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STATIONARITY CONDITIONS FOR LINEAR MODELS

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Abstract—The problem of building a linear stationary model for a process given by evenly spaced discrete or continuous observations is considered. Criteria are proposed for the existence of such a model governed by a vector difference or differential equation. Various model representations in discrete and continuous forms are studied and numerical methods for their identification are developed. This gives the order and dynamics of a model in the canonical form. To include processes in noisy environment, a moving average of observations is introduced into deterministic identification algorithms. Different integral forms of the moving average of continuous observations are proposed for identification of models governed by a system of linear stationary differential equations. Discussion of some experimental and computational results is presented.

1. INTRODUCTION

The problem of model building in the form of systems of linear stationary differential equations is ubiquitous in many areas of science. In engineering it arises in systems analysis. In biology it is found under the general heading of compartment analysis. It is found in many areas of economics (production models, etc.) and it plays the key role in the study of socioeconomic processes.

The usual line of research is as follows. Given a sequence of observed data, one assumes a linear stationary model

$$\frac{dx}{dt} = A(p)x, \quad x(t_0) = x_0(p), \quad t \geq t_0 \tag{1}$$

$$y(t) = h(p)x, \quad x \in R^m, \ y \in R^1 \tag{2}$$

with undetermined parameters $(p_1, \ldots, p_k) = p$ to be found by fitting the vector function $x(t, p) \in R^m$ to observed data $y_1, \ldots, y_s$; $y_i = y(t_i)$. For doing that the least-squares method is frequently used. Some authors, instead of taking a differential model (1), consider algebraic models in the form of polynomials [1] or some exponential functions like $x = at^b e^{ct}$, where a, b, c are constants to be determined [2]. Obviously, a differential model (1) represents far broader class of functions which includes all finite combinations of sine, cosine, and exponential functions with polynomial coefficients. Thereby, indirect measurements assumed by (2) and dependence on a vector-parameter $p = (p_1, \ldots, p_k)$ in (1, 2) add to the diversity of functions represented in the class of dynamic models (1, 2), this giving also a new and richer sense to mathematical modelling in terms of dynamic models.

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If the model is not known a priori (as it is known, e.g., in mechanics), then its order and structure depend on the experience of a researcher and the model is meant successful, if iterations converge to a unique vector-parameter p^* robustly under variations of the initial guess p_0. In many cases this technique serves well. However, it is easy to verify that such robust convergence is not sufficient for a model to be adequate.

In complex cases it is important to be able, prior to building a model, to check whether or not a model exists and, if it does, to determine the model and time intervals on which it exists. This paper offers necessary and sufficient conditions which must be satisfied, if a linear stationary model exists. The conditions are easily computable and are based solely on the observed data. An algorithm is developed to accomplish the computations which deliver the order and canonical form of a model and the intervals of time on which this model exists. It may well happen to be a model with variable structure (including variable order) as is common for complex biological and economic systems.

This research was inspired by the investigation of Jennrich and Bright [3] and its discussion by Wiggins [4], so the results are applied to the same case study of a catenary model concerning the distribution of sulfate in the body of a baboon named Brunhilda. The observed data are given as measurements of radioactivity in blood samples taken from Brunhilda at specified times after an initial bolus injection containing radioactive sulfate. The results of [3, 4] were further discussed in [5]. For discussion of structural identifiability see also [6–12].

2. DISCRETE OBSERVATIONS

We start with an exact sample-data representation of the system (1), (2):

$$x_{n+1} = Fx_n, \quad F = \exp(A\,\Delta t) = \sum_{k=0}^{\infty} \frac{A^k \Delta t^k}{k!} \tag{3}$$

$$y_n = hx_n, \quad x_n \in R^m, \quad y_n \in R^1, \quad n = 0, 1, \ldots \tag{4}$$

where $x_n = x(t_n)$, $y_n = y(t_n)$, $t_n = t_0 + n\Delta t$, $\Delta t = \text{const}$; y_n are given observations. The values of A, h, x_0, hence, F and x_n are not known. However, $F = \text{const}$, if $A = \text{const}$ and $\Delta t = \text{const}$.

Discrete system (3, 4) yields exact values $x(t)$, $y(t)$ of the system (1), (2) at times $t_n = t_0 + n\Delta t$. If one takes the first two terms of the series (3), then the system (3) with the matrix $F^* = I + \Delta t A$ (I = unit matrix) gives a discrete approximation to the system (1). The values of its state vector x_n^* do not coincide with $x(t)$ at times t_n but tend to $x(t)$ as $\Delta t \to 0$. So, if only discrete observations are available, the discrete model (3, 4) gives a complete and exact description of the behavior of the system (1) in regard to the information contained in the available discrete observations.

2.1 *Necessary conditions*

Some results discussed in these two subsections have been obtained by Lee [13]. We drop certain assumptions not justified by the available information. It is also expedient to present a simplified direct derivation which gives convenient expressions for computation and immediately leads to the continuous case.

Assume that for some finite m there exists a linear stationary system (3) with the output y_n (4).

The observations y_n are the only values that are known. We assume the constancy of m, F, h and ask what condition this constancy induces on the observations y_n.

The answer comes from one fundamental result of the theory of linear spaces: given a vector $h' \in R^m$ and a constant $m \times m$ matrix (linear operator) F', ($' =$ transpose) there is a unique cyclic subspace of dimension $r \le m$ invariant with respect to the operator F' and this subspace $\{M\} \subseteq R^m$ is generated by the first r linearly independent vectors of the chain h', $F' \cdot h', \ldots$, that is

$$\{M\} = \{h', F'h', \ldots, F'^{r-1}h'\} \subseteq R^m, \quad r \le m, \quad F'\{M\} \subseteq \{M\}. \tag{5}$$

The relations (5) can be formulated in the form that, whatever constant values of m, h, F, there is some $r \le m$ such that the first r vectors in the chain h', $F'h'$, $F'^2h', \ldots$ are linearly independent and all others depend on those first in the chain. For example, the $(r+1)$-th vector is given by the expression:

$$F'^r h' = a_1 h' + a_2 F'h' + \cdots + a_r F'^{r-1}h', \quad r \le m \tag{6}$$

where the coefficients a_i $(i = 1, \ldots, r)$ are uniquely determined by h and F.

Now, let us fix arbitrary x_s $(s \ge 0)$ as initial state and write $r+1$ successive observations, as follows from (3, 4):

$$\begin{aligned} y_s &= hx_s \\ y_{s+1} &= hx_{s+1} = hFx_s \\ &\cdots\cdots\cdots\cdots \\ &\cdots\cdots\cdots\cdots \\ &\cdots\cdots\cdots\cdots \\ y_{s+r-1} &= hx_{s+r-1} = hFx_{s+r-2} = hF^{r-1}x_s \\ y_{s+r} &= hx_{s+r} = hFx_{s+r-1} = hF^r x_s. \end{aligned} \tag{7}$$

If we transpose the equalities (7) and write the linear combination with coefficients from (6), we come to the equation:

$$\begin{aligned} \Delta_{sr} &= -y_{s+r} + a_1 y_s + a_2 y_{s+1} + \cdots + a_r y_{s+r-1} \\ &= x_s'(-F'^r h' + a_1 h' + a_2 F'h' + \cdots + a_r F'^{r-1}h') = 0, \quad (s = 0, 1, \ldots), \text{ whatever } x_s \end{aligned} \tag{8}$$

Conclusion 1. If the observations $y_0, y_1, \ldots, y_n, \ldots$ are produced by a linear stationary system (1, 2) or (3, 4) (which makes no difference in regard to the observations), then, whatever x_0, h, A, Δt, F in (1, 2) or (3, 4), there is a number r, $m \ge r \ge 1$, such that the observations satisfy a linear r-th order difference equation

$$y_{s+r} = a_1 y_s + a_2 y_{s+1} + \cdots + a_r y_{s+r-1}, \qquad s = 0, 1, 2, \ldots \tag{9}$$

Remark. If $r = m$ in (5) for some particular h, F, then the system (3, 4) is called completely observable [14]. The origin of this term is that in this case, given the first m observations and known matrices in (7), one can compute the (unknown) state x_s from (7): $x_s = M'^{(-1)}Y$, where M is the matrix with columns from (5), and Y is the left hand vector in (7).

The coefficients $a_1, \ldots, a_r$ in (9) depend on the (unknown) matrices h, F (see (6)). In most cases, however, they can be determined directly from the observations using (9). Writing (9) for $s = 0, 1, \ldots, r-1$, one gets the linear system:

$$\begin{bmatrix} y_r \\ y_{r+1} \\ y_{r+2} \\ \cdots \\ y_{2r-1} \end{bmatrix} = \begin{bmatrix} y_0 & y_1 & y_2 & \cdots y_{r-1} \\ y_1 & y_2 & y_3 & \cdots y_r \\ y_2 & y_3 & y_4 & \cdots y_{r+1} \\ \cdots & \cdots & \cdots & \cdots \\ y_{r-1} & y_r & y_{r+1} & \cdots y_{2r-2} \end{bmatrix} \cdot \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \cdots \\ a_r \end{bmatrix} = C_{0r} \cdot q \tag{10}$$

The matrix C_{sr} ($s = 0$ in (10)) can prove to be singular or not.

If the system (3, 4) is completely observable and the initial state x_0 generates all the modes of the system (in other words, x_0 does not belong to any of the root subspaces of the operator F), then the matrix $C_{sm}(r = m)$ is nonsingular. This is the result of Lee [13], which needs the correction that the time increment Δt must be appropriately chosen (see the sequel). Even in this case, however, x_0, h, F are not known in advance to make this conclusion. This is a major setback of the theory presented earlier [5]: all the information must be drawn from the observations.

The invariant subspace $\{M\}$ of (5), $F'\{M\} \subseteq \{M\}$, coincides with a certain root subspace of the operator F', if $r < m$. Denote the bases of the root subspaces of F' by $T'_1, \ldots, T'_k, \ldots, T'_u$; $\dim T'_i = r_i$, $\sum_{i=1}^{u} r_i = m$, and let the first k subspaces coincide with $\{M\}$:

$$\{T'_1, \ldots, T'_k\} = \{M\}, \{T'_{k+1}, \ldots, T'_u\} \cap \{M\} = \emptyset, \qquad \sum_{i=1}^{k} r_i = r < m. \tag{11}$$

Consider the transposed inverse of the matrix $[T'_1, \ldots, T'_k, \ldots, T'_u]$, that is, the matrix

$$\begin{aligned} T^* &= [T'_1, \ldots, T'_k, \ldots, T'_u]^{(-1)'} \\ &= [T_1^{-1}, \ldots, T_k^{-1}, \ldots, T_u^{-1}] \end{aligned} \tag{12}$$

which defines the root subspaces for the original operator F in (3). By construction we have the orthogonality

$$M'[T_{k+1}^{-1}, \ldots, T_u^{-1}] = 0, \quad \text{so} \quad h \cdot [T_{k+1}^{-1}, \ldots, T_u^{-1}] = 0 \tag{13}$$

where M is a basis in $\{M\}$.

Further, if $x_0 \in T_i^{-1}$ then $x_{n+1} = Fx_n \in T_i^{-1}$ and the vectors x_n span the entire subspace T_i^{-1} for $n = 0, 1, \ldots, r_i - 1$.

Now, consider the representation of an unknown initial state x_0:

$$x_0 = T_1^{-1}p_1 + \cdots + T_k^{-1}p_k + T_{k+1}^{-1}p_{k+1} + \cdots + T_u^{-1}p_u; \quad \dim p_i = r_i. \tag{14}$$

If for x_0 actually realized, it appeared that $p_1 = 0, \ldots, p_k = 0$, then $x_0 \in \{T_{k+1}^{-1}, \ldots, T_u^{-1}\}$, hence, it does not affect the observations which by virtue of (13) are all zero: $y_n = 0$, $n = 0, 1, \ldots$, and vice versa.

In non-trivial cases some of the p_i ($k \geq i \geq 1$) are nonzero, which implies nonzero output. Suppose $p_1 \neq 0$, $p_2 \neq 0, \ldots, p_t \neq 0$ ($t \leq k$). Then, if the time increment Δt is appropriately chosen (see the sequel), the rank of the matrix C_{sr} in (10) equals $r_1 + r_2 + \cdots + r_t \leq r$ ($=r$, if $t = k$) and remains constant for $s = 0, 1, 2, \ldots$. We come to the following proposition.

Conclusion 2. If the observations $y_0, y_1, \ldots, y_n, \ldots$, with Δt appropriately chosen, are produced by a linear stationary system (1, 2) or (3, 4), then the minor arrays C_{sn} ($s, n = 0, 1, \ldots$) of the infinite matrix

$$\begin{bmatrix} y_0 & y_1 & y_2 & \cdots & y_n & \cdots \\ y_1 & y_2 & y_3 & \cdots & y_{n+1} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix} \tag{15}$$

have the maximum rank $w = r_1 + r_2 + \cdots + r_t$ in the sense that all C_{sn} with $n \leq w$ have the rank n and all C_{sn} with $n \geq w$ have the rank w irrespective of s which indicates the start y_s of the minor array C_{sn}. So the rank of C_{sn} remains constant and not greater than $w = r_1 + \cdots + r_t$, where $r_1, \ldots, r_t$ are the dimensions of the root subspaces affected by the initial vector x_0. Since the maximum rank of C_{sn} is w , there are only w linearly independent observations in the chain (7), thus, the number r (8, 9) must be replaced by the number w, $w \leq r \leq m$, and exactly w coefficients can be determined from the system (10).

2.2. *Sufficiency*

To infer the existence of a linear stationary model (3, 4) from the available information, we assume a property which, if it exists, is easily computable given a series of observations $y_0, y_1, \ldots, y_n, \ldots$. Two convenient procedures mathematically equivalent but different in computation are considered.

2.2.1 *Horizontal sweep method.* Take the first nonzero observation, say y_0, and make a forward sweep to check the condition:

$$D_{s1} = y_{s+1}y_{s-1} - y_s^2 = 0, \quad s = 1, 2, \ldots \tag{16}$$

Usually this condition does not hold and it appears just at the first computation for D_{11}. Then take the first k rows in the matrix (15) and make successive forward sweeps for $k = 2, 3, \ldots$ to find the least k^* for which the following conditions are satisfied:

$$D_{sk^*} = C_{s+1,k^*} - C_{sk^*}C_{s-1,k^*}^{-1}C_{sk^*} = 0 \qquad (s = 1, 2, 3, \ldots) \tag{17}$$

Again, the fact that conditions (17) do not hold appears in the first computation; singularity of the matrix C_{sk}, that is $|C_{sk}| = 0$, obtained before arrival at certain k^* for which (17) are all satisfied means that for that current $k < k^*$ conditions (17) do not hold.

Suppose that eventually we arrive at some $k = k^*$ for which the conditions (17) hold for all the observations or at least for the first n observations within the time interval $[t_s, t_{s+n} = t_s + n\Delta t]$ of interest. Then on this interval $[t_s, t_{s+n}]$ there exists a linear stationary model with the output $y_s, y_{s+1}, \ldots, y_n$.

To prove this result, we rewrite the conditions (17) in the form

$$C_{sk^*}^{-1}C_{s+1,k^*} = C_{s-1,k^*}^{-1}C_{sk^*} = Q_{k^*} = \text{const}, \qquad (s = 1, 2, \ldots) \tag{18}$$

where by Q_k we denote a constant matrix which exists for $k = k^*$ when conditions (17) are all satisfied.

By inspection of the structure (15), it becomes clear that the matrix Q_{k^*} has the canonical form:

$$Q_{k^*} = \begin{bmatrix} 0 & 0 & \dots & 0 & a_1 \\ 1 & 0 & \dots & 0 & a_2 \\ 0 & 1 & \dots & 0 & a_3 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 & a_{k^*-1} \\ 0 & 0 & \dots & 1 & a_{k^*} \end{bmatrix} = \left[\begin{array}{c|c} 0 & \\ \hline & q \\ I & \end{array}\right], \quad q = \begin{bmatrix} a_1 \\ \vdots \\ a_{k^*} \end{bmatrix} \tag{19}$$

where the elements $[a_1, \dots, a_{k^*}] = q'$ are to be determined.

Now it is easily seen that conditions (17) satisfied for $k = k^*$ imply the recurrence relation (see (18)):

$$C_{s+1,k^*} = C_{sk^*} Q_{k^*}, \quad (s = 0, 1, 2, \dots) \tag{20}$$

The first $k^* - 1$ columns of the matrix equation (20) give trivial identities $y_i = y_i$ $(i = s+1, s+2, \dots, s+2k^*-2)$ and the last column yields the k^*th order difference equation

$$y_{s+k^*} = a_1 y_s + a_2 y_{s+1} + \dots + a_{k^*} y_{s+k^*-1}, \quad (s = 0, 1, 2, \dots) \tag{21}$$

This equation is equivalent to a system of k^* first-order difference equations which are given by the transpose of the relation (20):

$$C_{s+1,k^*} = Q'_{k^*} C_{sk^*}, \quad (s = 0, 1, 2, \dots) \tag{22}$$

Indeed, introducing the k^*-vector

$$\bar{x}'_s = \{y_s, y_{s+1}, \dots, y_{s+k^*-1}\} \tag{23}$$

one comes to the system equivalent to (22) with the (scalar) output $y_s = h\bar{x}_s = [1, 0, \dots, 0]\bar{x}_s$ evident by construction of the vector $\bar{x}_s$. So the recurrence relations (20) and (22) are equivalent both to difference equation (21) and to the following system which has the special form called canonical:

$$\bar{x}_{n+1} = Q'_{k^*}\bar{x}_n, \quad \bar{x}_n \in R^{k^*}, \quad Q'_{k^*} = \left[\begin{array}{c|c} 0 & I \\ \hline \multicolumn{2}{c}{q'} \end{array}\right] \tag{24}$$

$$y_n = h\bar{x}_n, \quad y_n \in R^1, \quad h = [1, 0, \dots, 0]. \tag{25}$$

This system has exactly the general form (3), (4), so sufficiency of conditions (17) for the existence of a linear stationary system (24, 25) is shown. The relation (20) by virtue of the structure (15) holds for any $k > k^*$ with the matrix Q_k of the same structure (19) and first $k - k^*$ elements a_i all zero: $a_1 = 0, \dots, a_{k-k^*} = 0$. So, if there exists a k^* for which (20) is satisfied, then (20) is valid for any $k > k^*$ with singular matrix Q_k, rank $Q_k = k - 1$, containing the same information (the same nontrivial elements $a_1, \dots, a_{k^*}$). So all C_{sk} $(s = 1, 2, \dots)$ are singular for $k > k^*$ and the condition (17) may hold only once for $k = k^*$, if any. Hence, there is no need for further search, once k^* has been found.

After finding k^*, the matrix Q_{k^*} can be computed:

$$Q_{k^*} = C_{sk^*}^{-1} \cdot C_{s+1,k^*}. \tag{26}$$

If one retains in the matrices Q_{k^*} and C_{s+1,k^*} of (20) only the last columns, one obtains the system identical to (10). So $a_1, \ldots, a_{k^*}$ calculated by (26) are equal to those of (9) with the note that $k^* = r = w$, since w is the maximum dimension of a nonsingular C_{sk} and k^* is the only dimension for which (17) is satisfied. This completes the following result.

Conclusion 3. The condition (17) is necessary and sufficient for the existence of a linear stationary model (3, 4) with the given output $y_n = y(t_n)$, $n = 0, 1, \ldots$. The model is identified in the canonical form (24, 25) with the matrix Q_{k^*} calculated by (26) and an initial state $\bar{x}_0$ given simply as the first k^* observations (23). The order $k^* = w$ of the model is minimal in the sense that no model of order $k < k^* = w$ exists and the infinity of stationary models with $k > w$ can be obtained by enlarging the state vector $\bar{x}_n$ and completing the matrices Q_k and h in the way that they preserve the structures (24), (25) with the same q' standing flush to the right and the first $k - w$ elements of the last row being all zero. Obviously, nonsingular linear transformations give other equivalent models of orders $k \geq w$, but the canonical model (24, 25) of minimal order w is unique.

2.2.2. *Vertical sweep method.* Compute the matrices Q_k according to (26) for $s = 0$ and $k = 1, 2, \ldots$. Generally, for $k = 1, 2, \ldots, w$ all Q_k appear in the form (19) and the form of Q_{w+1} will become distorted. It indicates that $C_{s,w+1}$ is almost singular (C_{sk} are rarely singular because of noise in y_n), so w is the minimal order of a supposed stationary model. Then make horizontal sweep for $k = w$ and $s = 1, 2, \ldots$ to determine the interval of its existence. If all Q_w appear identical, then the model (24, 25) exists on the interval beginning at $s = 0$, and, with $Q_w = \text{const}$ computed, this model is already identified. If Q_w will vary for $s = 1, 2, \ldots$, then on the interval with varying Q_w a model of order w does not exist. Start again computing Q_k for $s = 1$, $k = 1, 2, \ldots$. Then, if a model is not found, continue for $s = 2$, $k = 1, 2, \ldots$, etc.

2.3. *Moving average of observations*

Observations as well as a system itself contain noise, so the conditions (17) and correspondent relations are in practice always distorted. Zero mean noise in a measuring device can be eliminated by using a moving average of observations

$$Z_s = \frac{1}{N} \sum_{i=s}^{s+N-1} y_i, \qquad s = 0, 1, 2, \ldots \tag{27}$$

in place of original observations y_s ($s = 0, 1, 2, \ldots$). It follows from linearity of the model (3), (4) that the matrix Q_w identified by using Z_s in place of y_s will correspond to the mean values of the observations for sufficiently large number N. However, the initial state cannot be identified by placing Z_s for y_s in (23), so that $\bar{x}_s$ (23) becomes, as before, corrupted by a realization of the noise.

The measure of distortion or deviation from a linear stationary path is given by the value of the last element $\Delta_{kk}(s)$ of the matrix D_{sk} in (17) (all other elements of D_{sk} are zero whatever y_s employed). The value $\Delta_{kk}(s)$ equals exactly $-\Delta_{sr}$ (for $r = k$) of (8) and gives the current deviation from the path of a would-be linear stationary model identified at the moment t_s.

2.4. *Is there anything else to identify that can be identified?*

A model identified as above has the canonical form (23–25). What is actually identified is the characteristic polynomial

$$\begin{aligned} |Q_w - \lambda I| &= (-1)^{w+1} a_1 - \lambda[(-1)^w a_2 - \lambda[\ldots - \lambda(a_w - \lambda)]]\ldots] \\ &= (-1)^{w+1}(a_1 + a_2\lambda + \cdots + a_w \lambda^{w-1} + \lambda^w) \end{aligned}$$

(or the vector $q' = \{a_1, a_2, \ldots, a_w\}$ of its coefficients) corresponding to the part of the completely observable subsystem of (3, 4) affected by the (actually realized) initial state x_0 from (3). Its projection $\bar{x}_0$, $\dim \bar{x}_0 = w$ onto the completely observable subspace $\{M\}$ (5) is given by (23) where $k^* = w$ is the total dimension of those root subspaces within $\{M\}$ which are affected by x_0 in (3). The nonsingular transformation with the matrix T^* form (12), slightly modified in order to get real vectors instead of each pair of complex conjugate Jordan vectors, converts (3, 4) into a form with exhibited block-space structure. The additional transformation of the blocks actually producing the given set of observations converts the corresponding subsystem into the canonical form (23–25). Then it is easily seen there is nothing more to identify since the subsystem generating the observations is completely identified by (23–25) and all other blocks give just no trace on the observations.

However, canonical coordinates usually do not coincide with natural (physical) coordinates and it leads to the situation when the identified canonical model cannot be employed directly to control a process by some physical parameters distinct from the coefficients a_i ($i = 1, \ldots, w$), even in the case when the system is completely observable and the state x_0 affects all the modes. As an illustration, consider the example of a linear oscillator

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + kx = 0; \quad t \geq 0, \quad x(0) = x_0, \quad \frac{\mathrm{d}x(0)}{\mathrm{d}t} = \dot{x}_0 \tag{28}$$

$$y_n = y(t_n) = x(t_n), \quad t_n = n\Delta t, \quad n = 0, 1, \ldots, N; \quad \Delta t > 0. \tag{29}$$

Denoting $x_1 = x$, $x_2 = \mathrm{d}x/\mathrm{d}t$, $\omega^2 = k/m$, one gets the Cauchy form of the equation (28)

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\omega^2 & 0 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad \text{or} \quad \frac{\mathrm{d}x^*}{\mathrm{d}t} = Ax^*, \tag{30}$$

$$x^* = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad x^*(0) = \begin{bmatrix} x(0) \\ \mathrm{d}x(0)/\mathrm{d}t \end{bmatrix} = \begin{bmatrix} x_0 \\ \dot{x}_0 \end{bmatrix}$$

which appears already canonical. The system is completely observable and any real $x^*(0) \neq 0$ affects all the modes (since $\lambda = \pm\omega i$, $i^2 = -1$, and eigenvectors are complex conjugate).

Discrete observations come out as if they were produced by a discrete system of the structure

$$x_{n+1}^* = Fx_n^*, \quad F = \exp(\Delta t A), \quad x_0^* = x^*(0), \quad n = 0, 1, \ldots \tag{31}$$

$$y_n = [1, 0]x_n^* \tag{32}$$

which corresponds to (28–30) and yields exact sampled data $x_n^* = x^*(t_n)$ on the trajectories since $x_{n+1}^* = x^*(t_{n+1}) = e^{At_{n+1}}x^*(0) = e^{A(t_n + \Delta t)}x^*(0) = e^{\Delta t A}\,e^{At_n}x^*(0) = e^{\Delta t A}x_n^*$.

One can easily verify that the matrix $F = \exp(\Delta t \cdot A)$ of (31) is not in the canonical form as the matrix A is. Therefore, identification by the observed data y_n of (29) will identify not (31) but a transformed system which has the canonical form (cf. (23–25))

$$\bar{x}_{n+1} = Q_2'\bar{x}_n, \quad Q_2' = \begin{bmatrix} 0 & 1 \\ a_1 & a_2 \end{bmatrix}, \quad \bar{x}_0 = \begin{bmatrix} y_0 \\ y_1 \end{bmatrix}, \quad n = 0, 1, \ldots, \tag{33}$$

with a_1, a_2 computed by (10) or (26) where $r = k^* = 2$.

However, one needs to identify the parameters m, k, x_0, $\dot{x}_0$ of the original system (28), not its discrete equivalent (33) producing the same observed data. The reason is not only that the state vector $\bar{x}_n$ in (33) has no physical sense but that it is not clear from the values of

a_1, a_2 how the changes of yet unknown physical parameters, mass m and rigidity k, may affect the oscillations (the period is also unknown). So, if identification aims at prediction of observed data, then the procedure is completed upon arrival at (33). But if the aim is *identification and control of real trajectories*, then (33) completes just the first step of the research.

Suppose that the structure of a model (28) is known in advance and it remains to identify m, k and the realization of a trajectory. From (28) to (33) one calculates:

$$\lambda_A = \pm\, \omega i, \quad \mu_Q = \mu_F = e^{\Delta t \lambda_A} = e^{\pm \omega i \Delta t} = (\cos \omega \Delta t \pm i \sin \omega \Delta t), \quad (i^2 = -1)$$

$$|Q_2' - \mu I| = \begin{vmatrix} -\mu & 1 & \\ a_1 & a_2 & -\mu \end{vmatrix} = \mu^2 - a_2\mu - a_1 = 0$$

$$a_2 = \mu_1 + \mu_2 = 2\cos \omega \Delta t, \quad a_1 = -\mu_1\mu_2 = -1. \tag{34}$$

The condition $a_1 = -1$ gives the test for validation of the assumed structure (28) and the first equality of (34) yields the parameters

$$\omega = \frac{1}{\Delta t} \arccos \frac{a_2}{2}, \quad \text{period } T = \frac{2\pi}{\omega} = \frac{2\pi \Delta t}{\arccos (a_2/2)} \tag{35}$$

with the structure (28) and ω determined; the trajectory is identified by the initial conditions:

$$x_0 = y_0, \quad \dot{x}_0 = \frac{\omega}{\sin \omega \Delta t} (y_1 - y_0 \cos \omega \Delta t). \tag{36}$$

To avoid the integration of (28) with (36), one can predict the exact sample-data trajectory directly from the discrete model (33):

$$\begin{aligned} x(t_n) &= \bar{x}_n^{(1)}, \quad n = 0, 1, 2, \ldots, \\ V(t_n) &= \left.\frac{dx}{dt}\right|_{t_n} = \frac{\omega}{\sin \omega \Delta t} (\bar{x}_n^{(2)} - \bar{x}_n^{(1)} \cos \omega \Delta t) \end{aligned} \tag{37}$$

(which reduces to (36) for $n = 0$).

The physical parameters m, k are dynamically indeterminable, but the linear relation

$$k = m\omega^2 = m \left(\frac{1}{\Delta t} \arccos \left(\frac{a_2}{2} \right) \right)^2 \tag{38}$$

gives an effective means to control the oscillations.

This closed form solution was possible because of additional information given in the assumed structure of the model (28). In the general case, the final result of model identification is a set of nonlinear relations in the space of physical parameters R^γ ($\gamma = m^2 + m, m = \dim x$) which single out a variety of possible models equivalent in regard to the observations. From that variety one makes a choice on the basis of some additional information about the physical, biological, etc., properties of the phenomenon under consideration (cf. the Brunhilda case below).

2.5 *Proper discretization*

Poor choice of the time increment Δt may cause degeneracy of the observations as it does the incomplete observability and/or initial state not affecting some of the root subspaces. In the above example, if $\Delta t = \pi k/\omega$ ($k = 1, 2, \ldots$) were chosen, this would reduce the order of the canonical model (33) to $w = 1$ since in this case the observations (as follows from the solution of (28)) would appear $y_n = y_0 = \text{const}$ for even k and $y_n = (-1)^n y_0$ for odd k and, in either case, the rank of the matrix (15) is $w = 1$. So, with such Δt, the system (28) is not identifiable despite its complete observability and $x^*(0)$ affecting all the modes. The general rule for avoiding degeneracy is that Δt must not be a multiple of a half period of any of the periodic functions contained in a solution. Those periods are not known in advance, so, in the case of doubt, one should try several Δt taking such that brings the maximum rank in the matrix (15). Since degenerate increments form a countable set, it can be accomplished also by a small change of Δt. Nondegenerate variations of Δt affect the transformation from the canonical model onto original (physical) model as can be seen from (37). But they do not affect the root subspaces $\{T_i^{-1}\}$ in (12), so the structural properties of a model and of the set of observations are invariant with respect to the choice of nondegenerate increment Δt.

3. CONTINUOUS OBSERVATIONS

For a continuous system (1) with continuous output (2) available for observation it is expedient, especially in complex cases, to identify directly the matrix A of (1) without going through the matrix $F = \exp(\Delta t A)$ of its discrete representation (3).

3.1 *Criterion in differential form*

Differentiating the output $y(t)$ of (2), one comes to the sequence of relations

$$y^{(k)}(t) = \mathrm{d}^k y/\mathrm{d}t^k = hA^k x(t), \quad k = 0, 1, \ldots, r \tag{39}$$

which are identical to (7) with the matrix A employed in place of F. This justifies the same procedure as in Sec. 2 to determine the existence, order, dynamics, and initial state of a suppposed linear stationary model (1) for a plant generating the observed output $y(t)$. One employs the sequential derivatives (39) in place of discrete signals y_s in the matrices (10), (15) and proceeds with the same procedures. A linear stationary model exists if and only if the matrix (15) filled with $y^{(k)}(t)$ has a constant rank w whatever t and k employed. The number w is the minimal order of a model (1) and the constant coefficients $a_1, \ldots, a_w$ determined from (10) filled with $y^{(k)}(t)$ give its dynamics in the canonical form similar to (23, 24). To illustrate how it works, we take again the example (28) in which the observed signal is

$$y(t) = x(t) = C \sin(\omega t + \beta), \quad t \geq 0; \quad C, \omega, \beta \text{ yet unknown.} \tag{40}$$

Differentiating (40) and putting into (15), one can easily see that the matrix (filled with observations) will necessarily have the rank $w = 2$. So the dynamics of a model is determined by the constants a_1, a_2 given by the relation (cf. (10)):

$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} y(t) & \dot{y} \\ \dot{y} & \ddot{y} \end{bmatrix}^{-1} \cdot \begin{bmatrix} \ddot{y} \\ \dddot{y} \end{bmatrix}. \tag{41}$$

Making use of the assumed structure (28), (40), one can see that (41) gives the solution $a_1 = -\omega^2$, $a_2 = 0$ which corresponds to the canonical model (cf. (23, 24)):

$$\frac{\mathrm{d}Z}{\mathrm{d}t} = \begin{bmatrix} 0 & 1 \\ -\omega^2 & 0 \end{bmatrix} \cdot Z; \quad Z = \begin{bmatrix} y(t) \\ \mathrm{d}y/\mathrm{d}t \end{bmatrix}, \quad t \geq 0. \tag{42}$$

Physical model (28) also has the canonical structure (30), so $x^*(t) \equiv Z(t)$ and they coincide completely. With known ω, the constants C and β in (40) are determined by the relations:

$$C = \sqrt{y^2 + \frac{\dot{y}^2}{\omega^2}}, \quad \beta = \operatorname{Arctan}\frac{\omega y}{\dot{y}} - \omega t \quad \left(\text{take } |\beta| < \frac{\pi}{2}\right).$$

Because of noisy measurements, sequential derivatives are impractical in computations and should be approximated by integrals. We present also another method using the integrated output.

3.2 *Criterion in integral form*

Take a set of time intervals $t_s = t + \Delta t_s$ and compute the values:

$$y_0 = y(t), \quad y_s = \int_t^{t_s} y(\tau - t)\,\mathrm{d}\tau, \quad s = 1, 2, \ldots \tag{43}$$

to fill the matrix (15). It can be shown that a linear stationary model exists if and only if this matrix has a constant rank w whatever t and Δt_s (Δt_s must be properly chosen, otherwise the rank can appear less than w). The coefficients $a_1^*, \ldots, a_w^*$ computed from (10) filled with (43) determine the dynamics of a model but not in the canonical form. To obtain an approximation to a canonical model, one has to employ in place of (43) the values

$$\begin{aligned}
N_0 &= y(t), \quad N_1 = \frac{2}{\Delta t_1}\left[\frac{1}{\Delta t_1}\int_t^{t+\Delta t_1} y\,\mathrm{d}\tau - y(t)\right] = N_1(\Delta t_1),\\
N_2 &= \frac{3[N_1(\Delta t_2) - N_1(\Delta t_1)]}{\Delta t_2 - \Delta t_1} = N_2(\Delta t_1, \Delta t_2)\\
N_3 &= \frac{4[N_2(\Delta t_1, \Delta t_3) - N_2(\Delta t_1 \Delta t_2)]}{\Delta t_3 - \Delta t_2}\\
&= N_3(\Delta t_1, \Delta t_2, \Delta t_3), \text{etc.}
\end{aligned} \tag{44}$$

It can be verified, that if (10) is filled with the values (44) and all $\Delta t \to 0$ then $a_i^* \to a_i$ ($i = 1, \ldots, w$) where a_i are the coefficients of a model (1) in the canonical form.

Another procedure with greater smoothing effect employs, in place of (43), the successively integrated output with one common Δt:

$$y_0 = y(t), \quad y_s(\Delta t) = \int_t^{t+\Delta t} y_{s-1}(\tau - t)\,\mathrm{d}\tau, \quad s = 1, 2, \ldots.$$

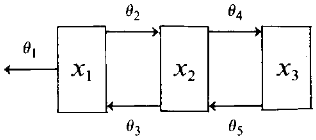
Using these values, one can obtain an approximation to a canonical model by means of a construction similar to (44) in which N_0 and N_1 remain the same but all following functionals are different, for example:

$$N_2^* = \frac{12}{\Delta t}\left\{N_1(\Delta t) - \frac{3}{\Delta t}\left[\frac{2}{\Delta t^2} y_2(\Delta t) - y_0\right]\right\}.$$

One can see that this construction as well as (44) present an integral form of the moving average of observations.

4. DISCUSSION OF THE BRUNHILDA MODEL

The catenary model studied by Jennrich and Bright [3] was of the form



which corresponds to the equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \begin{bmatrix} -\theta_1 - \theta_2, & \theta_3, & 0 \\ \theta_2, & -\theta_3 - \theta_4, & \theta_5 \\ 0, & \theta_4, & -\theta_5 \end{bmatrix} x, \; x(0) = (2 \cdot 10^5, 0, 0) \tag{45}$$

$$y(t) = [1, 0, 0]x = x_1(t), \quad t \geq 0 \tag{46}$$

containing unknown parameters $\theta_1, \ldots, \theta_5$. With $\theta_3 \cdot \theta_5 \neq 0$ (which is evident by construction of the model) the system (45, 46) is completely observable. There were given the values of 21 observations measured at different times. We took a set of evenly spaced observations measured at times $t_i = 10, 20, 30, \ldots, 90$ and computed the least squares fit of the difference equation (9) for orders 1, 2, 3, 4 which procedure gave a minimum MSE for the order 3. Another set of observations taken at time $t_i = 10, 30, 50, \ldots, 170$ yielded the order 4. This rules out the question of Wiggins [4] that the simpler two-compartment model might have served better and, on the contrary, suggests that the real process might have had a variable structure or one of compartments on the interval (90, 170] might have been functioning as a second-order system rather than the first-order one. There were too few observations to analyze that in detail.

Further, assuming a model of order 3 on [10, 90], one can obtain by (6) exactly three ($r = m = 3$) transcendental equations for θ_i where $F = \exp(\Delta t \cdot A)$, $\Delta t = 10$, $A(\theta_i)$, $h = \text{const}$ given by (45, 46) and a_1, a_2, a_3 computed from (10). Those equations in five-dimensional space R^5 of θ's do not determine a point but rather a two-dimensional manifold for θ_1, θ_2, θ_3, θ_4, θ_5 corresponding to the given observations. It leaves two degrees of freedom in θ's and even the reasonable demand suggested (but not confirmed) by the authors "that the first two compartments exchange at an equal rate, $\theta_2 = \theta_3$", would still leave one degree of freedom. This explains the result of Wiggins [4] who has obtained different estimates for θ's using the output $y^*(t) = x_3(t)$ instead of the original observations in the verification scheme:

$$\{y(t) = x_1(t)\} = > \{\hat{\theta}_i\} = > \{x_3(t) = y^*(t)\} = > \{\theta_i^*\} \neq \{\hat{\theta}_i\}.$$

In such a situation the results of weighted least-square fit are obviously model-dependent, compartment-dependent, even algorithm- and weights-dependent. The knowledge of initial state, seemingly useful in augmenting the goodness-of-fit, in reality does not contribute to estimation of dynamics (i.e., θ's). A poor initial state may only add to uncertainty causing degeneracy of the observations which, fortunately, is not the case in the Brunhilda model.

Finally, we have to mention that in order to predict further observations it is not necessary to identify θ's: a canonical model producing $y(t)$ is completely identified by (23), (24). However, to study an animal (to cure a sick person), a natural biological model (45) is to be identified to understand and control the process. For this task additional information is needed to identify all θ's. Griffiths [5] also points out the need of additional information to identify all θ's. He identifies the coefficients of the characteristic polynomial and of the powers of s in the Laplace transform representation. Thereby it is suggested to use the initial values of the first derivatives of $x_1(t)$, $x_2(t)$ and of the second derivative of $x_3(t)$ in (45) which we are hesitant to employ.

5. SOME EXPERIMENTAL RESULTS

The procedures developed in Section 2 were tested on various models with the observations generated on a computer. These experiments revealed the following general features:

1. The coefficients a_i computed by (10) are very sensitive to the noise in observations; 2. The use of a moving average (27) brings great improvement in computations; 3. The sum of squares due to errors is very sensitive with respect to the order and decreases sharply with the reach of the right order of a model; 4. The observations are not equally and uniformly good in time, e.g., they may degenerate with a decaying exponent in the solution which may cause an illusion of variable order in the case of noisy measurements.

As an illustration of the dependence of the SSE on the order of a supposed model, we present the following figures obtained when computing the least-squares fit of the difference equation (9) for the Brunhilda model within time interval [10,90]:

$$(\text{order} => 10^{-3} \times \text{MSE}): => (1 => 8360), (2 => 690), (3 => 64), (4 => 171).$$

6. CONCLUSIONS

The methods and computational procedures developed in this research present an effective means to solve the problem of the existence and identification of a linear stationary model on the basis of a set of continuous or evenly spaced discrete observations. The order and the canonical structure of the minimal model give a complete solution to the problem of prediction of further observations. Building a model in natural coordinates usually requires certain additional information unless natural coordinates coincide with the canonical ones. If the matrix of a model contains more unknown parameters than the dimension of the state vector, then the observations identify a set of models equivalent with respect to the output, from which set one makes a choice on the basis of some additional information. The least-squares fit methods like the one proposed by Jennrich and Bright [3] may converge to one of the models depending on a concrete algorithm, weights and an initial guess taken to start the computations. A certain level of noise always present in measurements brings in some statistical approach (see, e.g., [15–17]), however, the first step in noise elimination is simply to take a moving average in place of the separate observations to identify the dynamics of a model.

As concerns structural properties, it is established that there is no one-to-one correspondence between a model and the signal trajectory. To obtain such a map in canonical form, the following four conditions must be satisfied:

1. the system should be completely observable;
2. the initial state should affect all the modes;
3. the time increment Δt should be properly chosen;
4. the matrix of a model should contain the number of unknown parameters not greater than the order calculated as the rank of the matrix (15) filled by observations.

This matrix gives the answer on the question of the existence of a linear stationary model, and if affirmative, it determines its order and dynamics. The initial state of its canonical representation is then given by w successive observations where w is the order of the matrix (15) or, which is the same, of the difference equation (9).

Computational experiments have shown stability of the algorithm in respect to the calculation of the order in the presence of noise. The computation of dynamical coefficients a_i has proved to be very sensitive to the noise and requires the application of a moving average of observations. In the presence of noise one can observe the phenomenon of varying order due to degeneracy of observations when they become comparable in magnitude with the noise. Distinction should be made between this phenomenon and an order actually varying due to the features of a real system.

REFERENCES

1. C. Daniel and F. S. Wood, *Fitting Equations to Data*, Wiley-Interscience (1971).
2. A. E. Hoerl, Fitting Curves to Data. *Chemical Business Handbook* (edited by J. H. Perry), McGraw Hill (1954), Sec. 20, 55–57.
3. R. I. Jennrich and P. B. Bright, Fitting systems of linear differential equations using computer generated exact derivatives. *Technometrics*, **18**(4), 385–392 (1976).
4. A. D. Wiggins, Discussion. *Technometrics*, **18**(4), 393–399 (1976).
5. D. Griffiths, Structural identifiability for compartmental models. *Technometrics*, **21**(2), 257–259 (1979).
6. M. Berman and R. Shoenfeld, Invariants in experimental data on linear kinetics and the formulation of models. *Journal of Applied Physics*, **27**, 1361–1370 (1956).
7. R. Bellman and K. J. Astrom, On structural identifiability. *Mathematical Biosciences*, **7**, 329–339 (1970).
8. S. I. Rubinow and A. Winzer, Compartment analysis: an inverse problem. *Mathematical Biosciences*, **11**, 203–247 (1971).
9. S. I. Rubinow, On closed or almost closed compartment systems. *Mathematical Biosciences*, **18**, 245–253 (1973).
10. M. Milanese and G. P. Molino, Structural identifiability of compartmental models and pathophysiological information from the kinetics of drugs. *Mathematical Biosciences*, **26**, 175–190 (1975).
11. B. K. Shah, Data analysis problems in the area of pharmacokinetics research. *Biometrics*, **32**, 145–157 (1976).
12. E. Walter, G. Le Cardinal and P. Bertrand, On the identifiability of linear state systems. *Mathmatical Biosciences*, **31**, 131–141 (1976).
13. R. C. K. Lee, Optimal Estimation, Identification and Control. Research Monograph No. 28, M.I.T. Press, Cambridge, Massachusetts (1964).
14. R. E. Kalman, On the general theory of control systems. In *Proc. of the 1st IFAC Congress*, Vol. 2, Butterworths, London (1961).
15. J. H. Matis and H. O. Hartley, Stochastic compartmental analysis: model and least squares estimation from time series data. *Biometrics*, **27**, 77–102 (1971).
16. J. A. Jacquez, *Compartment Analysis in Biology and Medicine*, American Elsevier, New York (1972).
17. A. H. Markus, Power laws in compartmental analysis. Part I: a unified stochastic model. *Mathematical Biosciences*, **23**, 337–350 (1975).