Practical Realizations in Process Modeling:

KRISHNAMURTHY JAYARAMAN
and
LEON LAPIDUS
Department of Chemical Engineering
Princeton University
Princeton, New Jersey 08540

Part I. A New Approach to Practical Realization

A new approach is presented for the construction of linear, low-order stable, state-variable, dynamic models from experimental pulse response data of process systems: the problem of practical realization. This problem is solved by deriving and implementing constraints in the estimation of Markov parameters which are input to a realization algorithm. This is accomplished sequentially by using an algorithm for recursive partial realization. Bounds on the Markov parameters are derived from qualitative information about the smoothness of the response curve and used in a stagewise regression procedure. The present procedure identifies the faster modes first; hence the tail of the pulse response, if inordinately long and inaccurate, may be ignored while lower-order partial realizations are constructed.

SCOPE

With the increasing complexity of present day engineering systems, it has become necessary to develop time domain representations of their dynamic behavior for purposes of simulation and control. Such models, called state-variable models, emphasize the internal structure of the system and can incorporate nonzero initial conditions in predicting the transients in a system. The most tractable and popular class of state-variable models is that of linear, time-invariant, finite-dimensional (lumped) systems, represented by a set of ordinary, first-order, linear differential equations with constant coefficients. Many process systems may be modeled by repeated identification over periods of time invariance by using such realizations coupled with time delays, if necessary.

In the chemical engineering literature, the most widely quoted technique for identifying the internal dynamics of a system from observed input/output behavior is the method of moments. This approach to real systems has widely recognized disadvantages. In the present work, a different approach is presented for constructing linear, low-order, stable state-variable models for the dynamics of process systems from real response data (the problem of practical realization). This approach involves much less hypothesis and exploits qualitative information about the smoothness of the response curve. It operates in the framework of a recursive realization algorithm of Rissanen (1971) to estimate a set of Markov parameters which are the successive derivatives of the impulse response evaluated at $t = 0$. These parameters then yield a realization (a state-variable model) for the system.

Over the last decade, considerable attention has been given to the problem of translating an exact input/output representation of a system into a state-space representation for its dynamics. Starting with Kalman's canonical decomposition theorem (Kalman, 1963), which showed that the input/output description reveals only the controllable and observable part of a dynamical system, this area of linear system identification has progressed to the point where a number of algorithms are now available for constructing minimal realizations from a transfer function or from an impulse response function. In most algorithms, notably those of Ho (1966), Ackerman and Bucy (1971), and Rissanen (1971), this is done via a set of Markov parameters. When the input/output relation is in the form of experimental pulse response data, and especially for continuous time systems with intermittent measurements, the Markov parameters must be estimated with great care from the noisy data. The problem of practical realization is solved here by deriving and implementing constraints in the estimation of these Markov parameters. In the second paper of this two part series, the nature of the approximation thus obtained is discussed with examples.

We start this paper with a brief survey of the problem of realization and its solution. We outline the conceptual basis of realizations, describe the algebraic problems of minimal complete realization and minimal partial realization, indicate the importance of extension sequences of Markov parameters in the partial realization problem, and finally describe Rissanen's recursive realization algorithm in detail. Next, we present the composite scheme for practical realization, evolved in this work.

CONCLUSIONS AND SIGNIFICANCE

A specific procedure has been described in this paper for regularizing the ill-posed problem (in the sense of Hadamard) of identifying linear state-variable models starting from real impulse response curves, such as measured residence time densities for flow systems, in the face of uncertainty in model dimension. These impulse response curves are obtained from continuous time systems with intermittent measurements. The resulting composite scheme is simple and recursive; it combines stagewise estimation of Markov parameters by constrained, linear regression and their recursive partial realization by Rissanen's algorithm, with information flowing to and fro between these two component schemes.

The major contribution of this paper lies in the use of regularity assumptions on the impulse response functions considered, to derive bounds on Markov parameters, by

means of corresponding sign patterns in a factor matrix of Rissanen's realization algorithm. These regularity assumptions also ensure the stability of partial realizations of all orders. In addition, a useful connection has been established with previous work by chemical engineers in modeling flow systems—the class of impulse response functions satisfying these assumptions may be obtained as residence time densities from series-parallel networks of stirred tanks. This correspondence allows us to take into account an additional characteristic of the original system derived from its impulse response function, the intensity function.

REALIZATION THEORY AND ALGORITHMS

The realization problem is to derive a set of state-variable equations to describe the internal dynamics of a system from a set of input/output relations. In general, this is extremely difficult because of the multitude of possible system types—linear or nonlinear, stationary or time varying, finite or infinite dimensional—and the multitude of possible modes of input excitation used to study the response of the system.

A common approach is to postulate a priori that the system can be modeled by a finite set of linear, time invariant, state-variable equations, starting from the impulse response of the system. In this work, we shall further restrict ourselves to systems with a single input and a single output (but with a number of state variables) so that the model equations are of the form

$$\begin{aligned} \dot{x}(t) &= Ax(t) + bu(t) \\ y(t) &= cx(t) \end{aligned} \tag{1}$$

where $x(t) \in R^n$, $u(t)$, and $y(t)$ are scalars, and A, b, c have compatible dimensions. We must then determine the minimal dimension n of the state space which yields a canonical realization. The motivation for this was first established by Kalman (1963, 1969). The input/output relation for a system depends only on its reachable and observable parts. For a linear system, reachability is equivalent to controllability.

The basic question in examining controllability of a model is whether it can be decoupled such that some portions of it will not be affected by the inputs. Observability relates to the question of whether the outputs of the model can be related to all of the states. These two properties guarantee a proper model corresponding to input/output data, without extraneous information. A realization $\Sigma = (A, b, c)$ of an input/output relation is canonical if and only if it is both completely controllable and completely observable. All canonical realizations for the same input/output relation differ only by a change of basis in the state space. That is, if $\Sigma_1 = (A_1, b_1, c_1)$ and $\Sigma_2 = (A_2, b_2, c_2)$ are canonical realizations of the same impulse response function, there exists a nonsingular matrix T such that

$$A_2 = TA_1T^{-1}, \quad b_2 = Tb_1 \quad c_2 = c_1T^{-1} \tag{2}$$

The transfer function for (1) is given by

$$G(s) = c(sI - A)^{-1}b \quad G(\infty) = 0 \tag{3}$$

and the impulse response function by

$$g(t) = c \exp(At)b \tag{4}$$

Expansion of $G(s)$ about $s = \infty$, as a Taylor series in $1/s$ or expansion of $g(t)$ about $t = 0$, as a Taylor series in t yields the Markov parameters $\{Y_k\}$:

$$G(s) = \sum_{k=0}^{\infty} Y_k s^{-(k+1)} \tag{5}$$

$$g(t) = \sum_{k=0}^{\infty} Y_k t^k/k! \tag{6}$$

Combining (3) and (5) or (4) and (6), we obtain

$$Y_k = [d^k g(t)/dt^k]_{t=0} = cA^kb \tag{7}$$

The algebraic problems of realization may now be formulated in terms of the Markov parameters (Kalman, 1971) as follows.

(1) Minimal Complete Realization

Given a countably infinite sequence $\{Y_0, Y_1, Y_2, \ldots\}$, find a triple of matrices $\Sigma = (A, b, c)$ such that

(i) $Y_k = cA^kb \qquad k = 0, 1, 2, \ldots$
(ii) $n = \dim \Sigma = \text{size } A = \text{minimum}$

(2) Minimal Partial Realization

Given a finite sequence of length M, $\{Y_0, Y_1, \ldots, Y_{M-1}\}$, find a triple of matrices $\Sigma_M = (A, b, c)$ such that

(i) $Y_k = cA^kb \qquad k = 0, 1, \ldots, M-1$
(ii) $n_M = \text{size } A = \text{minimum}$

Minimal partial realizations are more useful, since for a continuous time system, only a finite number of Markov parameters (being the time derivatives of the impulse response at $t = 0$) can be estimated reliably. Also, the assumption that the original system considered is linear, time invariant, and finite dimensional may not be valid over a long period of time.

An appealing aspect of the realization approach to identification is that there is no need to fix a priori the dimension of the model. If the sequence of Markov parameters is derived from an exact input/output representation, the dimension of the original system can be obtained directly from the Markov parameters. The following theorem for the existence of a realization of the form of (1) was established by Ho (1966):

Theorem 1. The sequence $\{Y_k\}_{k=1}^{\infty}$ has a finite dimensional realization if and only if there exist an integer n and n constants $\alpha_1, \alpha_2, \ldots, \alpha_n$, such that

$$Y_{n+j} = \sum_{i=1}^{n} \alpha_i Y_{n-i+j} \quad \text{for all } j \geq 0 \tag{8}$$

Then n is the dimension of the minimal realization and $\{\alpha_i\}_{i=1}^{n}$ the coefficients of its characteristic polynomial. The realizability criterion for a partial sequence may be expressed more conventionally in terms of Hankel matrices of Markov parameters defined by

$$H(i,j) = \begin{bmatrix} Y_0 & Y_1 & \ldots & Y_{j-1} \\ Y_1 & Y_2 & \ldots & Y_j \\ \vdots & & & \vdots \\ Y_{i-1} & Y_i & \ldots & Y_{i+j-2} \end{bmatrix} \quad i, j = 1, 2, \ldots \tag{9}$$

Theorem 2 (Tether, 1970; Kalman, 1971). A minimal partial realization exists for a given finite sequence $\{Y_0, Y_1, \ldots, Y_{M-1}\}$ and is essentially unique (except for a change of basis in the state space) if and only if there exist positive integers β, α such that

(i) $\beta + \alpha = M$
(ii) $\text{rank } H_{\beta\alpha} = \text{rank } H_{\beta+1,\alpha} = \text{rank } H_{\beta,\alpha+1}$

The dimension n_M of the realization Σ_M is then equal to rank $H_{\beta\alpha}$. In addition to matching the given finite sequence, this realization generates a unique infinite extension sequence of Markov parameters given by

$$Y_k = c_{\Sigma_M} A^k{}_{\Sigma_M} b_{\Sigma_M} \qquad k \geq M \tag{10}$$

For a given finite length M, the above realizability criterion may not be satisfied. In this event, one must either obtain more Markov parameters from the response curve or specify a finite extension of the given sequence in order to meet the realizability criterion. This is the major step in partial realization. Once the realizability criterion is met, one may use any of the standard realization algorithms to calculate the minimal partial realization from the given finite sequence of Markov parameters.

$$\underset{H(4,4)}{\begin{bmatrix} 0 & 1 & -10 & 98 \\ 1 & -10 & 98 & -974 \\ -10 & 98 & -974 & 9\,726 \\ 98 & -974 & 9\,726 & -97\,230 \end{bmatrix}} = \underset{R(4,4)}{\begin{bmatrix} 1 & & & \\ -10 & 1 & & \\ 98 & -10 & 1 & \\ -974 & 98 & -13 & 1 \end{bmatrix}} \underset{Q(4,4)}{\begin{bmatrix} 0 & 1 & -10 & 98 \\ 1 & 0 & -2 & 6 \\ 0 & 0 & -14 & 182 \\ 0 & 0 & 0 & 0 \end{bmatrix}} \tag{16}$$

If the sequence of Markov parameters is generated by a triple $(A, b, c)_n$ whose j controllability matrix is given by

$$Q_j \equiv [b \; Ab \; A^2b \; \ldots \; A^{j-1}b] \tag{11}$$

and whose i observability matrix is given by

$$R_i \equiv [c' \; A'c' \; (A')^2c' \; \ldots \; (A')^{i-1}c']' \tag{12}$$

($'$ denotes transpose)

then

$$H(i, j) = R_iQ_j \tag{13}$$

This relationship underlies the role of the Hankel matrices in the realization problem. All solutions to the algebraic realization problem involve a factorization of the Hankel matrix into the observability matrix and the controllability matrix for the model:

$$H(n, n) = R_nQ_n \tag{14}$$

Different canonical forms can be obtained for the realization matrices by clever factorizations of the Hankel matrix.

The first algorithmic solution to the algebraic problem of realization was presented by Ho (1966). Later, other algorithms were presented by Silverman (1971), Ackerman and Bucy (1971), and Rissanen (1971). Rissanen's algorithm is recursive and solves a more general problem.

Given the partial sequence $Y_1, Y_2, \ldots, Y_N$ for each $N = 1, 2, 3, \ldots$, find a sequence of minimal partial realizations

$$\Sigma_N = (A_N, b_N, c_N)$$

such that $\ldots \; \Sigma_{N'} \subseteq \Sigma_N \subseteq \; \ldots$ if $N' < N$. Here the inclusion symbol means that the matrices in $\Sigma_{N'}$ appear as submatrices of the corresponding ones in Σ_N so that each of the prior partial sequence of Markov parameters can be realized by calculating just a few new elements in the corresponding realization.

The essence of Rissanen's algorithm is a recursive scheme for factorizing growing portions of the Hankel matrix of Markov parameters:

$$H(n+1, m) = R(n+1, n+1)Q(n+1, m) \quad m \geq n+1$$
$$\text{rank } H(n+1, m) \geq n \tag{15}$$

where $R(n+1, n+1)$ is lower triangular with 1's on the diagonal. The factorization scheme is related to a Gauss elimination scheme with a choice of the pivoting elements such that with recursion the following feature is obtained.

The last row of H is linearly dependent on the previous rows if and only if the last row of Q is a row of zeros. These two features ensure the uniqueness of the factor matrices R and Q.

The steps in the factorization scheme are outlined below (see Rissanen, 1971):

1. Set $q_{1i} = Y_i$ for all i
2. Proceeding recursively, we have at the i^{th} row all the r_{jk}'s and q_{jk}'s, $j = 0, 1, \ldots, i-1$, determined. Let $s(j)$ be the least integer such that $q_{j,s(j)} \neq 0, j < n$. $s(j)$ exists because of the rank condition on H. Set $q_{k,s(j)} = 0$ for $k > j$. Equation (15) then leads to a set of $i-1$ equations, one for each column $s(j)$, $j = 1, \ldots, i-1$. The unknowns $r_{i1}, \ldots, r_{i,i-1}$ (in the i^{th} row of R) may be computed recursively from the equations. The submatrix $R(i, i)$ then determines the remaining elements of the i^{th} row of Q, which completes the cycle.

As an illustration (Example 1)

Defining c as the first row of $R(n, n)$ and b as the first column of $Q(n, n)$, we obtain

$$A = R^{-1}(n, n) \; R_*(n, n) \tag{17}$$

where $R_*(n, n)$ is obtained by omitting the first row and the last column of $R(n+1, n+1)$. The matrix A thus obtained will be lower Hessenberg with 1's on the superdiagonal.

The recursive realization scheme with the factorization outlined above is described below. (It is assumed that from some source, the Markov parameters $Y_1, Y_2, \ldots, Y_N$ for any $N = 1, 2, \ldots$ are available.)

1. Let k be the least integer for which $Y_k \neq 0$. Take $N = 2k+1$ and form $H(k+1, k+1)$. It has rank $\geq k$.
2. Apply the factorizing algorithm and find $R(k+1, k+1)$ and $Q(k+1, k+1)$. If the last row of Q is nonzero, the rank of $H(k+1, k+1)$ is $k+1$. Increase N by 2, form $H(k+2, k+2)$, and continue the factorization. Repeat till say, for $N = 2n-1$, the last row of $Q(n, n)$ is zero.
3. From the formulas in (17), calculate the partial realization $\Sigma(n-1)$. The inverse of $R(n-1, n-1)$ can also be calculated recursively, since R and R^{-1} are both lower triangular.
4. If on adding some more Markov parameters, a nonzero element is introduced in the last row of Q, the dimension of the realization must be increased by the same procedure to match these later Markov parameters. The realization matrices from the factorization in example 1 are

$$A = \begin{bmatrix} -10 & 1 & 0 \\ -2 & 0 & 1 \\ -14 & 0 & -3 \end{bmatrix}; \quad b = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}; \quad c = [1 \;\; 0 \;\; 0] \tag{18}$$

In practice, the last row of Q is considered zero if

$$|q_{ni}| \,/\, ||q_i|| \leq \delta \tag{19}$$

a specified tolerance level, for all i. Here $||q_i||$ is the column norm of the i^{th} column of Q defined by

$$||q_i|| = \sum_{j=1}^{n} |q_{ji}| \tag{20}$$

At any stage of the recursive realization procedure, Q forms the controllability matrix for the realization at that stage. That is

$$Q = [b \; Ab \; A^2b \; \ldots .] \tag{21}$$

The response of the state vector $\mathbf{x}$ to an impulse in the input, $u = \delta(t)$ with $x(0) = 0$, is given by

$$x(t) = \exp(At)b \tag{22}$$

Expanding (21) in a Taylor series about $t = 0$, we obtain

$$x(t) = b + Ab\,t + A^2b\frac{t^2}{2!} + \ldots \tag{23}$$

Thus, A^ib represents the i^{th} derivative of the response of the state vector at $t = 0$. Each independent row of a general controllability matrix represents a component of the state. In the matrix Q of Rissanen's algorithm, each nonzero row represents a component of the state. So, with the criterion in (19), we are in effect omitting components of the state that are smaller than δ in relation to the rest. Thus, Rissanen's factorization scheme allows us to characterize the error of approximation by a lower dimensional model in a convenient way.

There is another useful feature that falls out of Rissanen's factorization scheme: $H(n, n) = R(n, n)\ Q(n, n)$. If the last row of $Q(n, n)$ is zero, then the last row of $D(n, n) \equiv R^{-1}(n, n)$ spans the space of solutions to the equation

$$x'H = 0 \qquad (R^{-1}H = Q) \tag{24}$$

By construction, R is nonsingular. If we now look back at theorem 1, it is evident that the last row of $D(n, n)$ then consists of the coefficients of the characteristic polynomial of A. In example 1,

$$D(4,4) = R^{-1}(4,4) = \begin{bmatrix} 1 & & & \\ 10 & 1 & & \\ 2 & 10 & 1 & \\ 20 & 32 & 13 & 1 \end{bmatrix} \tag{25}$$

The characteristic polynomial for the resulting third-order model is

$$\psi(s) \equiv s^3 + 13s^2 + 32s + 20 \tag{26}$$

Rissanen's algorithm is specially suited to the partial realization problem, since it allows us to test for the realizability criterion at each stage of the recursion in a simple, convenient way. Further, the overall strategy of generating as many initial zeros in each row of Q as possible allows us to generate an extension sequence of Markov parameters by adding zeros in the later columns of the last row of the Q matrix and preserving the Hankel pattern. This too is done recursively. For example, given the finite sequence $\{0, 1, -10, 98\}$, an extension sequence may be obtained as follows:

$$\begin{bmatrix} 0 & 1 & -10 & 98 & (-960) \\ 1 & -10 & 98 & (-960) & (9\,404) \\ -10 & 98 & (-960) & (9\,404) & (-92\,120) \end{bmatrix} = \begin{bmatrix} 1 & & \\ -10 & 1 & \\ 98 & -10 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & -10 & 98 & (-960) \\ 1 & 0 & -2 & (20) & (-196) \\ 0 & 0 & 0 & (0) & (0) \end{bmatrix} \tag{27}$$

First we arrange the given finite sequence in a Hankel matrix and apply the factorization scheme: $H(3, 3) = R(3, 3)\ Q(3, 3)$. h_{33} and hence q_{33} are missing, but all the elements of $R(3, 3)$ can be computed regardless. Using $R(3, 3)$ we shall generate the subsequent columns of H and Q by the following procedure. Set $q_{33} = 0 \rightarrow h_{33} = -960$. Therefore, $h_{24} = -960 \rightarrow q_{24} = 20$. Then set $q_{34} = 0 \rightarrow h_{34} = 9\,404$. Therefore $h_{15} = -960$, $h_{25} = +9\,404 \rightarrow q_{15} = -960$, $q_{25} = -196$. Then set $q_{35} = 0 \rightarrow h_{35} = -92\,120$, and so on. The extension thus obtained is -960, 9 404, $-92\,120$, ...

A Scheme for Practical Realization

The objective in the present work is to construct linear, low-order, stable state-variable models of the dynamics of process systems from real response data. This problem of practical realization is ill-posed because it includes an ill-defined step. A problem is well posed in the sense of Hadamard if it has a unique solution which depends continuously on its data. The problem of passing from an exact representation of the input/output relation to a state-space representation is well defined. As we have seen in the previous section, most algorithms for realization use an intermediate set of Markov parameters, which are the successive derivatives of the impulse response evaluated at $t = 0$. The estimation of these Markov parameters from noisy response data for continuous time systems with intermittent measurements is the ill-defined step (Audley and Lee, 1974) and must be done with care.

Previous workers have reported difficulties in attempts at solving the practical realization problem. Audley and Rugh (1973) have indicated, with an example, that if no structure is imposed on the model, an asymptotically stable n-dimensional system may have no lower dimensional asymptotically stable minimal partial realization. Rossen (1972) has shown how careless estimation of Markov parameters, or specification of a nonunique finite extension of a given partial sequence of Markov parameters, in order to meet the realizability criterion, without any structure in mind, may lead to unstable models for stable physical processes. Audley and Rugh have not proposed any procedure to overcome their difficulty. Neither has Rossen proposed any solution to the problem. He has, however, proposed "after the fact surgery," an involved procedure for constructing stable models from unstable models by replacing the positive eigenvalues by a larger number of negative eigenvalues chosen to preserve the condition of matching the initially given partial sequence of Markov parameters. The resulting realization is nonminimal, however.

To ensure that the resulting model retains the smoothness and stability of the original system response, we must incorporate these features into the set of Markov parameters. Also, since the number of Markov parameters that can be estimated reliably from noisy pulse response data of a continuous time system is limited, even after regularization, we would like to build these features into as short a sequence of Markov parameters as possible. Here we shall show how this can be done in the framework of Rissanen's algorithm for recursive partial realization.

We wish to estimate as many Markov parameters as possible, $\{Y_i\}^M_{i=1}$, from the pulse response of an output, $\{z(t_k)\}^N_{k=1}$, in the presence of noise. This is for a continuous time system with intermittent measurements, so that

$$y(t) = Y_0 + Y_1t + Y_2t^2/2! + \ldots = \sum_{i=0}^{\infty} Y_it^i/i! \tag{28}$$

$$z(t_k) = y(t_k) + \epsilon(t_k) \tag{29}$$

where the statistics of the noise ϵ are unknown. We are interested in good estimates for the first few Markov parameters rather than a good fit of the data with the Markov parameters over the entire range of the response. We require the minimum partial realization that will be derived from the first few Markov parameters, rather than the power series itself, to predict the response of the system closely. For instance, for a system specified by the impulse response function

$$g(t) = -0.35e^{-7t} + 5.25e^{-3t} - 8.4e^{-2t} + 3.5e^{-t} \tag{30}$$

with settling time around 6.5 units, a forty term Taylor series about $t = 0$ is required to predict the response accurately up to $t = 2$. However, to identify the exact model of dimension 4, only nine Markov parameters are required.

In the practical problem, a finite number of Chebyshev polynomials orthogonal on the continuous interval $(-1, 1)$ are used to estimate the Markov parameters. The error in representation by a finite power series is added onto the noise ϵ

$$z(t_k) = \sum_{i=0}^{M} Y_i t_k^i/i! + v(t_k) \tag{31}$$

or, in terms of the Chebyshev polynomials $\{T_i(\tau)\}$, where τ is the normalized argument

$$z(\tau_k) = \sum_{i=0}^{M} a_i T_i(\tau_k) + \eta(\tau_k) \tag{32}$$

v and η being the modified errors. With varying M, it is impossible to specify the statistics of the error η in any meaningful way. Hence, a filtering algorithm cannot be used here.

To obtain reliable estimates of the Markov parameters, we must now take recourse to constrained regression, using several successive lower degree fits with trend removal. The a priori information on the smoothness and stability of the original response must be used to derive constraints on the parameters (see Hunt, 1972). The characterization of the smoothness of the response and its use in deriving constraints on the parameters form the core of the present work.

We begin by outlining the preliminary steps in the estimation procedure.

1. A time scale is chosen for the process such that the *settling time* for the pulse response or the time range of interest is $O(1)$. Similarly, a scale is chosen for the observed variable such that the ordinates are $O(1)$.

2. At each stage of the regression procedure, the overall fitting function is written as

$$f(t) = g_k(t) + t^{k+1} h_k(t) \tag{33}$$

where $g_k(t)$ is of degree k and is made up of the previously identified Markov parameters.

3. From the initial stages of regression, the number of zero Markov parameters at the start of the sequence must be estimated.

The need for specifying the appropriate number of zero Markov parameters q may be seen from a correspondence between the Markov parameters and transfer functions. For a transfer function with n poles and m zeros

$$G(s) = \frac{K(s^m + \beta_1 s^{m-1} + \ldots + \beta_m)}{s^n + \alpha_1 s^{n-1} + \ldots + \alpha_n} \tag{34}$$

$$q = n - m - 1 \tag{35}$$

that is, if $g(t)$ is the impulse response function for the system

$$g(0) = g'(0) = \ldots = g^{(q-1)}(0) = 0 \tag{36}$$

where $g^{(k)}(t) \equiv d^k g/dt^k$ and the dimension of the lowest order partial realization is $q + 1$. This would correspond to a system with no finite zeros in its transfer function. The existence of q zero Markov parameters ensures that the response of the output considered has at least q independent derivatives. In the context of tracer kinetics in biological systems, the quantity q has been termed the minimum number of precursors (Rescigno and Segre, 1966). In addition, Brockett (1965) has characterized the quantity $(q + 1) = (n - m)$, the difference in degrees between the numerator and denominator polynomials of a rational transfer function, as an invariant under state feedback, called the relative order of the system.

Another important consideration in specifying the number of zero Markov parameters is the ratio of the first two nonzero Markov parameters. These may be obtained from (34) as

$$Y_{n-m} = K \quad \text{and} \quad Y_{n-m+1} = K(\beta_1 - \alpha_1) \tag{37}$$

It is well known that

$$\beta_1 = -\sum_{i=1}^{m} z_i \quad \text{and} \quad \alpha_1 = -\sum_{j=1}^{n} p_j \tag{38}$$

where $\{z_i\}^m_{i=1}$ and $\{p_j\}^n_{j=1}$ are the zeros and poles of the system, respectively. Therefore

$$Y_{n-m+1}/Y_{n-m} = \sum_{j=1}^{n} p_j - \sum_{i=1}^{m} z_i \tag{39}$$

If the magnitude of this ratio is some large number, say, of order 100 or 1 000, then with the proviso (explained later) that $\left|\sum_{i=1}^{m} z_i\right| < \left|\sum_{j=1}^{n} p_j\right|, \left|\sum_{j=1}^{n} p_j\right|$ must be at least of order 100 or 1 000. This would imply either that the model is of very large dimension or that the matrix A of the complete realization has a few extremely large eigenvalues. Both possibilities would obscure the identification process. So the number of zero Markov parameters must then be increased by one, and the ratio of the first two nonzero Markov parameters obtained with this modification must be checked again. It must be noted here that both the observed variable and the time have been scaled at the start of the estimation procedure.

Thus, the correct number of zero Markov parameters guarantees a minimal degree of smoothness and avoids spurious or undesirable stiffness in the model.

We may now pursue the stagewise regression procedure described in Equation (33) to obtain estimates for the subsequent Markov parameters. Here, since these are the higher-order derivatives of the impulse response evaluated at $t = 0$, we need bounds on them to be able to obtain reliable estimates reflecting the smoothness and stability of the given response.

To motivate further the specific characterization proposed here for the smoothness and stability of the impulse response function, let us recall the procedure described in the previous section for generating an extension sequence of Markov parameters from the factor matrix Q of Rissanen's factorization scheme. This was done recursively by setting the undetermined elements in the last row of Q to zero. The elements of the extension sequence obtained at any stage of the recursive realization procedure could be used as bounds on the subsequent Markov parameters if we could specify a sign pattern among the entries to be made in the matrix Q.

It is found that we can specify a sign pattern among the entries in the matrix Q and, in addition, ensure that all lower order partial realizations are asymptotically stable if we make the following assumptions.

1. The impulse response function g(t) is a probability density function that can be expressed as a finite linear combination of exponential density functions; that is

$$g(t) \geq 0 \quad \text{for} \quad t \geq 0$$

$$= 0 \quad \text{for} \quad t < 0 \qquad \int_0^\infty g(t)dt = 1 \tag{40}$$

and

$$g(t) = \sum_{i=1}^{n} A_i e^{-\gamma_i t} \qquad (41)$$

where $\{\gamma_i > 0\}$ and $\{A_i\}$ are real constants.

The transfer function $G(s)$ for the system is then the Laplace transform of a probability density function; hence, following Feller (1971), $G(0) = 1$ and $G(s)$ is completely monotone; that is, $G(s)$ defined on $(0, \infty)$ possesses derivatives $G^{(k)}(s)$ for all orders and

$$(-1)^k G^{(k)}(s) \geq 0 \quad s > 0 \quad k = 0, 1, 2, \ldots \qquad (42)$$

From (41) it is evident that the transfer function for the complete realization is a ratio of two polynomials in s with real and negative poles:

$$G(s) = \prod_{i=1}^{m} (s - z_i) / \prod_{j=1}^{n} (s - p_j) \qquad (43)$$

$$p_j \text{ real and } < 0 \quad \forall\ j \qquad (44)$$

Also, (42) implies that the zeros of the transfer function must have negative real parts:

$$Re(z_i) < 0 \quad \forall\ i \qquad (45)$$

2. The second assumption is that the magnitude of the sum of zeros for the complete realization is less than the magnitude of the sum of the poles; that is

$$\left| \sum_{i=1}^{m} z_i \right| < \left| \sum_{j=1}^{n} p_j \right| \qquad (46)$$

Equations (44) and (45) imply that

$$sgn \left[\sum_{i=1}^{m} z_i \right] = sgn \left[\sum_{j=1}^{n} p_j \right] \qquad (47)$$

Hence, equations (46) and (39) imply that the ratio of the first two nonzero Markov parameters is negative. Moreover, since $g(t) \geq 0$ for $t \geq 0$ [Equation (40)], the first nonzero derivative of $g(t)$ must be positive. Therefore

$$Y_{n-m} > 0 \qquad Y_{n-m+1} < 0 \qquad (48)$$

These inequalities are important in ensuring the stability of lower-order partial realizations.

Interestingly, the class of impulse responses satisfying the two assumptions stated above comprises residence time densities of series-parallel networks of stirred tanks (CSTR's), a popular class of models for flow systems in chemical engineering. This correspondence affords a significant advantage in allowing us to take into account, while constructing models, an additional characteristic of the original system derivable from its impulse response function, the intensity function (Naor and Shinnar, 1963; Bassingthwaite, 1970). In the context of residence time densities, the intensity function $\lambda(t)$ is defined such that the conditional probability of a particle with age t in the system leaving the system within the next time element dt is $\lambda(t)dt$:

$$\lambda(t) = g(t)/F^*(t) \qquad (49)$$

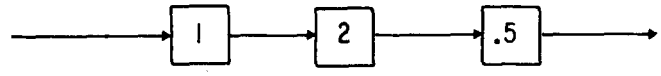
where

$$F^*(t) = 1 - \int_0^t g(t)dt \qquad (50)$$

The intensity function is especially useful in distinguishing among various nonsymmetrical probability density functions (see Barlow and Proschan, 1967).

For a single CSTR, represented by an exponential density function of residence times, the intensity function $\lambda(t)$ is constant with time. For a series combination of CSTR's, represented by a convolution of exponential density functions, the intensity function is monotone increasing. The

$$G(s) = \frac{1}{(s+1)(s+2)(s+.5)}$$



$$g(t) = \frac{4}{3} e^{-t/2} - 2e^{-t} + \frac{2}{3} e^{-2t}$$

Fig. 1. and example 2. A series combination of stirred tanks.

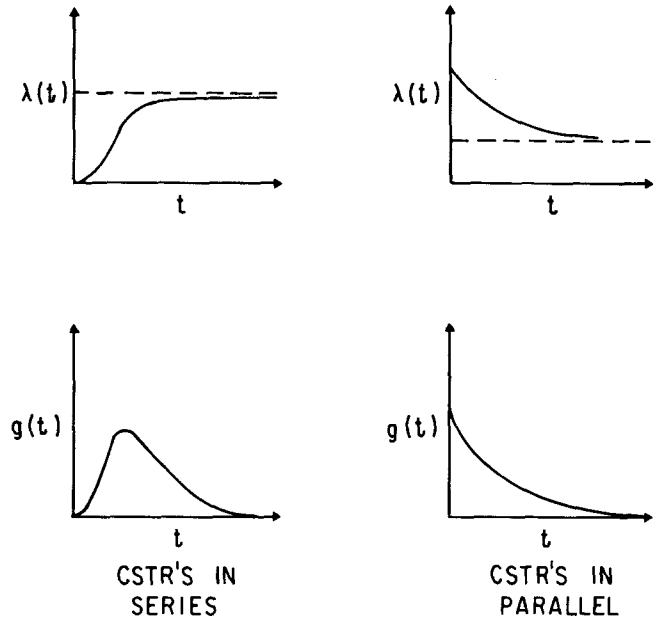


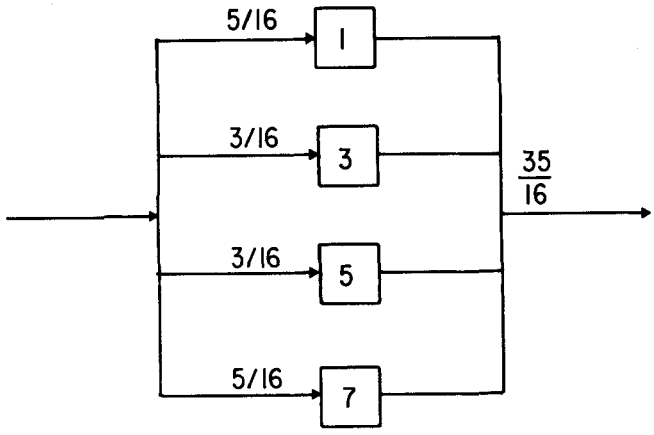
Fig. 2. and example 3. A parallel combination of stirred tanks.

corresponding transfer function has no zeros in the finite s plane (see example 2 and Figure 1). The intensity function is monotone decreasing for a parallel combination of CSTR's, with one CSTR in each branch, represented by a probabilistic mixture of exponential density functions (see Figure 2). Such an impulse response function is completely monotone, and the Markov parameters have alternating signs. The corresponding transfer function $G(s) = N(s)/D(s)$ where $D(s)$ and $N(s)$ are polynomials of degree n and $n - 1$, respectively, $N(0)/D(0) = 1$; and the roots $\{-\eta_r\}$ of $N(s)$ and $\{-\gamma_r\}$ of $D(s)$ are distinct, real, negative, and interlaced (see example 3 and Figure 3):

$$0 < \gamma_1 < \eta_1 < \gamma_2 < \eta_2 < \ldots < \eta_{n-1} < \gamma_n \qquad (51)$$

For a series parallel network of CSTR's, the intensity function may be monotone or nonmonotone depending on whether there exists a parallel pathway much slower than the other pathways in the system. Hence, when the intensity function is nonmonotone, the model must have some zeros in the finite s plane, which may be complex but with negative real parts. This is a useful guide in constructing realizations for such systems.

Having described the class of models to be used for the complete realization of the given impulse response function, we now proceed to specify the corresponding sign patterns in the factor matrix Q of Rissanen's factorization scheme. Following the present approach of imposing qualitative constraints on the input/output description of a dynamical system and examining their implications for the corresponding state space realization matrices, we may impose an additional such constraint, that of reciprocity (Wil-



$$G(s) = \frac{35}{16}\,\frac{(s+2)(s+4)(s+6)}{(s+7)(s+5)(s+3)(s+1)}$$

$$g(t) = \frac{35}{256}\,(5e^{-t} + 3e^{-3t} + 3e^{-5t} + 5e^{-7t})$$

Fig. 3. The intensity function $\lambda(t)$ and the impulse response function $g(t)$.

lems, 1972). A dynamical system is said to be externally reciprocal if its transfer function matrix is symmetric. The Markov parameter matrices will then be symmetric, and thus the Hankel matrix will be symmetric.

Single input-single output systems are automatically reciprocal. This property of single input-single output systems leads to an invariant diagonal matrix for all minimal realizations representing a given impulse response or transfer function. This invariant will be seen to be the signature matrix of the real, symmetric Hankel matrix of Markov parameters. It is found that in the factorization of the Hankel matrix, with Rissanen's scheme used, the information contained in this signature matrix is transmitted directly to the matrix Q. This observation is the basis of sign patterns observed in Q for the classes of systems discussed earlier.

We begin by summarizing the relevant results on reciprocity in state-space descriptions. A formal detailed description has been given by Willems (1972). If (A, b, c) is a minimal realization of a single input-single output transfer function, so is (A', c', b'). Hence, there exists a unique, nonsingular matrix T such that

$$A' = TAT^{-1} \quad c' = Tb \quad b' = cT^{-1} \tag{52}$$

Moreover, in this particular equivalence, T is symmetric:

$$T = T' \tag{53}$$

The equalities in (52) imply that

$$T[b\ Ab\ \ldots\ A^{n-1}b] = [c'\ A'c'\ \ldots\ (A')^{n-1}c'] \tag{54}$$

or

$$TQ = R'$$

Since T is a real symmetric matrix, it may be factored as $T = S'\Sigma_i S$ with S nonsingular and Σ_i a signature matrix (see Gantmacher, 1959, Part I, p. 298). A signature matrix is a diagonal matrix whose elements are $+1$, -1 or 0. Here, since T is nonsingular, Σ_i will have no zeros. The matrix S which yields this factorization is not unique, but by Sylvester's law of inertia (Gantmacher, 1959), the number of $+1$'s and -1's in Σ_i are both uniquely determined by T. Σ_i is critical in defining internal reciprocity:

$$T = S'\Sigma_i S \qquad \Sigma_i = I_{l_1} + (-I_{l_2}) \tag{55}$$

$$l_1 + l_2 = \dim A = n$$

Further, it has been shown that the integers l_1 and l_2 are uniquely determined by the transfer function $G(s)$ and are independent of the particular minimal realization used to generate T. Internal reciprocity may be defined by noting that a state-space realization (A, b, c) may be written as

$$\begin{bmatrix} \dot{x} \\ y \end{bmatrix} = \left[\begin{array}{c|c} A & b \\ \hline c & 0 \end{array}\right] \begin{bmatrix} x \\ u \end{bmatrix} \tag{56}$$

If there exists an $(n+1) \times (n+1)$ dimensional signature matrix such that

$$\Sigma \left[\begin{array}{c|c} A & b \\ \hline c & 0 \end{array}\right] = \left[\begin{array}{c|c} A & b \\ \hline c & 0 \end{array}\right]' \Sigma \tag{57}$$

(A, b, c) will be termed internally reciprocal with respect to Σ, and the state variables x will reflect internal reciprocity. The significance of Σ_i for internal reciprocity is that for the transfer function $G(s)$, there exists an internally reciprocal minimal realization with Σ of (57) given by

$$\Sigma = \left[\begin{array}{c|c} \Sigma_i & 0 \\ \hline 0 & 1 \end{array}\right] \tag{58}$$

Hence Σ_i is termed the internal signature matrix for the transfer function $G(s)$. This invariant matrix may be determined from the Hankel matrix of Markov parameters for the system. Let us consider, for an n-dimensional system, the factorization

$$H(n, n) = R(n, n)\ Q(n, n) \tag{59}$$

The matrix T of (52) for the resulting realization is given by

$$TQ = R' \tag{54}$$

with

$$T = T'$$

Therefore,

$$H = Q'T'Q = Q'TQ \tag{60}$$

Since $Q(n, n)$ is nonsingular, $H(n, n)$ is related to T by a congruence transformation. Also

$$T = S'\Sigma_i S \rightarrow H = (SQ)'\Sigma_i(SQ) \tag{61}$$

where SQ is nonsingular. Thus, the internal signature matrix for a given transfer function $G(s)$ is the same as the signature matrix congruent to the corresponding Hankel matrix of Markov parameters $H(n, n)$. Jacobi's theorem and a rule of Frobenius (Gantmacher, 1959, Part I, pp. 303 and 343) may now be invoked to determine l_1 and l_2 of (55) for an impulse response function from the signs of the leading principal minors of the corresponding Hankel matrix.

At each stage of the recursive factorization of the Hankel matrix, using Rissanen's algorithm, we may write the equation

$$|H(k, k)| = |R(k, k)|\,|Q(k, k)| \tag{62}$$

where $|\cdot| \equiv$ determinant of $\cdot$. By construction, R is a lower triangular matrix with 1's on the diagonal:

$$|R(k, k)| = 1 \qquad \forall\ k = 1, 2, \ldots \tag{63}$$

which implies that

$$|H(k, k)| = |Q(k, k)| \qquad k = 1, 2, \ldots \tag{64}$$

That is, the leading principal minors of the matrix Q have the same values (including signs) as the leading principal minors of the Hankel matrix H. The implications of this fact for realizing impulse response functions satisfying the two assumptions stated earlier will now be examined.

Among impulse response functions that are combinations

of exponential density functions, the parallel combination and the series combination are observed to be characterized by distinct sign patterns in the matrix Q. Let us first apply Rissanen's algorithm to the impulse response function of a parallel combination of CSTR's given in example 3. Such an impulse response function is completely monotone, and the Markov parameters follow an alternating sign sequence. The corresponding Hankel matrix with nine Markov parameters (normalized such that the first Markov parameter is 1) is factorized below:

$$H = \begin{bmatrix} 1 & -4 & 22 & -136 & 883 \\ -4 & 22 & -136 & 883 & -5\,884 \\ 22 & -136 & 883 & -5\,884 & 39\,832 \\ -136 & 883 & -5\,884 & 39\,832 & -272\,416 \\ 883 & -5\,884 & 39\,836 & -272\,416 & 1\,811\,520 \end{bmatrix}$$

$$= \underbrace{\begin{bmatrix} 1 & & & & \\ -4 & 1 & & & \\ 22 & -8 & 1 & & \\ -136 & 56.5 & -12 & 1 & \\ 883 & -392 & 106 & -16 & 1 \end{bmatrix}}_{R} \underbrace{\begin{bmatrix} 1 & -4 & 22 & -136 & 883 \\ 0 & 6 & -48 & 339 & -2352 \\ 0 & 0 & 15 & -180 & 1590 \\ 0 & 0 & 0 & 22.5 & -360 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}}_{Q} \quad (65)$$

There are no zero Markov parameters for this type of system, and hence Q is upper triangular. It may be shown (Widder, 1964, p. 167, Theorem 16) that the impulse response function is completely monotone if and only if the square symmetric Hankel matrices of Markov parameters of all dimensions are nonnegative definite; that is

$$H(k, k) = H^I(k, k) \geq 0 \qquad k = 1, 2, \ldots \quad (66)$$

This implies that the leading principal minors of the Hankel matrix are nonnegative. From (64), we then obtain

$$|Q(k, k)| \geq 0 \qquad k = 1, 2, \ldots \quad (67)$$

Since Q is upper triangular, (67) implies that the elements on the diagonal of Q are nonnegative; that is

$$q_{kk} \geq 0 \qquad k = 1, 2, \ldots \quad (68)$$

Among the nonzero rows of Q, corresponding to the independent rows of the Hankel matrix, the elements on the diagonal will be positive. The internal signature matrix for this type of system is the identity matrix $\Sigma_i = I$. The resulting realization matrices are

$$A = \begin{bmatrix} -4 & 1 & & \\ 6 & -4 & 1 & \\ 0 & 2.5 & -4 & 1 \\ 0 & 0 & 1.5 & -4 \end{bmatrix}; \quad b = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix};$$

$$c = [1 \quad 0 \quad 0 \quad 0] \quad (69)$$

For all systems of this type, with the Markov parameters normalized with respect to the first one, b will be a unit vector of appropriate dimension, with its first element equal to 1, like c. Then, the columns of Q are the first columns of successive powers of the matrix A. That is, if $e_1' = (1, 0, \ldots, 0)$

$$Q = [e_1 \quad Ae_1 \quad A^2e_1 \quad \ldots] \quad (70)$$

We shall now state two lemmas on the relation between A and Q, which may be proved by induction on n, the dimension of A. Let us denote by $a_{ij}^{(k)}$, the (i, j) entry of A^k.

Lemma 1. The columns of $Q(n, n) = [e_1 \; Ae_1 \ldots A^{n-1}e_1]$ will form an upper triangular matrix if and only if the elements in A below the first subdiagonal are zero; that is

$$\{a_{ij} = 0, \quad i > j + 1\} \leftrightarrow \{a_{i1}^{(k)} = 0, \quad i > k + 1\} \quad (71)$$

Combining this with the fact that in any realization obtained by Rissanen's algorithm, A is lower Hessenberg, we conclude that A must be a tridiagonal matrix, as in (69).

Lemma 2. Given that A is a tridiagonal matrix with 1's on the superdiagonal, the matrix $Q(n, n) = [e_1 \; Ae_1 \ldots A^{n-1}e_1]$ has positive diagonal elements if and only if the elements on the subdiagonal of A are positive; that is

$$q_{ii} > 0 \leftrightarrow a_{i+1,i} > 0 \quad (72)$$

Hence, for this type of system, A must be an input/output matrix (Beckenbach and Bellman, 1961) defined by the inequalities $a_{ij} \geq 0 \quad i \neq j$. Such a matrix has the property that e^{At} is nonnegative for $t \geq 0$; that is, all the components of the state vector are nonnegative for $t \geq 0$, if the initial condition is nonnegative. Further, for an input/output matrix A, e^{At} is asymptotically stable only if $a_{ii} < 0$ for all i (see Hearon, 1963). Thus, A is a tridiagonal matrix with 1's on the superdiagonal, satisfying

$$a_{ij} \geq 0 \quad i \neq j \quad \text{and} \quad a_{ii} < 0 \quad i, j = 1, 2, \ldots, n \quad (73)$$

This structure for A results in a regular sign pattern in all the columns of the rectangular matrix Q in (70), with n rows. The impulse response of the system may be viewed as a relaxation from the initial condition $x(0) = b = e_1$; that is

$$\dot{x} = Ax \quad x_1(0) = 1; \quad x_i(0) = 0, \quad i \neq 1 \quad (74)$$

The successive derivatives of each component of the state at $t = 0$ may then be related to $x_1(0) = 1$. With the given structure for A, we then obtain

$$x_i^{(l)}(0) = 0 \qquad l = 0, 1, \ldots, i - 2$$
$$(-1)^k x_i^{(k+i-1)}(0) > 0 \quad k = 0, 1, \ldots \quad (75)$$

where $x_i^{(j)}(0)$ denotes the j^{th} derivative of the impulse response of the i^{th} component of the state, evaluated at $t = 0$. It has been shown earlier [Equations (21) to (23)] that the i^{th} row of Q represents the i^{th} component of the state and that

$$q_{ij} = x_i^{(j-1)}(0) \qquad i, j = 1, 2, \ldots \quad (76)$$

Thus, in the i^{th} row of Q, the elements starting from the i^{th} column follow an alternating sign sequence. Looking back at the Q matrix for example 3 in (65), we note that this pattern is obtained. Let us define, for a vector $z = (z_1, z_2, \ldots, z_n)$ of real numbers $S^-(z)$ as the number of sign changes in the sequence obtained from $z_1, z_2, \ldots z_n$ by deleting all zero terms. The sign pattern in Q for the present type of system may be stated succinctly as follows.

In the realization of a completely monotone impulse response function, the first n columns among the n nonzero rows of Q form an upper triangular matrix with positive elements on the diagonal. For each column of Q among the nonzero rows of Q, $S^-(\cdot)$ has the maximum possible value.

Let us now turn to the series combination of CSTR's

and consider the impulse response function given in example 2. The 4×4 Hankel matrix formed from seven of the corresponding Markov parameters is factorized below:

$$\begin{bmatrix} 0 & 0 & 1 & 3.5 \\ 0 & 1 & -3.5 & 8.75 \\ 1 & -3.5 & 8.75 & -19.375 \\ -3.5 & 8.75 & -19.375 & 40.6875 \end{bmatrix} = \begin{bmatrix} 1 & & & \\ -3.5 & 1 & & \\ 8.75 & -3.5 & 1 & \\ -19.375 & 8.75 & -3.5 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 & -3.5 \\ 0 & 1 & 0 & -3.5 \\ 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{77}$$

If the factorization is continued after more columns are added in the Hankel matrix, the following rectangular matrix is obtained for Q (R being a square matrix is unchanged):

$$Q = \begin{array}{c} \begin{matrix} e_3 & e_2 & e_1 & Ae_1 & A^2e_1 & A^3e_1 \end{matrix} \\ \begin{bmatrix} 0 & 0 & 1 & -3.5 & 8.75 & -19.375 \\ 0 & 1 & 0 & -3.5 & 11.25 & -27.125 \\ 1 & 0 & 0 & -1 & 3.75 & -8.75 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array} \tag{78}$$

The number of zero Markov parameters is two, and the relative order of the system is three. The 3×3 matrix in the left upper section of Q is antidiagonal with 1's on the antidiagonal. This arises from the special pivoting technique employed in Rissanen's algorithm. In the subsequent columns of Q, a uniform sign pattern is observed; for each column of Q, $S^-(\cdot) = 0$.

The leading principal minors of H and hence the leading principal minors of Q here are given by

$$|Q(k,k)| = |H(k,k)| = 0 \qquad k < n \tag{79}$$

$$|Q(n,n)| = |H(n,n)| = (-1)^{n(n-1)/2} \tag{80}$$

Invoking the rule of Frobenius cited earlier and setting

$$|Q(k,k)| = |H(k,k)| = (-1)^{k(k-1)/2} \quad k = 1, 2, \ldots, n \tag{81}$$

we may obtain the internal signature matrix corresponding to the given impulse response.

Since the transfer function for this type of system has no zeros in the finite s plane and poles that are real and negative, the corresponding impulse response function $g(t)$ is a one-sided Polya density function of order n (see Karlin, 1968). Such a density function is unimodal and has the property that

$$\sigma_k \begin{vmatrix} g(t) & g'(t) & \ldots & g^{(k-1)}(t) \\ g'(t) & g''(t) & \ldots & g^{(k)}(t) \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ g^{(k-1)}(t) & g^{(k)}(t) & \ldots & g^{(2k-2)}(t) \end{vmatrix} > 0 \tag{82}$$

$$k = 1, 2, \ldots, n \qquad 0 < t < \infty$$

with

$$\sigma_k = (-1)^{k(k-1)/2}$$

Here, it is useful to note a more complete statement of the class of transfer functions representing Polya density functions; $g(t)$ is a one-sided Polya density function if and only if the reciprocal of its Laplace transform is an entire function of the form

$$\psi(s) = C\, s^k\, e^{\theta s} \prod_{i=1}^{\infty} (1 + \lambda_i s) \tag{83}$$

where $\theta \geq 0$, k is a nonnegative integer and $\lambda_i \geq 0 \; \forall \; i$ (see Karlin, 1968, p. 345, Theorem 3.2).

The realization matrices for example 2 are given by

$$A = \begin{bmatrix} -3.5 & 1 & 0 \\ -3.5 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}; \quad b = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}; \quad c = [1 \;\; 0 \;\; 0] \tag{84}$$

It is noted here that A is in companion form, and the corresponding transfer function may be written by inspection as

$$G(s) = \frac{1}{s^3 + 3.5s^2 + 3.5s + 1} \tag{85}$$

Moreover, A is such that

$$\begin{aligned} b &= e_n = (0, 0, \ldots, 0, 1) \\ Ab &= Ae_n = e_{n-1} \\ A^2b &= Ae_{n-1} = e_{n-2} \\ &\cdot \\ &\cdot \\ &\cdot \\ A^{n-1}b &= Ae_2 = e_1 \\ A^nb &= Ae_1 = -\alpha \end{aligned} \tag{86}$$

where $\mathbf{e}_j$ is a unit vector with the j^{th} component equal to 1, and $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n)$ is the set of coefficients of the characteristic polynomial of A:

$$\psi(s) \equiv \alpha^n + \alpha_1 s^{n-1} + \ldots + \alpha_n \tag{87}$$

Hence, the elements in the first column of A, which is the same as the column immediately following the antidiagonal submatrix in Q, must all be negative for A to be a stability matrix.

A stronger necessary condition for stability seems to hold in terms of the powers of A when the eigenvalues of the complete realization matrix A are real and distinct, as in the case of a Polya density function. Then A^m is observed to be column definite for all m. A matrix is said to be column definite (Hirschmann and Widder, 1955) if minors of the same order belonging to the same combination of columns are of the same sign. It is conjectured that this property of A^m arises from the fact that A^m may be written as

$$A^m = [A^m e_1, \quad A^{m-1}e_1, \ldots, A^{m-n+1}e_1] \tag{88}$$

This latter fact (88) may be seen by writing $A^m = [A^m\mathbf{e}_1 \; A^m e_2 \ldots A^m e_n]$ and by using the relations in (86); that is

$$A = [Ae_1 \quad e_1 \quad e_2 \quad \ldots \quad e_{n-1}]$$

$$A^2 = [A^2e_1 \quad Ae_1 \quad e_1 \quad \ldots \quad e_{n-2}]$$

and so on. Let us now define a real matrix $U = [u_{ij}]_1^n$ to be variation limiting if $y = Ux$ implies that $S^-(y) \leq \kappa(x) - 1$, where $\kappa(x)$ denotes the number of nonzero components of x. Hirschmann and Widder (1955) have proved a theorem stating that a real matrix is variation limiting if and only if it is column definite. Now e_1 has only one nonzero component, $\kappa(e_1) = 1$. So, if A^m is column definite for all m

$$S^-(A^m e_1) = 0 \qquad \forall\, m \tag{89}$$

However, the m^{th} column of the factor matrix Q is $A^{m-1}\mathbf{e}_1$. Hence, for each column of Q, $S^-(\cdot) = 0$.

Thus, for an impulse response function that is a convolution of n exponential density functions, the first $(n \times n)$ submatrix of Q is antidiagonal with 1's on the antidiagonal, and the subsequent columns satisfy $S^-(\cdot) = 0$.

For more general impulse response functions representing series-parallel networks of CSTR's, the recursive feature of Rissanen's algorithm results in a sign pattern in Q which is a composite of the two distinct sign patterns described above for the parallel and series combinations.

Let us consider the realization of the impulse response function in example 4 (the corresponding network of CSTR's is depicted in Figure 4). The Hankel matrix, with nine of the corresponding Markov parameters (normalized with respect to the first nonzero Markov parameter), is factorized below:

$$\begin{bmatrix} 0 & 1 & -10 & 82 & -628 \\ 1 & -10 & 82 & -628 & 4\,651 \\ -10 & 82 & -628 & 4\,651 & -33\,790 \\ 82 & -628 & 4\,651 & -33\,790 & 242\,472 \\ -628 & 4\,651 & -33\,790 & 242\,472 & -1\,727\,848 \end{bmatrix} = \begin{bmatrix} 1 & & & \\ -10 & 1 & & \\ 82 & -10 & 1 & \\ -628 & 82 & -12.75 & 1 \\ 4\,651 & -628 & 118 & -16 \end{bmatrix} \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & 12 & -153 & 1\,416 \\ & & & 11.25 & -180 \\ & & & & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & -10 & 82 & -628 \\ 1 & 0 & -18 & 192 & -1\,629 \\ 0 & 0 & 1 & -153 & 1\,416 \\ 0 & 0 & 0 & 11.25 & -180 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (90)$$

The controllability matrix $Q(n, n)$ here may be partitioned into four blocks

$$Q = \left[\begin{array}{cc} Q_L & Q_S \\ \hline 0 & Q_R \end{array}\right] \quad (91)$$

where Q_L is an antidiagonal matrix of dimension $q + 1$ with 1's on the antidiagonal, and Q_R is an upper triangular matrix of order $(n - q - 1)$. The leading principal minors of Q, and hence the leading principal minors of H, are given by the following relations:

$$\begin{aligned} |Q(k,k)| &= 0 \qquad k \leq q \\ |Q(q+1, q+1)| &= |Q_L| = (-1)^{q(q+1)/2} \\ |Q(k,k)| &= |Q_L|\ |Q_R(k,k)| \qquad k > q+1 \end{aligned} \quad (92)$$

$$\begin{bmatrix} 0 & 0 & 1 & -3.5 & 8.75 \\ 0 & 1 & -3.5 & 8.75 & \\ 1 & -3.5 & 8.75 & & \\ -3.5 & 8.75 & & & \end{bmatrix} = \begin{bmatrix} 1 & & & \\ -3.5 & 1 & & \\ 8.75 & -3.5 & 1 & \\ & 8.75 & -3.5 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 & -3.5 & 8.75 \\ 0 & 1 & 0 & -3.5 & \\ 1 & 0 & 0 & & \\ 0 & 0 & 0 & & \end{bmatrix} \quad (94)$$

The last relation is obtained from the fact that the partitioned matrix Q is upper quasitriangular (the block in the lower left section of Q is zero).

For the partial realization of dimension $(q + 1)$ to be stable, it is necessary that the elements in the first column of the block Q_s be all negative. In the lower block Q_R, the sign of the first entry is uncertain for a general series parallel combination. It may be $+1$ or -1; then the other diagonal elements of Q_R are observed to have the same sign. The sign pattern among the columns of Q_R, which is upper triangular, obeys the rule given for the parallel combination of CSTR's, that $S^-(\cdot)$ is the maximum possible in each column.

In general, the density functions considered in this work are all extended sign regular of order n (ESR_n) (Karlin, 1968, p. 70); that is, they obey the relation in (82), $\{\sigma_k\}_1^n$ now being some sequence of signs. For a parallel combination of CSTR's, $\sigma_k = +1\ \forall\ k$; for a series combination of CSTR's, $\sigma_k = (-1)^{k(k-1)/2}\ \forall\ k$. The sign regularity properties of such impulse response functions have been translated into sign patterns among the columns of the matrix Q.

We now proceed to illustrate the technique for deriving bounds on later Markov parameters. Let us consider the impulse response function of example 2 and assume that the number of zero Markov parameters and the first two nonzero Markov parameters have been estimated:

$$q = 2 \qquad Y_0 = Y_1 = 0$$

and

$$Y_2 = 1 \qquad Y_3 = -3.5$$

The factorization equation may be written as

$$\begin{bmatrix} 0 & 0 & 1 & -3.5 \\ 0 & 1 & -3.5 & \\ 1 & -3.5 & & \\ -3.5 & & & \end{bmatrix} = \begin{bmatrix} 1 & & & \\ -3.5 & 1 & & \\ & -3.5 & 1 & \\ & & -3.5 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 & -3.5 \\ 0 & 1 & 0 & \\ 1 & 0 & 0 & \\ 0 & 0 & 0 & \end{bmatrix} \quad (93)$$

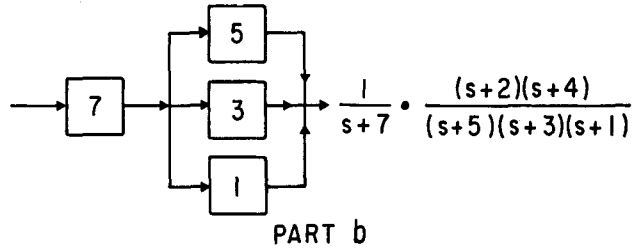
The fourth column of Q must have negative elements:

$$q_{24} < 0 \rightarrow Y_4 < 12.25$$

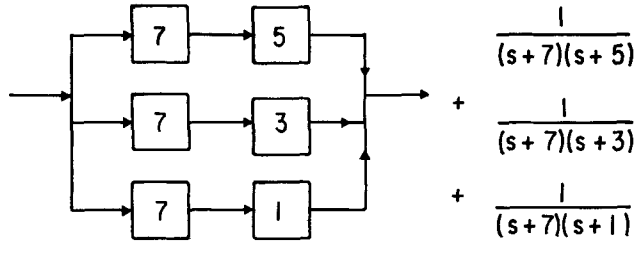
If we obtain the value of Y_4 satisfying this bound as $Y_4 = 8.75$, the exact value from the original system, we proceed further with

PART a

$$G(s) = (105/8)\frac{(s+2)(s+4)}{(s+7)(s+5)(s+3)(s+1)}$$



PART b



THE SCHEMATICS FOR PART a AND b ARE EQUIVALENT

THE IMPULSE RESPONSE FUNCTION IS

$$g(t) = \frac{105}{128}\left(e^{-t} + e^{-3t} + 3e^{-5t} - 5e^{-7t}\right)$$

Fig. 4. and example 4. The intensity function for a system which is monotone and has a maximum.

$$q_{34} < 0 \rightarrow Y_4 < -18.375$$

If we decide on the basis of the intensity function to model the given impulse response by a realization with no zeros, then the dimension of the model is three (since $q = 2$) and $S^-(\cdot) = 0$ for all columns of Q in the first three rows. Hence, $q_{25} > 0 \rightarrow Y_5 > -30.625$. We have thus obtained both lower and upper bounds on Y_5:

$$-30.625 < Y_5 < -18.375$$

These bounds contain the exact value of Y_5 for the original system, -19.375. We may not be able to estimate Y_4 so accurately; if the actual estimate obtained for Y_4 is 8.41, the bounds for Y_5 are changed accordingly to -16 and -29.5:

$$-29.5 < Y_5 < -16$$

In other cases, bounds calculated for Y_5 by using an approximate value for Y_4 may not contain the original exact value of Y_5. But, given that approximate value of Y_4, the calculated bounds on Y_5 must be obeyed by the estimate, regardless, for the overall realization to predict a smooth and stable response.

In the sequence of Markov parameters for a system, the bulk of the value of later Markov parameters comes, as we shall show in the following paper, from the partial realization determined from earlier Markov parameters. In this situation, a stagewise regression procedure with successive trend removal is very useful, particularly for a system with a large spread among its time constants, where the Markov parameters become very large quickly. Trend removal enables us to reduce the bias that may be required to satisfy the bounds on later Markov parameters, with lower degree fits (Beaton and Tukey, 1974). At each stage, twenty to thirty data points are used in a least-squares fit with eight to twelve Chebyshev polynomials $\{T_i(\tau)\}$ orthogonal on the continuous interval $(-1, 1)$. For the constrained regression, we use a ridge estimator (Hoerl, 1962) defined by

$$d^* = (X'X + kI)^{-1}(X'Z) \quad k \geq 0 \qquad (95)$$

when necessary, the original normal equation being

$$d = (X'X)^{-1}(X'Z) \qquad (96)$$

where Z is the vector of observations, X the Gram matrix, and d the vector of coefficients. The value of k used is the minimum required (say 0 to 0.2) to satisfy the constraints on d.

Thus, we have a composite algorithm combining stagewise estimation of Markov parameters and their recursive partial realization with information flowing to and fro between these two component schemes. The number of zero Markov parameters and the first two nonzero Markov parameters are first estimated; then a bound is obtained from the realization algorithm on the next parameter. The next stage of regression yields one or two more parameters; these are then used in the realization algorithm to obtain a higher-order realization as well as bounds on the subsequent Markov parameters which will be estimated in the next stage, and so on.

In the following paper, the use of this algorithm is illustrated with pulse responses from numerical examples of lumped and distributed systems, as well as an empirically measured residence time density function.

NOTATION

A, b, c = matrices in realization, Equation (1), Part I
C = concentration in liquid phase
C_s = concentration in solid phase
D = matrix defined in Equation (25), Part I
$\mathcal{D}$ = diffusivity of adsorbate in the fluid, Equation (23), Part II
d = vector of coefficients in Equation (96), Part I
d^* = vector of coefficients in Equation (95), Part I
e_i = unit vector with i^{th} component equal to 1
F^* = response to a unit step-down at the inlet of a linear system
F = response to a unit step-up at the inlet of a linear system
$f(t)$ = overall fitting function, Equation (33), Part I
$g(t)$ = impulse response function
$g_k(t)$ = constraint function of degree k, Equation (33), Part I
$G(s)$ = transfer function
$h_k(t)$ = fitted function at $(k+1)^{th}$ stage of regression, Equation (33), Part I
$H(i, j)$ = Hankel matrix with i rows and j columns, Equation (9), Part I
K = constant in Equation (34), Part I
k = constant in Equation (22), Part II
k_1, k_2 = constants in Equation (23), Part II
l_1, l_2 = integers in Equation (55), Part I
L = operator in Equation (21), Part II
L_1 = operator in Equation (22), Part II
m = degree of numerator polynomial of a rational transfer function
M = number of Markov parameters used to construct a partial realization, Equation (10), Part I
n = number of poles of a transfer function
p_j = j^{th} pole of a transfer function
q = number of zero Markov parameters for a given impulse response function, Equations (35) and (36), Part I
Q = controllability matrix, one of the factors of Rissanen's factorization scheme
R = observability matrix, the other factor of Rissanen's factorization scheme
R_* = matrix defined in Equation (17), Part I
S = matrix defined in Equation (55), Part I
s = Laplace transform variable
T = matrix defined in Equation (54), Part I
$T_i(\tau)$ = i^{th} degree Chebyshev polynomial
t = time
$u(t)$ = input, scalar, Equation (1), Part I
$v(t)$ = error, Equation (31), Part I
V = interstitial velocity, Equation (23), Part II
X = Gram matrix, Equations (95) and (96), Part I
$\mathbf{x}$ = state vector, Equation (1), Part I
y = output, scalar, Equation (1), Part I
Y_k = $(k+1)^{th}$ Markov parameter, Equation (5), Part I
Z = spatial coordinate, axial direction
$z(t)$ = measured output, with measurement error
z_i = i^{th} zero of a transfer function
$\mathbb{Z}$ = vector of observations of output at different times

Greek Letters

α_i = coefficient of s^{n-i} in the characteristic polynomial of A
β_i = coefficient of s^{m-i} in the numerator of a transfer function
β = fractional void volume, Equation (23), Part II
γ_i = i^{th} mode, Equation (41), Part I
δ = tolerance level, Equation (19), Part I
$\epsilon(t)$ = measurement noise, Equation (21), Part I
$\eta(t)$ = error, Equation (32), Part I
θ = time delay
$\kappa(x)$ = number of nonzero components of x
λ_i = parameter in Equation (83), Part I
ν = parameter in Equation (26), Part II

$\Pi(Z)$ = function in Equation (21), Part II
$\rho(Z)$ = function in Equation (21), Part II
σ_k = sign of k^{th} determinant in Equation (82), Part I
$\psi(s)$ = characteristic polynomial of A

Manuscript received September 15, 1975; revision received and accepted November 25, 1975.

Part II. The Approximation Problem

The composite algorithm derived in Part I is used to construct models from pulse responses of lumped and distributed systems, as well as an empirically measured residence time density. Along the way, salient points in the numerical implementation of the algorithm are indicated. In the present recursive procedure, the initial transient is predicted accurately by lower-order partial realizations; successive partial realizations involve progressively longer tails of the pulse response. The zeroth moment of the impulse response is used to advantage when realizations with no zeros are appropriate

SCOPE

In Part I of this two-part series, a sequential algorithm was derived for obtaining practical realizations from realistic response data of continuous time systems with intermittent measurements. In Part II, the modeling procedure will be illustrated with impulse responses from numerical examples of lumped and distributed systems, as well as an empirically measured residence time density.

The question that arises in evaluating these models is: In what sense is the input/output relation of a partial realization an approximation to the given input/output relation? The answer depends on the data set used to derive these realizations. In earlier work, the moments of the impulse response have been used to derive realizations. This is possible, since the moments form a set of parameters related to powers of A^{-1} in the same way that the Markov parameters are related to powers of A in the realization (A, b, c) (Bruni, 1969). If moments are used in the realization algorithm, a low frequency approximation is obtained which may not bring out the initial transient of the original response. The Markov parameters yield a high frequency approximation which may not bring out the long time behavior of the system. Rossen (1972) has used a combined set of parameters with some moments preceding the Markov parameters to obtain in some cases a better long-time approximation. However, for other cases, he obtained unstable models for stable physical processes. The regularization procedure presented in Part I, and used here, is based on the use of Markov parameters alone. Here, we shall compare partial realizations of different dimensions in terms of their impulse responses. In this comparison, the different data sets are finite sequences of Markov parameters of increasing length. In addition, we shall discuss the range of modes that may be identified from a given impulse response.

CONCLUSIONS AND SIGNIFICANCE

The present recursive realization algorithm identifies the faster modes first and then identifies the slower modes; that is, the initial transient is predicted accurately by lower-order partial realizations; successive partial realizations have progressively longer tails. Hence, the tail of the response, if inordinately long and inaccurate, may be ignored while lower-order partial realizations are constructed. This feature is a definite improvement over the method of moments, which is extremely sensitive to the tail of the response.

A distributed system may be modeled by a finite dimensional realization coupled with a time delay. The number of zero Markov parameters estimated then depends on the time delay chosen; in selecting this combination, we seek to ensure a minimal degree of smoothness in the predicted response, keeping the dimension of the realization low (at most 5).

The intensity function provides useful information for both lumped and distributed systems. As illustrated by the examples, systems with monotone increasing intensity functions are easier to model, partly because the zeroth moment can then be taken into account. When the zeroth moment is used, the value of the first nonzero Markov parameter assumes increased importance.

CHARACTERIZING THE APPROXIMATION

Sequential model building methods such as the dominant pole technique and the present recursive realization procedure may be compared with respect to the order of identification of the system's response modes. In the dominant pole technique, the slowest mode or the largest time constant is identified first; then this is peeled off from the response curve to identify the next slower mode, and so on (Sheppard, 1962, Chapter 11). In the recursive realization procedure, however, as the dimension of the partial realization increases, slower modes are added on. The impulse responses of higher-order partial realizations have progressively longer tails. This is illustrated by the partial realizations of the impulse response function (see example 4 of Part I):

$$g(t) = \frac{1}{16}\left(e^{-t} + e^{-3t} + 3e^{-5t} - 5e^{-7t}\right) \qquad (1)$$

with transfer function

$$G(s) = \frac{(s+2)(s+4)}{(s+7)(s+5)(s+3)(s+1)} \qquad (2)$$

The complete realization matrices, obtained from the first nine Markov parameters, are:

$$A = \begin{bmatrix} -10 & 1 & 0 & 0 \\ -18 & 0 & 1 & 0 \\ 12 & 0 & -2.75 & 1 \\ 0 & 0 & 0.9375 & -3.25 \end{bmatrix}; \quad b = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}; \quad c = [1 \quad 0 \quad 0 \quad 0] \qquad (3)$$