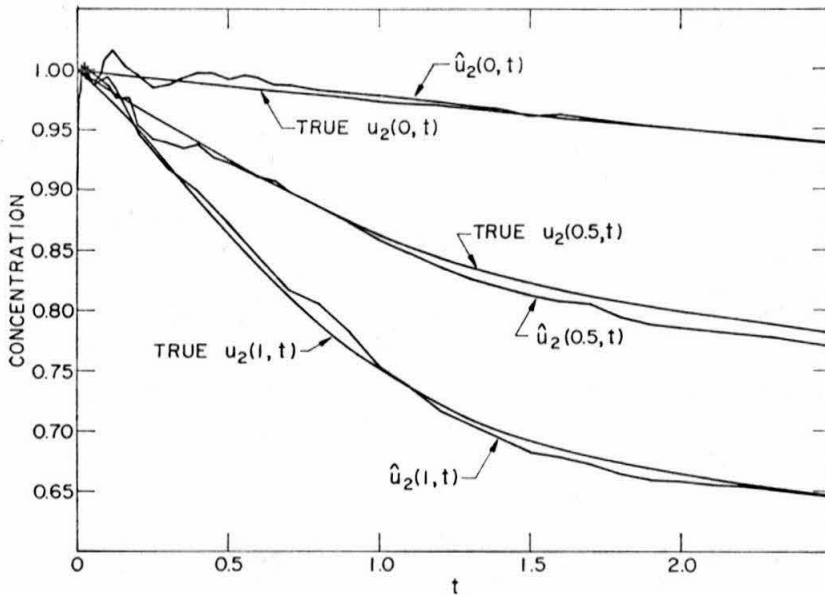


Fig. 3. True and filtered values of concentration at locations $x = 1$, $x = 0.5$, and $x = 0$ at 10% observation noise with three observations and $u_e(t) = 1.16667$.

4.2. Feedback Control. We now study the dynamics of the closed loop including the nonlinear filter. The system is highly sensitive to $u_c(t)$. Improper application of $u_c(t)$ can cause system instability, as we saw in Fig. 1 for the case of 20% measurement errors. Clearly, the less the uncertainty in \hat{u}_{1_0} and \hat{u}_{2_0} and the lower the measurement noise level, the better the performance of the filter and the control. We note from Figs. 2 and 3 that there is an initial period of time required for \hat{u}_1 and \hat{u}_2 [and, in particular, $\hat{u}_1(1, t)$] to converge to the actual values. Because of the exothermic nature of the system, during this initial period it is better to overestimate than underestimate $u_1(1, t)$. Underestimating $u_1(1, t)$ for too long a period of time may cause $u_c(t)$ to assume u_c^{\max} for too long and drive the system unstable. Consequently, we will always make sure that $\hat{u}_{1_0} > u_{1_0}$ and $\hat{u}_{2_0} < u_{2_0}$. This is possible because in practice we know the temperature bounds and the initial concentration fairly well anyway. Thus, the initial conditions for Eqs. (40)-(41) should not be expected to be a problem.

The number of observations required depends on our objective. One observation $y_1(t)$ may be sufficient if our sole purpose is for $\hat{u}_1(1, t)$ to be close to $u_1(1, t)$. Additional observations can be expected to improve not only $\hat{u}_1(x, t)$ and $\hat{u}_2(x, t)$ but also $\hat{u}_1(1, t)$.

Figures 4 and 5 show the temperature response at 10% and 20%

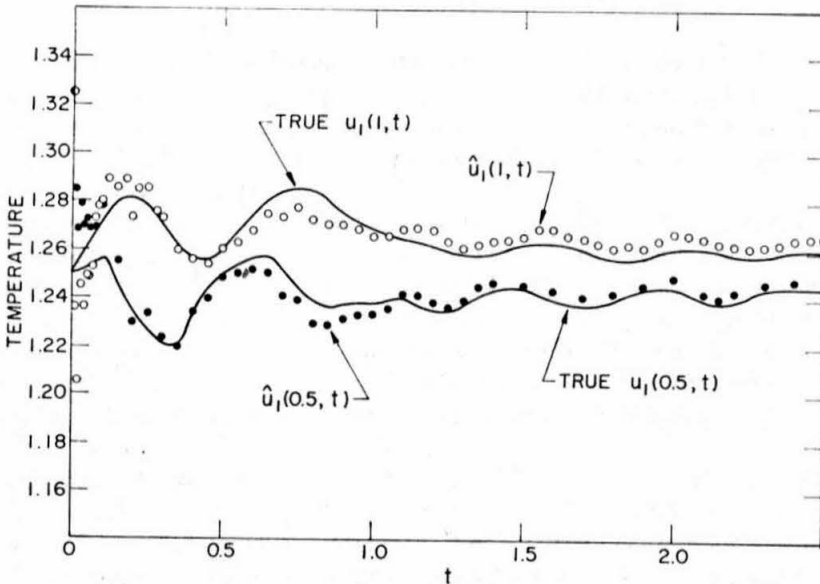


Fig. 4. True and filtered values of temperature at locations $x = 1$ and $x = 0.5$ at 10% observation noise with three observations under feedback proportional control.

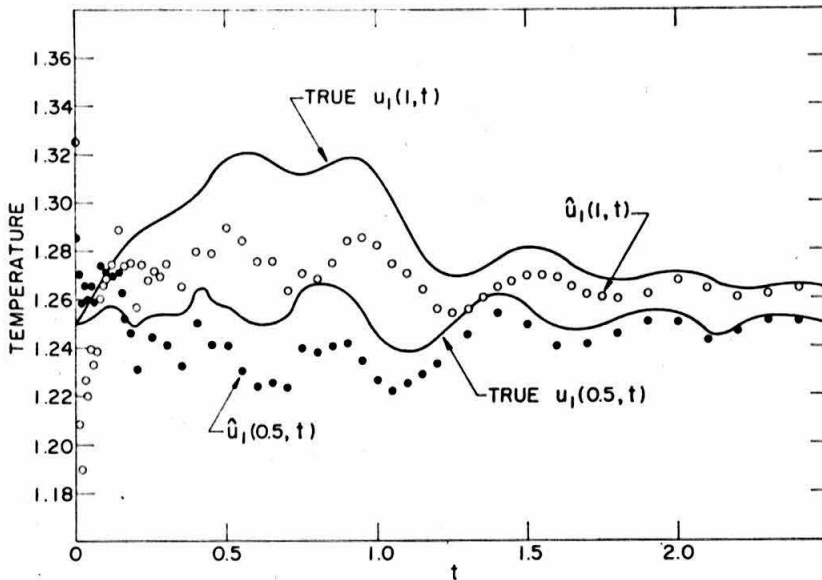


Fig. 5. True and filtered values of temperature at locations $x = 1$ and $x = 0.5$ at 20% observation noise with three observations under feedback proportional control.

measurement noise, respectively, with the filter in the control loop. In each case, we show $u_1(1, t)$ and $u_1(0.5, t)$ the actual temperatures in the reactor, as well as the estimated values of these temperatures from the filter. Figures 4 and 5 were generated on the basis of the three observations [Eqs. (37)–(39)].

Figure 6 presents a comparison of the completely deterministic response (curve 2 of Fig. 1), $u_1(1, t)$ at 10% measurement noise and no filter (curve 3 of Fig. 1), and $u_1(1, t)$ at 10% measurement noise with a filter in the loop (curve 1 of Fig. 4). Likewise, Fig. 7 presents the same comparisons for 20% measurement noise. In this case, even at the unusually high level of error of 20%, the feedback control scheme employing a filter prevents the system from becoming unstable.

4.3. Approximate Filter. For this two-state variable system, the filter consists of six coupled nonlinear partial differential equations. In general, the necessity to integrate the covariance equations will greatly diminish its practical utility for any system with even a modest number of state variables. A significant reduction in computing time could be achieved by avoiding the integration of the covariance equations.

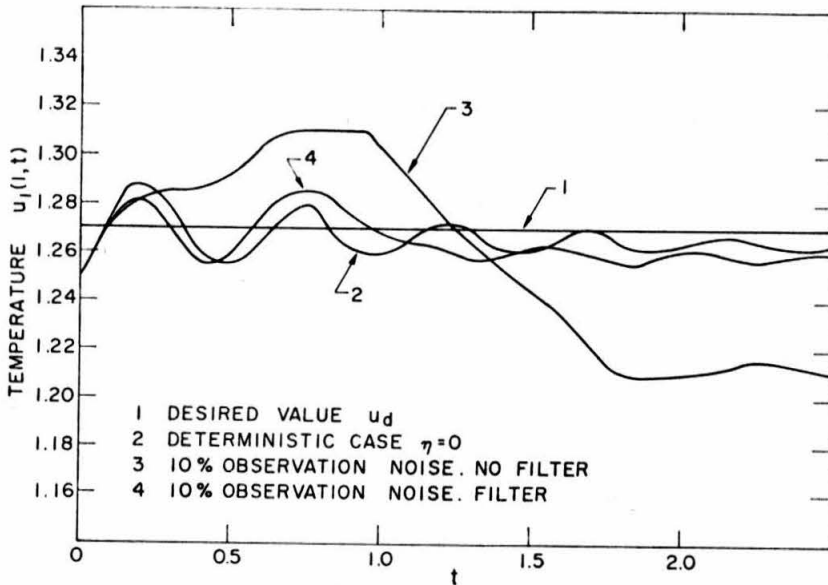


Fig. 6. Comparison of true centerline temperature under feedback proportional control at 0% observation noise (curve 2), 10% observation noise with no filter (curve 3), and 10% observation noise with filter and three observations (curve 4).

One approach is to assume directly the form of the solution. We note that, for a linear system with white noise disturbances,

$$P_{ij}^{(vv)}(x, s, t) = \mathcal{E}[(u_i(x, t) - \hat{u}_i(x, t))(u_j(s, t) - \hat{u}_j(s, t))]. \quad (46)$$

In the nonlinear case, relations such as (46) do not apply; however, Eq. (46) may be used as a qualitative guide to choosing the form of $P^{(vv)}(x, s, t)$.

Let us consider the formation of an approximate filter for the polymerization reactor system. The boundary conditions that must be satisfied are [we drop superscript (vv) for convenience]

$$\begin{aligned} P_{11}(0, s, t) &= 0, & P_{11}(x, 0, t) &= 0, \\ P_{12}(0, s, t) &= 0, & P_{21}(x, 0, t) &= 0, \\ [P_{11_2}]_{x=1} &= 0, & [P_{11_1}]_{s=1} &= 0, \\ [P_{12_2}]_{x=1} &= 0, & [P_{21_1}]_{s=1} &= 0. \end{aligned} \quad (47)$$

Since the system exhibits the behavior of exothermicity, concentra-

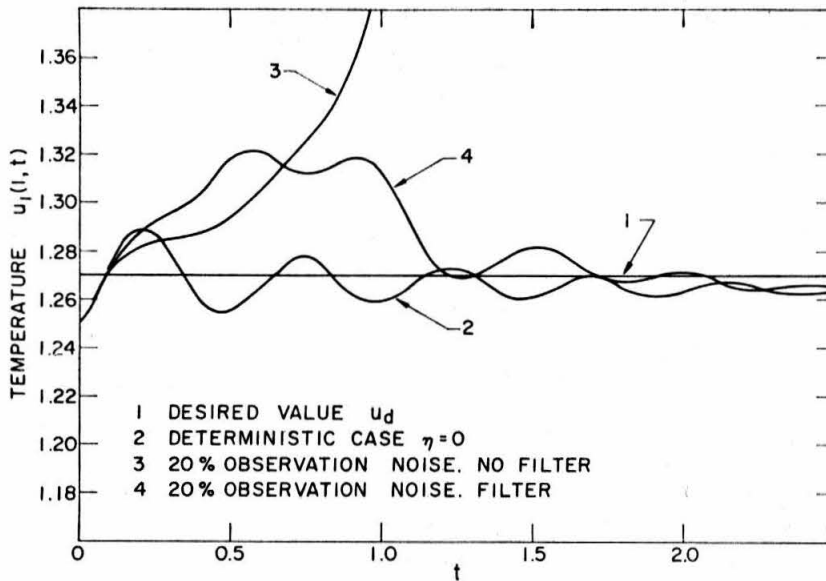


Fig. 7. Comparison of true centerline temperature under feedback proportional control at 0% observation noise (curve 2), 20% observation noise with no filter (curve 3), and 20% observation noise with filter and three observations (curve 4).

tion and temperature should have negative correlation. Therefore, we can assume

$$P_{11}, P_{22} \geq 0, \quad P_{12}, P_{21} \leq 0. \quad (48)$$

Since $u_1(0, t)$ is known precisely for all t , it is reasonable to assume that $P_{11}(x, s, t)$ decreases as x and s decrease. On the other hand, there is no reason to assume that u_2 will be estimated more accurately at one location than another. So we assume that $P_{22}(x, s, t)$ is independent of x and s . Thus, we make the following assumptions:

- (i) $|P_{11}(x, s, t)|$ should decrease as x and s decrease;
- (ii) $|P_{12}(x, s, t)|$ should decrease as x decreases and be independent of s ;
- (iii) $|P_{21}(x, s, t)|$ should decrease as s decreases and be independent of x ;
- (iv) $|P_{22}(x, s, t)|$ should be independent of x and s ; and
- (v) since the estimates should improve with t , $P_{ij}(x, s, t) \rightarrow 0$ as t increases.

A set of approximations which satisfy these requirements are:

$$P_{11}(x, s, t) = C_{11}xs \exp[-|x-s|][k_1 \exp(-\alpha_1 t) + k_2 \exp(-\alpha_2 t) + k_3 \exp(-\alpha_3 t)], \quad (49)$$

$$P_{12}(x, s, t) = C_{12}[1 - (x-1)^2][k_4 \exp(-\alpha_4 t) + k_5 \exp(-\alpha_5 t) + k_6 \exp(-\alpha_6 t)], \quad (50)$$

$$P_{21}(x, s, t) = C_{21}[1 - (s-1)^2][k_7 \exp(-\alpha_7 t) + k_8 \exp(-\alpha_8 t) + k_9 \exp(-\alpha_9 t)], \quad (51)$$

$$P_{22}(x, s, t) = C_{22}[k_{10} \exp(-\alpha_{10} t) + k_{11} \exp(-\alpha_{11} t) + k_{12} \exp(-\alpha_{12} t)]. \quad (52)$$

Figure 8 shows a comparison of $P_{11}(1, 1, t)$ and $P_{12}(1, 1, t)$ for the full and the approximate filter. The values shown are those for the feedback control case with three observations and 10% noise. As we see, the key characteristic of the function $P_{ij}(x, s, t)$ is its rapid initial decline in magnitude and asymptotic tendency toward zero. An approximate representation of $P_{ij}(x, s, t)$ exhibiting this behavior can be expected to be a useful alternative to integration of the full filter. The computation

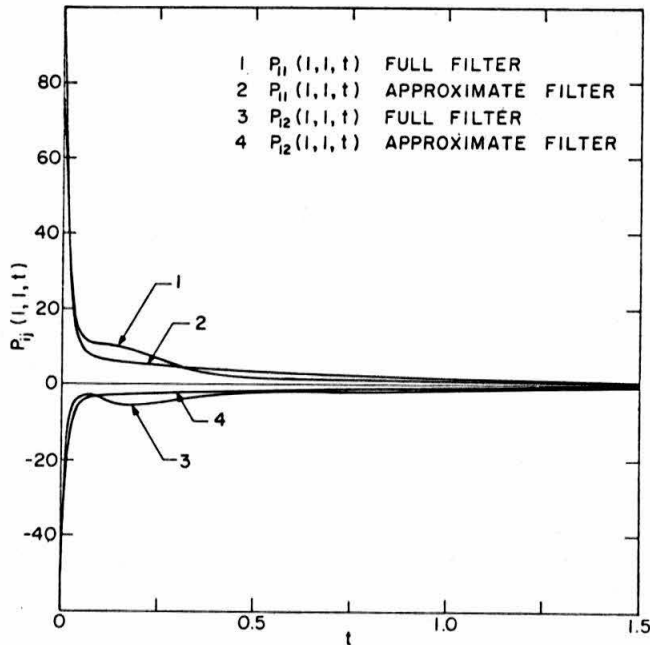


Fig. 8. Comparison of $P_{ij}(1, 1, t)$ of full and approximate filter under feedback proportional control at 10% observation noise with three observations.

time for the feedback control case using Eqs. (49)–(52) was 28 sec as opposed to over 6 min for the full filter. The curves of \hat{u}_1 and \hat{u}_2 for the approximate filter are very close to those for the full filter, and are not shown.

The parameter values for Fig. 8 are $C_{11} = 75$, $C_{12} = -37.5$, $C_{21} = -37.5$, $C_{22} = 75$, and Eqs. (49)–(52) are of the general form

$$P_{ij} = C_{ij}[0.9 \exp(-66t) + 0.09 \exp(-2t) + 0.01 \exp(-0.5t)]. \quad (53)$$

5. Summary

We have presented a scheme for the feedback control of stochastic distributed systems. The scheme involves the inclusion in the loop of a computer performing on-line filtering to provide optimal state estimates for the controller. We have presented a theoretical comparison of feedback proportional control of a styrene polymerization reactor with and without filtering. Finally, we showed how the integration of the filter covariance equations could be avoided by assuming the form of $P_{ij}(x, s, t)$. For the particular example, the approximate filter required only 28 sec of computing time to control the reactor for 17 h of real time. Thus, this scheme offers promise for the control of processes that contain elements of uncertainty and for which a time-shared process control computer is available.

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Chapter III

OPTIMAL FILTERING FOR SYSTEMS GOVERNED BY FUNCTIONAL DIFFERENTIAL EQUATIONS

1. Introduction

In this chapter, within a single framework we obtain new optimal filters for the following classes of systems:

1. Nonlinear lumped parameter systems containing multiple constant and time-varying delays;
2. Mixed nonlinear lumped and hyperbolic distributed parameter systems; and
3. Nonlinear systems with functional time delays.

Several known [16,19] and new linear filters evolve as special cases of the more general nonlinear results. Figure 1 illustrates the classes of systems for which filters are derived in this paper.

We begin by formulating the general problem which can be shown to include each of the above as special cases. We shall then present the derivation of the filter for this class of problems. After doing so, we shall illustrate the computational application of the general filter for a chemical-reactor heat-exchanger system.

2. Formulation of the Problem

Let us consider the problem of filtering for the class of well-posed systems governed by the coupled ordinary and partial functional differential equations

$$\dot{x}(t) = f(x(t), z(r_1, t), \dots, z(r_\beta, t), t) + \int_0^1 K(z(r, t), r, t) dr + \xi(t) \quad (1)$$

$$z_t(r, t) = -M(r, t)z_r(r, t) + g(z(r, t), r, t) + \zeta(r, t) \quad (2)$$

defined for $t \geq 0$ on the normalized spatial domain $r \in (0, 1)$.

$x(t)$ and $z(r, t)$ are n_1 - and n_2 -dimensional state vectors, respectively, and $\xi(t)$ and $\zeta(r, t)$ are zero-mean random processes with arbitrary statistical properties. z_t and z_r denote $\partial z / \partial t$ and $\partial z / \partial r$, respectively. Observations of the system consist of the n_3 -dimensional vector $y(t)$, related to the states by

$$y(t) = h(x(t), z(r_1^*, t), \dots, z(r_\gamma^*, t), t) + \int_0^1 H(z(r, t), r, t) dr + \eta(t) \quad (3)$$

where $\eta(t)$ is a zero-mean measurement error with arbitrary statistical properties and $0 < r_1 < \dots < r_\beta \leq 1$ and $0 < r_1^* < \dots < r_\gamma^* \leq 1$.

One should note that there is no loss of generality in having the observations y depend only on t ; for example, the vector y could be expanded and partitioned so that all interior measurements $z(r_i^*, t)$ could be observed within this framework. Initial conditions for (1) and (2) are

$$x(0) = x_0 \quad (4)$$

$$z(r, 0) = z_0(r) \quad (5)$$

The boundary condition at $r = 0$ for (2) is

$$z(0, t) = b(x(t)) \quad (6)$$

We shall now show that by appropriate modification of the system (1)-(6), four important classes of time delay and mixed lumped and distributed parameter systems result.

2.1 Nonlinear systems with multiple constant time delays

The system (1)-(6) can be reduced to the following nonlinear lumped parameter system containing multiple constant time delays:

$$\dot{x}(t) = f(x(t), x(t-\alpha_1), \dots, x(t-\alpha_\beta), t) + \xi(t) \quad (7)$$

$$y(t) = h(x(t), x(t-\alpha_1^*), \dots, x(t-\alpha_\gamma^*), t) + \eta(t) \quad (8)$$

$$x(t) = \phi(t), \quad -\alpha_{\max} \leq t \leq 0$$

$$\alpha_{\max} = \max(\alpha_\beta, \alpha_\gamma^*) \quad (9)$$

where $0 < \alpha_1 < \dots < \alpha_\beta$ and $0 < \alpha_1^* < \dots < \alpha_\gamma^*$. This can be done by setting $K = H = g = \zeta = 0$, $b(x(t)) = x(t)$, (and hence $n_2 = n_1$), $M(r, t) = \alpha_{\max}^{-1}$, $r_i = \alpha_i / \alpha_{\max}$, $r_j^* = \alpha_j^* / \alpha_{\max}$, and $z(r, 0) = \phi(-r\alpha_{\max})$. Then $z(r_i, t) = x(t - \alpha_i)$ and $z(r_j^*, t) = x(t - \alpha_j^*)$. In the formulation (7)-(9) there are β constant time delays in the state equation and γ constant time delays in the observation equation. These delays need not be equal.

2.2 Nonlinear systems with multiple time-varying delays

The system (1)-(6) can be reduced to the following nonlinear lumped parameter system containing multiple time-varying delays:

$$\dot{x}(t) = f(x(t), x(t-\alpha_1(t)), \dots, x(t-\alpha_\rho(t)), t) + \xi(t) \quad (10)$$

$$y(t) = h(x(t), x(t-\alpha_1^*(t)), \dots, x(t-\alpha_\omega^*(t)), t) + \eta(t) \quad (11)$$

$$\dot{\alpha}_i(t) < 1 \quad i = 1, 2, \dots, \rho \quad (12)$$

$$\dot{\alpha}_j^*(t) < 1 \quad j = 1, 2, \dots, \omega \quad (13)$$

$$x(t) = \phi(t) \quad -\alpha_{\max} \leq t \leq 0 \quad (14)$$

$$\alpha_{\max} = \max(\alpha_1(0), \dots, \alpha_\rho(0), \alpha_1^*(0), \dots, \alpha_\omega^*(0)) \quad (15)$$

To do so we set $K = H = g = \zeta = 0$, $\beta = \gamma = 1$, $r_1 = r_1^* = 1$, $b(x(t)) = [x^T(t), x^T(t), \dots, x^T(t)]^T$, an $n_2 = (\rho + \omega)n_1$ -dimensional vector consisting of $\rho + \omega$ identical vector elements $x(t)$, $M(r, t) = [M_{ij}(r, t)]$ an $n_2 \times n_2$ -matrix with $n_1 \times n_1$ -matrix components M_{ij} defined by

$$M_{ij} = \begin{cases} 0 & i \neq j \\ \frac{1 - r\dot{\alpha}_i}{\alpha_i} I & i = 1, 2, \dots, \rho \\ & i = j \\ \frac{1 - r\dot{\alpha}_{i-\rho}^*}{\alpha_{i-\rho}^*} I & i = \rho + 1, \dots, \rho + \omega \end{cases} \quad (16)$$

Also we let the n_2 -dimensional vector $z(r, t) = [z_1^T(r, t), \dots, z_\rho^T(r, t), z_1^{*T}(r, t), \dots, z_\omega^{*T}(r, t)]^T$ where each $z_i(r, t)$ or $z_j^*(r, t)$ is an n_1 -dimensional vector, and set $z_i(r, 0) = \phi(-r\alpha_i(0))$, $z_j^*(r, 0) = \phi(-r\alpha_j^*(0))$. Then $z_i(1, t) = x(t - \alpha_i(t))$ and $z_j^*(1, t) = x(t - \alpha_j^*(t))$. Conditions (12) and (13) insure that the time delays do not increase faster than time itself.

2.3 Mixed nonlinear lumped and hyperbolic distributed parameter systems

Setting $K = H = 0$, $\beta = 1$, and $r_1 = 1$, we obtain the mixed lumped and hyperbolic distributed system

$$\dot{x}(t) = f(x(t), z(1,t), t) + \xi(t) \quad (17)$$

$$z_t(r,t) = -M(r,t)z_r(r,t) + g(z(r,t), r, t) + \zeta(r,t) \quad (18)$$

$$y(t) = h(x(t), z(r_1^*, t), \dots, z(r_\gamma^*, t), t) + \eta(t) \quad (19)$$

subject to (4)-(6). Thus, (17)-(19) represents processes in which transportation lags are accompanied by phenomena such as dissipation of mass and energy, fluid mixing, and chemical reactions. In such cases, differential-difference equations are inadequate in describing the system. The importance of this class of systems has been previously discussed by Hiratsuka and Ichikawa [9] and Aggarwal [1].

2.4 Nonlinear systems with functional time delays

The system (1)-(6) can be reduced to the following nonlinear lumped parameter system containing functional time delay

$$\begin{aligned} \dot{x}(t) = & f(x(t), x(t-\alpha_1), \dots, x(t-\alpha_\beta), t) \\ & + \int_0^{\alpha_{\max}} K_0(x(t-\alpha), \alpha, t) d\alpha + \xi(t) \end{aligned} \quad (20)$$

$$\begin{aligned} y(t) = & h(x(t), x(t-\alpha_1^*), \dots, x(t-\alpha_\gamma^*), t) \\ & + \int_0^{\alpha_{\max}} H_0(x(t-\alpha), \alpha, t) d\alpha + \eta(t) \end{aligned} \quad (21)$$

$$\begin{aligned} x(t) = & \phi(t), \quad -\alpha_{\max} \leq t \leq 0 \\ & \alpha_{\max} = \max(\alpha_\beta, \alpha_\gamma^*) \end{aligned} \quad (22)$$

where $0 < \alpha_1 < \dots < \alpha_\beta$ and $0 < \alpha_1^* < \dots < \alpha_\gamma^*$. This can be done by setting $g = \zeta = 0$, $b(x(t)) = x(t)$, (and hence $n_2 = n_1$),

$M(r,t) = \alpha_{\max}^{-1}$, $r_i = \alpha_i / \alpha_{\max}$, $r_j^* = \alpha_j^* / \alpha_{\max}$, $r = \alpha / \alpha_{\max}$,
 $K(z(r,t), r, t) = \alpha_{\max} K_0(z(r,t), \alpha_{\max} r, t)$, $H(z(r,t), r, t) =$
 $\alpha_{\max} H_0(z(r,t), \alpha_{\max} r, t)$, and $z(r,0) = \phi(-r\alpha_{\max})$. Then $z(r_i, t) =$
 $x(t - \alpha_i)$, $z(r_j^*, t) = x(t - \alpha_j^*)$, and $z(r, t) = x(t - \alpha)$.

3. Derivation of the Filter

We shall derive the optimal least square filtering and smoothing equations for the system (1)-(6) through the use of differential sensitivities and a decomposition algorithm. In this section we shall present the detailed derivation for the case of $K = H = 0$ in (1)-(6). We do this only for the convenience of the reader so as to avoid details which are more cumbersome than need be given. We shall, however, present the filter for the completely general form of (1)-(6) in Section 4.

The derivation of the filter for the system of (1)-(6) consists of two parts. First, we formulate the problem of fixed time smoothing and derive the necessary conditions for optimality. Second, we convert the smoothing problem into the filtering problem using a formulation based on differential sensitivities [22].

3.1 Statement of the problem

Consider the system (1)-(6) with $K = H = 0$. The state estimation problem is: Given any fixed $T > 0$ and observations $y(t)$, $0 \leq t \leq T$, it is desired to estimate $x(t)$ and $z(r,t)$ for $0 \leq t \leq T$, $0 \leq r \leq 1$. This is the smoothing problem. The estimation criterion shall be to minimize

$$\begin{aligned}
 \Psi = & \int_0^T \langle \dot{x} - f, R_0(t)(\dot{x} - f) \rangle dt + \int_0^T \langle y - h, \\
 & Q(t)(y - h) \rangle dt + \int_0^T \int_0^1 \int_0^1 \langle z_t(r,t) + M(r,t)z_r(r,t) \\
 & - g(z(r,t),r,t), R_1(r,s,t)(z_t(s,t) + M(s,t)z_s(s,t) \\
 & - g(z(s,t),s,t)) \rangle dr ds \Bigg\} dt \quad (23)
 \end{aligned}$$

where the weighting matrices $R_0(t)$ and $Q(t)$ are symmetric positive-definite. $R_1(r,s,t)$ is defined by [21,33]

$$\int_0^1 R_1^+(r,\rho,t) R_1(\rho,s,t) d\rho = I\delta(r-s) \quad (24)$$

where $R^+(r,s,t)$ is a positive-definite, symmetric matrix: $R^+(r,s,t) = (R^+(s,r,t))^T$. $\delta(\cdot)$ is the Dirac delta function and I is the identity matrix. Although $R_0(t)$, $Q(t)$ and $R_1^+(r,s,t)$ are only restricted to be symmetric positive-definite, they can be chosen to reflect the statistical properties of the stochastic variables $\xi(t)$, $\zeta(r,t)$ and $\eta(t)$ if statistical information about these errors is known.

We first reformulate this problem as an optimal control problem, i.e., it is desired to minimize

$$\begin{aligned}
 \Psi_1 = & \int_0^T \langle u(t), R_0(t) u(t) \rangle dt + \int_0^T \langle y - h, Q(t)(y - h) \rangle dt \\
 & + \int_0^T \int_0^1 \int_0^1 \langle v(r,t), R_1(r,s,t) v(s,t) \rangle dr ds \Bigg\} dt \quad (25)
 \end{aligned}$$

subject to the constraints

$$\dot{x}(t) = f(x(t), z(r_1, t), \dots, z(r_\beta, t), t) + u(t) \quad (26)$$

$$z_t(r, t) = -M(r, t)z_r(r, t) + g(z(r, t), r, t) + v(r, t) \quad (27)$$

$$z(0, t) = b(x(t)) \quad (28)$$

The necessary conditions for optimality corresponding to (25)-(28) are readily derived through adjoining (26)-(28) to the objective (25) by Lagrange multipliers $\lambda(t)$ and $\sigma(r, t)$ and then taking first variations (see Appendix III-B). Only the results are presented here, where we use the circumflex $\hat{\cdot}$ to indicate the optimal values, and the notation (\cdot/T) in the arguments to denote the dependence of the optimal solution on the observation interval $[0, T]$. The optimal values of $\hat{x}(t/T)$ and $\hat{z}(r, t/T)$ result from the solution of the following two-point boundary value problem:

$$\hat{x}_t(t/T) = \hat{f} - \frac{1}{2} R_0^{-1}(t) \hat{\lambda}(t/T) \quad (29)$$

$$\hat{z}_t(r, t/T) = -\hat{M}z_r + \hat{g} - \frac{1}{2} \int_0^1 R_1^+(r, s, t) \hat{\sigma}(s, t/T) ds \quad (30)$$

$$\hat{\lambda}_t(t/T) = 2\hat{h}_x^T Q(t)(y - \hat{h}) - \hat{f}_x^T \hat{\lambda}(t/T) - \hat{b}_x^T M^T(0, t) \hat{\sigma}(0, t/T) \quad (31)$$

$$\begin{aligned} \hat{\sigma}_t(r, t/T) = & 2 \sum_{i=1}^Y \hat{h}_{z(r_i^*, t/T)}^T Q(t)(y - \hat{h}) \delta(r - r_i^*) \\ & - \sum_{i=1}^{\beta} \hat{f}_{z(r_i, t/T)}^T \hat{\lambda}(t/T) \delta(r - r_i) \\ & - \hat{g}_{z(r, t/T)}^T \hat{\sigma}(r, t/T) - (M^T(r, t) \hat{\sigma}(r, t/T))_r \end{aligned} \quad (32)$$

$$\hat{\lambda}(0/T) = \hat{\lambda}(T/T) = 0 \quad (33)$$

$$\hat{\sigma}(r,0/T) = \hat{\sigma}(r,T/T) = 0 \quad (34)$$

$$\hat{z}(0,t/T) = b(\hat{x}(t/T)) \quad (35)$$

$$\hat{\sigma}(1,t/T) = 0 \quad (36)$$

where \hat{f} denotes $f(\hat{x}(t/T), \hat{z}(r_1, t/T), \dots, \hat{z}(r_\beta, t/T), t)$, etc.

Equations (29)-(36) represent the boundary value problem which must be solved to produce the optimal least square smoothed estimates of $x(t)$ and $z(r, t)$ when data are given over $0 \leq t \leq T$. The optimal smoothing results for each of the special cases discussed in Section 2 can be determined from the appropriate simplification of these equations.

3.2 Differential sensitivities

In the above two-point boundary value problem we can express the solutions $\hat{x}(t/T)$ and $\hat{z}(r, t/T)$ in terms of the Lagrange multipliers by

$$\hat{x}(t/T) = x[\hat{\lambda}(t/T), \hat{\sigma}(s, t/T)] \quad (37)$$

$$\hat{z}(r, t/T) = z[r, \hat{\lambda}(t/T), \hat{\sigma}(s, t/T)] \quad s \in [0, 1] \quad (38)$$

Let $\delta/\delta\hat{\sigma}$ denote the functional derivative and define the first order differential sensitivity matrices P^{XX} , P^{XZ} , P^{ZX} and P^{ZZ} by

$$P^{XX}(t/T) = -2 \frac{\partial \hat{x}(t/T)}{\partial \hat{\lambda}(t/T)} \quad (39)$$

$$P^{XZ}(s, t/T) = -2 \frac{\delta \hat{x}(t/T)}{\delta \hat{\sigma}(s, t/T)} \quad (40)$$

$$P^{ZX}(r, t/T) = -2 \frac{\partial \hat{z}(r, t/T)}{\partial \hat{\lambda}(t/T)} \quad (41)$$

$$P^{ZZ}(r, s, t/T) = -2 \frac{\delta \hat{z}(r, t/T)}{\delta \hat{\sigma}(s, t/T)} \quad (42)$$

Then, using the chain rule of calculus, the partial derivatives of \hat{x} , \hat{z} and \hat{z}_r with respect to T can be expressed as

$$\hat{x}_T(t/T) = -\frac{1}{2} \left\{ P^{XX}(t/T) \hat{\lambda}_T(t/T) + \int_0^1 P^{XZ}(s, t/T) \hat{\sigma}_T(s, t/T) ds \right\} \quad (43)$$

$$\hat{z}_T(r, t/T) = -\frac{1}{2} \left\{ \int_0^1 P^{ZZ}(r, s, t/T) \hat{\sigma}_T(s, t/T) ds + P^{ZX}(r, t/T) \hat{\lambda}_T(t/T) \right\} \quad (44)$$

$$\hat{z}_{rT}(r, t/T) = -\frac{1}{2} \left\{ \int_0^1 P_r^{ZZ}(r, s, t/T) \hat{\sigma}_T(s, t/T) ds + P_r^{ZX}(r, t/T) \hat{\lambda}_T(t/T) \right\} \quad (45)$$

These equations describe the time evolution of the optimal solutions \hat{x} and \hat{z} as the length of the observation interval T varies.

Now let $q(t/T)$ be whatever we desire to estimate in the system, based on observations $y(\tau)$, $\tau \in [0, T]$, and denote the optimal estimate of $q(t/T)$ by $\hat{q}(t/T)$. Since we are interested in the optimal filter estimate, we seek $\hat{q}(T/T)$ and, in particular, the total derivative $d\hat{q}(T/T)/dT$. We note that

$$\frac{d\hat{q}(T/T)}{dT} = \hat{q}_t(t/T) \Big|_{t=T} + \hat{q}_T(t/T) \Big|_{t=T}$$

which we write for convenience as

$$\frac{d\hat{q}(T/T)}{dT} = \hat{q}_t(T/T) + \hat{q}_T(T/T) \quad (46)$$

Thus, the total derivative of the quantity $\hat{q}(T/T)$ is a sum of two terms, one representing the dynamics of the system $\hat{q}_t(t/T)|_{t=T}$, and the second the updating of the estimate in the face of new observations $\hat{q}_T(t/T)|_{t=T}$. This result was demonstrated for lumped parameter systems by Padmanabhan [22].

When \hat{q} is also a function of one or more spatial variables $\hat{q}(r,s,t/T)$, then (46) becomes

$$\frac{\partial \hat{q}(r,s,T/T)}{\partial T} = \hat{q}_t(r,s,t/T)|_{t=T} + \hat{q}_T(r,s,t/T)|_{t=T} \quad (47)$$

which we write for convenience as

$$\frac{\partial \hat{q}(r,s,T/T)}{\partial T} = \hat{q}_t(r,s,T/T) + \hat{q}_T(r,s,T/T) \quad (48)$$

We emphasize that each term in (47), and hence (48), represents a different partial derivative. In particular, the L.H.S. of (47) and (48) is the analog to the total derivative in (46), whereas the R.H.S. of (47) and (48) consists of partial derivatives with respect to each of the arguments t and T in $(\cdot, t/T)$, respectively.

3.3 State filter equations

We now wish to derive the dynamical equations for $dx(T/T)/dT$ and $\partial \hat{z}(r,T/T)/\partial T$ which represent the rate of change of the filtered estimates with T . Using (46) and (48), these can be expressed as

$$\frac{d\hat{x}(T/T)}{dT} = \hat{x}_t(T/T) + \hat{x}_T(T/T) \quad (49)$$

$$\frac{\partial \hat{z}(r,T/T)}{\partial T} = \hat{z}_t(r,T/T) + \hat{z}_T(r,T/T) \quad (50)$$

Equations (33) and (34) imply that

$$\frac{d\hat{\lambda}(T/T)}{dT} = \frac{\partial \hat{\sigma}(s, T/T)}{\partial T} = 0 \quad (51)$$

Using (46) and (48), (51) can be written

$$\hat{\lambda}_T(T/T) + \hat{\lambda}_t(T/T) = 0 \quad (52)$$

$$\hat{\sigma}_T(s, T/T) + \hat{\sigma}_t(s, T/T) = 0 \quad (53)$$

Then (31)-(34) and (52)-(53) give

$$\hat{\lambda}_T(T/T) = -2\hat{h}_x^T Q(T)(y - \hat{h}) \quad (54)$$

$$\hat{\sigma}_T(s, T/T) = -2 \sum_{i=1}^Y \hat{h}_{z_i}^T(r_i^*, T/T) Q(T)(y - \hat{h}) \delta(s - r_i^*) \quad (55)$$

Substituting (54) and (55) into (43) and (44), we obtain

$$\hat{x}_T(T/T) = P^{XX}(T/T)\hat{h}_x^T Q(T)(y - \hat{h}) + \sum_{i=1}^Y P^{XZ}(r_i^*, T/T)\hat{h}_{z_i}^T(r_i^*, T/T)Q(T)(y - \hat{h}) \quad (56)$$

$$\begin{aligned} \hat{z}_T(r, T/T) = & \sum_{i=1}^Y P^{ZZ}(r, r_i^*, T/T)\hat{h}_{z_i}^T(r_i^*, T/T) Q(T)(y - \hat{h}) \\ & + P^{ZX}(r, T/T)\hat{h}_x^T Q(T)(y - \hat{h}) \end{aligned} \quad (57)$$

On the other hand, (29), (30), (33) and (34) give

$$\hat{x}_t(T/T) = \hat{f} \quad (58)$$

$$\hat{z}_t(r, T/T) = -Mz_r + \hat{g} \quad (59)$$

Hence (49), (50), (56)-(59) constitute the state filter equations.

The boundary condition for $\hat{z}(0, T/T)$ is

$$\hat{z}(0, T/T) = b(\hat{x}(T/T)) \quad (60)$$

3.4 Covariance equations

We now need to derive the dynamic equations for the differential sensitivities $P^{XX}(T/T)$, $P^{XZ}(s, T/T)$, $P^{ZX}(r, T/T)$ and $P^{ZZ}(r, s, T/T)$ to complete the specification of the filter. These equations are usually referred to as the covariance equations by analogy to the linear case, although they are not the true covariances in the nonlinear case. In order to derive these equations, we need the total derivatives with respect to T of the four differential sensitivities as in (49) and (50) for the state filter equations. As we know, each $\partial P(\cdot, T/T)/\partial T$ will be a sum of two terms, $P_t(\cdot, T/T)$ and $P_T(\cdot, T/T)$. For the general nonlinear case we are considering, it can be shown that $P_T(\cdot, T/T)$ involves the second order differential sensitivities, and, likewise, the second order differential sensitivities involve the third order differential sensitivities, etc. Thus, in general, it is not possible to close the system of equations. For this reason, we will approximate $\partial P(\cdot, T/T)/\partial T$ by $P_t(\cdot, T/T)$, enabling us to obtain a closed set of equations.

The basic approach is that we shall derive two expressions for each of the quantities

$$\frac{\partial}{\partial t} [\hat{x}_T(t/T)] \quad \frac{\partial}{\partial t} [\hat{z}_T(r, t/T)] \quad (61)$$

and equate the two expressions for each of the quantities while setting $t = T$. Since each of the quantities above is a continuous function of t and T , we can write

$$\frac{\partial}{\partial t} [\hat{x}_T(t/T)] = \frac{\partial}{\partial T} [\hat{x}_t(t/T)] \quad (62)$$

$$\frac{\partial}{\partial t} [\hat{z}_T(r, t/T)] = \frac{\partial}{\partial T} [\hat{z}_t(r, t/T)] \quad (63)$$

Substituting (29) in the R.H.S. of (62) gives

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{x}_T(t/T)] &= \hat{f}_x \hat{x}_T(t/T) + \int_0^1 \left\{ \sum_{i=1}^{\beta} \hat{f}_z(r_i, t/T) \delta(r-r_i) \right\} \hat{z}_T(r, t/T) dr \\ &\quad - \frac{1}{2} R_0^{-1}(t) \hat{\lambda}_T(t/T) \end{aligned} \quad (64)$$

which, with the help of (43) and (44), can be written as

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{x}_T(t/T)] &= -\frac{1}{2} \left[\hat{f}_x P^{xx}(t/T) + \sum_{i=1}^{\beta} \hat{f}_z(r_i, t/T) P^{zx}(r_i, t/T) + R_0^{-1}(t) \right] \\ &\times \hat{\lambda}_T(t/T) - \frac{1}{2} \int_0^1 \left\{ \sum_{i=1}^{\beta} \hat{f}_z(r_i, t/T) P^{zz}(r_i, s, t/T) + \hat{f}_x P^{xz}(s, t/T) \right\} \hat{\sigma}_T(s, t/T) ds \end{aligned} \quad (65)$$

On the other hand, using (43) we can write

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{x}_T(t/T)] &= -\frac{1}{2} \left[P_t^{xx}(t/T) \hat{\lambda}_T(t/T) + \int_0^1 P_t^{xz}(s, t/T) \hat{\sigma}_T(s, t/T) ds \right] \\ &\quad - \frac{1}{2} \left[P^{xx}(t/T) \frac{\partial}{\partial t} [\hat{\lambda}_T(t/T)] + \int_0^1 P^{xz}(s, t/T) \frac{\partial}{\partial t} [\hat{\sigma}_T(s, t/T)] ds \right] \end{aligned} \quad (66)$$

which gives us two expressions for the first quantity in (61).

To obtain two relations for the second quantity in (61) we first substitute (30) in the R.H.S. of (63), giving

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{z}_T(r, t/T)] &= -M\hat{z}_T + \hat{g}_z(r, t/T) \hat{z}_T(r, t/T) \\ &\quad - \frac{1}{2} \int_0^1 R_1^+(r, s, t) \hat{\sigma}_T(s, t/T) ds \end{aligned} \quad (67)$$

which, with the help of (44) and (45), can be written as

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{z}_T(r, t/T)] &= -\frac{1}{2} [-M(r, t) P_r^{ZX}(r, t/T) + \hat{g}_z(r, t/T) P^{ZX}(r, t/T)] \\ &\quad \times \hat{\lambda}_T(t/T) - \frac{1}{2} \left[\int_0^1 \left\{ -M(r, t) P_r^{ZZ}(r, s, t/T) + \hat{g}_z(r, t/T) P^{ZZ}(r, s, t/T) \right. \right. \\ &\quad \left. \left. + R_1^+(r, s, t) \right\} \hat{\sigma}_T(s, t/T) ds \right] \end{aligned} \quad (68)$$

On the other hand, using (44) we can write

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{z}_T(r, t/T)] &= -\frac{1}{2} \left[\int_0^1 P_t^{ZZ}(r, s, t/T) \hat{\sigma}_T(s, t/T) ds \right. \\ &\quad \left. + P_t^{ZX}(r, t/T) \hat{\lambda}_T(t/T) \right] - \frac{1}{2} \left[\int_0^1 P^{ZZ}(r, s, t/T) \frac{\partial}{\partial t} [\hat{\sigma}_T(s, t/T)] ds \right. \\ &\quad \left. + P^{ZX}(r, t/T) \frac{\partial}{\partial t} [\hat{\lambda}_T(t/T)] \right] \end{aligned} \quad (69)$$

Now we equate (65) and (66) setting $t = T$. For the equality to hold, the coefficients of $\hat{\lambda}_T(t/T)$, $\hat{\sigma}_T(s, t/T)$ and $\hat{\sigma}_T(0, t/T)$ must be zero at $t = T$. (The last two terms of (66) are evaluated in Appendix III-A.) Doing so, we obtain

$$\begin{aligned} P_t^{XX}(T/T) &= \hat{f}_X P^{XX}(T/T) + P^{XX}(T/T) \hat{f}_X^T \\ &\quad + \sum_{i=1}^{\beta} \hat{f}_z(r_i, T/T) P^{ZX}(r_i, T/T) + \sum_{i=1}^{\beta} P^{XZ}(r_i, T/T) \hat{f}_z^T(r_i, T/T) \end{aligned}$$

$$\begin{aligned}
 & + p^{XX}(T/T) V^{XX}(T/T) P^{XX}(T/T) \\
 & + \sum_{i=1}^Y P^{XX}(T/T) V^{Xi}(T/T) P^{ZX}(r_i^*, T/T) \\
 & + \sum_{i=1}^Y P^{XZ}(r_i^*, T/T) V^{iX}(T/T) P^{XX}(T/T) \\
 & + \sum_{i=1}^Y \sum_{j=1}^Y P^{XZ}(r_i^*, T/T) V^{ij}(T/T) P^{ZX}(r_j^*, T/T) + R_0^{-1}(T) \quad (70)
 \end{aligned}$$

$$\begin{aligned}
 P_t^{XZ}(s, T/T) & = \hat{f}_X P^{XZ}(s, T/T) + P^{XZ}(s, T/T) \hat{g}_Z^T(s, T/T) - P_s^{XZ}(s, T/T) M^T(s, T) \\
 & + \sum_{i=1}^{\beta} \hat{f}_Z(r_i, T/T) P^{ZZ}(r_i, s, T/T) + P^{XX}(T/T) V^{XX}(T/T) P^{XZ}(s, T/T) \\
 & + \sum_{i=1}^Y P^{XX}(T/T) V^{Xi}(T/T) P^{ZZ}(r_i^*, s, T/T) \\
 & + \sum_{i=1}^Y P^{XZ}(r_i^*, T/T) V^{iX}(T/T) P^{XZ}(s, T/T) \\
 & + \sum_{i=1}^Y \sum_{j=1}^Y P^{XZ}(r_i^*, T/T) V^{ij}(T/T) P^{ZZ}(r_j^*, s, T/T) \quad (71)
 \end{aligned}$$

$$P^{XZ}(0, T/T) = P^{XX}(T/T) \hat{b}_X^T \quad (72)$$

Similarly, equating (68) and (69) we obtain (the last two terms of (69) are evaluated in Appendix III-A)

$$\begin{aligned}
 P_t^{ZZ}(r, s, T/T) & = \hat{g}_Z(r, T/T) P^{ZZ}(r, s, T/T) + P^{ZZ}(r, s, T/T) \hat{g}_Z^T(s, T/T) \\
 & - M(r, T) P_r^{ZZ}(r, s, T/T) - P_s^{ZZ}(r, s, T/T) M^T(s, T) \\
 & + P^{ZX}(r, T/T) V^{XX}(T/T) P^{XZ}(s, T/T) \\
 & + \sum_{i=1}^Y P^{ZX}(r, T/T) V^{Xi}(T/T) P^{ZZ}(r_i^*, s, T/T)
 \end{aligned}$$

$$\begin{aligned}
 & + \sum_{i=1}^{\gamma} p^{ZZ}(r, r_i^*, T/T) v^{ix}(T/T) p^{XZ}(s, T/T) \\
 & + \sum_{i=1}^{\gamma} \sum_{j=1}^{\gamma} p^{ZZ}(r, r_i^*, T/T) v^{ij}(T/T) p^{ZZ}(r_j^*, s, T/T) \\
 & + R_1^+(r, s, T)
 \end{aligned} \tag{73}$$

$$\begin{aligned}
 p_t^{ZX}(r, T/T) & = p^{ZX}(r, T/T) \hat{f}_x^T + \hat{g}_z(r, T/T) p^{ZX}(r, T/T) \\
 & - M(r, T) p_r^{ZX}(r, T/T) \\
 & + \sum_{i=1}^{\beta} p^{ZZ}(r, r_i, T/T) \hat{f}_z^T(r_i, T/T) \\
 & + p^{ZX}(r, T/T) v^{XX}(T/T) p^{XX}(T/T) \\
 & + \sum_{i=1}^{\gamma} p^{ZZ}(r, r_i^*, T/T) v^{ix}(T/T) p^{XX}(T/T) \\
 & + \sum_{i=1}^{\gamma} p^{ZX}(r, T/T) v^{xi}(T/T) p^{ZX}(r_i^*, T/T) \\
 & + \sum_{i=1}^{\gamma} \sum_{j=1}^{\gamma} p^{ZZ}(r, r_i^*, T/T) v^{ij}(T/T) p^{ZX}(r_j^*, T/T)
 \end{aligned} \tag{74}$$

$$p^{ZZ}(r, 0, T/T) = p^{ZX}(r, T/T) \hat{b}_x^T \tag{75}$$

The quantities v^{XX} , v^{ix} , v^{xi} and v^{ij} are defined by

$$v^{XX}(T/T) = [\hat{h}_x^T Q(T) (y(T) - \hat{h})]_x \tag{76}$$

$$v^{ix}(T/T) = [\hat{h}_z^T(r_i^*, T/T) Q(T) (y(T) - \hat{h})]_x \quad i=1, 2, \dots, \gamma \tag{77}$$

$$v^{xi}(T/T) = [\hat{h}_x^T Q(T) (y(T) - \hat{h})]_{z(r_i^*, T/T)} \quad i=1, 2, \dots, \gamma \tag{78}$$

$$v^{ij}(T/T) = [\hat{h}_{z(r_i^*, T/T)}^T Q(T)(y(T) - \hat{h})]_{z(r_j^*, T/T)} \quad (79)$$

$i, j=1, 2, \dots, \gamma$

The remaining boundary conditions for (70), (71), (73) and (74) can be obtained by differentiating (35) with respect to T ,

$$\begin{aligned} \frac{\partial \hat{z}(0, t/T)}{\partial \hat{\lambda}(t/T)} \hat{\lambda}_T(t/T) + \int_0^1 \frac{\delta \hat{z}(0, t/T)}{\delta \hat{\sigma}(s, t/T)} \hat{\sigma}_T(s, t/T) ds \\ = \hat{b}_x \frac{\partial \hat{x}(t/T)}{\partial \hat{\lambda}(t/T)} \hat{\lambda}_T(t/T) + \hat{b}_x \int_0^1 \frac{\delta \hat{x}(t/T)}{\delta \hat{\sigma}(s, t/T)} \hat{\sigma}_T(s, t/T) ds \end{aligned} \quad (80)$$

and then equating the coefficients of $\hat{\lambda}_T(t/T)$ and $\hat{\sigma}_T(s, t/T)$ to zero at $t = T$; the result is

$$P^{ZX}(0, T/T) = \hat{b}_x P^{XX}(T/T) \quad (81)$$

$$P^{ZZ}(0, s, T/T) = \hat{b}_x P^{XZ}(s, T/T) \quad (82)$$

The entire filter is summarized in Table 1. In the column of initial conditions, $\hat{x}(0/0)$ and $\hat{z}(r, 0/0)$ represent our best initial guesses of x_0 and $z_0(r)$. The initial conditions $P^{XX}(0/0)$, $P^{XZ}(s, 0/0)$, $P^{ZX}(r, 0/0)$ and $P^{ZZ}(r, s, 0/0)$ are basically arbitrary. In the linear, white noise case it can be shown that

$$P^{XX}(T/T) = E[(x(T) - \hat{x}(T/T))(x(T) - \hat{x}(T/T))^T] \quad (83)$$

$$P^{XZ}(r, T/T) = E[(x(T) - \hat{x}(T/T))(z(r, T) - \hat{z}(r, T/T))^T] \quad (84)$$

$$P^{ZX}(r, T/T) = E[(z(r, T) - \hat{z}(r, T/T))(x(T) - \hat{x}(T/T))^T] \quad (85)$$

$$P^{ZZ}(r, s, T/T) = E[(z(r, T) - \hat{z}(r, T/T))(z(s, T) - \hat{z}(s, T/T))^T] \quad (86)$$

Table 1. Filter for the System of (1)-(6) with $K=H=0$

	Equations	Initial Conditions	Boundary Conditions
<u>Estimates</u>			
$\hat{x}(T/T)$	(49), (56), (58)	$\hat{x}(0/0)$	None
$\hat{z}(r, T/T)$	(50), (57), (59)	$\hat{z}(r, 0/0)$	(60)
<u>First Order Differential Sensitivities</u>			
$P^{XX}(T/T)$	(70)	$P^{XX}(0/0)$	None
$P^{XZ}(s, T/T)$	(71)	$P^{XZ}(s, 0/0)$	(72)
$P^{ZX}(r, T/T)$	(74)	$P^{ZX}(r, 0/0)$	(81)
$P^{ZZ}(r, s, T/T)$	(73)	$P^{ZZ}(r, s, 0/0)$	(75), (82)

These relations may be used as a guide in choosing $P^{XX}(0/0), \dots, P^{ZZ}(r, s, 0/0)$.

3.5 Discussion of the filter

The exact equations for the four covariance matrices are of the form

$$\frac{dP(T/T)}{dT} = P_t(T/T) + P_T(T/T) \quad (87)$$

where P can denote P^{XX}, P^{XZ}, P^{ZX} or P^{ZZ} . We noted earlier that we would neglect the second terms on the R.H.S. of these equations. Let us give some indication as to how these neglected terms might be calculated. Employing the chain rule, we have for $P_T^{XZ}(r, t/T)$, for example,

$$P_T^{XZ}(r, t/T) = \frac{\partial P^{XZ}(r, t/T)}{\partial \hat{\lambda}(t/T)} \hat{\lambda}_T(t/T) + \int_0^1 \frac{\delta P^{XZ}(r, t/T)}{\delta \hat{\sigma}(v, t/T)} \hat{\sigma}_T(v, t/T) dv \quad (88)$$

The terms

$$\frac{\partial P^{XZ}(r, t/T)}{\partial \hat{\lambda}(t/T)}, \quad \frac{\delta P^{XZ}(r, t/T)}{\delta \hat{\sigma}(v, t/T)}$$

are $n_1 \times n_2 \times n_1$ and $n_1 \times n_2 \times n_2$ matrices, respectively, which are the second order differential sensitivities. Thus, the neglected terms in (87) involve second order differential sensitivities, which in turn depend on third order differential sensitivities, etc. As with other nonlinear stochastic problems in mathematics, the exact solution of the nonlinear filtering problem is unavailable due to a closure problem. In the linear, white noise case it can be shown that the second and higher order differential sensitivities are identically zero.

4. Filtering in Nonlinear Systems Described by Functional Differential Equations

In principle, the method of derivation of Section 3 can be used in the case when K and H are nonzero in (1) and (3). However, an easier way to deduce the form of the filter is to express the integrals as summations,

$$\int_0^1 K(z(r, t), r, t) dr = \lim_{\substack{N_1 \rightarrow \infty \\ \Delta_i^+ \rightarrow 0}} \sum_{i=1}^{N_1} K(z(r_i^+, t), r_i^+, t) \Delta_i^+ \quad (89)$$

$$\int_0^1 H(z(r, t), r, t) dr = \lim_{\substack{N_2 \rightarrow \infty \\ \Delta_i^- \rightarrow 0}} \sum_{i=1}^{N_2} H(z(r_i^-, t), r_i^-, t) \Delta_i^- \quad (90)$$

and apply the results of Section 3 with the appropriate limiting procedures. The filter for this case is summarized below. The state filter is

$$\begin{aligned} \frac{d\hat{x}(T/T)}{dT} = & \hat{f} + \int_0^1 K[\hat{z}(\theta, T/T), \theta, T] d\theta + P^{XX}(T/T) \hat{h}_X^T Q(T) \hat{\phi}(T/T) \\ & + \sum_{i=1}^{\gamma} P^{XZ}(r_i^*, T/T) \hat{h}_{Z(r_i^*, T/T)}^T Q(T) \hat{\phi}(T/T) \\ & + \int_0^1 P^{XZ}(\theta, T/T) \hat{H}_{Z(\theta, T/T)}^T(\theta) Q(T) \hat{\phi}(T/T) d\theta \end{aligned} \quad (91)$$

$$\begin{aligned} \frac{\partial \hat{z}(r, T/T)}{\partial T} = & -M \hat{z}_r + \hat{g} + \sum_{i=1}^{\gamma} P^{ZZ}(r, r_i^*, T/T) \hat{h}_{Z(r_i^*, T/T)}^T Q(T) \hat{\phi}(T/T) \\ & + P^{ZX}(r, T/T) \hat{h}_X^T Q(T) \hat{\phi}(T/T) \\ & + \int_0^1 P^{ZZ}(r, \theta, T/T) \hat{H}_{Z(\theta, T/T)}^T(\theta) Q(T) \hat{\phi}(T/T) d\theta \end{aligned} \quad (92)$$

$$\hat{z}(0, T/T) = b(\hat{x}(T/T)) \quad (93)$$

where

$$\begin{aligned} \hat{\phi}(T/T) = & y(T) - h(\hat{x}(T/T), \hat{z}(r_1^*, T/T), \dots, \hat{z}(r_\gamma^*, T/T), T) \\ & - \int_0^1 H(\hat{z}(\theta, T/T), \theta, T) d\theta \end{aligned} \quad (94)$$

The covariance equations are (corresponding to (70), (71), (73) and (74) for $K = H = 0$)

$$\begin{aligned}
 P_t^{XX}(T/T) &= [\text{R.H.S. of (70)}] + \int_0^1 \hat{K}_Z(\theta, T/T)(\theta) P^{ZX}(\theta, T/T) d\theta \\
 &+ \int_0^1 P^{XZ}(\theta, T/T) \hat{K}_Z^T(\theta, T/T)(\theta) d\theta + W^{XX}(T/T) \quad (95)
 \end{aligned}$$

$$\begin{aligned}
 P_t^{XZ}(s, T/T) &= [\text{R.H.S. of (71)}] + \int_0^1 \hat{K}_Z(\theta, T/T)(\theta) P^{ZZ}(\theta, s, T/T) d\theta \\
 &+ W^{XZ}(s, T/T) \quad (96)
 \end{aligned}$$

$$\begin{aligned}
 P_t^{ZX}(r, T/T) &= [\text{R.H.S. of (74)}] + \int_0^1 P^{ZZ}(r, \theta, T/T) \hat{K}_Z^T(\theta, T/T)(\theta) d\theta \\
 &+ W^{ZX}(r, T/T) \quad (97)
 \end{aligned}$$

$$P_t^{ZZ}(r, s, T/T) = [\text{R.H.S. of (73)}] + W^{ZZ}(r, s, T/T) \quad (98)$$

where the terms $V(T/T)$ will be defined below (the definitions differ slightly from those in Section 3.) The terms $W^{\mu\lambda}(\cdot, \cdot, T/T)$ are defined by

$$\begin{aligned}
 W^{\mu\lambda}(\cdot, \cdot, T/T) &= \int_0^1 P^{\mu X}(\cdot, T/T) V^{XZ}(\zeta, T/T) P^{Z\lambda}(\zeta, \cdot, T/T) d\zeta \\
 &+ \int_0^1 P^{\mu Z}(\cdot, \zeta, T/T) V^{ZX}(\zeta, T/T) P^{X\lambda}(\cdot, T/T) d\zeta \\
 &+ \sum_{i=1}^{\gamma} \int_0^1 P^{\mu Z}(\cdot, r_i^*, T/T) V^{iZ}(\zeta, T/T) P^{Z\lambda}(\zeta, \cdot, T/T) d\zeta \\
 &+ \sum_{i=1}^{\gamma} \int_0^1 P^{\mu Z}(\cdot, \zeta, T/T) V^{Zi}(\zeta, T/T) P^{Z\lambda}(r_i^*, \cdot, T/T) d\zeta \\
 &+ \int_0^1 \int_0^1 P^{\mu Z}(\cdot, \zeta, T/T) V_1^{ZZ}(\zeta, \nu, T/T) P^{Z\lambda}(\nu, \cdot, T/T) d\zeta d\nu
 \end{aligned}$$

$$\begin{aligned}
 & + \int_0^1 \int_0^1 P^{\mu z}(\cdot, \zeta, T/T) V_2^{zz}(\zeta, \nu, T/T) P^{z\lambda}(\zeta, \cdot, T/T) d\zeta d\nu \\
 & + \int_0^1 P^{\mu z}(\cdot, \zeta, T/T) V_3^{zz}(\zeta, T/T) P^{z\lambda}(\zeta, \cdot, T/T) d\zeta
 \end{aligned} \tag{99}$$

where $\mu = x$ or z and $\lambda = x$ or z . The unspecified left argument of each term is r if $\mu = z$ and does not exist if $\mu = x$. The unspecified right argument of each term is s if $\lambda = z$ and does not exist if $\lambda = x$.

In this case the V matrices are defined as follows (we suppress the dependence on T for convenience):

$$\begin{aligned}
 V^{xx} &= [\hat{h}_x^T Q \hat{\Phi}]_x & V^{xi} &= [\hat{h}_x^T Q \hat{\Phi}]_{z(r_i^*)} \\
 V^{xz}(\theta) &= -\hat{h}_x^T Q \hat{H}_{z(\theta)}(\theta) & V^{ix} &= [\hat{h}_{z(r_i^*)}^T Q \hat{\Phi}]_x \\
 V^{ij} &= [\hat{h}_{z(r_i^*)}^T Q \hat{\Phi}]_{z(r_j^*)} & V^{iz}(\theta) &= -\hat{h}_{z(r_i^*)}^T Q \hat{H}_{z(\theta)}(\theta) \\
 V^{zx}(\theta) &= -\hat{H}_{z(\theta)}^T(\theta) Q \hat{h}_x & V^{zi}(\theta) &= -\hat{H}_{z(\theta)}^T(\theta) Q \hat{h}_{z(r_i^*)} \\
 V_1^{zz}(\theta, \nu) &= -\hat{H}_{z(\theta)}^T(\theta) Q \hat{H}_{z(\nu)}(\nu) \\
 V_2^{zz}(\theta, \nu) &= -[\hat{H}_{z(\theta)}^T(\theta) Q \hat{H}(\nu)]_{z(\theta)} \\
 V_3^{zz}(\theta) &= [\hat{H}_{z(\theta)}^T(\theta) Q (y - \hat{h})]_{z(\theta)}
 \end{aligned} \tag{100}$$

The filter in this case is summarized in Table 2.

Table 2. Filter for the System (1)-(6) with $K \neq 0, H \neq 0$

<u>Estimates</u>	<u>Equations</u>	<u>Initial Conditions</u>	<u>Boundary Conditions</u>
$\hat{x}(T/T)$	(91)	$\hat{x}(0/0)$	None
$\hat{z}(r,T/T)$	(92)	$\hat{z}(r,0/0)$	(93)
<u>First Order Differential Sensitivities</u>			
$P^{XX}(T/T)$	(95)	$P^{XX}(0/0)$	None
$P^{XZ}(s,T/T)$	(96)	$P^{XZ}(s,0/0)$	(72)
$P^{ZX}(r,T/T)$	(97)	$P^{ZX}(r,0/0)$	(81)
$P^{ZZ}(r,s,T/T)$	(98)	$P^{ZZ}(r,s,0/0)$	(75),(82)

5. A Computational Example

We consider a system consisting of a well-stirred chemical reactor, a portion of the output from which is recycled through a heat exchanger back to the reactor. We assume that there is a zero order exothermic chemical reaction taking place in the fluid in both the reactor and the heat exchanger. The temperature of the reactor is controlled by recycling a fixed fraction of the effluent through the heat exchanger.

The dynamic behavior of the system is governed by

$$\dot{x}(t) = -0.05x + 0.2z(1,t) - 0.001 \left[\exp\left(\frac{20x}{1+x}\right) - 1 \right]$$

$$z_t(r,t) = -z_r(r,t) + 0.1 - 0.001 \exp\left(\frac{20z}{1+z}\right) \quad 0 \leq r \leq 1$$

$$z(0,t) = x(t) \quad t \geq 0$$

$$x(0) = z(r,0) = -0.1 \quad (\text{unknown})$$

where the states $x(t)$ and $z(r,t)$ are the dimensionless temperatures in the reactor and heat exchanger, respectively. We neglect any sources of dynamical noise in either the reactor or the heat exchanger. We desire to estimate $x(t)$ and $z(r,t)$ based on the observations

$$y_1(t) = x(t) + \eta_1(t)$$

$$y_2(t) = z(0.5,t) + \eta_2(t)$$

which are noisy measurements of the reactor temperature and the temperature at the midpoint of the heat exchanger. For the purpose of numerical simulation the observation errors were generated by $\eta_i(t) = 0.3G(0,1)$, $i=1,2$, where $G(0,1)$ is a normally distributed random variable with zero mean and unit standard deviation produced by a random number generator.

The filter equations with $Q(t) = 1$ are (for convenience, the dependence on the observation interval $[0,T]$ is suppressed, i.e., (\cdot, t) is to be read as $(\cdot, t/t)$)

$$\hat{x}_t(t) = -0.05\hat{x} + 0.2\hat{z}(1,t) - 0.001 \left[\exp\left(\frac{20\hat{x}}{1+\hat{x}}\right) - 1 \right]$$

$$+ P^{XX}(t)[y_1(t) - \hat{x}(t)] + P^{XZ}(0.5,t)[y_2(t) - \hat{z}(0.5,t)]$$

$$\hat{z}_t(r,t) = -\hat{z}_r(r,t) + 0.1 - 0.001 \exp\left(\frac{20\hat{z}}{1+\hat{z}}\right) + P^{ZZ}(r,0.5,t)[y_2(t)$$

$$- \hat{z}(0.5,t)] + P^{XZ}(r,t)[y_1(t) - \hat{x}(t)]$$

$$\hat{z}(0,t) = \hat{x}(t)$$

$$\dot{p}^{xx}(t) = -0.1 p^{xx}(t) - \frac{0.04}{(1+\hat{x})^2} \exp\left(\frac{20\hat{x}}{1+\hat{x}}\right) p^{xx}(t) \\ + 0.4 p^{xz}(1,t) - p^{xx}(t)^2 - p^{xz}(0.5,t)^2$$

$$p_t^{xz}(s,t) = -0.05 p^{xz}(s,t) - \frac{0.02}{(1+\hat{x})^2} \exp\left(\frac{20\hat{x}}{1+\hat{x}}\right) p^{xz}(s,t) \\ - \frac{0.02}{(1+\hat{z})^2} \exp\left(\frac{20\hat{z}}{1+\hat{z}}\right) p^{xz}(s,t) - p_s^{xz}(s,t) + 0.2 p^{zz}(1,s,t) \\ - p^{xx}(t) p^{xz}(s,t) - p^{xz}(0.5,t) p^{zz}(0.5,s,t)$$

$$p_t^{zz}(r,s,t) =$$

$$\left\{ \frac{-0.02}{(1+\hat{z}(r,t))^2} \exp\left(\frac{20\hat{z}(r,t)}{1+\hat{z}(r,t)}\right) - \frac{0.02}{(1+\hat{z}(s,t))^2} \exp\left(\frac{20\hat{z}(s,t)}{1+\hat{z}(s,t)}\right) \right\} p^{zz}(r,s,t)$$

$$- p_r^{zz}(r,s,t) - p_s^{zz}(r,s,t) - p^{xz}(r,t) p^{xz}(s,t) - p^{zz}(r,0.5,t) p^{zz}(0.5,s,t)$$

$$p^{xz}(0,t) = p^{xx}(t) ; \quad p^{zz}(r,0,t) = p^{xz}(r,t) ; \quad p^{zz}(0,s,t) = p^{xz}(s,t)$$

Note that we have made use of the symmetrical properties of the covariances, i.e., $p^{xx} = p^{xxT}$, $p^{xz} = p^{zxT}$, and $p^{zz}(r,s,t) = p^{zz}(s,r,t)^T$. We chose $\hat{x}(0) = \hat{z}(r,0) = 0.25$, $p^{xx}(0) = 2.0$, $p^{xz}(s,0) = 2.0$, $p^{zz}(r,s,0) = 2.0$ as initial conditions for the filter. The filter performance is shown in Figure 3 where the true states $x(t)$, $z(0.5,t)$, $z(1,t)$ and their estimates $\hat{x}(t)$, $\hat{z}(0.5,t)$, $\hat{z}(1,t)$ are compared. Numerical solution of the state and filter was carried out using a finite difference scheme and required about 40 seconds on an IBM 370/155 for an experimental time of $t = 40$. It is clear that the filter tracks the state variables very quickly in spite of the relatively

poor initial guess and large measurement noise.

6. Figures

Figure 1 Classes of Filters Derived in this Chapter

Figure 2 Well-Stirred Chemical Reactor with External Heat Exchanger

Figure 3 Comparison of Actual and Estimated Temperatures in Reactor, at Midpoint and Exit of Heat Exchanger, $x(t)$, $z(0.5,t)$, $z(1,t)$, respectively.

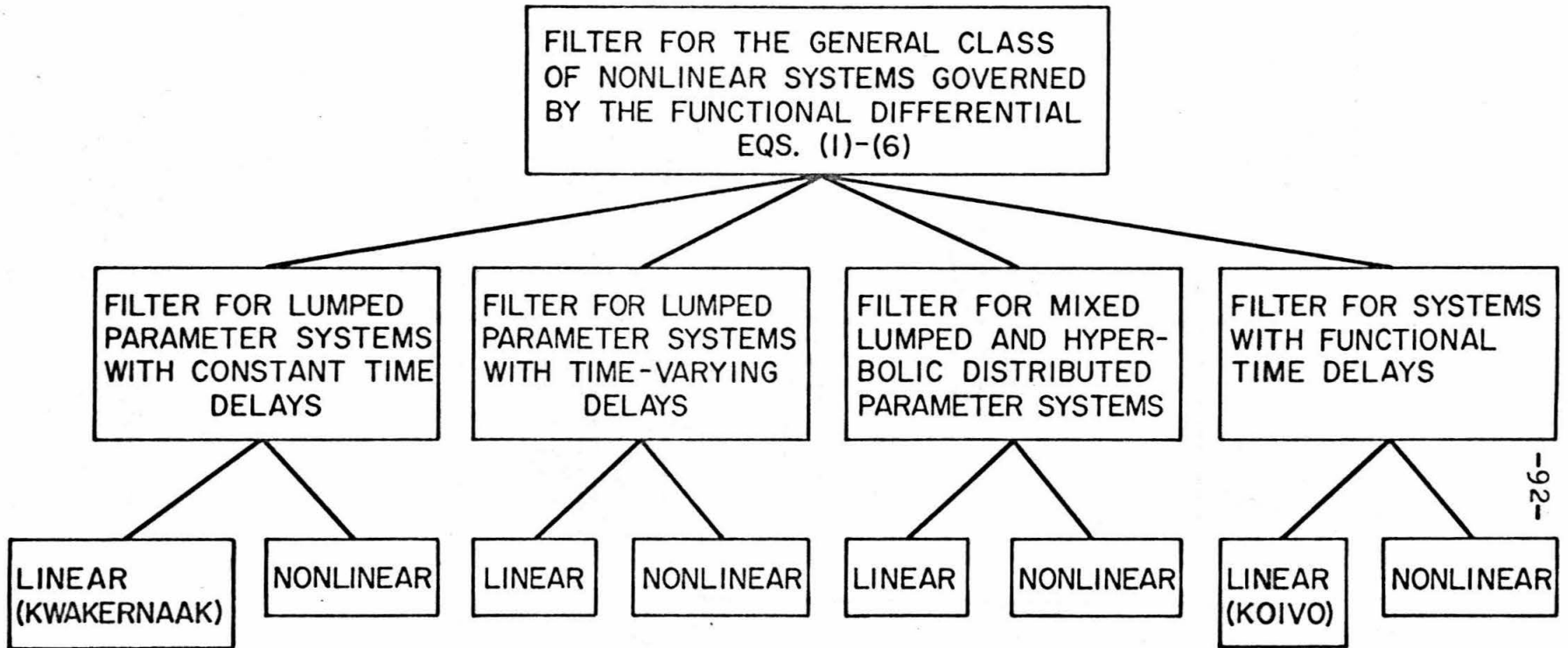


FIGURE 1

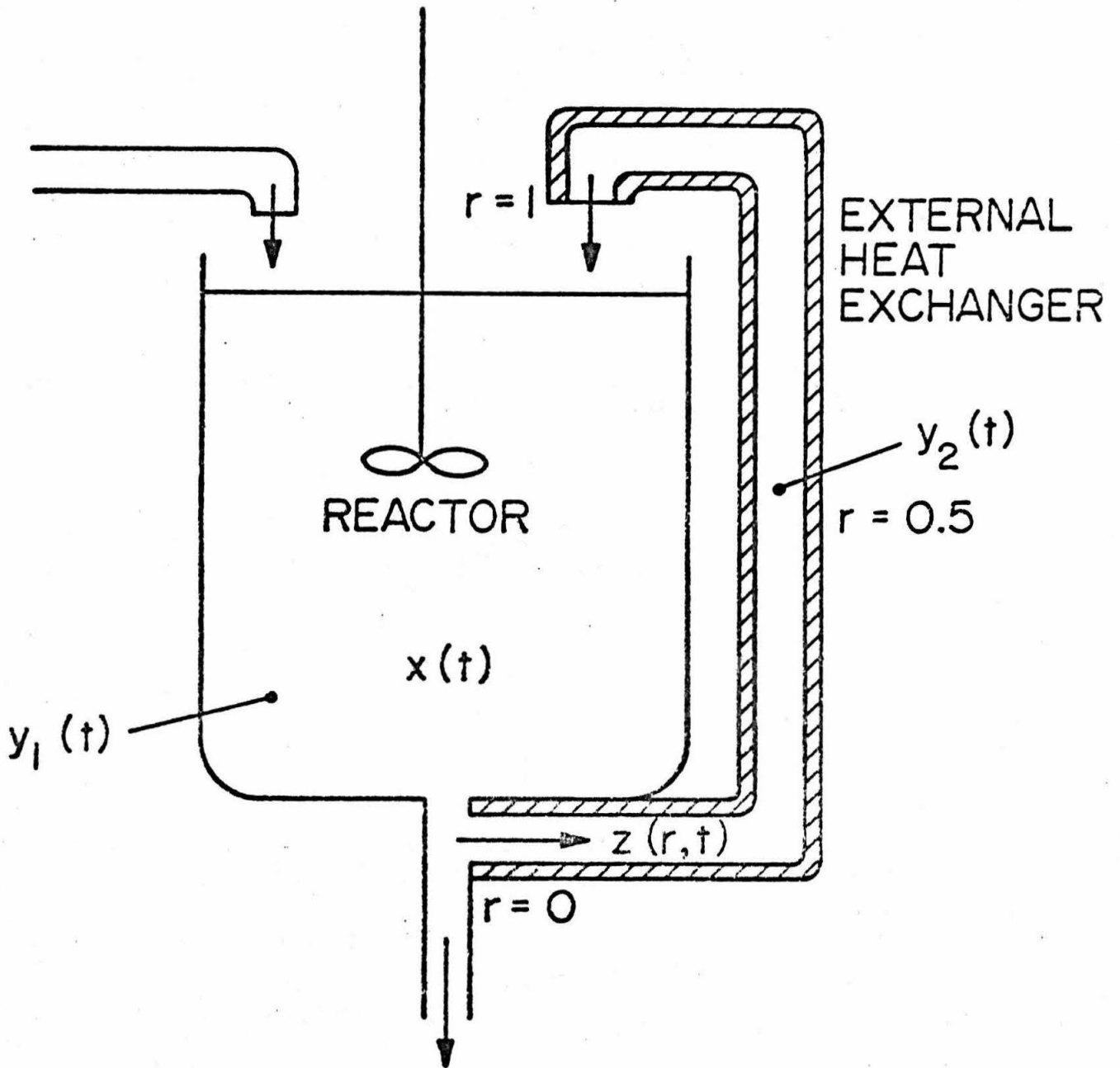


FIGURE 2

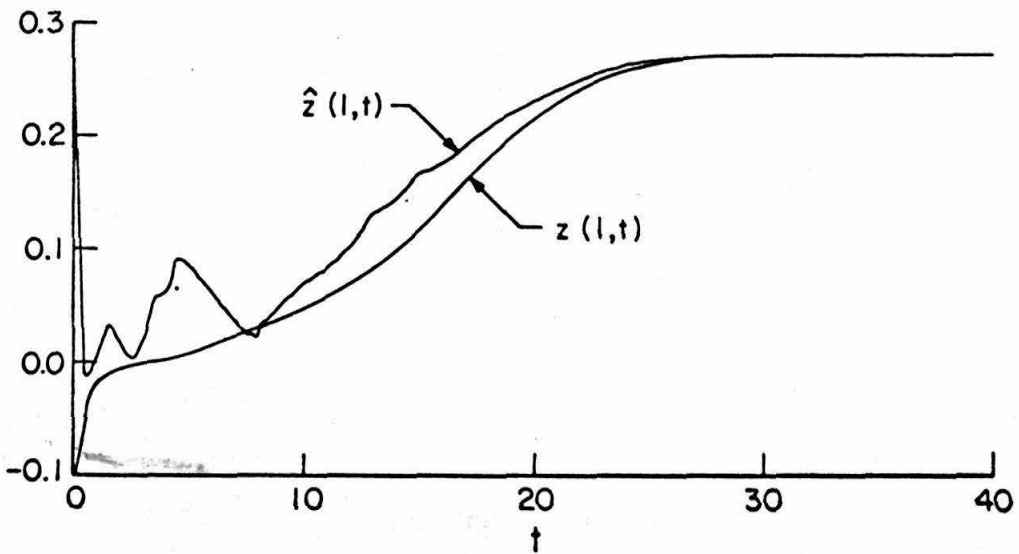
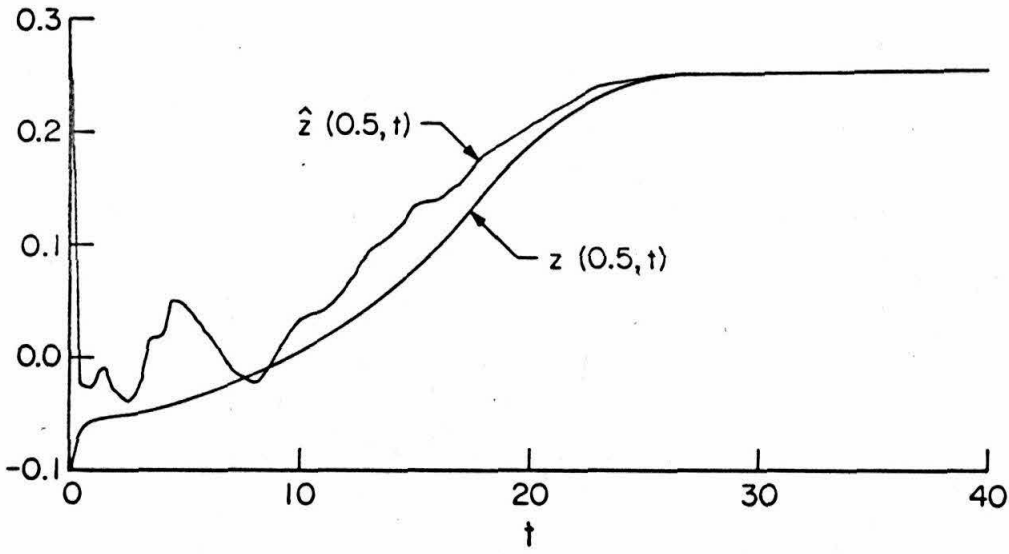
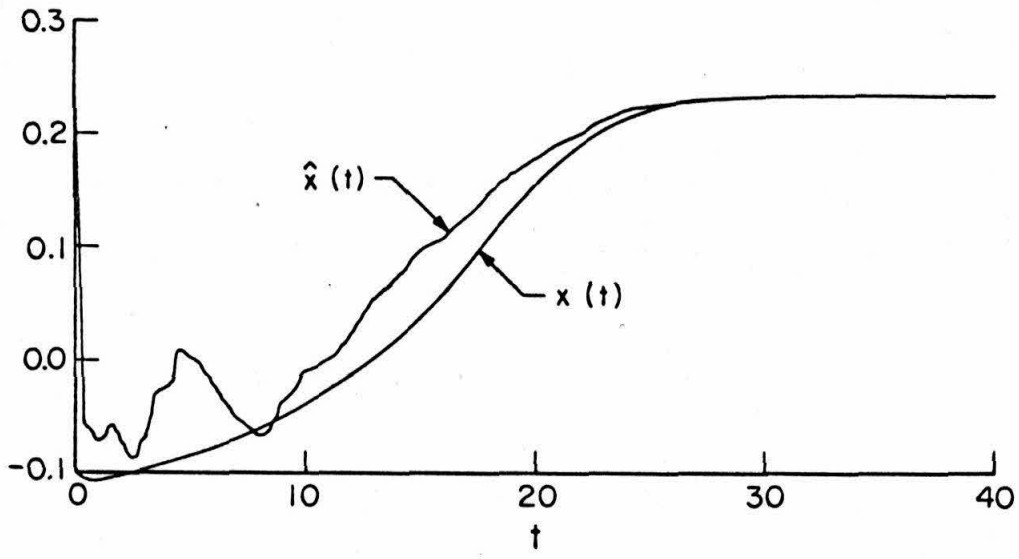


FIGURE 3

Appendix III-A

We first consider the quantity

$$P \frac{\partial}{\partial t} [\hat{\lambda}(t/T)] \quad (A.1)$$

where P can either be $P^{XX}(t/T)$ or $P^{ZX}(r,t/T)$. Let us define the vector

$$V^X(t/T) = \hat{h}_X^T Q(t)(y - \hat{h}) \quad (A.2)$$

and the matrices

$$V^{XX}(t/T) = [\hat{h}_X^T Q(t)(y - \hat{h})]_X \quad (A.3)$$

$$V^{Xi}(t/T) = [\hat{h}_X^T Q(t)(y - \hat{h})]_{Z(r_i^*, t/T)} \quad (A.4)$$

$i=1, \dots, \gamma$

Using (31), (A.1) can be expressed as

$$\begin{aligned} P \frac{\partial}{\partial t} [\hat{\lambda}_T(t/T)] &= P \frac{\partial}{\partial T} [\hat{\lambda}_t(t/T)] \\ &= P \frac{\partial}{\partial T} [2\hat{h}_X^T Q(t)(y - \hat{h}) - \hat{f}_X^T \hat{\lambda}(t/T) - \hat{b}_X^T M^T(0,t) \hat{\sigma}(0,t/T)] \\ &= P 2V^{XX}(t/T) \hat{x}_T(t/T) + P 2 \sum_{i=1}^{\gamma} V^{Xi}(t/T) \hat{z}_T(r_i^*, t/T) \\ &\quad - P \hat{f}_X^T \hat{\lambda}_T(t/T) - P \hat{b}_X^T M^T(0,t) \hat{\sigma}_T(0,t/T) \\ &\quad - P (\hat{f}_X^T)_T \hat{\lambda}(t/T) - P (\hat{b}_X^T)_T M^T(0,t) \hat{\sigma}(0,t/T) \end{aligned} \quad (A.5)$$

The last two terms of (A.5) will not contribute to the final results of the equations governing $P^{XX}(T/T), \dots, P^{ZX}(r,T/T)$ since $\hat{\lambda}(T/T) = 0$ and $\hat{\sigma}(0, T/T) = 0$. Neglecting these two terms (A.5) can be rewritten as

$$\begin{aligned}
 & P \frac{\partial}{\partial t} [\hat{\lambda}_T(t/T)] \\
 &= P 2V^{XX}(t/T)\hat{x}_T(t/T) + P 2 \int_0^1 \left(\sum_{i=1}^Y V^{Xi}(t/T) \delta(r - r_i^*) \right) \hat{z}_T(r, t/T) dr \\
 & - P \hat{f}_X^T \hat{\lambda}_T(t/T) - P \hat{b}_X^T M^T(0, t) \hat{\sigma}_T(0, t/T) \tag{A.6}
 \end{aligned}$$

Inserting (43) and (44) into (A.6) gives

$$\begin{aligned}
 & P \frac{\partial}{\partial t} [\hat{\lambda}_T(t/T)] \\
 &= - [PV^{XX}(t/T) P^{XX}(t/T) + \sum_{i=1}^Y PV^{Xi}(t/T) P^{ZX}(r_i^*, t/T)] \hat{\lambda}_T(t/T) \\
 & - \int_0^1 [PV^{XX}(t/T)P^{XZ}(s, t/T) + \sum_{i=1}^Y PV^{Xi}(t/T) P^{ZZ}(r_i^*, s, t/T)] \hat{\sigma}_T(s, t/T) ds \\
 & - P \hat{f}_X^T \hat{\lambda}_T(t/T) - P \hat{b}_X^T M^T(0, t) \hat{\sigma}_T(0, t/T) \tag{A.7}
 \end{aligned}$$

We now consider the quantity

$$\int_0^1 P(s) \frac{\partial}{\partial t} [\hat{\sigma}_T(s, t/T)] ds \tag{A.8}$$

where $P(s)$ can either be $P^{XZ}(s, t/T)$ or $P^{ZZ}(r, s, t/T)$. Let us define the vector

$$v^i(t/T) = \hat{h}_z^T(r_i^*, t/T) Q(t)(y - \hat{h}) \tag{A.9}$$

and the matrices

$$v^{ix}(t/T) = [\hat{h}_z^T(r_i^*, t/T) Q(t)(y - \hat{h})]_x \tag{A.10}$$

$$v^{ij}(t/T) = [\hat{h}_z^T(r_i^*, t/T) Q(t)(y - \hat{h})]_{z(r_j^*, t/T)} \tag{A.11}$$

Using (32), (A.8) can be expressed as

$$\begin{aligned}
 & \int_0^1 P(s) \frac{\partial}{\partial t} [\hat{\sigma}_T(s, t/T)] ds = \int_0^1 P(s) \frac{\partial}{\partial T} [\hat{\sigma}_t(s, t/T)] ds \\
 & = \int_0^1 P(s) \frac{\partial}{\partial T} \left[2 \sum_{i=1}^Y \hat{h}_Z^T(r_i^*, t/T) Q(t)(y - \hat{h}) \delta(s - r_i^*) \right. \\
 & \quad - \sum_{i=1}^{\beta} \hat{f}_Z^T(r_i, t/T) \hat{\lambda}(t/T) \delta(s - r_i) - \hat{g}_Z^T(s, t/T) \hat{\sigma}(s, t/T) \\
 & \quad \left. - (M^T(s, t) \hat{\sigma}(s, t/T))_s \right] ds \tag{A.12}
 \end{aligned}$$

Again, due to the fact that $\hat{\lambda}(T/T) = 0$ and $\hat{\sigma}(s, T/T) = 0$, some of the terms in (A.12) will not contribute to the final results of the equations governing $P_t^{XX}(T/T), \dots, P_t^{ZX}(r, T/T)$. Neglecting these terms, we can write (A.12) as

$$\begin{aligned}
 & \int_0^1 P(s) \frac{\partial}{\partial T} [\hat{\sigma}_T(s, t/T)] ds \\
 & = \int_0^1 P(s) \left[2 \sum_{i=1}^Y v^{ix}(t/T) \delta(s - r_i^*) \hat{x}_T(t/T) \right. \\
 & \quad + 2 \sum_{i=1}^Y \sum_{j=1}^Y v^{ij}(t/T) \delta(s - r_i^*) \hat{z}_T(r_j^*, t/T) \\
 & \quad - \sum_{i=1}^{\beta} \hat{f}_Z^T(r_i, t/T) \delta(s - r_i) \hat{\lambda}_T(t/T) - \hat{g}_Z^T(s, t/T) \hat{\sigma}_T(s, t/T) \\
 & \quad \left. - \frac{\partial}{\partial T} (M^T(s, t) \hat{\sigma}(s, t/T))_s \right] ds \tag{A.13}
 \end{aligned}$$

Using (43) and (44) in (A.13) and integrating the last term of (A.13) by parts, we obtain

$$\begin{aligned}
 & \int_0^1 P(s) \frac{\partial}{\partial t} [\hat{\sigma}_T(s, t/T)] ds \\
 = & - \left[\sum_{i=1}^Y P(r_i^*) v^{ix}(t/T) p^{xx}(t/T) + \sum_{i=1}^Y \sum_{j=1}^Y P(r_i^*) v^{ij}(t/T) p^{zx}(r_j^*, t/T) \right. \\
 & \left. + \sum_{i=1}^B P(r_i) \hat{f}_{zT}^T(r_i, t/T) \right] \hat{\lambda}_T(t/T) \\
 - & \int_0^1 \left[\sum_{i=1}^Y P(r_i^*) v^{ix}(t/T) p^{xz}(s, t/T) + \sum_{i=1}^Y \sum_{j=1}^Y P(r_i^*) v^{ij}(t/T) p^{zz}(r_j^*, s, t/T) \right. \\
 & \left. + P(s) \hat{g}_{zT}^T(s, t/T) - P_s(s) M^T(s, t) \right] \hat{\sigma}_T(s, t/T) ds \\
 & - P(s) M^T(s, t) \hat{\sigma}_T(s, t/T) \Big|_{s=0}^{s=1} \tag{A.14}
 \end{aligned}$$

Appendix III-B

In this appendix we derive the necessary conditions for optimality corresponding to the minimization of (25) subject to (26)-(28). This is achieved by setting the first variation of the Lagrangian L to zero [14] where

$$\begin{aligned}
 L = & \int_0^T \langle u(t), R_0(t) u(t) \rangle dt + \int_0^T \langle y - h, Q(t)(y - h) \rangle dt \\
 & + \int_0^T \left\{ \int_0^1 \int_0^1 \langle v(r,t), R_1(r,s,t) v(s,t) \rangle dr ds \right\} dt \\
 & + \int_0^T \langle -\lambda(t), \dot{x} - f - u \rangle dt \\
 & + \int_0^T \left\{ \int_0^1 \langle -\sigma(r,t), z_t(r,t) + M(r,t) z_r(r,t) - g(z(r,t), r, t) \right. \\
 & \qquad \qquad \qquad \left. - v(r,t) \rangle dr \right\} dt \\
 & + \int_0^T \langle +\mu(t), z(0,t) - b(x(t)) \rangle dt
 \end{aligned}$$

$u(t)$ and $v(r,t)$ are the vector controls. $\lambda(t)$, $\sigma(r,t)$ and $\mu(t)$ are the vector Lagrange multipliers. Let δL denote the first variation of L and we emphasize the fact that δL is the total first variation. Suppose L depends functionally on parameters p_i , $i=1,2,\dots,J$, then we can write $\delta L = \sum_{i=1}^J \delta L(p_i)$ where $\delta L(p_i)$ is the first variation of L with respect to a variation of p_i (denoted by δp_i) over the appropriate domain. In this way we can write

$$\begin{aligned}
 \delta L &= \delta L(\lambda(t)) + \delta L(\sigma(r,t)) + \delta L(\mu(t)) \\
 &+ \delta L(u(t)) + \delta L(v(r,t)) + \delta L(v(s,t)) \\
 &+ \delta L(x(t)) + \delta L(\dot{x}(t)) + \delta L(z(0,t)) \\
 &+ \delta L(z(r,t)) + \delta L(z_t(r,t)) + \delta L(z_r(r,t))
 \end{aligned}$$

We proceed to evaluate various variations.

$$\delta L(\lambda(t)) = \int_0^T \langle -\delta\lambda(t), \dot{x} - f - u \rangle dt$$

$$\delta L(\sigma(r,t)) = \int_0^T \int_0^1 \langle -\delta\sigma(r,t), z_t + Mz_r - g - v \rangle dr dt$$

$$\delta L(\mu(t)) = \int_0^T \langle +\delta\mu(t), z(0,t) - b(x(t)) \rangle dt$$

$$\delta L(u(t)) = \int_0^T \langle \delta u(t), 2R_0(t) u(t) + \lambda(t) \rangle dt$$

$$\delta L(v(r,t)) + \delta L(v(s,t))$$

$$\begin{aligned}
 &= \int_0^T \left\{ \int_0^1 \int_0^1 \langle \delta v(r,t), 2R_1(r,s,t) v(s,t) \rangle dr ds \right. \\
 &\quad \left. + \int_0^1 \langle \delta v(r,t), \sigma(r,t) \rangle dr \right\} dt
 \end{aligned}$$

$$\delta L(x(t)) = \int_0^T \langle \delta x(t), -2h_x^T Q(t)(y-h) \rangle dt$$

$$+ \int_0^T \langle \delta x(t), f_x^T \lambda(t) \rangle dt + \int_0^T \langle \delta x(t), -b_x^T \mu(t) \rangle dt$$

$$\delta L(\dot{x}(t)) = \int_0^T \langle -\delta \dot{x}(t), \lambda(t) \rangle dt$$

$$= \langle -\delta x(t), \lambda(t) \rangle \Big|_0^T + \int_0^T \langle \delta x(t), \dot{\lambda}(t) \rangle dt$$

$$\delta L(z(0,t)) = \int_0^T \langle \delta z(0,t), \mu(t) \rangle dt$$

$$\begin{aligned} \delta L(z(r,t)) = & \int_0^T \left\{ \int_0^1 \langle \delta z(r,t), -\sum_{i=1}^{\gamma} 2h_{z(r_i^*,t)}^T Q(t)(y-h) \delta(r-r_i^*) \rangle dr \right. \\ & + \int_0^1 \langle \delta z(r,t), \sum_{i=1}^{\beta} f_{z(r_i,t)}^T \lambda(t) \delta(r-r_i) \rangle dr \\ & \left. + \int_0^1 \langle \delta z(r,t), g_{z(r,t)}^T \sigma(r,t) \rangle dr \right\} dt \end{aligned}$$

$$\begin{aligned} \delta L(z_t(r,t)) = & \int_0^1 \int_0^T \langle -\delta z_t(r,t), \sigma(r,t) \rangle dt dr \\ = & \int_0^1 \langle -\delta z(r,T), \sigma(r,T) \rangle dr + \int_0^1 \langle +\delta z(r,0), \sigma(r,0) \rangle dr \\ & + \int_0^T \int_0^1 \langle \delta z(r,t), \sigma_t(r,t) \rangle dr dt \end{aligned}$$

$$\begin{aligned} \delta L(z_r(r,t)) = & \int_0^T \int_0^1 \langle -\delta z_r(r,t), M^T(r,t) \sigma(r,t) \rangle dr dt \\ = & \int_0^T \langle \delta z(0,t), M^T(0,t) \sigma(0,t) \rangle dt \\ & + \int_0^T \langle \delta z(1,t), -M^T(1,t) \sigma(1,t) \rangle dt \\ & + \int_0^T \int_0^1 \langle \delta z(r,t), +M^T(r,t) \sigma(r,t) \rangle_r dr dt \end{aligned}$$

In order that $\delta L = 0$ for arbitrary δp_i , the coefficient of each of the following δp_i must identically be zero. Let $\phi(\delta p_i)$ denote the coefficient of δp_i , then

$$\phi(\delta \lambda(t)) = 0 \implies \dot{x} = f + u(t)$$

$$\phi(\delta \sigma(r,t)) = 0 \implies z_t = -Mz_r + g + v(r,t)$$

$$\phi(\delta \mu(t)) = 0 \implies z(0,t) = b(x(t))$$

$$\phi(\delta u(t)) = 0 \implies u(t) = -\frac{1}{2} R_0^{-1}(t) \lambda(t)$$

$$\phi(\delta v(r,t)) = 0 \implies v(r,t) = -\frac{1}{2} \int_0^1 R_1^+(r,s,t) \sigma(s,t) ds$$

$$\phi(\delta x(t)) = 0 \implies \dot{\lambda}(t) = 2h_X^T Q(t)(y-h) - f_X^T \lambda(t) + b_X^T \mu(t)$$

$$\begin{aligned} \phi(\delta z(r,t)) = 0 \implies \sigma_t(r,t) = & 2 \sum_{i=1}^{\gamma} h_{z(r_i^*,t)}^T Q(t)(y-h) \delta(r-r_i^*) \\ & - \sum_{i=1}^{\beta} f_{z(r_i,t)}^T \lambda(t) \delta(r-r_i) \\ & - g_{z(r,t)}^T \sigma(r,t) - (M^T(r,t) \sigma(r,t))_r \end{aligned}$$

$$\phi(\delta z(0,t)) = 0 \implies \mu(t) + M^T(0,t) \sigma(0,t) = 0$$

$$\phi(\delta z(1,t)) = 0 \implies \sigma(1,t) = 0$$

$$\phi(\delta x(0)) = 0 \implies \lambda(0) = 0$$

$$\phi(\delta x(T)) = 0 \implies \lambda(T) = 0$$

$$\phi(\delta z(r,0)) = 0 \implies \sigma(r,0) = 0$$

$$\phi(\delta z(r,T)) = 0 \implies \sigma(r,T) = 0$$

Chapter IV

OPTIMAL FILTERING FOR SYSTEMS GOVERNED BY COUPLED ORDINARY
AND PARTIAL DIFFERENTIAL EQUATIONS

1. Introduction

In this chapter an optimal filter is derived for a class of systems governed by coupled ordinary and parabolic and hyperbolic partial differential equations with additive volume, boundary and observation disturbances. The formulation here is sufficiently general that it includes as a special case the class of $H = K = 0$ systems studied in Chapter III.

2. Statement of Problem

We consider the class of well-posed systems governed by

$$\dot{x}(t) = f(x(t), z(r_1, t), \dots, z(r_\beta, t), t) + \xi(t)$$

$$z_t(r, t) = g(r, t, z, z_r, z_{rr}, x) + \zeta(r, t)$$

$$b_0(t, x, z, z_r) + \zeta_0(t) = 0 \quad r = 0$$

$$b_1(t, x, z, z_r) + \zeta_1(t) = 0 \quad r = 1$$

$$y(t) = h(x(t), z(r_1^*, t), \dots, z(r_\gamma^*, t), t) + \eta(t) \quad (1)$$

defined for time $t \geq 0$ on the normalized spatial domain $r \in (0, 1)$. $x(t)$ is an n_1 -vector state, $z(r, t)$ is an n_2 -vector state and $y(t)$ is an n_3 -vector of observations. The boundary conditions b_0 and b_1 are ℓ_0 - and ℓ_1 -vector functions, respectively.

$\xi(t)$, $\zeta(r,t)$, $\zeta_0(t)$, $\zeta_1(t)$ and $\eta(t)$ are zero-mean random processes with unknown statistical properties. r_i and r_j^* are discrete points on the spatial domain; we assume that $0 \leq r_1 < \dots < r_\beta \leq 1$ and $0 \leq r_1^* < \dots < r_\gamma^* \leq 1$. The initial conditions $x(0)$ and $z(r,0)$ are in general not known.

The smoothing problem is: given any fixed $T > 0$ and observations $y(t)$, $0 \leq t \leq T$, it is desired to estimate $z(r,t)$ and $x(t)$ for $0 \leq t \leq T$ such that the least square error functional

$$\begin{aligned} \psi = & \int_0^T \langle \dot{x} - f, R(t)(\dot{x} - f) \rangle dt + \int_0^T \langle y - h, Q(t)(y - h) \rangle dt \\ & + \int_0^T \left\{ \int_0^1 \int_0^1 \langle z_t(r,t) - g(r,t, z, z_r, z_{rr}, x), \right. \\ & \left. R(r,s,t)(z_t(s,t) - g(s,t, z, z_s, z_{ss}, x)) \rangle dr ds \right\} dt \\ & + \int_0^T \langle b_0(t, x, z, z_r), R_0(t)(b_0(t, x, z, z_r)) \rangle dt \\ & + \int_0^T \langle b_1(t, x, z, z_r), R_1(t)(b_1(t, x, z, z_r)) \rangle dt \end{aligned} \quad (2)$$

is minimized. The weighting matrices $R(t)$, $R_0(t)$, $R_1(t)$ and $Q(t)$ are symmetric positive-definite. $R(r,s,t)$ is defined by [21,33]

$$\int_0^1 R^+(r,\rho,t) R(\rho,s,t) d\rho = I\delta(r-s) \quad (3)$$

where $R^+(r,s,t)$ is a positive-definite, symmetric matrix: $R^+(r,s,t) = (R^+(s,r,t))^T$. $\delta(\cdot)$ is the Dirac delta function and I is the identity matrix.

3. Necessary Conditions of Optimality

The problem of smoothing can be reformulated as an unconstrained minimization problem. The performance index becomes

$$\begin{aligned}
 L = & \int_0^T \langle u(t), R(t) u(t) \rangle dt + \int_0^T \langle y - h, Q(t)(y - h) \rangle dt \\
 & + \int_0^T \left\{ \int_0^1 \int_0^1 \langle v(r,t), R(r,s,t) v(s,t) \rangle dr ds \right\} dt \\
 & + \int_0^T \langle v_0(t), R_0(t) v_0(t) \rangle dt + \int_0^T \langle v_1(t), R_1(t) v_1(t) \rangle dt \\
 & + \int_0^T \langle -\lambda(t), \dot{x} - f - u \rangle dt \\
 & + \int_0^T \left\{ \int_0^1 \langle -\sigma(r,t), z_t(r,t) - g(r,t,z,z_r,z_{rr},x) - v(r,t) \rangle dr \right\} dt \\
 & + \int_0^T \langle \mu_0(t), b_0(t,x,z,z_r) + v_0(t) \rangle dt \\
 & + \int_0^T \langle \mu_1(t), b_1(t,x,z,z_r) + v_1(t) \rangle dt \tag{4}
 \end{aligned}$$

The $u(t)$, $v(r,t)$, $v_0(t)$ and $v_1(t)$ are the control vectors, whereas the $\lambda(t)$, $\sigma(r,t)$, $\mu_0(t)$ and $\mu_1(t)$ are the vector Lagrange multipliers.

We assume that the inverses of $b_{0z_r}^T$ and $b_{1z_r}^T$ (denoted by $b_{0z_r}^{-1}$ and $b_{1z_r}^{-1}$) exist when they are square matrices. If not square, $b_{0z_r}^{-1}$ and $b_{1z_r}^{-1}$ are to be interpreted as the left pseudo inverses

$$b_{0z_r}^{-1} = (b_{0z_r} \quad b_{0z_r}^T)^{-1} b_{0z_r}$$

$$b_{1z_r}^{-1} = (b_{1z_r} \quad b_{1z_r}^T)^{-1} b_{1z_r} \quad (5)$$

The necessary conditions for optimality, obtained from the vanishing of the first variation of L (see Appendix IV-B) assume the form of a two-point boundary value problem and are

$$\hat{x}_t(t/T) = \hat{f} - \frac{1}{2} R^{-1}(t) \hat{\lambda}(t/T) \quad (6)$$

$$\hat{z}_t(r, t/T) = \hat{g} - \frac{1}{2} \int_0^1 R^+(r, s, t) \hat{\sigma}(s, t/T) ds \quad (7)$$

$$\begin{aligned} \hat{\lambda}_t(t/T) = & 2\hat{h}_x^T Q(t)(y - \hat{h}) - \hat{f}_x^T \hat{\lambda}(t/T) - \hat{b}_{0x}^T \hat{\mu}_0(t/T) \\ & - \hat{b}_{1x}^T \hat{\mu}_1(t/T) - \int_0^1 \hat{g}_x^T \hat{\sigma}(s, t/T) ds \end{aligned} \quad (8)$$

$$\begin{aligned} \hat{\sigma}_t(r, t/T) = & 2 \sum_{i=1}^{\gamma} \hat{h}_{z_i}^T(r_i^*, t/T) Q(t)(y - \hat{h}) \delta(r - r_i^*) \\ & - \sum_{i=1}^{\beta} \hat{f}_{z_i}^T(r_i, t/T) \hat{\lambda}(t/T) \delta(r - r_i) - \hat{g}_{z_r}^T(r, t/T) \hat{\sigma}(r, t/T) \\ & + (\hat{g}_{z_r}^T \hat{\sigma})_r - (\hat{g}_{z_{rr}}^T \hat{\sigma})_{rr} \end{aligned} \quad (9)$$

$$\hat{b}_0 - \frac{1}{2} R_0^{-1}(t) \hat{\mu}_0(t/T) = 0 \quad r = 0 \quad (10)$$

$$\hat{b}_1 - \frac{1}{2} R_1^{-1}(t) \hat{\mu}_1(t/T) = 0 \quad r = 1 \quad (11)$$

$$\hat{\lambda}(0/T) = \hat{\lambda}(T/T) = 0 \quad (12)$$

$$\hat{\sigma}(r, 0/T) = \hat{\sigma}(r, T/T) = 0 \quad (13)$$

$$\hat{\mu}_0(t/T) = \hat{b}_{0z_r}^{-1} \hat{g}_{z_{rr}}^T \hat{\sigma} \quad r = 0 \quad (14)$$

$$\hat{\mu}_1(t/T) = -\hat{b}_{1z_r}^{-1} \hat{g}_{z_{rr}}^T \hat{\sigma} \quad r = 1 \quad (15)$$

$$\hat{b}_{0z}^T \hat{b}_{0z_r}^{-1} \hat{g}_{z_{rr}}^T \hat{\sigma} - \hat{g}_{z_r}^T \hat{\sigma} + (\hat{g}_{z_{rr}}^T \hat{\sigma})_r = 0 \quad r = 0 \quad (16)$$

$$\hat{b}_{1z}^T \hat{b}_{1z_r}^{-1} \hat{g}_{z_{rr}}^T \hat{\sigma} - \hat{g}_{z_r}^T \hat{\sigma} + (\hat{g}_{z_{rr}}^T \hat{\sigma})_r = 0 \quad r = 1 \quad (17)$$

4. Differential Sensitivities

Expressing the solutions $\hat{x}(t/T)$ and $\hat{z}(r,t/T)$ in terms of the Lagrange multipliers by

$$\begin{aligned} \hat{x}(t/T) &= x[\hat{\lambda}(t/T), \hat{\sigma}(s,t/T)] \\ \hat{z}(r,t/T) &= z[r, \hat{\lambda}(t/T), \hat{\sigma}(s,t/T)] \end{aligned} \quad s \in [0,1] \quad (18)$$

we define the first order differential sensitivity matrices P^{XX} , P^{XZ} , P^{ZX} and P^{ZZ} by

$$\begin{aligned} P^{XX}(t/T) &= -2 \frac{\partial \hat{x}(t/T)}{\partial \hat{\lambda}(t/T)} \\ P^{XZ}(s,t/T) &= -2 \frac{\delta \hat{x}(t/T)}{\delta \hat{\sigma}(s,t/T)} \\ P^{ZX}(r,t/T) &= -2 \frac{\partial \hat{z}(r,t/T)}{\partial \hat{\lambda}(t/T)} \\ P^{ZZ}(r,s,t/T) &= -2 \frac{\delta \hat{z}(r,t/T)}{\delta \hat{\sigma}(s,t/T)} \end{aligned} \quad (19)$$

Then, using the chain rule of calculus, the partial derivatives of \hat{x} , \hat{z} , \hat{z}_r and \hat{z}_{rr} with respect to T can be expressed as

$$\hat{x}_T(t/T) = -\frac{1}{2} \left\{ P^{XX}(t/T) \hat{\lambda}_T(t/T) + \int_0^1 P^{XZ}(s,t/T) \hat{\sigma}_T(s,t/T) ds \right\} \quad (20)$$

$$\hat{z}_T(r,t/T) = -\frac{1}{2} \left\{ \int_0^1 P^{ZZ}(r,s,t/T) \hat{\sigma}_T(s,t/T) ds + P^{ZX}(r,t/T) \hat{\lambda}_T(t/T) \right\} \quad (21)$$

$$\hat{z}_{rT}(r,t/T) = -\frac{1}{2} \left\{ \int_0^1 P_r^{ZZ}(r,s,t/T) \hat{\sigma}_T(s,t/T) ds + P_r^{ZX}(r,t/T) \hat{\lambda}_T(t/T) \right\} \quad (22)$$

$$\hat{z}_{rrT}(r,t/T) = -\frac{1}{2} \left\{ \int_0^1 P_{rr}^{ZZ}(r,s,t/T) \hat{\sigma}_T(s,t/T) ds + P_{rr}^{ZX}(r,t/T) \hat{\lambda}_T(t/T) \right\} \quad (23)$$

5. Decomposition of the Filtering Process

We merely restate here (46) and (48) of Chapter III

$$\frac{d\hat{q}(T/T)}{dT} = \hat{q}_t(T/T) + \hat{q}_T(T/T) \quad (24)$$

$$\frac{\partial \hat{q}(r,s,T/T)}{\partial T} = \hat{q}_t(r,s,T/T) + \hat{q}_T(r,s,T/T) \quad (25)$$

6. State Filter Equations

We want to derive the dynamical equations which govern $\frac{d\hat{x}(T/T)}{dT}$ and $\frac{\partial \hat{z}(r,T/T)}{\partial T}$. Using (24) and (25), these can be expressed as

$$\frac{d\hat{x}(T/T)}{dT} = \hat{x}_t(T/T) + \hat{x}_T(T/T)$$

$$\frac{\partial \hat{z}(r, T/T)}{\partial T} = \hat{z}_t(r, T/T) + \hat{z}_T(r, T/T) \quad (26)$$

Equations (12) and (13) imply that

$$\begin{aligned} \frac{d\hat{\lambda}(T/T)}{dT} &= 0 \\ \frac{\partial \hat{\sigma}(s, T/T)}{\partial T} &= 0 \end{aligned} \quad (27)$$

Using (24) and (25), (27) can be rewritten as

$$\begin{aligned} \hat{\lambda}_T(T/T) + \hat{\lambda}_t(T/T) &= 0 \\ \hat{\sigma}_T(s, T/T) + \hat{\sigma}_t(s, T/T) &= 0 \end{aligned} \quad (28)$$

Then, (8), (9), (12)-(15) and (28) give

$$\begin{aligned} \hat{\lambda}_T(T/T) &= -2\hat{h}_x^T Q(T)(y - \hat{h}) \\ \hat{\sigma}_T(s, T/T) &= -2 \sum_{i=1}^Y \hat{h}_z^T(r_i^*, T/T) Q(T)(y - \hat{h}) \delta(s - r_i^*) \end{aligned} \quad (29)$$

Substituting (29) into (20) and (21), we obtain

$$\hat{x}_T(T/T) = P^{XX}(T/T)\hat{h}_x^T Q(T)(y - \hat{h}) + \sum_{i=1}^Y P^{XZ}(r_i^*, T/T)\hat{h}_z^T(r_i^*, T/T) Q(T)(y - \hat{h}) \quad (30)$$

$$\begin{aligned} \hat{z}_T(r, T/T) &= \sum_{i=1}^Y P^{ZZ}(r, r_i^*, T/T)\hat{h}_z^T(r_i^*, T/T) Q(T)(y - \hat{h}) + P^{ZX}(r, T/T) \\ &\quad \times \hat{h}_x^T Q(T)(y - \hat{h}) \end{aligned} \quad (31)$$

On the other hand, (6), (7), (12), (13) give

$$\hat{x}_t(T/T) = \hat{f} \quad (32)$$

$$\hat{z}_t(r, T/T) = \hat{g} \quad (33)$$

Hence, (26), (30)-(33) constitute the state filter equations. The boundary conditions are obtained by setting $t = T$ in (10)-(15) and are

$$\begin{aligned} b_0(T, \hat{x}, \hat{z}, \hat{z}_r) &= 0 \\ b_1(T, \hat{x}, \hat{z}, \hat{z}_r) &= 0 \end{aligned} \quad (34)$$

7. Dynamical Equations for the Differential Sensitivities

We need to derive the dynamical equations which govern $P_t^{XX}(T/T)$, $P_t^{XZ}(s, T/T)$, $P_t^{ZX}(r, T/T)$ and $P_t^{ZZ}(r, s, T/T)$. We shall derive two expressions for each of the quantities

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{x}_T(t/T)] \\ \frac{\partial}{\partial t} [\hat{z}_T(r, t/T)] \end{aligned} \quad (35)$$

and equate the two expressions for each of the quantities and set $t = T$. Since each of the quantities above is a continuous function of t and T , we can write

$$\frac{\partial}{\partial t} [\hat{x}_T(t/T)] = \frac{\partial}{\partial T} [\hat{x}_t(t/T)] \quad (36)$$

$$\frac{\partial}{\partial t} [\hat{z}_T(r, t/T)] = \frac{\partial}{\partial T} [\hat{z}_t(r, t/T)] \quad (37)$$

7.1 Derivation of two expressions for $\frac{\partial}{\partial t} [\hat{x}_T(t/T)]$

Substituting (6) in the right hand side of (36) gives

$$\begin{aligned}
 \frac{\partial}{\partial t} [\hat{x}_T(t/T)] &= \frac{\partial}{\partial T} [\hat{f} - \frac{1}{2} R^{-1}(t) \hat{\lambda}(t/T)] \\
 &= \hat{f}_x \hat{x}_T(t/T) + \sum_{i=1}^{\beta} \hat{f}_z(r_i, t/T) \hat{z}_T(r_i, t/T) - \frac{1}{2} R^{-1}(t) \hat{\lambda}_T(t/T) \\
 &= \hat{f}_x \hat{x}_T(t/T) + \int_0^1 \left(\sum_{i=1}^{\beta} \hat{f}_z(r_i, t/T) \delta(r-r_i) \right) \hat{z}_T(r, t/T) dr \\
 &\quad - \frac{1}{2} R^{-1}(t) \hat{\lambda}_T(t/T) \tag{38}
 \end{aligned}$$

which, with the help of (20)-(21), can be rewritten as

$$\begin{aligned}
 \frac{\partial}{\partial t} [\hat{x}_T(t/T)] &= - \frac{1}{2} [\hat{f}_x P^{xx}(t/T) + \sum_{i=1}^{\beta} \hat{f}_z(r_i, t/T) P^{zx}(r_i, t/T) \\
 &\quad + R^{-1}(t)] \hat{\lambda}_T(t/T) \\
 &\quad - \frac{1}{2} \left[\int_0^1 \left(\sum_{i=1}^{\beta} \hat{f}_z(r_i, t/T) P^{zz}(r_i, s, t/T) + \hat{f}_x P^{xz}(s, t/T) \right) \hat{\sigma}_T(s, t/T) ds \right] \tag{39}
 \end{aligned}$$

On the other hand, we can write using (20),

$$\begin{aligned}
 \frac{\partial}{\partial t} [\hat{x}_T(t/T)] &= - \frac{1}{2} \frac{\partial}{\partial t} [P^{xx}(t/T) \hat{\lambda}_T(t/T) + \int_0^1 P^{xz}(s, t/T) \hat{\sigma}_T(s, t/T) ds] \\
 &= - \frac{1}{2} [P_t^{xx}(t/T) \hat{\lambda}_T(t/T) + \int_0^1 P_t^{xz}(s, t/T) \hat{\sigma}_T(s, t/T) ds] \\
 &\quad - \frac{1}{2} [P^{xx}(t/T) \frac{\partial}{\partial t} [\hat{\lambda}_T(t/T)] + \int_0^1 P^{xz}(s, t/T) \frac{\partial}{\partial t} [\hat{\sigma}_T(s, t/T)] ds] \tag{40}
 \end{aligned}$$

7.2 Derivation of two expressions for $\frac{\partial}{\partial t} [\hat{z}_T(r, t/T)]$

Substituting (7) in the right hand side of (37) gives

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{z}_T(r, t/T)] &= \frac{\partial}{\partial T} \left[\hat{g} - \frac{1}{2} \int_0^1 R^+(r, s, t) \hat{\sigma}(s, t/T) ds \right] \\ &= \hat{g}_z(r) \hat{z}_T(r, t/T) + \hat{g}_{z_r}(r) \hat{z}_{r_T}(r, t/T) \\ &\quad + \hat{g}_{z_{rr}}(r) \hat{z}_{rr_T}(r, t/T) + \hat{g}_x \hat{x}_T(t/T) - \frac{1}{2} \int_0^1 R^+(r, s, t) \hat{\sigma}_T(s, t/T) ds \end{aligned} \quad (41)$$

where $\hat{g}(r)$ denotes $g(r, t, \hat{z}, \hat{z}_r, \hat{z}_{rr}, \hat{x})$. Using (20)-(23) we can rewrite (41) as

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{z}_T(r, t/T)] &= - \frac{1}{2} [\hat{g}_z(r) P^{ZX}(r, t/T) + \hat{g}_{z_r}(r) P_r^{ZX}(r, t/T) + \hat{g}_{z_{rr}}(r) P_{rr}^{ZX}(r, t/T) \\ &\quad + \hat{g}_x P^{XX}(t/T)] \hat{\lambda}_T(t/T) \\ &\quad - \frac{1}{2} \left[\int_0^1 (\hat{g}_z(r) P^{ZZ}(r, s, t/T) + \hat{g}_{z_r}(r) P_r^{ZZ}(r, s, t/T) \right. \\ &\quad \left. + \hat{g}_{z_{rr}}(r) P_{rr}^{ZZ}(r, s, t/T) + \hat{g}_x P^{XZ}(s, t/T) \right. \\ &\quad \left. + R^+(r, s, t) \hat{\sigma}_T(s, t/T) ds \right] \end{aligned} \quad (42)$$

On the other hand, using (21), we can write

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{z}_T(r, t/T)] &= - \frac{1}{2} \frac{\partial}{\partial t} \left[\int_0^1 P^{ZZ}(r, s, t/T) \hat{\sigma}_T(s, t/T) ds + P^{ZX}(r, t/T) \hat{\lambda}_T(t/T) \right] \end{aligned}$$

$$\begin{aligned}
 &= -\frac{1}{2} \left[\int_0^1 p_t^{ZZ}(r,s,t/T) \hat{\sigma}_T(s,t/T) ds + p_t^{ZX}(r,t/T) \hat{\lambda}_T(t/T) \right] \\
 &\quad - \frac{1}{2} \left[\int_0^1 p_t^{ZZ}(r,s,t/T) \frac{\partial}{\partial t} [\hat{\sigma}_T(s,t/T)] ds + p_t^{ZX}(r,t/T) \frac{\partial}{\partial t} [\hat{\lambda}_T(t/T)] \right]
 \end{aligned}
 \tag{43}$$

7.3 The equations for $p_t^{XX}(T/T), \dots, p_t^{ZX}(r,T/T)$

Bearing in mind that $\hat{\lambda}$ and $\hat{\sigma}$ are being considered as independent vector Lagrange multipliers in our formulation of (18), we first equate (39) and (40) and set $t = T$. For equality to hold, the coefficients of $\hat{\lambda}_T(t/T), \hat{\sigma}_T(s,t/T), \hat{\sigma}_T(1,t/T)$ and $\hat{\sigma}_T(0,t/T)$ must identically be zero at $t = T$. The last two terms of (40) are evaluated in Appendix IV-A. We obtain

$$\begin{aligned}
 p_t^{XX}(T/T) &= \hat{f}_x P^{XX}(T/T) + P^{XX}(T/T) \hat{f}_x^T \\
 &+ \sum_{i=1}^{\beta} \hat{f}_z(r_i, T/T) P^{ZX}(r_i, T/T) + \sum_{i=1}^{\beta} P^{XZ}(r_i, T/T) \hat{f}_z^T(r_i, T/T) \\
 &+ P^{XX}(T/T) V^{XX}(T/T) P^{XX}(T/T) \\
 &+ \sum_{i=1}^{\gamma} P^{XX}(T/T) V^{Xi}(T/T) P^{ZX}(r_i^*, T/T) \\
 &+ \sum_{i=1}^{\gamma} P^{XZ}(r_i^*, T/T) V^{iX}(T/T) P^{XX}(T/T) \\
 &+ \sum_{i=1}^{\gamma} \sum_{j=1}^{\gamma} P^{XZ}(r_i^*, T/T) V^{ij}(T/T) P^{ZX}(r_j^*, T/T) \\
 &+ R^{-1}(t)
 \end{aligned}
 \tag{44}$$

$$\begin{aligned}
 P_t^{XZ}(s, T/T) &= \hat{f}_X P^{XZ}(s, T/T) + P^{XX}(T/T) \hat{g}_X^T + P^{XZ}(s, T/T) \hat{g}_Z^T(s) \\
 &+ P_s^{XZ}(s, T/T) \hat{g}_{Z_s}^T(s) + P_{ss}^{XZ}(s, T/T) \hat{g}_{Z_{ss}}^T(s) \\
 &+ \sum_{i=1}^{\beta} \hat{f}_Z(r_i, T/T) P^{ZZ}(r_i, s, T/T) \\
 &+ P^{XX}(T/T) V^{XX}(T/T) P^{XZ}(s, T/T) \\
 &+ \sum_{i=1}^{\gamma} P^{XX}(T/T) V^{Xi}(T/T) P^{ZZ}(r_i^*, s, T/T) \\
 &+ \sum_{i=1}^{\gamma} P^{XZ}(r_i^*, T/T) V^{iX}(T/T) P^{XZ}(s, T/T) \\
 &+ \sum_{i=1}^{\gamma} \sum_{j=1}^{\gamma} P^{XZ}(r_i^*, T/T) V^{ij}(T/T) P^{ZZ}(r_j^*, s, T/T) \quad (45)
 \end{aligned}$$

$$P^{XZ}(s, T/T) \hat{b}_{1_z}^T + P_s^{XZ}(s, T/T) \hat{b}_{1_{z_s}}^T + P^{XX}(T/T) \hat{b}_{1_x}^T = 0 \quad s = 1 \quad (46)$$

$$P^{XZ}(s, T/T) \hat{b}_{0_z}^T + P_s^{XZ}(s, T/T) \hat{b}_{0_{z_s}}^T + P^{XX}(T/T) \hat{b}_{0_x}^T = 0 \quad s = 0 \quad (47)$$

Similarly, equating (42) and (43) gives

$$\begin{aligned}
 P_t^{ZZ}(r, s, T/T) &= \hat{g}_Z(r) P^{ZZ}(r, s, T/T) + \hat{g}_{Z_r}(r) P_r^{ZZ}(r, s, T/T) \\
 &+ \hat{g}_{Z_{rr}}(r) P_{rr}^{ZZ}(r, s, T/T) + \hat{g}_X(r) P^{XZ}(s, T/T) \\
 &+ P^{ZZ}(r, s, T/T) \hat{g}_Z^T(s) + P_s^{ZZ}(r, s, T/T) \hat{g}_{Z_s}^T(s) \\
 &+ P_{ss}^{ZZ}(r, s, T/T) \hat{g}_{Z_{ss}}^T(s) + P^{ZX}(r, T/T) \hat{g}_X^T(s)
 \end{aligned}$$

$$\begin{aligned}
 & + P^{ZX}(r, T/T) V^{XX}(T/T) P^{XZ}(s, T/T) \\
 & + \sum_{i=1}^Y P^{ZX}(r, T/T) V^{Xi}(T/T) P^{ZZ}(r_i^*, s, T/T) \\
 & + \sum_{i=1}^Y P^{ZZ}(r, r_i^*, T/T) V^{iX}(T/T) P^{XZ}(s, T/T) \\
 & + \sum_{i=1}^Y \sum_{j=1}^Y P^{ZZ}(r, r_i^*, T/T) V^{ij}(T/T) P^{ZZ}(r_j^*, s, T/T) \\
 & + R^+(r, s, t)
 \end{aligned} \tag{48}$$

$$\begin{aligned}
 P_t^{ZX}(r, T/T) & = P^{ZX}(r, T/T) \hat{f}_x^T + \hat{g}_x P^{XX}(T/T) + \hat{g}_z(r) P^{ZX}(r, T/T) \\
 & + \hat{g}_{z_r}(r) P_r^{ZX}(r, T/T) + \hat{g}_{z_{rr}}(r) P_{rr}^{ZX}(r, T/T) \\
 & + \sum_{i=1}^{\beta} P^{ZZ}(r, r_i, T/T) \hat{f}_z^T(r_i, T/T) \\
 & + P^{ZX}(r, T/T) V^{XX}(T/T) P^{XX}(T/T) \\
 & + \sum_{i=1}^Y P^{ZZ}(r, r_i^*, T/T) V^{iX}(T/T) P^{XX}(T/T) \\
 & + \sum_{i=1}^Y P^{ZX}(r, T/T) V^{Xi}(T/T) P^{ZX}(r_i^*, T/T) \\
 & + \sum_{i=1}^Y \sum_{j=1}^Y P^{ZZ}(r, r_i^*, T/T) V^{ij}(T/T) P^{ZX}(r_j^*, T/T)
 \end{aligned} \tag{49}$$

$$P^{ZZ}(r, s, T/T) \hat{b}_{z_s}^T + P_s^{ZZ}(r, s, T/T) \hat{b}_{z_s}^T + P^{ZX}(r, T/T) \hat{b}_x^T = 0 \quad s = 1 \tag{50}$$

$$P^{ZZ}(r, s, T/T) \hat{b}_{o_z}^T + P_s^{ZZ}(r, s, T/T) \hat{b}_{o_z}^T + P^{ZX}(r, T/T) \hat{b}_{o_x}^T = 0 \quad s = 0 \tag{51}$$

We proceed to determine the $r = 0$ and $r = 1$ boundary conditions for (44), (45), (48) and (49). For $r = 0$, combine (10) and

$$\hat{b}_{1z} p^{zx}(r, T/T) + \hat{b}_{1z_r} p_r^{zx}(r, T/T) + \hat{b}_{1x} p^{xx}(T/T) = 0 \quad (57)$$

$$\begin{aligned} \hat{b}_{1z} p^{zz}(r, s, T/T) + \hat{b}_{1z_r} p_r^{zz}(r, s, T/T) + \hat{b}_{1x} p^{xz}(s, T/T) & \quad r = 1 \\ - R_1^{-1}(T) \hat{b}_{1z_r}^{-1} \hat{g}_{z_{rr}}^T \delta(s-1) = 0 & \quad (58) \end{aligned}$$

By simple inspection, one can observe that the following symmetrical properties hold for the sensitivity matrices

$$\begin{aligned} p^{xx}(T/T) &= p^{xx}(T/T)^T \\ p^{xz}(r, T/T) &= p^{zx}(r, T/T)^T \\ p^{zz}(r, s, T/T) &= p^{zz}(s, r, T/T)^T \end{aligned} \quad (59)$$

Finally, we note that the boundary conditions (50) and (51) hold only for the open interval $r \in (0, 1)$. To include the end points $r = 0$ and $r = 1$, we (by inspecting (56) and (58)) replace (50) and (51) by

$$\begin{aligned} p^{zz}(r, s, T/T) \hat{b}_{1z}^T + p_s^{zz}(r, s, T/T) \hat{b}_{1z_s}^T + p^{zx}(r, T/T) \hat{b}_{1x}^T \\ - (R_1^{-1}(T) \hat{b}_{1z_s}^{-1} \hat{g}_{z_{ss}}^T)^T \delta(r-1) = 0 \quad s = 1 \end{aligned} \quad (60)$$

$$\begin{aligned} p^{zz}(r, s, T/T) \hat{b}_{0z}^T + p_s^{zz}(r, s, T/T) \hat{b}_{0z_s}^T + p^{zx}(r, T/T) \hat{b}_{1x}^T \\ + (R_0^{-1}(T) \hat{b}_{0z_s}^{-1} \hat{g}_{z_{ss}}^T)^T \delta(r) = 0 \quad s = 0 \end{aligned} \quad (61)$$

The entire filter is summarized in Table 1. In the column of initial conditions, $\hat{x}(0/0)$ and $\hat{z}(r,0/0)$ represent our best initial guesses of $x(0)$ and $z(r,0)$. The initial conditions $P^{XX}(0/0)$, $P^{XZ}(s,0/0)$, $P^{ZX}(r,0/0)$ and $P^{ZZ}(r,s,0/0)$ are basically arbitrary.

Table 1. Optimal Filter for System (1)

	Equations	Initial Conditions	Boundary Conditions
<u>Estimates</u>			
$\hat{x}(T/T)$	(26),(30),(32)	$\hat{x}(0/0)$	None
$\hat{z}(r,T/T)$	(26),(31),(33)	$\hat{z}(r,0/0)$	(34)
<u>First Order Differential Sensitivities</u>			
$P^{XX}(T/T)$	(44)	$P^{XX}(0/0)$	None
$P^{XZ}(s,T/T)$	(45)	$P^{XZ}(s,0/0)$	(46),(47)
$P^{ZX}(r,T/T)$	(49)	$P^{ZX}(r,0/0)$	(55),(57)
$P^{ZZ}(r,s,T/T)$	(48)	$P^{ZZ}(r,s,0/0)$	(56),(58) (60),(61)

In the linear white noise case, it can be shown that

$$P^{XX}(T/T) = E[(x(T) - \hat{x}(T/T))(x(T) - \hat{x}(T/T))^T]$$

$$P^{XZ}(r,T/T) = E[(x(T) - \hat{x}(T/T))(z(r,T) - \hat{z}(r,T/T))^T]$$

$$P^{ZX}(r,T/T) = E[(z(r,T) - \hat{z}(r,T/T))(x(T) - \hat{x}(T/T))^T]$$

$$P^{ZZ}(r,s,T/T) = E[(z(r,T) - \hat{z}(r,T/T))(z(s,T) - \hat{z}(s,T/T))^T]$$

This may be used as a guide for choosing $P^{XX}(0/0), \dots, P^{ZX}(r,0/0)$.

When solving the sensitivity equations, one can eliminate either (45)

or (49) by using properties (59).

If $b_{0z_r} = 0$, then we should replace $\hat{b}_{0z_r}^{-1}$ by \hat{b}_{0z}^{-1} and $\delta(s)$ by $\frac{d}{ds} \delta(s)$ in (56), $\hat{b}_{0z_s}^{-1}$ by \hat{b}_{0z}^{-1} and $\delta(r)$ by $\frac{d}{dr} \delta(r)$ in (61). If $b_{1z_r} = 0$, then we should replace $\hat{b}_{1z_r}^{-1}$ by \hat{b}_{1z}^{-1} and $\delta(s-1)$ by $\frac{d}{ds} \delta(s-1)$ in (58), $\hat{b}_{1z_s}^{-1}$ by \hat{b}_{1z}^{-1} and $\delta(r-1)$ by $\frac{d}{dr} \delta(r-1)$ in (60).

Appendix IV-A

We first consider the quantity

$$P \frac{\partial}{\partial t} [\hat{\lambda}(t/T)] \quad (A.1)$$

where P can either be $P^{XX}(t/T)$ or $P^{ZX}(r,t/T)$. Let us define the vector

$$V^X(t/T) = \hat{h}_X^T Q(t)(y - \hat{h}) \quad (A.2)$$

and the matrices

$$V^{XX}(t/T) = [\hat{h}_X^T Q(t)(y - \hat{h})]_X \quad (A.3)$$

$$V^{Xi}(t/T) = [\hat{h}_X^T Q(t)(y - \hat{h})]_{Z(r_i^*, t/T)} \quad i = 1, \dots, \gamma \quad (A.4)$$

Using (8), (A.1) can be expressed as

$$\begin{aligned} P \frac{\partial}{\partial t} [\hat{\lambda}_T(t/T)] &= P \frac{\partial}{\partial T} [\hat{\lambda}_t(t/T)] \\ &= P \frac{\partial}{\partial T} [2\hat{h}_X^T Q(t)(y - \hat{h}) - \hat{f}_X^T \hat{\lambda}(t/T) - \hat{b}_{0X}^T \hat{\mu}_0(t/T) \\ &\quad - \hat{b}_{1X}^T \hat{\mu}_1(t/T) - \int_0^1 \hat{g}_X^T \hat{\sigma}(s, t/T) ds] \\ &= P 2V^{XX}(t/T) \hat{x}_T(t/T) + P 2 \sum_{i=1}^{\gamma} V^{Xi}(t/T) \hat{z}_T(r_i^*, t/T) \\ &\quad - P \hat{f}_X^T \hat{\lambda}_T(t/T) - P \hat{b}_{0X}^T \hat{\mu}_{0T}(t/T) - P \hat{b}_{1X}^T \hat{\mu}_{1T}(t/T) \end{aligned}$$

$$\begin{aligned}
 & - P(\hat{f}_x^T)_T \hat{\lambda}(t/T) - P(\hat{b}_{0x}^T)_T \hat{\mu}_0(t/T) - P(\hat{b}_{1x}^T)_T \hat{\mu}_1(t/T) \\
 & - \int_0^1 P \hat{g}_x^T \hat{\sigma}_T(s, t/T) ds - \int_0^1 P(\hat{g}_x^T)_T \hat{\sigma}(s, t/T) ds
 \end{aligned} \tag{A.5}$$

Note that from (12)-(14) we have $\hat{\lambda}(T/T) = 0$, $\hat{\sigma}(r, T/T) = 0$, $\hat{\mu}_0(T/T) = 0$ and $\hat{\mu}_1(T/T) = 0$. Hence, some of the terms in (A.5) will not contribute to the final equations governing $P_t^{XX}(T/T), \dots, P_t^{ZX}(r, T/T)$. Neglecting these terms and using (14) and (15), we can rewrite (A.5) as

$$\begin{aligned}
 P \frac{\partial}{\partial t} [\hat{\lambda}_T(t/T)] &= P 2V^{XX}(t/T) \hat{x}_T(t/T) \\
 &+ P 2 \int_0^1 \left(\sum_{i=1}^Y V^{Xi}(t/T) \delta(r - r_i^*) \right) \hat{z}_T(r, t/T) dr \\
 &- P \hat{f}_x^T \hat{\lambda}_T(t/T) - P \hat{b}_{0x}^T \hat{b}_{0z_r}^{-1} \hat{g}_{z_{rr}}^T \hat{\sigma}_T(0, t/T) \\
 &+ P \hat{b}_{1x}^T \hat{b}_{1z_r}^{-1} \hat{g}_{z_{rr}}^T \hat{\sigma}_T(1, t/T) \\
 &+ \int_0^1 P \hat{g}_x^T \hat{\sigma}_T(s, t/T) ds
 \end{aligned} \tag{A.6}$$

Inserting (20) and (21) into (A.6) gives

$$\begin{aligned}
 P \frac{\partial}{\partial t} [\hat{\lambda}_T(t/T)] &= -[P V^{XX}(t/T) P^{XX}(t/T) + \sum_{i=1}^Y P V^{Xi}(t/T) P^{ZX}(r_i^*, t/T)] \hat{\lambda}_T(t/T) \\
 &- \int_0^1 [P V^{XX}(t/T) P^{XZ}(s, t/T) + \sum_{i=1}^Y P V^{Xi}(t/T) P^{ZZ}(r_i^*, s, t/T) \\
 &\quad + P \hat{g}_x^T] \hat{\sigma}_T(s, t/T) ds
 \end{aligned}$$

$$\begin{aligned}
 - P \hat{f}_x^T \hat{\lambda}_T(t/T) - P \hat{b}_0^T \hat{b}_0^{-1} \hat{g}_{z_{rr}}^T \hat{\sigma}_T(0, t/T) \\
 + P \hat{b}_1^T \hat{b}_1^{-1} \hat{g}_{z_{rr}}^T \hat{\sigma}_T(1, t/T)
 \end{aligned} \tag{A.7}$$

We now consider the quantity

$$\int_0^1 P(s) \frac{\partial}{\partial t} [\hat{\sigma}_T(s, t/T)] ds \tag{A.8}$$

where $P(s)$ can either be $P^{xz}(s, t/T)$ or $P^{zz}(r, s, t/T)$.

Let us define the vector

$$V^i(t/T) = \hat{h}_{z(r_i^*, t/T)}^T Q(t)(y - \hat{h}) \tag{A.9}$$

and the matrices

$$V^{ix}(t/T) = [\hat{h}_{z(r_i^*, t/T)}^T Q(t)(y - \hat{h})]_x \tag{A.10}$$

$$V^{ij}(t/T) = [\hat{h}_{z(r_i^*, t/T)}^T Q(t)(y - \hat{h})]_{z(r_j^*, t/T)} \tag{A.11}$$

Using (9), (A.8) can be expressed as

$$\begin{aligned}
 & \int_0^1 P(s) \frac{\partial}{\partial t} [\hat{\sigma}_T(s, t/T)] ds = \int_0^1 P(s) \frac{\partial}{\partial T} [\hat{\sigma}_t(s, t/T)] ds \\
 & = \int_0^1 P(s) \frac{\partial}{\partial T} \left[2 \sum_{i=1}^{\gamma} \hat{h}_{z(r_i^*, t/T)}^T Q(t)(y - \hat{h}) \delta(s - r_i^*) \right. \\
 & \quad \left. - \sum_{i=1}^{\beta} \hat{f}_{z(r_i, t/T)}^T \hat{\lambda}(t/T) \delta(s - r_i) \right. \\
 & \quad \left. - \hat{g}_z^T \hat{\sigma}(s, t/T) + (\hat{g}_z^T \hat{\sigma})_s - (\hat{g}_{z_{ss}}^T \hat{\sigma})_{ss} \right] ds
 \end{aligned}$$

$$\begin{aligned}
 &= \int_0^1 P(s) \left[2 \sum_{i=1}^Y V^{ix}(t/T) \delta(s - r_i^*) \hat{x}_T(t/T) \right. \\
 &\quad \left. + 2 \sum_{i=1}^Y \sum_{j=1}^Y V^{ij}(t/T) \delta(s - r_i^*) \hat{z}_T(r_j^*, t/T) \right. \\
 &\quad \left. - \sum_{i=1}^{\beta} \hat{f}_z^T(r_i, t/T) \delta(s - r_i) \hat{\lambda}_T(t/T) - \sum_{i=1}^{\beta} (\hat{f}_z^T(r_i, t/T))_T \delta(s - r_i) \hat{\lambda}(t/T) \right] ds \\
 &+ \int_0^1 P(s) (-\hat{g}_z^T \hat{\sigma} + (\hat{g}_{z_s}^T \hat{\sigma})_s - (\hat{g}_{z_{ss}}^T \hat{\sigma})_{ss})_T ds \tag{A.12}
 \end{aligned}$$

The last three terms of (A.12) may be evaluated using integration by parts. Neglecting terms which will not contribute to the final equations governing $P_t^{xx}(T/T), \dots, P_t^{zx}(r, T/T)$ and using (20) and (21), we obtain

$$\begin{aligned}
 &\int_0^1 P(s) \frac{\partial}{\partial t} [\hat{\sigma}_T(s, t/T)] ds \\
 &= - \left[\sum_{i=1}^Y P(r_i^*) V^{ix}(t/T) P^{xx}(t/T) + \sum_{i=1}^Y \sum_{j=1}^Y P(r_i^*) V^{ij}(t/T) P^{zx}(r_j^*, t/T) \right. \\
 &\quad \left. + \sum_{i=1}^{\beta} P(r_i) \hat{f}_z^T(r_i, t/T) \right] \hat{\lambda}_T(t/T) \\
 &- \int_0^1 \left[\sum_{i=1}^Y P(r_i^*) V^{ix}(t/T) P^{xz}(s, t/T) + \sum_{i=1}^Y \sum_{j=1}^Y P(r_i^*) V^{ij}(t/T) P^{zz}(r_j^*, s, t/T) \right. \\
 &\quad \left. + P(s) \hat{g}_z^T + P_s(s) \hat{g}_{z_s}^T + P_{ss}(s) \hat{g}_{z_{ss}}^T \right] \hat{\sigma}(s, t/T) ds \\
 &+ [P(1) \hat{b}_{1_z}^T \hat{b}_{1_{z_s}}^{-1} \hat{g}_{z_{ss}}^T + P_s(1) \hat{g}_{z_{ss}}^T] \hat{\sigma}_T(1, t/T) \\
 &- [P(0) \hat{b}_{0_z}^T \hat{b}_{0_{z_s}}^{-1} \hat{g}_{z_{ss}}^T + P_s(0) \hat{g}_{z_{ss}}^T] \hat{\sigma}_T(0, t/T) \tag{A.13}
 \end{aligned}$$

In (53), (A.5) and (A.12) there are terms which have $\hat{\lambda}(t/T)$, $\hat{\sigma}(s,t/T)$, $\hat{\sigma}(1,t/T)$ or $\hat{\sigma}(0,t/T)$ as coefficient (note that $\hat{\mu}_0(t/T)$ and $\hat{\mu}_1(t/T)$ can be expressed in terms of $\hat{\sigma}(0,t/T)$ and $\hat{\sigma}(1,t/T)$ by (14) and (15)), e.g., the last term of (53). These terms do not contribute to the filter because they vanish at $t = T$. To show this, we consider a matrix \hat{H} which can be expressed as

$$\hat{H} = H[r, t, \hat{x}(t/T), \hat{z}(r, t/T), \hat{z}_r(r, t/T), \hat{z}_{rr}(r, t/T)]$$

Let $\hat{x}(t/T)$ and $\hat{z}(r, t/T)$ be functionals of the Lagrange multipliers as in (18). Let the vector \hat{e} denote either $\hat{\lambda}(t/T)$ or $\hat{\sigma}(r, t/T)$. Hence, $\hat{e} = 0$ at $t = T$. Further, let the operation $\hat{H}\hat{e}$ be defined. Then, there exist matrices \hat{H}_i , $i=1,2$, such that

$$\hat{H}_T \hat{e} = \int_0^1 \hat{H}_1 \hat{\sigma}_T(v, t/T) dv + \hat{H}_2 \hat{\lambda}_T(t/T)$$

and $\hat{H}_1 = \hat{H}_2 = 0$ at $t = T$. (Suppose \hat{H} has p columns and let \hat{h}_i be the column vectors and \hat{e}_i the scalar components such that

$$\hat{H} = [\hat{h}_1, \hat{h}_2, \dots, \hat{h}_p]$$

$$\hat{e}^T = [\hat{e}_1, \hat{e}_2, \dots, \hat{e}_p]$$

then

$$\hat{H}_T \hat{e} = \sum_{i=1}^p \hat{h}_{iT} \hat{e}_i$$

We can express

$$\begin{aligned}
 \hat{h}_{i_T} \hat{e}_i &= \hat{e}_i \left[\hat{h}_{i_x} \frac{\partial \hat{x}(t/T)}{\partial \hat{\lambda}(t/T)} \hat{\lambda}_T(t/T) + \hat{h}_{i_x} \int_0^1 \frac{\partial \hat{x}(t/T)}{\partial \hat{\sigma}(v,t/T)} \hat{\sigma}_T(v,t/T) dv \right. \\
 &+ \hat{h}_{i_z} \frac{\partial \hat{z}(r,t/T)}{\partial \hat{\lambda}(t/T)} \hat{\lambda}_T(t/T) + \hat{h}_{i_z} \int_0^1 \frac{\partial \hat{z}(r,t/T)}{\partial \hat{\sigma}(v,t/T)} \hat{\sigma}_T(v,t/T) dv \\
 &+ \hat{h}_{i_{z_r}} \frac{\partial \hat{z}_r(r,t/T)}{\partial \hat{\lambda}(t/T)} \hat{\lambda}_T(t/T) + \hat{h}_{i_{z_r}} \int_0^1 \frac{\partial \hat{z}_r(r,t/T)}{\partial \hat{\sigma}(v,t/T)} \hat{\sigma}_T(v,t/T) dv \\
 &\left. + \hat{h}_{i_{z_{rr}}} \frac{\partial \hat{z}_{rr}(r,t/T)}{\partial \hat{\lambda}(t/T)} \hat{\lambda}_T(t/T) + \hat{h}_{i_{z_{rr}}} \int_0^1 \frac{\partial \hat{z}_{rr}(r,t/T)}{\partial \hat{\sigma}(v,t/T)} \hat{\sigma}_T(v,t/T) dv \right] \\
 &= \hat{H}_{i2} \hat{\lambda}_T(t/T) + \int_0^1 \hat{H}_{i1} \hat{\sigma}_T(v,t/T) dv
 \end{aligned}$$

where $\hat{H}_{i1} = \hat{H}_{i2} = 0$ at $t = T$. Hence, $\hat{H}_k = \sum_{i=1}^p \hat{H}_{ik}$.

Appendix IV-B

In this appendix we obtain the necessary conditions for optimality corresponding to the minimization of (4). This is achieved by setting the first variation of L^* (denoted by δL) to zero [14]. We emphasize that δL is the total first variation. Suppose L depends functionally on parameters p_i , $i=1,2,\dots,J$, then we can write $\delta L = \sum_{i=1}^J \delta L(p_i)$ where $\delta L(p_i)$ is the first variation of L with respect to a variation of p_i (denoted by δp_i) over the appropriate domain. In this way, we can write

$$\begin{aligned} \delta L = & \delta L(\lambda(t)) + \delta L(\sigma(r,t)) + \delta L(\mu_0(t)) + \delta L(\mu_1(t)) \\ & + \delta L(u(t)) + \delta L(v(r,t)) + \delta L(v(s,t)) + \delta L(v_0(t)) \\ & + \delta L(v_1(t)) + \delta L(x(t)) + \delta L(\dot{x}(t)) + \delta L(z(0,t)) + \delta L(z(1,t)) \\ & + \delta L(z_r(0,t)) + \delta L(z_r(1,t)) + \delta L(z(r,t)) + \delta L(z_t(r,t)) \\ & + \delta L(z_r(r,t)) + \delta L(z_{rr}(r,t)) \end{aligned}$$

We proceed to evaluate various variations.

$$\begin{aligned} \delta L(\lambda(t)) &= \int_0^T \langle -\delta\lambda(t), \dot{x} - f - u \rangle dt \\ \delta L(\sigma(r,t)) &= \int_0^T \int_0^1 \langle -\delta\sigma(r,t), z_t - g - v \rangle dr dt \\ \delta L(\mu_0(t)) &= \int_0^T \langle +\delta\mu_0(t), b_0 + v_0 \rangle dt \end{aligned}$$

$$\delta L(\mu_1(t)) = \int_0^T \langle \delta\mu_1(t), b_1 + v_1 \rangle dt$$

$$\delta L(u(t)) = \int_0^T \langle \delta u(t), 2R(t) u(t) + \lambda(t) \rangle dt$$

$$\delta L(v(r,t)) + \delta L(v(s,t))$$

$$= \int_0^T \left\{ \int_0^1 \int_0^1 \langle \delta v(r,t), 2R(r,s,t) v(s,t) \rangle dr ds + \int_0^1 \langle \delta v(r,t), \sigma(r,t) \rangle dr \right\} dt$$

$$\delta L(v_0(t)) = \int_0^T \langle \delta v_0(t), 2R_0(t) v_0(t) + \mu_0(t) \rangle dt$$

$$\delta L(v_1(t)) = \int_0^T \langle \delta v_1(t), 2R_1(t) v_1(t) + \mu_1(t) \rangle dt$$

$$\delta L(x(t)) = \int_0^T \langle \delta x(t), -2h_x^T Q(t)(y-h) \rangle dt$$

$$+ \int_0^T \langle \delta x(t), f_x^T \lambda(t) \rangle dt + \int_0^T \langle \delta x(t), b_{0x}^T \mu_0(t) + b_{1x}^T \mu_1(t) \rangle dt$$

$$+ \int_0^T \langle \delta x(t), \int_0^1 g_x^T \sigma(s,t) ds \rangle dt$$

$$\delta L(\dot{x}(t)) = \int_0^T \langle -\delta \dot{x}(t), \lambda(t) \rangle dt$$

$$= \langle -\delta x(t), \lambda(t) \rangle \Big|_0^T + \int_0^T \langle \delta x(t), \dot{\lambda}(t) \rangle dt$$

$$\delta L(z(0,t)) = \int_0^T \langle \delta z(0,t), b_{0z}^T \mu_0(t) \rangle dt$$

$$\delta L(z(1,t)) = \int_0^T \langle \delta z(1,t), b_{1z}^T \mu_1(t) \rangle dt$$

$$\delta L(z_r(0,t)) = \int_0^T \langle \delta z_r(0,t), b_{0z_r}^T \mu_0(t) \rangle dt$$

$$\delta L(z_r(1,t)) = \int_0^T \langle \delta z_r(1,t), b_{1z_r}^T \mu_1(t) \rangle dt$$

$$\begin{aligned} \delta L(z(r,t)) = & \int_0^T \left\{ \int_0^1 \langle \delta z(r,t), - \sum_{i=1}^{\gamma} 2h_{z(r_i^*,t)}^T Q(t)(y-h) \delta(r-r_i^*) \rangle dr \right. \\ & + \int_0^1 \langle \delta z(r,t), \sum_{i=1}^{\beta} f_{z(r_i,t)}^T \lambda(t) \delta(r-r_i) \rangle dr \\ & \left. + \int_0^1 \langle \delta z(r,t), g_{z(r,t)}^T \sigma(r,t) \rangle dr \right\} dt \end{aligned}$$

$$\begin{aligned} \delta L(z_t(r,t)) = & \int_0^1 \int_0^T \langle -\delta z_t(r,t), \sigma(r,t) \rangle dt dr \\ = & \int_0^1 \langle -\delta z(r,T), \sigma(r,T) \rangle dr + \int_0^1 \langle +\delta z(r,0), \sigma(r,0) \rangle dr \\ & + \int_0^T \int_0^1 \langle \delta z(r,t), \sigma_t(r,t) \rangle dr dt \end{aligned}$$

$$\begin{aligned} \delta L(z_r(r,t)) = & \int_0^T \int_0^1 \langle \delta z_r(r,t), g_{z_r}^T \sigma(r,t) \rangle dr dt \\ = & \int_0^T \langle \delta z(r,t), g_{z_r}^T \sigma(r,t) \rangle \Big|_{r=0}^{r=1} dt \end{aligned}$$

$$- \int_0^T \int_0^1 \langle \delta z(r,t), (g_{z_r}^T \sigma(r,t))_r \rangle dr dt$$

$$\begin{aligned} \delta L(z_{rr}(r,t)) &= \int_0^T \int_0^1 \langle \delta z_{rr}(r,t), g_{z_{rr}}^T \sigma(r,t) \rangle dr dt \\ &= \int_0^T \langle \delta z_r(r,t), g_{z_{rr}}^T \sigma(r,t) \rangle \Big|_{r=0}^{r=1} dt \\ &\quad - \int_0^T \langle \delta z(r,t), (g_{z_{rr}}^T \sigma(r,t))_r \rangle \Big|_{r=0}^{r=1} dt \\ &\quad + \int_0^T \int_0^1 \langle \delta z(r,t), (g_{z_{rr}}^T \sigma(r,t))_{rr} \rangle dr dt \end{aligned}$$

In order that $\delta L = 0$ for arbitrary δp_i , the coefficient of each of the following δp_i must identically be zero. Let $\phi(\delta p_i)$ denote the coefficient of δp_i , then

$$\phi(\delta \lambda(t)) = 0 \implies \dot{x} = f + u(t)$$

$$\phi(\delta \sigma(r,t)) = 0 \implies z_t = g + v$$

$$\phi(\delta \mu_0(t)) = 0 \implies b_0 + v_0 = 0$$

$$\phi(\delta \mu_1(t)) = 0 \implies b_1 + v_1 = 0$$

$$\phi(\delta u(t)) = 0 \implies u(t) = -\frac{1}{2} R^{-1}(t) \lambda(t)$$

$$\phi(\delta v(r,t)) = 0 \implies v(r,t) = -\frac{1}{2} \int_0^1 R^+(r,s,t) \sigma(s,t) ds$$

$$\phi(\delta v_0(t)) = 0 \implies v_0(t) = -\frac{1}{2} R_0^{-1}(t) \mu_0(t)$$

$$\phi(\delta v_1(t)) = 0 \implies v_1(t) = -\frac{1}{2} R_1^{-1}(t) \mu_1(t)$$

$$\phi(\delta x(t)) = 0 \implies \dot{\lambda}(t) = 2h_x^T Q(t)(y-h) - f_x^T \lambda(t) - b_{0x}^T \mu_0(t) - b_{1x}^T \mu_1(t) - \int_0^1 g_x^T \sigma(s,t) ds$$

$$\begin{aligned} \phi(\delta z(r,t)) = 0 \implies \sigma_t(r,t) &= 2 \sum_{i=1}^Y h_{z(r_i^*,t)}^T Q(t)(y-h) \delta(r-r_i^*) \\ &\quad - \sum_{i=1}^{\beta} f_{z(r_i,t)}^T \lambda(t) \delta(r-r_i) \\ &\quad - g_z^T(r,t) \sigma(r,t) + (g_{z_r}^T \sigma(r,t))_r \\ &\quad - (g_{z_{rr}}^T \sigma(r,t))_{rr} \end{aligned}$$

$$\phi(\delta z(0,t)) = 0 \implies b_{0z}^T \mu_0 - g_{z_r}^T \sigma + (g_{z_{rr}}^T \sigma)_r = 0 \quad r = 0$$

$$\phi(\delta z(1,t)) = 0 \implies b_{1z}^T \mu_1 + g_{z_r}^T \sigma - (g_{z_{rr}}^T \sigma)_r = 0 \quad r = 1$$

$$\phi(\delta z_r(0,t)) = 0 \implies b_{0z_r}^T \mu_0 - g_{z_{rr}}^T \sigma = 0 \quad r = 0$$

$$\phi(\delta z_r(1,t)) = 0 \implies b_{1z_r}^T \mu_1 + g_{z_{rr}}^T \sigma = 0 \quad r = 1$$

$$\phi(\delta x(0)) = 0 \implies \lambda(0) = 0$$

$$\phi(\delta x(T)) = 0 \implies \lambda(T) = 0$$

$$\phi(\delta z(r,0)) = 0 \implies \sigma(r,0) = 0$$

$$\phi(\delta z(r,T)) = 0 \implies \sigma(r,T) = 0$$

Chapter V

OBSERVABILITY AND OPTIMAL MEASUREMENT LOCATION IN LINEAR DISTRIBUTED PARAMETER SYSTEMS

1. Introduction

In this chapter we develop the concepts of observability and filter convergence for a class of stochastic linear distributed parameter systems whose solutions can be expressed as eigenfunction expansions. Since observations of a distributed system can, in principle, be placed anywhere in the spatial domain of the system, an important related question is the effect of the measurement locations on observability. Also, it is appropriate to ask what are the measurement locations that lead to the best estimates of the state of the system. These two questions are both addressed in this study.

2. System Description

Consider the class of stochastic, linear, distributed parameter systems governed by

$$\frac{\partial u(r,t)}{\partial t} = L_r u(r,t) + Ku(r,t) + \xi(r,t) \quad r \in D \quad (1)$$

$$B_r u(r,t) = 0 \quad r \in \partial D \quad (2)$$

defined for $t \geq 0$ on a spatial domain D (a connected, bounded subset of n -dimensional Euclidean space) with boundary ∂D , in which r is a point in the n -dimensional region $D + \partial D$. $u(r,t)$ is the m -vector state; $\xi(r,t)$ is an m -vector white noise (in time only)

disturbance; L_r is an $m \times m$ diagonal matrix, each element of which is a well-posed, linear, time-invariant, spatial partial differential operator. For example, a common form of L_r in the scalar case is $a_1 \partial^2 / \partial r^2 + a_2 \partial / \partial r + a_3$. K is an $m \times m$ constant matrix with zero diagonal elements (these are included in L_r); B_r is an $m_1 \times m$ matrix operator, each row of which has only one nonzero element, which is a well-posed, linear, time-invariant, spatial partial differential operator.

If there exists an $m \times m$ constant, diagonal matrix Λ and a corresponding scalar function $\phi(r)$ such that

$$L_r \phi(r) = \Lambda \phi(r) \quad r \in D \quad (3)$$

$$B_r \phi(r) = 0 \quad r \in \partial D \quad (4)$$

then Λ is an eigenvalue matrix of the system (1) and $\phi(r)$ is the corresponding eigenfunction.*

We now require (1) to have the following properties:

P1. The eigenvalue matrices $\Lambda_1, \Lambda_2, \dots$ are real. Denote the j th diagonal element of Λ_i by λ_{ji} . Then, for each j ,

$$\lambda_{j1} \geq \lambda_{j2} \geq \dots \quad \text{and} \quad \lim_{i \rightarrow \infty} \lambda_{ji} = -\infty.$$

P2. The corresponding eigenfunctions $\phi_1(r), \phi_2(r), \dots$ are real, complete, and orthonormal, i.e.,

$$\int_D \phi_i(r) \phi_j(r) dr = \delta_{ij}$$

* Note: The unusual nomenclatures introduced here are for the convenience of giving a compact presentation of the materials in this chapter.

P3. The initial condition for (1), $u(r,0)$, can be expressed as a linear combination of the first N eigenfunctions

$$u(r,0) = \sum_{i=1}^N \rho_i(0) \phi_i(r) \quad (5)$$

where the $\rho_i(0)$ are constant m -vectors.

P4. The dynamical disturbance $\xi(r,t)$ can be expressed as

$$\xi(r,t) = \sum_{i=1}^N \xi_i(t) \phi_i(r) \quad (6)$$

where the $\xi_i(t)$ are zero-mean, m -vector white noise processes.

The covariance matrix of the mN -vector white noise process

$\xi(t) = [\xi_1^T(t), \dots, \xi_N^T(t)]^T$ is $E[\xi(t)\xi(\tau)^T] = Q(t)\delta(t-\tau)$, where

$Q(t)$ is non-negative definite and continuously differentiable in

t . We denote the covariance matrix $E[\xi(r,t) \xi^T(s,\tau)] =$

$Q(r,s,t)\delta(t-\tau)$.

Note that we have assumed that (5) and (6) are equalities for N sufficiently large. Although there will, in fact, be some discrepancy between the left and right hand sides of (5) and (6), we assume N is large enough to neglect this and therefore take (5) and (6) as part of the specification of our basic system.

A wide class of real systems described by (1) possesses properties P1 and P2. We now show that properties P3 and P4 impose, in fact, no major constraints on the system (1) with respect to the initial conditions or the nature of the dynamical disturbance.

First, it is well known [5] if the $\phi_i(r)$ are complete in D , then any piecewise continuous m -vector function $f(r)$ can be

approximated by $f(r,N) = \sum_{i=1}^N f_i \phi_i(r)$, where $f_i = \int_D f(r) \phi_i(r) dr$, such that

$$\lim_{N \rightarrow \infty} \int_D \|f(r) - f(r,N)\|^2 dr = 0$$

where $\|\cdot\|$ denotes the norm. Therefore, by choosing N sufficiently large, any realistic $u(r,0)$ can be approximated by (5) to arbitrary accuracy in the mean square sense.

Second, if the $\phi_i(r)$ are complete in D , then $\phi_i(r) \phi_j(s)$ are complete in $D \times D$ [5]. As a consequence, let $\xi(r,t)$ be a zero-mean, m -vector white noise process with covariance matrix

$$E[\xi(r,t) \xi^T(s,\tau)] = Q^+(r,s,t) \delta(t-\tau) \text{ where, for all } t, Q^+(r,s,t) \text{ is}$$

- i) Symmetric in r and s , i.e., $Q^+(r,s,t) = Q^+(s,r,t)^T$
- ii) Piecewise continuous in r and s
- iii) Continuously differentiable in t
- iv) Non-negative definite, i.e., for any piecewise continuous m -vector function $g(r)$

$$\int_D \int_D g(r)^T Q^+(r,s,t) g(s) dr ds \geq 0$$

Actually, properties (i)-(iv) are not very restrictive, and have been assumed in other studies of stochastic distributed systems [28,29].

Let us define an m -vector random process $\xi(r,N,t) = \sum_{i=1}^N \xi_i(t) \phi_i(r)$, where $E[\xi_i(t)] = 0$, $E[\xi_i(t) \xi_j^T(\tau)] = Q_{ij}(t) \delta(t-\tau)$ and

$$Q_{ij}(t) = \int_D \int_D Q^+(r,s,t) \phi_i(r) \phi_j(s) dr ds \tag{7}$$

and let $E[\xi(r,N,t)\xi^T(s,N,\tau)] = Q(r,s,N,t)\delta(t-\tau)$. Then it follows directly from the completeness property of $\phi_i(r)\phi_j(s)$ that

$$\lim_{N \rightarrow \infty} \int_D \int_D \|Q^+(r,s,t) - Q(r,s,N,t)\|^2 dr ds = 0$$

We note that the $mN \times mN$ matrix $Q(t)$, whose elements are defined by (7), indeed possesses the basic properties of a covariance matrix, namely, it is symmetric and non-negative definite [12,13]. The key result is that the spatially distributed white noise disturbance $\xi(r,t)$ can be approximated by (6), such that for sufficiently large N , the covariance matrix of $\xi(r,t)$, $Q^+(r,s,t)$, can be approximated arbitrarily closely in the mean square sense.

We assume that observations of the state $u(r,t)$ are made continuously in time at discrete spatial locations. We assume that at each measurement point one or more of the m components of the state are observed directly. This corresponds to the most common situation with respect to experimental data (e.g., thermocouple measurements of temperature). We represent the observations in the following way:

$$y(r_i,t) = h_i u(r_i,t) + \eta_i(t) \quad r_i \in D + \partial D \quad (8)$$

$$i = 1, 2, \dots, d$$

where y is a scalar and each h_i is an m -dimensional row vector with only one nonzero component, whose value is one, corresponding to the component of $u(r,t)$ that is measured at that point. In order that more than one component may be measured at the same point, r_i and r_j may be identical for $i \neq j$. The $\eta_i(t)$ are zero-mean

white noise measurement errors. The covariance matrix of the d-vector process $\eta(t) = [\eta_1(t), \eta_2(t), \dots, \eta_d(t)]^T$ is $R(t)\delta(t-\tau)$, where $R(t)$ is positive definite and continuously differentiable in t .

We make two final assumptions: $\xi(t)$ and $\eta(t)$ are independent, hence $E[\xi(t)\eta^T(\tau)] = 0$, and there exist constants c_i such that $c_1 < \|R(t)\| < c_2$ and $c_3 < \|Q(t)\| < c_4$ for all t . The latter assumption is required for convergence of the Kalman filter [12,13].

Known volume and boundary inputs can be included in the formulation of the system. Let $\psi(r,t)$ and $b(r,t)$ be m -vector and m_1 -vector known functions, respectively. Rewrite (1) as

$$\frac{\partial u}{\partial t} = L_r u(r,t) + Ku(r,t) + \psi(r,t) + \xi(r,t) \quad (1a)$$

$$B_r u(r,t) = b(r,t) ; \quad u(r,0) = u_0(r) \quad (2a)$$

If we define

$$\frac{\partial u^+}{\partial t} = L_r u^+(r,t) + Ku^+(r,t) + \xi(r,t) \quad (1b)$$

$$B_r u^+(r,t) = 0 ; \quad u^+(r,0) = u_0(r) \quad (2b)$$

and

$$\frac{\partial u^-}{\partial t} = L_r u^-(r,t) + Ku^-(r,t) + \psi(r,t) \quad (1c)$$

$$B_r u^-(r,t) = b(r,t) ; \quad u^-(r,0) = 0 \quad (2c)$$

then by superposition, $u(r,t) = u^+(r,t) + u^-(r,t)$. Equations (1c) and (2c) can be solved to give $u^-(r,t)$. If we denote

$$y^+(r_i,t) = y(r_i,t) - h_i u^-(r_i,t)$$

then

$$y^+(r_i, t) = h_i u^+(r_i, t) + \eta_i(t) \quad (8a)$$

Thus, a system described by (1a), (2a) and (8) can always be reduced to one described by (1b), (2b) and (8a), a form suitable for application of later results.

The system (1), (8) with properties P1-P4 will be referred to as S .

3. Modal Representation of S

The solution of S is spanned by the first N eigenfunctions in the form

$$u(r, t) = \sum_{i=1}^N \rho_i(t) \phi_i(r) \quad (9)$$

where each $\rho_i(t)$ is an m -vector function. Substituting (9) into (1) and multiplying both sides of the resulting equation by $\phi_k(r)$ and integrating over D , we obtain

$$\dot{\rho}_k(t) = \Lambda_k \rho_k(t) + K \rho_k(t) + \xi_k(t) \quad (10)$$

If $\rho(t) = [\rho_1^T(t), \rho_2^T(t), \dots, \rho_N^T(t)]^T$, then $\rho(t)$ is governed by

$$\dot{\rho}(t) = A \rho(t) + F \rho(t) + \xi(t) \quad (11)$$

where A and F are the $mN \times mN$ matrices,

$$A = \begin{bmatrix} \Lambda_1 & & 0 \\ & \Lambda_2 & \\ 0 & & \ddots \\ & & & \Lambda_N \end{bmatrix} \quad F = \begin{bmatrix} K & & 0 \\ & K & \\ 0 & & \ddots \\ & & & K \end{bmatrix} \quad (12)$$

The observation (8) has the form

$$y(t) = M\rho(t) + \eta(t) \quad (13)$$

where $y(t) = [y(r_1, t), y(r_2, t), \dots, y(r_d, t)]^T$, and M is a $d \times mN$ matrix,

$$M = \begin{bmatrix} M_{11} & M_{12} & \dots & M_{1N} \\ M_{21} & & & \\ \vdots & & & \\ M_{d1} & \dots & & M_{dN} \end{bmatrix}$$

where each M_{ij} is the m -dimensional row vector, $h_i \phi_j(r_i)$.

Due to the orthonormality of the $\phi_i(r)$, it is easy to show that the correspondence between the original state $u(r, t)$ and the state $\rho(t)$ is one-to-one. We refer to (11) and (13) as the modal representation of S , which is an equivalent lumped parameter representation of the original distributed system. The modal representation of distributed systems has been used in a number of cases with respect to control of distributed systems [8,24].

We now state a few well-known results for linear, time-invariant lumped parameter systems that will later be needed. The system (11), (13) is completely observable iff the rank of $[M^T, (A^T + F^T)M^T, \dots, (A^T + F^T)^{mN-1} M^T]$ is mN [12,13]. The system (11), (13) is detectable

iff there exists a real matrix B such that $(A^T + F^T) + M^T B$ is asymptotically stable, i.e., all eigenvalues are negative [36].

Detectability essentially refers to the observability of the unstable modes of a system.

As mentioned in the Introduction, our primary reason for considering observability is as a prerequisite to estimating the state $u(r,t)$ of the system based on the noisy observations $y(r_i,t)$. Since S has been reduced to the modal system (11),(13), the classic Kalman filter can be applied to (11) and (13). It is

$$\dot{\hat{\rho}}(t) = (A+F)\hat{\rho}(t) + P(t) M^T R^{-1}(t) [y(t) - M\hat{\rho}(t)] \quad (14)$$

$$\dot{P}(t) = (A+F)P(t) + P(t)(A^T + F^T) - P(t)M^T R^{-1}(t)MP(t) + Q(t) \quad (15)$$

where $\hat{\rho}$ is the estimate of ρ . These equations are integrated simultaneously with the gathering of data $y(t)$ and provide continuously updated estimates $\hat{\rho}(t)$. The Kalman filter is said to be convergent if (14) is uniformly asymptotically stable and there exists a unique $\bar{P}(t)$ such that $\lim_{t \rightarrow \infty} P(t) = \bar{P}(t)$ for every symmetric, non-negative definite $P(0)$. If $Q(t)$ and $R(t)$ are time-invariant, $\bar{P}(t) = \bar{P}$, a constant matrix, the solution of

$$(A+F)\bar{P} + \bar{P}(A^T + F^T) - \bar{P}M^T R^{-1} M\bar{P} + Q = 0 \quad (16)$$

If the system (11),(13) is completely observable, then the Kalman filter is convergent. If Q and R are time-invariant, the Kalman filter is convergent iff the system (11),(13) is detectable [17].

We will define S to be completely observable and detectable when its modal representation is completely observable and detectable. An estimate of the original state will be obtained from (9) by

$$\hat{u}(r,t) = \sum_{i=1}^N \hat{\rho}_i(t) \phi_i(r) \quad (17)$$

The distributed filter for S is defined by (14), (15) and (17) and is defined to be convergent when its modal filter is convergent.

Finally, if we define $P(r,s,t) = E[(u(r,t) - \hat{u}(r,t))(u(s,t) - \hat{u}(s,t))^T]$, the modal filter (14)-(15), together with (17) can be shown to be equivalent to the distributed parameter filters of Tzafestas and Nightingale [28,29] and Seinfeld et al. [10,26]:

$$\begin{aligned} \frac{\partial \hat{u}}{\partial t} &= L_r \hat{u}(r,t) + K \hat{u}(r,t) \\ &+ \sum_{i=1}^d \sum_{j=1}^d P(r,r_i,t) h_i^T R_{ij}^{-1}(t) [y(r_j,t) - h_j \hat{u}(r_j,t)] \quad r \in D \end{aligned} \quad (18)$$

$$B_r \hat{u}(r,t) = 0 \quad r \in \partial D \quad (19)$$

$$\begin{aligned} \frac{\partial P}{\partial t} &= L_r P(r,s,t) + K P(r,s,t) + P(r,s,t) L_s^T + P(r,s,t) K^T \\ &+ \sum_{i=1}^d \sum_{j=1}^d P(r,r_i,t) h_i^T R_{ij}^{-1}(t) h_j P(r_j,s,t) + Q(r,s,t) \end{aligned} \quad (20)$$

$r, s \in D$

$$B_r P(r,s,t) = 0 \quad r \in \partial D, s \in D \quad (21)$$

$$B_s^T P(r,s,t) = 0 \quad s \in \partial D, r \in D \quad (22)$$

where $R_{ij}^{-1}(t)$ is the i,j th element of the matrix $R^{-1}(t)$ and $P(r,s,t) L_S^T = (L_S P^T(r,s,t))^T$.

4. Effect of Measurement Locations on Observability

The modal representation of S enables us to relate the observability and detectability of S to that of the modal system. Our basic objective is to use the modal representation to determine the effect of measurement locations on observability and filter convergence for S . When S is deterministic ($\xi(r,t) = \eta_i(t) = 0$), in order to determine $u(r,t)$ uniquely, measurements and their locations must be chosen such that complete observability is achieved. When S is stochastic, to guarantee meaningful estimates of $u(r,t)$, the modal filter must be convergent. Hence, again measurements and their locations must be chosen such that S is completely observable (if Q and R are time-varying) or detectable (if Q and R are time-invariant).

Two key questions can be posed: (1) Can we always find some finite set of measurements such that S is observable, and (2) Is there some minimum number of measurements sufficient for observability of S ? The principal results of this section attempt to answer these two questions. The results are embodied in two theorems.

Before stating the theorems, we make some slight changes in notation which will facilitate the proofs of the theorems. Let the measurement locations r_1, r_2, \dots, r_d be relabeled as $r_{ij}, i=1, \dots, m, j=1, \dots, d_i$ such that $\sum_{i=1}^m d_i = d$. Thus, the i th component of the state $u_i(r,t)$ is observed at d_i locations $r_{ij}, j=1, 2, \dots, d_i$. Let the

components of the m -vector ρ_i be ρ_{ji} , $j=1,2,\dots,m$, and denote the N -vector $\alpha_j = [\rho_{j1}, \rho_{j2}, \dots, \rho_{jN}]^T$ and the mN -vector $\alpha = [\alpha_1^T, \alpha_2^T, \dots, \alpha_m^T]^T$.

The deterministic forms of (11) and (13) then become

$$\dot{\alpha}(t) = G(t) \alpha(t) \quad (23)$$

$$z(t) = W(t) \alpha(t) \quad (24)$$

where the $mN \times mN$ constant matrix

$$G = \begin{bmatrix} G_{11} & G_{12} & \dots & G_{1m} \\ \vdots & & & \\ \vdots & & & \\ G_{m1} & \dots & & G_{mm} \end{bmatrix}$$

with each diagonal element G_{ii} an $N \times N$ diagonal matrix with elements λ_{ik} , $k=1,2,\dots,N$, and each off-diagonal element G_{ij} an $N \times N$ diagonal matrix with elements k_{ij} (the i,j th element of K).

The d -dimensional column vector $z(t) = [z_1^T(t), \dots, z_m^T(t)]^T$ with each element a d_i -dimensional row vector $z_i^T(t) = [y(r_{i1}, t), y(r_{i2}, t), \dots, y(r_{id_i}, t)]$. W is a $d \times mN$ constant diagonal matrix with each diagonal element W_i a $d_i \times N$ matrix,

$$W_i = \begin{bmatrix} \phi_1(r_{i1}) & \phi_2(r_{i1}) & \dots & \phi_N(r_{i1}) \\ \vdots & & & \\ \vdots & & & \\ \phi_1(r_{id_i}) & \phi_2(r_{id_i}) & \dots & \phi_N(r_{id_i}) \end{bmatrix} \quad i=1,2,\dots,m$$

In this formulation, S is completely observable iff the rank of $[W^T, G^T W^T, \dots, (G^T)^{mN-1} W^T] = mN$.

Theorem 1. There always exist spatial measurement points r_{ij} , $i=1,2,\dots,m$, $j=1,2,\dots,N$ such that S is completely observable.

Proof of Theorem 1. We want to show that, with a finite number of measurement locations, it is always possible to construct a measurement scheme that will make S completely observable. To do this, we will show that we can always choose N measurement locations at each of which all m components of $u(r,t)$ are observed to lead to an observable system. Thus, let $r_{ij} = r_j^*$, $i=1,2,\dots,m$, $j=1,2,\dots,N$, i.e., all components of $u(r,t)$ are measured at each r_j^* . In this case all W_i are identical, so set $W_i = W^*$. Since $\det W = (\det W^*)^m$ and S is completely observable if W is nonsingular, all we need to show is that r_j^* , $j=1,2,\dots,N$ exist such that W^* is nonsingular. We do this by induction. Define W_ℓ^* by

$$W_\ell^* = \begin{bmatrix} \phi_1(r_1^*) & \phi_2(r_1^*) & \dots & \phi_\ell(r_1^*) \\ \vdots & & & \\ \phi_1(r_\ell^*) & \dots & & \phi_\ell(r_\ell^*) \end{bmatrix}$$

We shall show that r_j^* , $j=1,2,\dots,N$ exist such that W_ℓ^* is nonsingular for all $\ell=1,2,\dots,N$. $W_1^* \neq 0$ since $\phi_1(r)$ cannot be identically zero for all $r \in D + \partial D$. Assume $\phi_1(r_1^*) \neq 0$. If W_2^* is singular for all r_2^* , then there exists some fixed constant b such that for all r_2^* ,

$$\begin{bmatrix} \phi_2(r_1^*) \\ \phi_2(r_2^*) \end{bmatrix} = b \begin{bmatrix} \phi_1(r_1^*) \\ \phi_1(r_2^*) \end{bmatrix}$$

which implies $\phi_2(r) = b\phi_1(r)$ for all r . This contradicts the orthonormality of ϕ_1 and ϕ_2 . Hence, an r_2^* must exist such that W_2^* is nonsingular. Now, assume W_ℓ^* is nonsingular and $W_{\ell+1}^*$ is singular for all $r_{\ell+1}^*$. Then there exists a set of fixed constants b_1, b_2, \dots, b_ℓ such that for all $r_{\ell+1}^*$

$$\begin{bmatrix} \phi_{\ell+1}(r_1^*) \\ \vdots \\ \phi_{\ell+1}(r_{\ell+1}^*) \end{bmatrix} = \sum_{j=1}^{\ell} b_j \begin{bmatrix} \phi_j(r_1^*) \\ \vdots \\ \phi_j(r_{\ell+1}^*) \end{bmatrix}$$

which implies $\phi_{\ell+1}(r) = \sum_{j=1}^{\ell} b_j \phi_j(r)$ for all r . This contradicts the orthonormality of $\phi_1, \phi_2, \dots, \phi_{\ell+1}$. Hence, an $r_{\ell+1}^*$ must exist such that $W_{\ell+1}^*$ is nonsingular. Q.E.D.

Theorem 1 represents only a sufficient condition for choosing measurements such that S can be made observable. Therefore, it may be possible to have an observable system with fewer measurements than prescribed in the proof of Theorem 1.

The second question we pose is, are there some circumstances under which we can use fewer than the number of measurements prescribed in the proof of Theorem 1 and still have an observable system? Theorem 2 presents this situation.

Theorem 2. If K is triangular (i.e., either $k_{ij} = 0$ for $i \geq j$ or $k_{ij} = 0$ for $i \leq j$) and if each component of u , $u_i(r, t)$, is measured at only one point r_i^* , $i=1, 2, \dots, m$, then S is completely observable if for all i

- a. $\phi_1(r_i^*) \neq 0$, $\phi_2(r_i^*) \neq 0$, \dots , $\phi_N(r_i^*) \neq 0$
- b. $\lambda_{i1}, \lambda_{i2}, \dots, \lambda_{iN}$ are distinct.

Proof of Theorem 2. Let $T = [W^T, G^T W^T, \dots, (G^T)^{N-1} W^T]$. It is straight-forward to show that $|\det T| = \prod_{i=1}^m |\det T_i|$ where $T_i = \Phi_i V_i$ and

$$\Phi_i = \begin{bmatrix} \phi_1(r_i^*) & & & & 0 \\ & \cdot & & & \\ & & \cdot & & \\ 0 & & & \cdot & \\ & & & & \phi_N(r_i^*) \end{bmatrix}$$

$$V_i = \begin{bmatrix} 1 & \lambda_{i1} & \lambda_{i1}^2 & \dots & \lambda_{i1}^{N-1} \\ 1 & \lambda_{i2} & \lambda_{i2}^2 & & \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & \lambda_{iN} & & & \lambda_{iN}^{N-1} \end{bmatrix}$$

If a. and b. hold for all i , then $\det T_i \neq 0$ for all i , implying T is nonsingular and hence S is completely observable. If $m = 1$, conditions a. and b. are both necessary and sufficient for observability, where for $m > 1$, a. and b. are only sufficient. If K is not triangular, conditions a. and b. are not, in general, required for observability. Q.E.D.

Lemma 1. If K is triangular and $\lambda_{ji} < 0$ for all $j=1,2,\dots,m$ and $i=1,2,\dots,N$, then S is detectable.

Proof of Lemma 1. Set $B = 0$ in the detectability test of Section 3. Then the eigenvalues of $(A+F)$ are λ_{ji} , $j=1,2,\dots,m$, $i=1,2,\dots,N$.

Q.E.D.

We now present a few simple examples to illustrate the application of Theorems 1 and 2.

Example 1. Consider the scalar, one-dimensional heat conduction system

$$\frac{\partial u}{\partial t} = \mu u_{rr}(r,t) \quad r \in (0,1), \mu > 0$$

$$u(r,t) = 0 \quad r = 0,1$$

The eigenfunctions and eigenvalues are $\phi_i(r) = \sqrt{2} \sin i\pi r$ and $\lambda_i = -\mu(i\pi)^2$, $i=1,2,\dots,N$. Let u be measured at only one point r^* . From Theorem 2, we see that complete observability of the system is achieved iff r^* does not belong to the set of locations, $\sin i\pi r^* = 0$, $i=1,2,\dots,N$.

Example 2. Consider the scalar, two-dimensional heat conduction system [4]

$$\frac{\partial u}{\partial t} = u_{rr}(r,s,t) + u_{ss}(r,s,t) \quad r,s \in (0,1)$$

$$u(r,s,t) = 0 \quad \left\{ \begin{array}{l} r = 0,1, s \in [0,1] \\ s = 0,1, r \in [0,1] \end{array} \right.$$

For $N = 4$ the eigenfunctions and eigenvalues are:

$$\phi_1(r,s) = 2 \sin \pi r \sin \pi s \quad \lambda_1 = -2\pi^2$$

$$\phi_2(r,s) = 2 \sin \pi r \sin 2\pi s \quad \lambda_2 = -5\pi^2$$

$$\phi_3(r,s) = 2 \sin 2\pi r \sin \pi s \quad \lambda_3 = -5\pi^2$$

$$\phi_4(r,s) = 2 \sin 2\pi r \sin 2\pi s \quad \lambda_4 = -8\pi^2$$

Since $\lambda_2 = \lambda_3$, Theorem 2 indicates that we will need more than one

measurement point. If we choose, for example, the two points $(r_1^*, s_1^*) = (\frac{1}{6}, \frac{1}{3})$ and $(r_2^*, s_2^*) = (\frac{1}{6}, \frac{1}{6})$, then $\det[W^T, G^T W^T] \neq 0$ and hence complete observability is achieved (given that $N = 4$ is an acceptable representation of the system).

Example 3. Consider the m -vector, one-dimensional system

$$\begin{aligned} \frac{\partial u}{\partial t} &= L_r u(r,t) + Ku(r,t) \quad , \quad r \in (0,1) \\ L_{i_r} &= \mu_i \frac{\partial^2}{\partial r^2} - \sigma_i \quad , \quad \mu_i > 0 \quad , \quad \sigma_i > 0 \quad , \quad i=1,2,\dots,m \\ \frac{\partial u_i}{\partial r} &= 0 \quad , \quad r = 0,1 \quad , \quad i=1,2,\dots,m \end{aligned}$$

where K has elements $k_{ij} \geq 0$ for $i < j$ and $k_{ij} = 0$ for $i \geq j$, $i, j=1,2,\dots,m$. This system represents the combined diffusion and first order decomposition of m chemical species, in which there is no flux of mass across the boundaries of the system. The eigenfunctions for this system are $\phi_1(r) = 1$, $\phi_i(r) = \sqrt{2} \cos(i-1) \pi r$, $i=2,\dots,N$. The j th diagonal element of Λ_i is $\lambda_{ji} = -\mu_j(i-1)^2 \pi^2 - \sigma_j$, $j=1,2,\dots,m$, $i=1,2,\dots,N$.

Let $u_i(r,t)$ be measured at r_i^* , $i=1,2,\dots,m$. Applying Theorem 2, it is clear that complete observability is achieved as long as r_i^* does not belong to the set of locations, $\cos k\pi r_i^* = 0$, $k=0,1,\dots,N-1$.

If K is not triangular, Theorem 2 cannot be applied. Theorem 1, however, will always guarantee that there exists a completely observable measurement scheme.

5. Optimal Location of Measurements

If S is deterministic ($\xi(r,t) = \eta_i(t) = 0$), the question of optimal measurement locations is irrelevant, since a set of measurements either provides sufficient information for the unique determination of $u(r,t)$ or not. The question of optimal measurement locations does have relevance, however, when one considers filtering for a stochastic distributed system. First, of course, the measurements must be chosen so that the system is completely observable (if Q and R are time-varying) or detectable (if Q and R are time-invariant). Then, the measurements can be positioned such that the resulting state estimates are in some sense optimal.

Consider the case in which R and Q are time-invariant. In this case a reasonable criterion of the accuracy of the state estimates is the trace of the steady state covariance matrix \bar{P} . In general, we could divide $D + \partial D$ into J grid points and examine all possible arrangements of the d measurements at these grid points. For each detectable arrangement the trace of \bar{P} can be computed and the set yielding the smallest value of the trace be chosen. This approach is clearly too time consuming for practical use.

We now present a suboptimal scheme for measurement locations in the case of scalar ($m=1$) one-dimensional ($n=1$) systems in which $\lambda_1 > \lambda_2 \cdots > \lambda_N$ and $\phi_i(r) = 0$ at a finite number of points. The method can be extended to the vector, multidimensional case, although for simplicity we present only the scalar, one-dimensional case here.

Say we wish to choose d locations, r_1, r_2, \dots, r_d , at which to observe $u(r, t)$ such that $\text{tr } \bar{P}$ is minimized. The following algorithm can be used:

1. Begin with one observation point r . Find that value of r that minimizes $\text{tr } \bar{P}$ and denote it by r_1 . (Here we first need to find the points of undetectability where $\text{tr } \bar{P} = \infty$).
2. Fix r_1 . Add a second measurement point r and find that value of r that minimizes $\text{tr } \bar{P}$ and denote it by r_2 .
3. Fix r_1 and r_2 . Add a third point and continue until all d points are chosen.

Although this approach clearly does not necessarily lead to an optimal set of points, it should produce results not far removed from an optimal set. This is because the first point is at its best location. Adding another point decreases $\text{tr } \bar{P}$, and we generally would expect that with two points at least one would be located near the optimum position for a single point.

In order to utilize this algorithm, we need to determine how \bar{P} varies with a measurement location r . First, we express \bar{P} as $\bar{P}(r)$, i.e., \bar{P} depends implicitly on the parameter r . Upon differentiating (16) with respect to r , we obtain an ordinary differential equation governing $\bar{P}(r)$ (the procedure was first suggested by Jamshidi [11])

$$\begin{aligned} \frac{d\bar{P}}{dr} [A^T - M^T(r)R^{-1}M(r)\bar{P}(r)] + [A - \bar{P}(r)M^T(r)R^{-1}M(r)] \frac{d\bar{P}}{dr} \\ = \bar{P}(r) \frac{dM^T}{dr} R^{-1}M(r) \bar{P}(r) + \bar{P}(r)M^T(r)R^{-1} \frac{dM}{dr} \bar{P}(r) \end{aligned} \quad (25)$$

where, since $m = 1$, $F = 0$.

Equation (25) is simply a matrix O.D.E. which may be integrated either forward or backward in r to obtain $\bar{P}(r)$ in any interval in which $\bar{P}(r)$ is continuous. To initiate the integration, $\bar{P}(r)$ must first be calculated independently at one arbitrary point in the given interval. This may be done by solving (16) by an iterative technique suggested by Kleinman [15].

We now apply this algorithm to an example.

Example 4. Consider the heat conduction system

$$u_t(r,t) = \sigma_1 u_{rr}(r,t) + \sigma_2 u(r,t) + \xi(r,t) \quad r \in (0,1)$$

$$u_r(r,t) = 0 \quad r = 0,1$$

We choose for illustration $N = 3$, for which the eigenfunctions and eigenvalues are $\phi_1(r) = 1$, $\phi_2(r) = \sqrt{2} \cos \pi r$, $\phi_3(r) = \sqrt{2} \cos 2\pi r$, and $\lambda_1 = \sigma_2$, $\lambda_2 = \sigma_2 - \sigma_1 \pi^2$, $\lambda_3 = \sigma_2 - 4\sigma_1 \pi^2$, respectively. We choose

$$Q = \begin{bmatrix} 0.005 & 0 & 0 \\ 0 & 2.0 & 0 \\ 0 & 0 & 2.0 \end{bmatrix}$$

and $R = 2$ for one measurement and

$$R = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

for two measurements.

From Theorem 2 we know that this system is unobservable iff $r = 1/4$, $1/2$ or $3/4$. Let us consider the optimal location of two

observations in two cases: (i) $\sigma_1 = 0.1, \sigma_2 = 0$, and (ii) $\sigma_1 = 0.1, \sigma_2 = 1.1$.

In case (i), it can be shown that for one observation the system is detectable at any r . The trace of \bar{P} in case (i) for one observation and two observations, one of which is at $r_1 = 0$, is shown in Figure 1. With only one observation, $\text{tr } \bar{P}$ is minimum either at $r = 0$ or $r = 1$. With the first observation fixed at $r_1 = 0$, curve 2 indicates that the best placement of the second point is at $r_2 = 1$.

In case (ii), it can be shown that for one observation the system is detectable for any r except $r = 1/2$. Figure 2 shows the trace of \bar{P} for one observation and two observations, one of which is at $r_1 = 0.36$. Curve 2 indicates that $r_2 = 1.0$ minimizes $\text{tr } \bar{P}$ given that $r_1 = 0.36$. Thus, for case (ii), with one point, its best location is $r_1 = 0.36$ or 0.64 ; with two points, one fixed at 0.36 , the best location of the second point is 1.0 . This is somewhat unexpected since it would appear from curve 1 in Figure 2 that with two measurements we would have to place them at 0.36 and 0.64 . Placing one at 0.36 , however, we are apparently required to put the second point as far away from the first one as possible.

6. Figures

Figure 1 Example 4, Case (i)

Curve 1: One measurement location at r .

Curve 2: First measurement location at $r_1 = 0$,
second measurement location at r .

Figure 2 Example 4, Case (ii)

Curve 1: One measurement location at r .

Curve 2: First measurement location at $r_1 = 0.36$,
second measurement location at r .

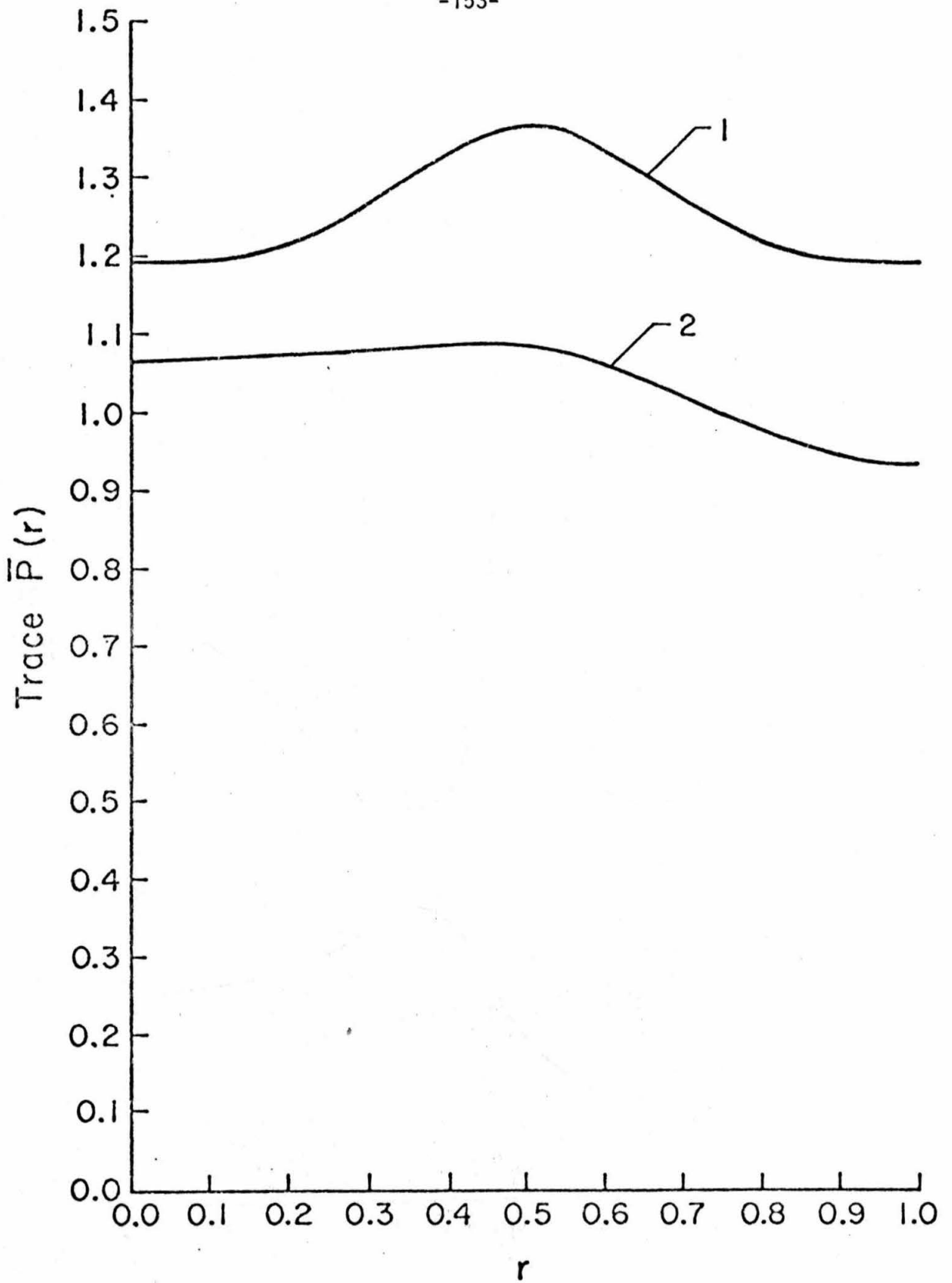


FIGURE 1

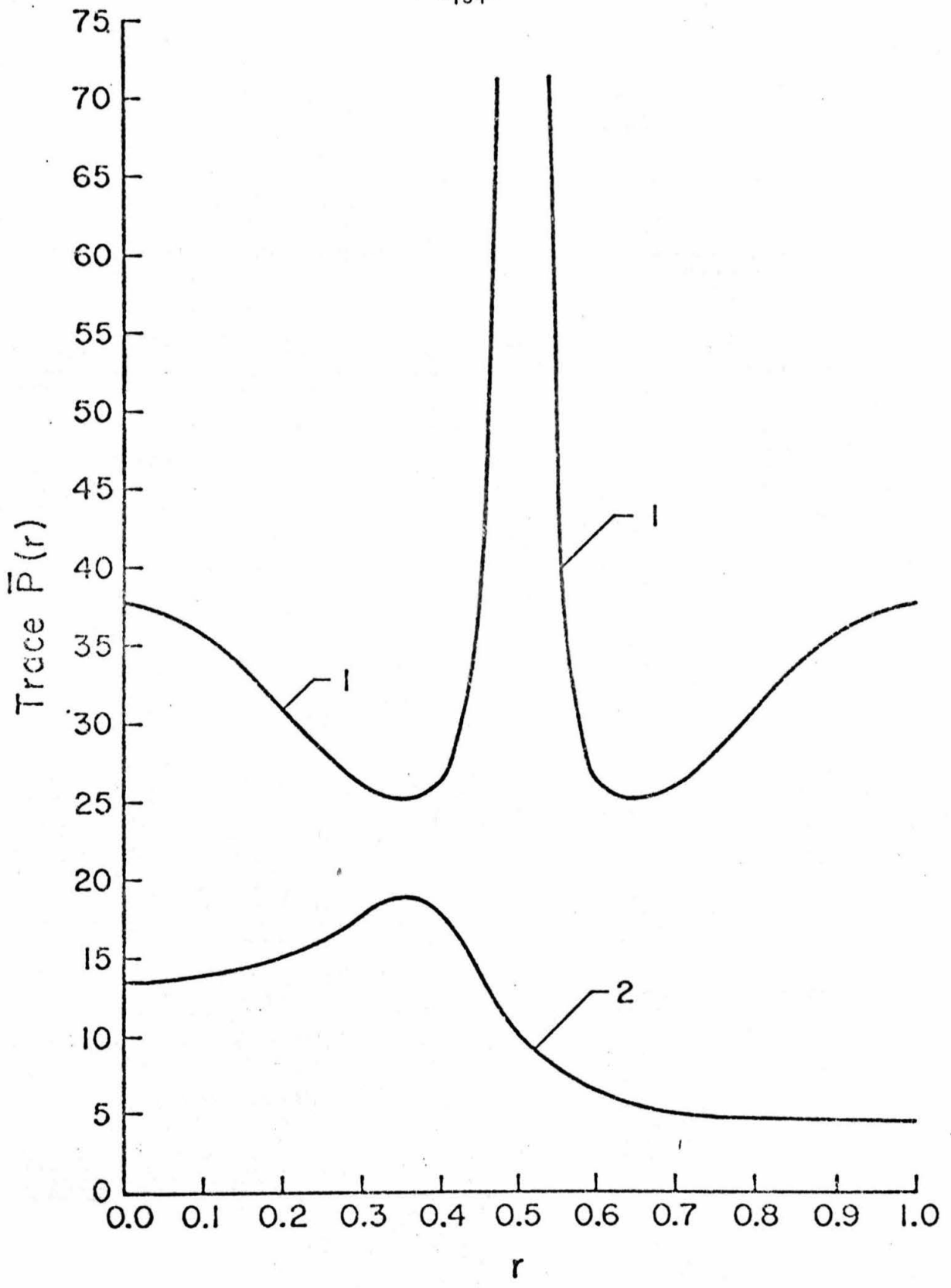


FIGURE 2

Appendix V-A

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Observability of a Class of Hyperbolic Distributed Parameter Systems

T. K. YU AND J. H. SEINFELD

Abstract—Necessary and sufficient conditions are presented for the observability of a class of linear hyperbolic distributed parameter systems. Observations are assumed to be made along paths intersecting the characteristic curves of the system.

In this correspondence we present some new results on the observability of a class of linear hyperbolic distributed parameter systems. The results are embodied in necessary and sufficient conditions for the recovery of the state of this class of systems. In order to develop the conditions, we present first an extension of the well-known conditions¹ for the observability of linear lumped parameter systems.

Consider the class of systems described by

$$\dot{u}(t) = F(t)u(t), \quad t \in [0, T] \quad (1)$$

where $u(t)$ is an $(n \times 1)$ state vector and $F(t)$ is an $(n \times n)$ matrix. Let $\Phi(t, 0)$ be the fundamental matrix for system (1). Suppose observations of this system are made at h discrete times in the form

$$y_i = H_i u(t_i), \quad i = 1, 2, \dots, h \quad (2)$$

where the y_i are $(m_i \times 1)$ vectors of observations and the H_i are $(m_i \times n)$ constant matrices. Therefore, the dimension of y_i and of H_i can change at different measurement times. This system is said to be *observable* if we can recover the initial state $u(0)$ from y_i , $i = 1, 2, \dots, h$. We present the following theorem.

Theorem 1: A necessary and sufficient condition for the observability of (1) is that the $(n \times \sum_{i=1}^h m_i)$ matrix, $M = [\Phi(t_i, 0)^T H_1^T, \dots, \Phi(t_h, 0)^T H_h^T]$, has rank n .

Proof: Let $r = \sum_{i=1}^h m_i$ and v_i denote the i th column vector of M . Also, let $Y = [y_1^T, \dots, y_h^T]^T = [Y_1, Y_2, \dots, Y_h]^T$. Form the $(n \times n)$ matrix Q from any n columns of M , $Q = [v_{i_1}, v_{i_2}, \dots, v_{i_n}]$. Then there is an $(n \times 1)$ vector $g = [Y_{i_1}, \dots, Y_{i_n}]^T$ such that $g = Q^T u(0)$. For any $t \in [0, T]$, we can write $g = Q^T \Phi(t, 0)^{-1} u(t)$. Hence, to recover $u(t)$ for all $t \in [0, T]$, it is necessary and sufficient that there exists a matrix Q with rank n or, equivalently, M must have rank n .

Example 1: Let us apply this theorem to system (1) with

$$F(t) = \begin{pmatrix} 0 & t \\ -t & 0 \end{pmatrix} \quad (3)$$

Suppose only u_1 can be measured. Say we measure u_1 at two times, t_1 and t_2 . Thus, $H_1 = H_2 = [1 \ 0]$ (i.e., $n = 2$, $m_1 = 1$, $m_2 = 1$, $r = 2$) and

$$M = \begin{bmatrix} \cos(t_1/2) & \cos(t_2/2) \\ \sin(t_1/2) & \sin(t_2/2) \end{bmatrix} \quad (4)$$

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 The authors are with the Department of Chemical Engineering, California Institute of Technology, Pasadena, Calif. 91109.
¹E. B. Lee and L. Marcus, *Foundations of Optimal Control Theory*. New York: Wiley, 1967.

Let t_i be chosen arbitrarily. Then, in order that M may have rank 2, it is necessary that $t_i \neq (t_j^2 + 2k\pi)^{1/2}$, $k = 1, 2, 3, \dots$, for the system to be observable.

OBSERVABILITY OF A CLASS OF HYPERBOLIC SYSTEMS

Consider the class of linear hyperbolic systems governed by

$$\frac{\partial u}{\partial t} + \beta \frac{\partial u}{\partial x} = Au, \quad x \in [0, 1], \quad t \geq 0 \quad (5)$$

where u is an $(n \times 1)$ state vector, β is a positive scalar constant, and A is an $(n \times n)$ constant matrix. The system (5) has only one type of characteristic line, namely, $dt/dx = 1/\beta$. Let $\Phi(\tau, 0)$ be the $(n \times n)$ fundamental matrix of the system, $\dot{w} = \frac{1}{\beta} A w$, $\tau \in [0, 1]$. Also, let R_α denote the closed region in the (x, t) plane bounded by $x = 0$, $x = 1$, $t = 0$, and $t = \beta^{-1}x + \alpha$, $\alpha \geq 0$.

Definition: The i th observation path $z_i(t)$ is a line in the (x, t) plane with the following properties: $z_i(0) = 1$, $z_i(t)$ crosses each characteristic line in R_α once, and $z_i(t)$ terminates at a point on the characteristic line $t = \beta^{-1}x + \alpha$.

Let there be h distinct observation paths, $z_i(t)$, $i = 1, 2, \dots, h$, that is, $z_i(t)$ and $z_j(t)$ have no common points for $i \neq j$ and $t > 0$. We will denote the value of the state along the i th observation path as $u_i(t)$. We assume that the observations $y_i(t)$ of the system (5) are made continuously along the h observation paths in the form

$$y_i(t) = H_i u_i(t), \quad i = 1, 2, \dots, h, \quad t > 0 \quad (6)$$

where the H_i are constant $(m_i \times n)$ matrices. The observation at the point $(x = 1, t = 0)$ is in the form $y_i(0) = H_0 u_i(0)$, $i = 1, 2, \dots, h$, where H_0 is a constant $(n \times n)$ matrix. We will call the system of (5) and (6) *observable* in R_α if $u(x, t)$ in R_α can be recovered from $y_i(t)$.

Theorem 2: A sufficient condition for the observability of (5) and (6) in R_α is: 1) if for any $\tau_1 \neq \tau_2 \neq \dots \neq \tau_h$, $0 \leq \tau_i \leq 1$, the $(n \times \sum_{i=1}^h m_i)$ matrix $L = [\Phi(\tau_1, 0)^T H_1^T, \dots, \Phi(\tau_h, 0)^T H_h^T]$ has rank n and 2) H_0 is nonsingular.

Proof: The proof follows directly from that for Theorem 1.

Example 2: Consider the system (5) with $n = 2$, $\beta = 1$, and

$$A = \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix} \quad (7)$$

Let $\alpha = 1/2$. Assume there are two paths in the (x, t) plane along which observations are made:

$$z_1(t) = 1 - t, \quad 0 \leq t \leq 1/2 \\ \quad \quad \quad 1/2, \quad 1/2 \leq t \leq 1 \quad (8)$$

$$z_2(t) = 1, \quad 0 \leq t \leq 1.5. \quad (9)$$

We choose the following observation matrices: $H_0 = I$, $H_1 = [1 \ 0]$, and $H_2 = [0 \ 1]$. Thus, at $x = 1$ and $t = 0$, both states are measured, but along $z_1(t)$ only u_1 is measured and along $z_2(t)$ only u_2 is measured. It is straightforward to show that

$$L = \begin{bmatrix} 1 & 0 \\ 1 - e^{-\tau_1} & e^{-\tau_1} \\ 1 - e^{-\tau_2} & e^{-\tau_2} \end{bmatrix} \quad (10)$$

has rank 2 for any $\tau_1 \neq \tau_2, 0 \leq \tau_1, \tau_2 \leq 1$; hence, the system is observable.

Finally, we consider another class of linear hyperbolic systems, namely, those governed by

$$\frac{\partial u}{\partial t} + A_1 \frac{\partial u}{\partial x} = A_2 u, \quad x \in [0,1], t \geq 0 \quad (11)$$

where A_1 and A_2 are $(n \times n)$ diagonal matrices with diagonal elements $\lambda_{11}, \dots, \lambda_{1n}$ and $\lambda_{21}, \dots, \lambda_{2n}$, respectively. Therefore, (11) represents n uncoupled hyperbolic systems, each having its own characteristic line, with slope $dt/dx = \lambda_{ii}^{-1}, i = 1, 2, \dots, n$. We assume $\lambda_{11} > \lambda_{12} > \dots > \lambda_{1n}$.

We define $R_\alpha(i)$ as the closed region on the (x,t) plane bounded by $x = 0, x = 1, t = 0$, and $t = \lambda_{1i}^{-1}x + \alpha, \alpha \geq 0$. We also define the single observation path $z^+(t)$ by: 1) $z^+(0) = 1$; 2) $z^+(t)$ crosses each characteristic line of type i in $R_\alpha(i)$ once, $i = 1, 2, \dots, n$; and 3) $z^+(t)$ terminates at a point on the characteristic line $t = \lambda_{1n}^{-1}x + \alpha$. $z_1^+(t)$ will denote the segment of $z^+(t)$ that begins at the point $(x = 1, t = 0)$ and terminates on the line $t = \lambda_{11}^{-1}x + \alpha$. Similarly, $z_i^+(t)$ is the segment of $z^+(t)$ that initiates from the line $t = \lambda_{1i}^{-1}x + \alpha$ and terminates on the line $t = \lambda_{1i}^{-1}x + \alpha$. The observation along path segment $z_i^+(t)$ is in the form

$$y_i^+(t) = H_i^+ u_{z_i^+}(t) \quad (12)$$

where H_i^+ is a constant $(m_i \times n)$ matrix.

Theorem 3: A necessary and sufficient condition for the observ-

ability of (11) and (12) in the region $R_\alpha(1)$ is that for each $(m_i \times n)$ matrix H_i^+ a new $(n - i + 1 \times n)$ matrix P_i^+

$$P_i^+ = \begin{bmatrix} p_{i,1} & p_{i,2} & \dots & p_{i,n} \\ p_{i+1,1} & p_{i+1,2} & \dots & p_{i+1,n} \\ \vdots & \vdots & \ddots & \vdots \\ p_{n,1} & & & p_{n,n} \end{bmatrix} \quad (13)$$

can be formed that has the properties $p_{j,k} \neq 0$ for all $j = k$ and $p_{j,k} = 0$ for $j > k$, and each row of P_i^+ is formed by some linear combination of rows of H_i^+ .

Proof: Let the $(n - i + 1 \times m_i)$ matrix B_i represent the transformation such that $B_i H_i^+ = P_i^+$. Then there exists a $g_i^+ = B_i y_i^+(t)$ such that $g_i^+ = P_i^+ u_{z_i^+}(t)$. Let $v_i^+(t)$ be a vector formed from deleting the first $i - 1$ components of $u_{z_i^+}(t)$ and W_i be the matrix formed from deleting the first $i - 1$ columns (all zeros) of P_i^+ . Then we can write $g_i^+ = W_i v_i^+$. Since W_i will be nonsingular, $v_i^+ = W_i^{-1} g_i^+$. This implies that u_i, \dots, u_n can be recovered along $z_i^+(t)$ and therefore u_i can be recovered along $z_1^+(t), z_2^+(t), \dots, z_i^+(t)$. Hence, u_i can be recovered along every characteristic line of type i in $R_\alpha(i)$ and the system is observable in $R_\alpha(1)$, proving sufficiency. Suppose for a particular H_i^+ a new matrix P_i^+ having the properties of Theorem 3 cannot be formed. This implies that some $u_j (i \leq j \leq n)$ cannot be recovered along $z_i^+(t)$. Hence, u_j cannot be recovered along some characteristic lines of type j in the region $R_\alpha(j)$, proving necessity.

Chapter VI

CONCLUSION

In this dissertation optimal filters have been derived for three important classes of nonlinear stochastic dynamical systems.

The first class of systems is governed by stochastic nonlinear hyperbolic and parabolic partial differential equations with boundary and volume disturbances of both additive and nonadditive nature. The form of the system enables the recursive estimation of both states and constant parameters. The performance of the filter was demonstrated computationally in an example for the feedback control of a styrene polymerization reactor.

The second class of systems encompasses, within a single framework, three types of stochastic time delay systems:

1. Nonlinear lumped parameter systems with multiple constant and time-varying delays;
2. Nonlinear systems of coupled ordinary and hyperbolic partial differential equations; and
3. Nonlinear lumped parameter systems having functional time delays.

The general filter was applied in a numerical example to a chemical reactor-heat exchanger system.

The third class of systems is a generalization of the second class by including systems described by mixed nonlinear lumped and parabolic partial differential equations with both volume and boundary disturbances.

Along with filtering, the related concept of observability and optimal measurement location was studied for a class of stochastic linear distributed parameter systems whose solutions can be expressed as eigenfunction expansions. The two questions examined are: (1) the effect of measurement locations on observability, and (2) the optimal location of measurements for state estimation. It was shown that a scheme of finite measurements can always be constructed such that the system is observable. Also, it was shown that for a special class of systems, only a few measurements will suffice for observability, as long as they are not placed at the "nodes" of the system. An algorithm was developed for determining a suboptimal set of measurement locations with respect to state estimates.

Finally, necessary and sufficient conditions for observability was derived for a separate class of linear hyperbolic distributed parameter systems.

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