

A Contribution to the Parameter Estimation of a Certain Class of Dynamical Systems

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The paper derives a procedure for the determination of the number of dynamical system parameters which are determinable on the bases of the input-output behaviour.

1. INTRODUCTION

An investigated biological object is in medical praxis often approximated by a multicompartmental system [6, 7]. It is supposed that

- a) the system consists of n compartments (Fig.1);
- b) mass transport exists between each of the two compartments and from each compartment to the exterior;
- c) the mass flow rate from the i -th to the j -th compartment or to the exterior is proportionate to the mass amount in the i -th compartment;
- d) mass is applied into compartments i_1, i_2, \dots, i_p ; $1 \leq i_1 < i_2 < \dots < i_p \leq n$;
- e) mass is measured in compartments j_1, j_2, \dots, j_q ; $1 \leq j_1 < j_2 < \dots < j_q \leq n$.

The multicompartmental system is described by the following equations:

$$(1) \quad \dot{\mathbf{x}} = \mathbf{Ax} + \mathbf{Bu}, \quad \mathbf{x}(0) = \mathbf{x}_0,$$

$$(2) \quad \mathbf{y} = \mathbf{Cx}$$

where $\mathbf{x} \in R^n$, $\mathbf{u} \in R^p$, $\mathbf{y} \in R^q$ and $\mathbf{A}, \mathbf{B}, \mathbf{C}$ are real constant matrices of appropriate dimensions.* The mathematical model (1) and (2) will be called the *dynamical system* $\mathcal{S} \equiv \{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$.

The symbols in Fig. 1 have the following meanings:

x_i — the mass amount in the i -th compartment,

* The output \mathbf{y} represents a set of measured $x_i, i = j_1, j_2, \dots, j_q$.

166 k_{ij} — the transfer constant from compartment i to j or to the exterior; $k_{ij} \geq 0$.
 u_{ik} — the inflow applied into compartment i .

In the terms of the above notation it is seen that:

$$(3) \quad \mathbf{A} = (a_{ij}), \quad i, j = 1, 2, \dots, n,$$

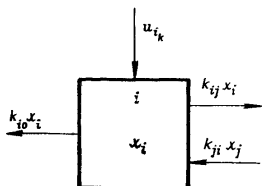


Fig. 1.

where

$$(4) \quad a_{ij} = \begin{cases} k_{ji}, & i \neq j, \\ -\sum_{\substack{r=0 \\ r \neq i}}^n k_{ir}, & i = j. \end{cases}$$

$$(5) \quad \mathbf{B} = (b_{ij}), \quad i = 1, 2, \dots, n; \quad j = 1, 2, \dots, p,$$

where

$$(6) \quad b_{ij} = \begin{cases} 1, & (i, j) \in \{(i_1, 1), (i_2, 2), \dots, (i_p, p)\}, \\ 0, & \text{otherwise.} \end{cases}$$

$$(7) \quad \mathbf{C} = (c_{ij}), \quad i = 1, 2, \dots, q; \quad j = 1, 2, \dots, n$$

where

$$(8) \quad c_{ij} = \begin{cases} 1, & (i, j) \in \{(1, j_1), (2, j_2), \dots, (q, j_q)\} \\ 0, & \text{otherwise.} \end{cases}$$

In a compartmental analysis the most interesting problem is the determination of the transfer constants k_{ij} of the model on the bases of an experiment. The experiment enables us to determine only the input-output relations. The object of this paper is to develop the procedure for the determination of the number of transfer constants which are determinable on the bases of the given experiment. The explicit formula is given for the system with one input as well as one output.

If it is not possible to determine (in a unique way) all the transfer constants, it is necessary either to rearrange the experiment or to suggest a simpler mathematical model. It is obvious that the rearrangement of the experiment is equivalent to a change of the \mathbf{B} and \mathbf{C} matrices.

2. THE TRANSFER FUNCTION MATRIX OF A DYNAMICAL SYSTEM

Let $\mathbf{x}(t)$, $\mathbf{y}(t)$, $\mathbf{u}(t)$ be Laplace transformable functions. Let us denote $\hat{\mathbf{x}}(s)$, $\hat{\mathbf{y}}(s)$, $\hat{\mathbf{u}}(s)$ the Laplace transforms of the $\mathbf{x}(t)$, $\mathbf{y}(t)$, $\mathbf{u}(t)$. Let us express a dependence of output \mathbf{y} on input \mathbf{u} from equations (1) and (2) by means of Laplace transform:

$$(9) \quad \hat{\mathbf{y}}(s) = \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1} \mathbf{B} \hat{\mathbf{u}}(s) + \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1} \mathbf{x}_0.$$

A $q \times p$ matrix $\mathbf{G}(s) = \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1} \mathbf{B}$ is called the *transfer function matrix* of the dynamical system $\mathcal{S} \equiv \{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$. Elements of the transfer function matrix are relatively prime rational functions and the degree of the numerator is less than the degree of the denominator. It is very well known that a dynamical system is *completely characterized* by its transfer function matrix $\mathbf{G}(s)$ if and only if (iff) this dynamical system is controllable and observable [1, 2]. The controllability and observability conditions are given in the

Theorem 1. *The dynamical system $\mathcal{S} \equiv \{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ is controllable and observable iff*

$$(10) \quad r(\mathbf{P}) = r(\mathbf{Q}) = n$$

where $r(\cdot)$ denotes the rank of matrix (\cdot) and

$$(11) \quad \mathbf{P} = [\mathbf{B}, \mathbf{AB}, \dots, \mathbf{A}^{n-1}\mathbf{B}]$$

$$(12) \quad \mathbf{Q} = [\mathbf{C}^T, \mathbf{A}^T \mathbf{C}^T, \dots, (\mathbf{A}^T)^{n-1} \mathbf{C}^T].$$

The proof is given e.g. in [1].

In the case when \mathbf{y} and \mathbf{u} are scalars ($p = q = 1$) the transfer function matrix $\mathbf{G}(s)$ is reduced to the point matrix and if seen scalarly, we briefly speak of the *transfer function* $G(s)$. From the equation (9) follows that

$$(13) \quad G(s) = \frac{M(s)}{\det(s\mathbf{I} - \mathbf{A})}$$

where

$$(14) \quad M(s) = \mathbf{C} \operatorname{adj}(s\mathbf{I} - \mathbf{A}) \mathbf{B}.$$

The maximum degree of the polynomial $M(s)$ is $n - 1$. We shall further define what is meant by *cancellations* in the transfer function $\mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1} \mathbf{B}$.

Definition 1. The transfer function $\mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B}$, where \mathbf{A} is $n \times n$ matrix, \mathbf{B} is $n \times 1$ matrix, \mathbf{C} is $1 \times n$ matrix, is said to *have no cancellation* iff the polynomials $M(s)$ and $\det(s\mathbf{I} - \mathbf{A})$ have no common factor.

The following theorem gives a necessary and sufficient condition for cancellations in the transfer function.

Theorem 2. Consider the transfer function $G(s) = \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B}$, where the matrices \mathbf{A} , \mathbf{B} , \mathbf{C} have the same dimensions as in definition 1. Transfer function $G(s)$ has no cancellation iff the corresponding dynamical system $\mathcal{S} \equiv \{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ is controllable and observable.

The proof is given in [3].

An extremely convenient formula for the transfer function which does not require matrix inversion was given by Brockett [4]. Let us define

$$(15) \quad \alpha = i \text{ if } \mathbf{C}\mathbf{A}^{i-1}\mathbf{B} \neq 0 \text{ and } \mathbf{C}\mathbf{A}^j\mathbf{B} = 0 \text{ for } 0 \leq j < i - 1$$

and

$$(16) \quad m^{-1} = \mathbf{C}\mathbf{A}^{\alpha-1}\mathbf{B}.$$

Then

$$(17) \quad G(s) = \frac{\det(s\mathbf{I} - \mathbf{A} + m\mathbf{B}\mathbf{C}\mathbf{A}^\alpha)}{ms^\alpha \det(s\mathbf{I} - \mathbf{A})}.$$

Since the identity (13) holds and the characteristic polynomial of an $n \times n$ matrix is of degree n , this identity places in evidence the fact that the numerator and denominator polynomials in (13) are of order $n - \alpha$ and n , respectively.

From the facts given above the following theorem results.

Theorem 3. Let us consider a controllable and observable dynamical system $\mathcal{S} \equiv \{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ with one input and one output. Then

- a) $M(s)$ and $\det(s\mathbf{I} - \mathbf{A})$ in (13) have no common factor,
- b) $M(s)$ and $\det(s\mathbf{I} - \mathbf{A})$ are of order $n - \alpha$ and n , respectively. α is defined in (15).

Proof. The theorem is the direct consequence of theorem 2 and Brockett's formula (17).

Now, we are going to proceed to the main part of the paper.

As it was pointed out in part 2 elements of the transfer function matrix are relatively prime rational functions:

$$(18) \quad G_{ij}(s) = \frac{\sum_{l=0}^m b_{ij} s^l}{\sum_{k=0}^r a_{ijk} s^k}, \quad m < r; \quad i = 1, 2, \dots, q; \quad j = 1, 2, \dots, p; \quad a_{ijr} = 1.$$

All the coefficients a_{ijk} and b_{ijl} are functions of transfer constants k_{ij} . The transfer function matrix is determined in a unique way by all of coefficients a_{ijk} and b_{ijl} .

Let us consider a dynamical system $\mathcal{L} \equiv \{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ which is described in detail in part 1. Which elements of matrix \mathbf{A} are determinable from the input-output behaviour in a unique way and under which conditions?

How to solve the above stated problem is given by the following procedure.

1. Transfer constants $k_{ij} \geq 0$, $i = 1, 2, \dots, n$; $j = 0, 1, \dots, n$ must fulfil the controllability and observability conditions (10). Derive these conditions in terms of k_{ij} .
2. Derive the transfer function matrix $\mathbf{G}(s)$ and point out all the mutually independent coefficients a_{ijk} , b_{ijl} for all i, j, k, l . The number of mutually independent coefficients a_{ijk} and b_{ijl} gives the number of determinable transfer constants k_{ij} .
3. Express transfer constants k_{ij} in terms of a_{ijk} and b_{ijl} if necessary.

We shall comment first the two points of the procedure.

1. The controllability and observability conditions ensure the dynamical system being completely characterized by its transfer function matrix. If these conditions were not fulfilled there would exist a part of the dynamical system which would not participate on the input-output behaviour [1].

2. The set of mutually independent coefficients a_{ijk} and b_{ijl} represent the set of equations for the determination of k_{ij} . It is evident that if the number of unknown elements of matrix \mathbf{A} is greater than the number of equations, matrix \mathbf{A} is not determined in a unique way. It is necessary to mention that some of k_{ij} may be given a priori e.g. zero.

For the single-input single-output dynamical system the following theorem holds:

Theorem 4. Let us consider a controllable and observable dynamical system $\mathcal{L} \equiv \{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ with one input and one output. The maximum number of determinable transfer constants k_{ij} is

- a) $2n - 1$ for $m = 1$
- b) $2n - \alpha + 1$ for $m \neq 1$

where α and m are defined in (15) and (16), respectively.

Proof. It is shown in [5] that the rank of $[CB, CAB, \dots, CA^{n-1}B]$ must be 1 if the transfer function is to be nonzero. If $\alpha = 1$ then $m = 1$. The numerator and denominator in (18) are both monic polynomials. Point a) is the direct consequence of theorem 3. If $\alpha > 1$ then m is a function of some k_{ij} . The numerator in (18) is a polynomial with m^{-1} as the leading coefficient. So the point b) is also the direct consequence of theorem 3.

In the following part of the paper several examples will serve as an illustration.

4. EXAMPLES

Example 1. Let us consider a three-compartment system which is pictured on Fig. 2. Let us suppose that only x_2 is measured. Then matrices A, B, C in the dynamical system $\mathcal{S} \equiv \{A, B, C\}$ are as follows:

$$A = \begin{bmatrix} -k_{10} - k_{12} & k_{21} & 0 \\ k_{12} & -k_{20} - k_{21} - k_{23} & k_{32} \\ 0 & k_{23} & -k_{30} - k_{32} \end{bmatrix},$$

$$B = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad \text{and} \quad C = [0 \ 1 \ 0].$$

The dynamical system \mathcal{S} is controllable and observable iff the following conditions hold simultaneously:

$$k_{12} > 0, \quad k_{21} > 0, \quad k_{23} > 0, \quad k_{32} > 0, \quad k_{10} + k_{12} \neq k_{30} + k_{32}.$$

(It is supposed in part 1 that $k_{ij} \geq 0$.) Because $m = 1$ the maximum number of determinable transfer constants k_{ij} is five (Theorem 4). Matrix A is not determined in a unique way for this matrix contains seven unknown elements.

Example 2. Let us consider a three-compartment system which is pictured on Fig. 2. Let us suppose that x_1 and x_3 are measured. Matrices A and B of the dynamical system $\mathcal{S} \equiv \{A, B, C\}$

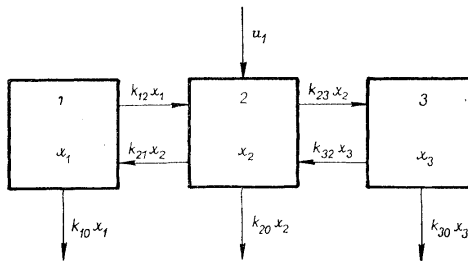


Fig. 2.

are the same as in example 1. Matrix \mathbf{C} has form

$$\mathbf{C} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

The dynamical system \mathcal{S} is contrrollable and observable iff the following conditions hold simultaneously:

$$k_{21} > 0, \quad k_{23} > 0, \quad k_{10} + k_{12} \neq k_{30} + k_{32}.$$

It is easy to derive that the transfer function matrix

$$(19) \quad \mathbf{G}(s) = \frac{1}{\det(s\mathbf{I} - \mathbf{A})} \begin{bmatrix} k_{21}(s + k_{30} + k_{32}) \\ k_{23}(s + k_{10} + k_{12}) \end{bmatrix}$$

contains seven independent coefficients $a_{ijk}, b_{ij}; i = 1, 2; j = 1; k = 0, 1, 2; l = 0, 1$. Matrix \mathbf{A} is determinable in a unique way.

Example 3. Let us consider a three-compartment system which is pictured on Fig. 2. Let us suppose that only x_2 is measured and that a mass is applied into compartments 1 and 3. Matrices \mathbf{A} and \mathbf{C} of the dynamical system $\mathcal{S} \equiv \{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ are the same as in example 1. Matrix \mathbf{B} has form

$$\mathbf{B} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix}.$$

The dynamical system \mathcal{S} is contrrollable and observable iff the following conditions hold simultaneously:

$$k_{12} > 0, \quad k_{32} > 0, \quad k_{10} + k_{12} \neq k_{30} + k_{32}.$$

It is easy to derive that the transfer function matrix

$$(20) \quad \mathbf{G}(s) = \frac{1}{\det(s\mathbf{I} - \mathbf{A})} \begin{bmatrix} k_{12}(s + k_{30} + k_{32}); & k_{32}(s + k_{10} + k_{12}) \end{bmatrix}$$

contains seven independent coefficients similarly as in example 2. So matrix \mathbf{A} is again determinable in a unique way.

It is seen from examples 2 and 3 that, from the theoretical point of view, there are several possible rearrangements of the experiment for the unique determination of matrix \mathbf{A} . The actual arrangement of the experiment must suit both theoretical conditions of unique determinability and practical realizability.

5. CONCLUSIONS

The object of this paper has been to find the theoretical number of determinable elements of matrix \mathbf{A} of a dynamical system $\mathcal{S} \equiv \{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ on the bases of an input-

output behaviour. The procedure has been described in part 3. For a single-input single-output system the explicit formula has been given in Theorem 4.

The paper is not concerned with the way of the best fitting of experimental data. It is necessary to emphasize that if the dynamical system was more complicated and some disturbances arose, the number of practically estimable parameters could have been less than a theoretical one. Not much work has been done in this field up to the present.

The results of the paper, of course, do not concern biological systems only and hold for practically all real systems with lumped parameters.

(Received June 9, 1971.)

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Příspěvek k problému odhadu parametrů určité třídy dynamických systémů

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V lékařské praxi jsou zkoumané biologické objekty často modelovány jako více-kompartmentové systémy. Nejdůležitějším problémem v kompartmentové analýze je určení přenosových konstant k_{ij} modelu na základě experimentu. Experimentálně však nelze přenosové konstanty určit přímo, neboť experiment nám umožňuje určit pouze závislost výstupních veličin systému na veličinách vstupních. V článku je odvozen postup pro zjištění teoretického počtu parametrů dynamického systému, které je možno určit na základě znalosti odezvy výstupu v závislosti na vstupu. Pro systémy s jedním vstupem a jedním výstupem je uvedena explicitní formule. V závěru práce je pro ilustraci uvedeno několik příkladů. Výsledky práce se ovšem netýkají pouze biologických systémů, ale platí prakticky pro všechny reálné systémy se soustředěnými parametry.

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